Fortran 90 & 95 Array and Pointer Techniques

Objects, Data Structures, and Algorithms

with subsets e-LF90 and F

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16 September 1998

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Preface

This book covers modern Fortran array and pointer techniques, including facilities provided by Fortran 95, with attention to the subsets e-LF90 and F as well. It provides coverage of Fortran based data structures and algorithm analysis.

The principal data structure that has traditionally been provided by Fortran is the array. Data structuring with Fortran has always been possible — although not always easy: one of the first textbooks on the subject (by Berztiss, in 1971) used Fortran for its program examples. Fortran 90 significantly extended the array features of the language, especially with syntax for whole arrays and array sections and with many new intrinsic functions. Also added were data structures, pointers, and recursion. Modern Fortran is second to none in its support of features required for efficient and reliable implementation of algorithms and data structures employing linked lists and trees as well as arrays.

Examples shown in this book use some features of Fortran 95, notably derived type component initialization, pointer initialization with **null**, and **pure** functions. Electronically distributed program examples include the Fortran 95 versions printed in the book, as well as alternative versions acceptable to the Fortran 90 subsets e-LF90 and F. Each of these subsets supports all essential features of Fortran 90 but omits obsolete features, storage association, and many redundancies that are present in the full Fortran language; furthermore, they are available at a very reasonable price to students and educators. Information concerning e-LF90 (“essential Lahey Fortran 90”) is available from Lahey Computer Systems, Inc.; 865 Tahoe Blvd.; Incline Village, NV 89450; (702) 831-2500; **<www.lahey.com>**; **<sales@lahey.com>**. Information concerning the F subset is available from Imagine1; 11930 Menaul Blvd. NE, Suite 106; Albuquerque, NM 87112; (505) 323-1758; **<www.imagine1.com/imagine1>**; **<info@imagine1.com>**.

The programming style used in this book, and in all three electronically distributed variant versions of the programming examples, is close to that required by F (the more restrictive of the two subsets). F version examples conform to the “common subset” described in *essential Fortran 90 & 95: Common Subset Edition*, by Loren P. Meissner (Unicomp, 1997), except that short-form **read** and **print** statements replace the more awkward form that common subset conformance requires. The e-LF90 version examples incorporate extensions described in Appendix C of *essential Fortran*, namely: initialization and type definition in the main program, simple logical **if** statements, **do while**, and internal procedures. Fortran 95 version examples (including those printed in the text) do not employ any further extensions except for facilities that are new in Fortran 95. All versions of the examples have been tested; the Fortran 95 versions were run under DIGITAL Visual Fortran v 5.0c: see **<www.digital.com/ fortran>**.

Bill Long, Clive Page, John Reid, and Chuckson Yokota reviewed earlier drafts of this material and suggested many improvements.

Chapter 1 Arrays and Pointers

1.1 WHAT IS AN ARRAY?

Think of a group of objects that are all to be treated more or less alike — automobiles on an assembly line, boxes of Wheaties on the shelf at a supermarket, or students in a classroom. A family with five or six children may have some boys and some girls, and their ages will vary over a wide range, but the children are similar in many ways. They have a common set of parents; they probably all live in the same house; and they might be expected to look somewhat alike.

In computer applications, objects to be processed similarly may be organized as an *array*. Fortran is especially noted for its array processing facilities. Most programming languages including Ada, C, and Pascal provide statements and constructs that support operations such as the following:

- Create an array with a given name, shape, and data type
- Assign values to one or more designated *elements* of an array
- Locate a specific element that has been placed in the array
- Apply a specified process to all elements of a particular array, either sequentially (one element at a time) or in parallel (all at once).

Two important properties make arrays useful.

1. An array is a *homogeneous* collection — all of its elements are alike in some important ways. In programming language terms, all elements of a given array have the same *data type*.[1] This has two consequences:

   First, it means that all elements of an array permit the same *operations* — those that are defined for the data type. For example, if the array elements are integers, operations of arithmetic such as addition and multiplication can be performed upon them. If their data type is logical, the applicable operations include *and, or,* and *not.*

   Second, having a common data type implies that all the elements of a given array have the same *storage representation*. The elements each occupy the same amount of space, which means that they can be stored in a linear sequence of equal-sized storage areas.

2. Each element is identified by a sequential number or *index*. Along with the fact that each element occupies some known amount of space in computer storage, this means that the addressing mechanisms in the computer hardware can easily locate any element of a particular array when its index number is known. A process to be applied to the array elements can proceed sequentially according to the index numbers, or a parallel process can rely upon the index numbers to organize the way in which all elements are processed.

[1] A Fortran data type can have *type parameters.* All elements of a given array have the same data type and the same type parameters.

Subscripts

In mathematical writing, the index number for an array element appears as a *subscript* — it is written in a smaller type font and on a lowered type baseline: A_1 for example. Most programming languages, including Fortran, have a more restricted character set that does not permit this font variation, so the index number is enclosed in parentheses that follow the array name, as **`A(1)`**. Some languages use square brackets instead of parentheses for the array index, as **`A[1]`**. Regardless of the notation, array indices are called subscripts for historical reasons.

A subscript does not have to be an integer constant such as **`1`**, **`17`**, or **`543`**; rather, in most contexts it can be an arbitrary expression of integer type. For example, the array element name A_{i+1} is written in Fortran as **`A(I + 1)`**. The value of a subscript expression is important, but its form is not. A specific array element is uniquely identified (at a particular point in a program) by the *name* of the array along with the *value* of the subscript. The subscript value is applied as an *ordinal* number (first, second, third, . . .) to designate the position of a particular element with relation to others in the array element sequence.

In the simplest case, subscripts have positive integer values from 1 up to a specific *upper bound;* for example, the upper bound is 5 in an array that consists of the elements

```
A(1)     A(2)     A(3)     A(4)     A(5)
```

The lower bound may have a different value, such as 0 or –3 in the following arrays:

```
A(0)     A(1)     A(2)     A(3)     A(4)
A(-3)    A(-2)    A(-1)    A(0)     A(1)
```

In any case, the subscript values consist of *consecutive* integers ranging from the lower bound to the upper bound.[2] The *extent* is the number of different permissible subscript values; the extent is 5 in each of the foregoing examples. More generally (for consecutive subscripts), the extent is the upper bound plus one minus the lower bound.

It should be noted that an array can consist of a single element: its upper and lower bounds can be the same. Perhaps surprisingly, Fortran (like a few other programming languages) permits an array to have no elements at all. In many contexts, such an array is considered to have lower bound 1 and upper bound 0.

Multidimensional Arrays

An array may be multidimensional, so that each element is identified by more than one subscript. The *rank* of an array is the number of subscripts required to select one of the elements. A rank-2 array is two-dimensional and is indexed by two subscripts; it might have six elements:

```
B(1, 1)  B(2, 1)  B(3, 1)  B(1, 2)  B(2, 2)  B(3, 2)
```

On paper, a one-dimensional array is usually written as a sequence of elements from left to right, such as any of the arrays named *A* in the previous examples. A two-dimensional array can be displayed as a *matrix* in which the first subscript is invariant across each row and the second subscript is invariant down each column, as in mathematics:

```
B(1, 1)  B(1, 2)  B(1, 3)
B(2, 1)  B(2, 2)  B(2, 3)
```

There is no convenient way to display an array of three or more dimensions on a single sheet of paper. A three-dimensional array can be imagined as a booklet with a matrix displayed on each page. The third subscript is invariant on each page, while the first two subscripts designate the row and column of the matrix on that page.

[2] Array subscripts are normally consecutive. Special Fortran *array section* notation supports nonconsecutive subscript values.

```
C(1, 1, 1)   C(1, 2, 1)   C(1, 3, 1)   (first page)
C(2, 1, 1)   C(2, 2, 1)   C(2, 3, 1)

C(1, 1, 2)   C(1, 2, 2)   C(1, 3, 2)   (second page)
C(2, 1, 2)   C(2, 2, 2)   C(2, 3, 2)

C(1, 1, 3)   C(1, 2, 3)   C(1, 3, 3)   (third page)
C(2, 1, 3)   C(2, 2, 3)   C(2, 3, 3)

C(1, 1, 4)   C(1, 2, 4)   C(1, 3, 4)   (fourth page)
C(2, 1, 4)   C(2, 2, 4)   C(2, 3, 4)
```

The *shape* of an array is a list of its extents along each dimension. Among the arrays just mentioned, *A* has shape (5), *B* has shape (2, 3), and *C* has shape (2, 3, 4). The total *size* of an array is the product of the extents along all its dimensions, so the size of *A* is 5, the size of *B* is 6, and the size of *C* is 24. Note that the size of a one-dimensional array is the same as its extent (number of elements).

Arrays as Objects

An array is an *object* with three principal attributes: its data type, its name, and its shape.[3] An array object can be a constant, a variable, an argument to a procedure, or an input or output list item. Here are some examples of array applications:

Lists. One-dimensional arrays are useful for storing *lists*. For example, Professor Smythe-Heppelwaite, who studies the thickness of butterflies' wings, might store each wing thickness as the value of one element of a one-dimensional array of real data type. The size of the array is determined by the number of butterflies in the collection.

As another example, a list of names could be stored as a one-dimensional array of character strings.

Tables. A *table* can be implemented as a one-dimensional array of structures. As a simple example, consider a table of 20 California cities containing the name, the latitude, and the longitude of each. Each row of the table is a structure consisting of a character string for the name and two integers for the latitude and longitude. Twenty of these structures in a one-dimensional array form the following table:

[3] Modern Fortran views arrays as objects: a procedure dummy argument that is an *assumed-shape* array matches the data type and the shape of the corresponding actual argument. Traditional Fortran dialects viewed an array argument as an area of storage whose attributes were established by declarations in the procedure and were independent of the referencing program unit.

```
Jacumba            33        116
Alturas            41        120
Woodside           37        122
Imperial Valley    33        116
Mira Loma          34        117
Glendora           34        118
Herlong            40        120
Temple City        34        118
Big Sur            36        122
Lafayette          38        122
Winterhaven        33        115
Nicolaus           39        122
Dobbins            39        121
Flintridge         34        118
Oakdale            38        121
Corona             34        117
Kensington         38        122
San Luis Obispo    35        121
Pacifica           38        123
Crescent City      42        124
```

Matrices. Two-dimensional arrays are useful in physical and mathematical applications. An example is illustrated Fig. 1.1. A horizontal beam supports a system of n vertical forces at positions $x_1, x_2, \ldots,$ x_n. Each force f_i produces a deflection $y_i = y(x_i)$ at each position x_i. We may represent the forces by a vector $\mathbf{f}$ of length n and the deflections by a vector $\mathbf{y}$ of length n. The deflections are related to the forces by the matrix equation $\mathbf{y} = A \cdot \mathbf{f}$, where A is an n by n matrix of coefficients of influence or of flexibility.

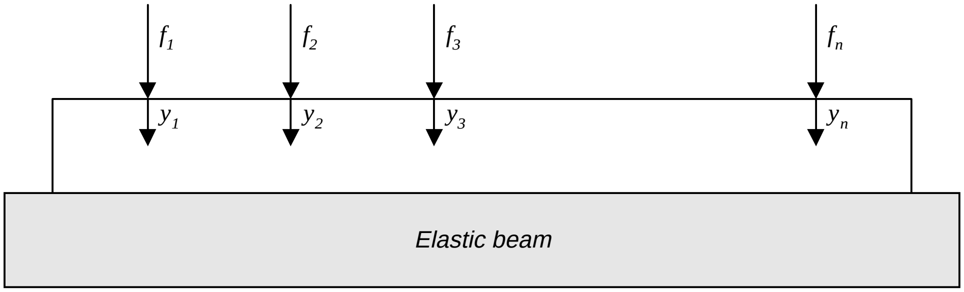


FIGURE 1.1. Elastic beam with forces and deflections

More generally, an n-by-m matrix can represent a *linear transformation* from an m-dimensional *vector space* to an n-dimensional vector space. In particular, an n-by-n square matrix can represent a linear transformation of an n-dimensional vector space onto itself. Multiplication of a matrix by a vector or by another matrix is defined mathematically so that it works correctly for this interpretation.

Three or more dimensions. A multi-dimensional array might be used for tallying the results of a survey of physical characteristics. For example, a 6-by-5-by-4 array might be used to count the number of individuals having any of six hair colors, five eye colors, and four skin colors.

Say It with Fortran

Fortran statements and constructs support operations such as the following:

- Create an array with a given name, shape, and data type
- Assign values to one or more designated *elements* of an array
- Locate a specific element that has been placed in the array
- Apply a specified process to all elements of a particular array.

Modern array facilities employed in this book include the three array classes: explicit shape (declared with bounds written as *specification expressions*, which may have fixed or varying values), assumed shape (procedure dummy arguments that take their shape from the corresponding actual argument), and deferred shape (allocatable or pointer target arrays). Programs here show examples of whole arrays and array sections, array constructors, and array-valued constants; how to combine arrays with derived-type structures, and arrays with the pointer attribute. Detailed descriptions of modern Fortran array facilities appear in other books such as *Fortran 90/95 Explained,* by Metcalf and Reid (Oxford Univ., 1996).

Whole Arrays and Array Sections

An array is a variable; thus, the array name (without a subscript) represents all elements of the array. For example, an array name in an input or output list causes input or output of all the array elements. For a vector, the elements are read or written in the obvious sequence. The *standard array element sequence* for arrays of higher rank is described later in this section.

There is a rich set of operations on whole arrays; most scalar operations are extended to whole-array operands. A whole-array operation is applied to all elements of the array. For example, if *B* and *C* are arrays that have the same shape, the expression **B + C** means that each element of *B* is to be added to the corresponding element of *C*. The operations of arithmetic and the elementary mathematical intrinsic functions apply *elementwise* to whole arrays. (See Elemental Intrinsic Functions later in this section.)

Furthermore, there is a large set of intrinsic functions for performing operations that would otherwise require indexed **do** loops. Whole-array constants, as a form of array constructors, are also provided.

Whole-Array Operations

A whole array, denoted by the array name without a subscript, is an *array variable*. Fortran permits an array variable in most contexts where a scalar variable is permitted.

Assignment is permitted between whole arrays of the same shape:

1. The shape of an array is determined by its rank (number of dimensions) and by its extent (number of elements) along each dimension.
2. Two arrays have the same shape if they have the same rank and if their extents agree along each dimension. The upper and lower subscript bounds are not required to agree.

The left and right sides of a whole-array assignment statement may have different types and other type properties, if the type, kind, and character length coercion rules that apply to assignment of scalars are observed.

```
! Example of whole-array assignment.
    implicit none
    real, dimension(5, 7) :: A, B
    real, dimension(0: 4, 0: 6) :: C
    integer, dimension(5, 7) :: I
! start
    read *, B
    C = B
    I = C
! Elementwise type coercion, with truncation, occurs.
    A = I
    print *, A
```

Whole arrays may be combined in *array expressions* by any operator that can be applied to variables whose type is that of the array elements. All arrays in such an expression must have the same shape. Each operator in an array expression denotes an elementwise operation upon corresponding elements of each array in the expression.

```
! Arithmetic and relational operations on whole arrays.
    implicit none
    real, dimension(5, 7) :: A, B, C
    logical, dimension(5, 7) :: T
    real, dimension(20) :: V, V_Squared
! start
    read *, B, C, V
    A = B + C
    T = B > C
    C = A * B
    V_Squared = V * V
    print *, T, C, V, V_Squared
```

Note that **A * B** denotes elementwise whole-array multiplication, *not* matrix multiplication as defined in linear algebra.

Shape conformance rules for whole-array expressions are extended to permit *scalar* subexpressions along with whole array operands. (All array operands in an expression must have the same shape.) The shapes of two operands are *conformable* if they are both whole arrays and have the same shape, or if either of the expressions is a scalar. When an operator has a scalar operand and a whole-array operand, the result is an array of the same shape as the whole-array operand. Each element of the result is obtained by combining the scalar with the corresponding element of the whole array. For example, the whole-array operation

```
A = 2.0 * B
```

combines the scalar **2.0** with each element of *B* and assigns the result to the corresponding element of *A*.

As we shall see, *array sections* are also conformable with whole arrays of the same shape and with scalars. This same extended definition of shape conformance also applies to assignment when the object on the left is a whole array and the expression on the right is scalar valued. Furthermore, actual arguments to certain intrinsic functions may combine scalars with arrays.

An array may be initialized with a scalar; a scalar is interpreted in much the same way in whole-array initialization as in whole-array assignment.

Of great importance for supercomputers that perform operations in *parallel* is the fact that Fortran does not artificially impose any particular element sequence upon whole-array assignment. Although conceptually all of the elements are processed in parallel, the actual sequence is arbitrary. The point is that assignment to the array variable named on the left side must not affect the evaluation of the right side in any way:

```
real, dimension(L) :: First, Second
  :
First = First + Second
```

A possible model for whole-array assignment assumes a temporary "array-sized register," or *shadow* of the left side, whose elements are assigned as they are calculated. As a final step, the shadow register is copied into the designated left side array. It is important to note, however, that whole-array assignment can often be implemented without incurring the extra space or time penalties implied by this model.

Elemental Intrinsic Functions

Many intrinsic functions, notably including the mathematical functions, are classified as *elemental*. An elemental intrinsic function accepts either a scalar or an array as its argument. When the argument is an array, the function performs its operation elementwise, applying the scalar operation to every array element and producing a result array of the same shape. For elemental intrinsic functions with more than one array argument, all actual arguments that are arrays must have the same shape. The following statements apply the intrinsic functions **max** and **sin** elementwise to whole arrays:

```
implicit none
real, dimension(5, 7) :: A, B, C, D
logical, dimension(5, 7) :: T
  :
A = max( B, C )
C = max( A, 17.0 )
T = sin( A ) > 0.5
```

Array Sections

An especially useful feature permits operations on all the elements in a designated portion of an array. An *array section* is permitted in most situations that accept a whole array. Most operations that are valid for scalars of the same type may be applied (elementwise) to array sections as well as to whole arrays. In particular, an array section may be an actual argument to an elemental intrinsic function.

The simplest form of array section is a sequence of consecutive elements of a vector. Such an array section is designated by the array name followed by a *pair* of subscript expressions that are separated by a colon and represent the subscript limits of the array section. Either expression (but not the colon) may be omitted; the default limits are the declared array bounds:

```
real, dimension(40) :: Baker
real, dimension(5, 17) :: John
real, dimension(144) :: Able
  :
Baker(1: 29)
Baker(: 29)  ! Default lower limit is 1.
John(5: 11)
John(: 11) ! Default is declared lower bound.
Able(134: 144)
Able(134: )  ! Default is declared upper bound.
```

An array section may be combined in an expression with whole arrays or other array expressions (of the same shape) and with scalars, and it may appear on the left side in an assignment statement. Each of the following assignment statements moves a consecutive subset of the elements of a vector.

```
real, dimension(100) :: X
real, dimension(5) :: Y, Z
X(1: 50) = X(51: 100)
Y(2: 5) = Y(1: 4)
Z(1: 4) = Z(2: 5)
```

An array section designator may include a third expression. This *increment* (in this context, often called the *stride*) gives the spacing between those elements of the underlying parent array that are to be selected for the array section:

```
real, dimension(8) :: A
real, dimension(18) :: V
A = V(1: 15: 2)
```

Values assigned to *A* are those of V_1, V_3, . . . , $V_{15.}$ A negative increment value reverses the normal array element sequence:

```
A = B(9: 2: -1)
```

Here, elements of the reversed array section — the eight elements B_9, B_8, B_7, . . . , B_2, in that order — are assigned to the consecutive elements of *A*.

A more complicated example is the following:

```
real, dimension(3, 5) :: E
real, dimension(2, 3) :: F
F = E(1: 3: 2, 1: 5: 2)
```

Here, on the last line, the first subscript of *E* takes on values 1, 3 and the second subscript of *E* takes on values 1, 3, 5. The array section is a two-dimensional array object whose shape matches that of *F*.

Any of the three components of an array section designator may be omitted. The final colon must be omitted if the third component is omitted:

```
real, dimension(100) :: A
A(: 50)                                    ! Same as A(1: 50) or A(1: 50: 1)
A(: 14: 2)                                                ! Same as A(1: 14: 2)
A(2: )                                   ! Same as A(2: 100) or A(2: 100: 1)
A(2: : 3)                                                ! Same as A(2: 100: 3)
A(: : 2)                                                 ! Same as A(1: 100: 2)
A(:)                                  ! Same as A(1: 100) or A(1: 100: 1) or A
A(: : -1)                        ! Same as A(1: 100: -1); array section of zero size
A(1: 100: )                                                          ! Prohibited
```

The default values for these components are, respectively, the lower subscript bound for the array dimension, the upper bound for the array dimension, and 1.

Array section designators may be combined with single subscripts to designate an array object of lower rank:

```
V(: 5) = M(2, 1: 5)
```

Here, the elements $M_{2,1}$ through $M_{2,5}$ form a one-dimensional array section that is assigned to the first five elements of *V*. As another example, `A(3, :)` designates the third row of the matrix *A* (all elements whose first subscript is 3), and `A(:, 5)` designates the fifth column of the matrix *A* (all elements whose second subscript is 5).

The *rank* of an array section is the number of subscript positions in which at least one colon appears; a colon in a subscript position signals that there is a *range* of subscript values for that dimension. The extent along each dimension is simply the number of elements specified by the section designator for that dimension.

In the absence of a colon, a fixed subscript value must appear; fixing one subscript value reduces the rank by 1. If *Fours* is an array of rank 4, then `Fours(:, :, :, 1)` denotes the rank-3 array that consists of all elements of *Fours* whose fourth subscript is 1. `Fours(:, :, 1, 1)` denotes the matrix (rank-2 array) that consists of all elements of *Fours* whose third and fourth subscripts are both 1. `Fours(:, 1, 1, 1)` denotes the vector (rank-1 array) that consists of all elements of *Fours* whose second, third, and fourth subscripts are all 1. Finally, `Fours(1, 1, 1, 1)` names a scalar, which, for most purposes, may be considered a rank-0 array. Note that `Fours(1: 1, 1: 1, 1: 1, 1: 1)` is not a scalar but an array whose rank is 4 and whose size is 1. This latter array may also be denoted as `Fours(: 1, : 1, : 1, : 1)`.

See also Vector Subscripts, later in this Section.

Array Input and Output

An *Input list* or an *Output list* may include a reference to a whole array. The elements are transmitted according to a standard sequence, defined immediately below. For an array of rank 1, this sequence consists of the elements in increasing subscript order. A rank-one array section without a stride designator also causes transmission of a set of contiguous array elements in increasing subscript order.

```
! Input and output of whole arrays and array sections.
  implicit none
  integer, parameter :: ARRAY_SIZE = 5
  integer, dimension(ARRAY_SIZE) :: Data_Array
! start
  read *, Data_Array                                         ! Whole array
  print *, " The first four values: ", Data_Array(: 4)     ! Array section
```

Standard Array Element Sequence

Some operations and intrinsic functions on whole arrays require that a *standard element sequence* be defined. The standard sequence depends on the subscript values: The leftmost subscript is varied first, then the next subscript, and so on.

Let the declaration for an array be

Type **, dimension(** $UBound_1$ **,** $UBound_2$ **,** $UBound_3$ **) ::** *Array name*

Then, a reference to

*Array name***(** $Subscript_1$, $Subscript_2$, $Subscript_3$)

will designate the element whose sequential position is

$$S_1 + U_1 \cdot (S_2 - 1) + U_1 \cdot U_2 \cdot (S_3 - 1)$$

where U represents an upper bound value in the declaration and S represents a subscript in the reference.

For arrays with explicit lower subscript bounds as well as upper bounds, the formula of course involves the bound values. If an array is declared with lower bounds L_1, L_2, L_3 and upper bounds U_1, U_2, U_3, and an element is referenced with subscript values S_1, S_2, S_3, the sequential position of this element is given by the following formula:

$$1 \ + \ (S_1 - L_1) \ + \ (U_1 - L_1 + 1) \cdot (S_2 - L_2) \ + \ (U_1 - L_1 + 1) \cdot (U_2 - L_2 + 1) \cdot (S_3 - \ L_3)$$

This formula can easily be generalized to more than three dimensions.

Note that U_3, the upper subscript range bound for the last dimension, does not appear in this formula. This last upper bound value has a role in determining the total size of the array, but it has no effect on the array element sequence.

Array Constructors and Array-Valued Constants

Fortran provides a method for constructing a vector by specifying its components as individual expressions or expression sequences. An array constructor consists of a *List* of expressions and implied **do** loops, enclosed by the symbols **(/** and **/)** :

(/ *List* **/)**

The expressions in the *List* may be scalar expressions or array expressions.

Array constructors are surprisingly versatile. For example, two or more vectors may be concatenated, or joined end to end, with an array constructor. In the following statement, suppose that **X**, **Y**, and **Z** are vectors:

```
Z = (/ X, Y /)
```

The usual conformance requirements of array assignment apply. Here, the length of **Z** must be the sum of the lengths of **X** and **Y**, and other attributes of the data must be compatible.

Array constructors are especially useful for constructing array-valued constants, as illustrated by the following examples. The first two of the following array constructors form constant vectors of real type, while the third is a constant vector of integer type.

```
(/ 3.2, 4.01, 6.4 /)
(/ 4.5, 4.5 /)
(/ 3, 2 /)
```

A named constant may be a whole array:

```
integer, dimension(5), parameter :: PRIMES = (/ 2, 3, 5, 7, 11 /)
```

A whole-array variable may be initialized in a type declaration, giving the initial value of the array by means of a scalar or an array constructor:

```
real, dimension(100), save :: Array = 0.0
integer,dimension(5), save :: Initial_Primes = (/ 2, 3, 5, 7, 11 /)
```

The implied **do** loop form that is permitted in an array constructor is so called because of its resemblance to the control statement of an indexed **do** construct:

(*Sublist* **,** *Index* **=** *Initial value* **,** *Limit* [**,** *Increment*] **)**

For example,

```
(J + 3, J + 2, J + 1, J = 1, N)
```

The *Sublist* consists of a sequence of items of any form that is permitted in the *List*; an implied **do** loop may be included in a sublist within an outer implied **do** loop. The Index variable (called an array constructor implied-**do** variable or ACID variable) should not be used for any other purpose; furthermore, it should be a local variable and should not have the pointer attribute.

Constructing an array of higher rank

An array constructor always creates an array of rank 1, but the intrinsic function **reshape** can be applied to create an array of higher rank. For example, the following expression constructs an **N** by **N** identity matrix:

```
reshape( (/ ((0.0, J = 1, I - 1), 1.0, (0.0, J = I + 1, N), I = 1, N) /), (/ N, N /) )
```

The intrinsic function **reshape** has two arguments, **source** and **shape**. The first argument, **source**, is an array of rank 1, of any type, with the correct total number of elements. The the second argument, **shape**, is a vector of one to seven positive integer elements. The number of elements in the **shape** vector determines the rank of the result from **reshape**. Each element of **shape** gives the size along one dimension of the result array; thus, the product of the element values of **shape** gives the total size of the result.

```
    integer, parameter :: N = 10
    integer, dimension(2), parameter :: Y_SHAPE = (/ 3, 2 /), &
      Z_SHAPE = (/ N, N /)
    integer :: I, J                          ! I and J are ACID variables.
    real, dimension(2) :: X
    real, dimension(3, 2) :: Y
    real, dimension(N * N) :: Q
    real, dimension(N, N) :: Z
! start
    X = (/ 4.5, 4.5 /)
    Y = reshape( (/ (I + 0.2, I = 1, 3), X, 2.0 /), Y_SHAPE )
    Q = (/ ((0.0, J = 1, I - 1), 1.0, (0.0, J = I + 1, N), I = 1, N) /)
    Z = reshape( Q, Z_SHAPE )
```

Here **Y_SHAPE** and **Z_SHAPE** are named array constants. Another array constant is assigned to **X**. In the assignment to **Y**, the source argument to the reshape function is an array constructor with six components: The first three are given by an implied **do** loop, the next two come from the vector **X**, and the sixth is the constant **2.0**. An array constructor is assigned to the vector **Q**, which is then reshaped to form **Z** and becomes an **N** by **N** identity matrix.

Vector Subscripts

A *vector* of integer type may appear as a subscript in an array section designator, along with any of the other allowed forms. The designated array section is formed by applying the elements of the vector subscript in sequence as subscripts to the parent array. Thus, the value of each element of the vector subscript must be within the array bounds for the parent array.

For example, suppose that *Z* is a 5 by 7 matrix and that *U* and *V* are vectors of lengths 3 and 4, respectively. Assume that the elements of *U* and *V* have the following values:

```
U   1, 3, 2
V   2, 1, 4, 3
```

Then, **Z(3, V)** consists of elements from the third row of *Z* in the following order:

```
Z(3, 2), Z(3, 1), Z(3, 4), Z(3, 3)
```

Also, **Z(U, 2)** consists of elements from the second column:

```
Z(1, 2), Z(3, 2), Z(2, 2)
```

And, **Z(U, V)** consists of the following elements:

```
Z(1, 2), Z(1, 1), Z(1, 4), Z(1, 3),
Z(3, 2), Z(3, 1), Z(3, 4), Z(3, 3),
Z(2, 2), Z(2, 1), Z(2, 4), Z(2, 3)
```

In the most useful applications, the elements of the subscript vector consist of a permutation of consecutive integers, as in these examples. The same integer may appear more than once in a subscript vector, but this practice is error-prone and should be done only with great care.

Vector subscripts are prohibited in certain situations. In particular, an actual argument to a procedure must not be an array section with a vector subscript if the corresponding dummy argument array is given a value in the procedure. Furthermore, an array section designated by a vector subscript with a repeated value must not appear on the left side of an assignment statement nor as an input list item.

The rank of an array section is the number of subscript positions that contain either a colon or the name of an integer vector (vector subscript). The extent of an array section along each dimension is simply the number of elements specified by the section designator for that dimension. For a vector subscript, the extent is determined by the number of elements in the vector.

1.2 ARRAY TECHNIQUES

This section examines some array processing techniques that are generally useful; many of these will be applied in later chapters.

Operation Counts and Running Time

An important purpose of this textbook is to compare different methods of accomplishing the same result. Several different factors in this comparison are discussed in Chapter 4, but the major one is *running time*. For numerical work, as in most traditional Fortran “number crunching” applications, running time is dominated by floating point operations (especially by multiplication time). On the other hand, for the nonnumerical applications that are the subject of this text it is more useful to count *comparison* operations and *move* operations.

It is assumed here that comparisons and moves account for most of the running time, or else that these are typical operations and that total running time is proportional to some combination of these. This assumption is unrealistic in actual practice, of course, for several reasons. First, it ignores the overhead of loop control, procedure reference, etc., which can dominate the "useful" operations in a tight loop or in a short procedure. Furthermore, as Bill Long has pointed out, memory loads are probably a more relevant factor than moves because the processor must wait for their completion, whereas most processors accomplish memory stores asynchronously.

Consider a procedure for exchanging two array elements with the aid of an auxiliary variable. This example illustrates the methods and notation that will be used. Declarations and other nonexecutable statements are omitted. Line numbers are given at the right for reference.

Operation Counts for Swap Subroutine

```
Aux = Array(I)                                                    ! 1
Array(I) = Array(J)                                               ! 2
Array(J) = Aux                                                    ! 3
```

The subroutine performs three move operations and no comparisons.

If *I* and *J* have the same value, **Swap** accomplishes nothing. At the cost of one comparison, the three move operations might be saved:

```
if (I /= J) then                                                  ! 1
  Aux = Array(I)                                                  ! 2
  Array(I) = Array(J)                                             ! 3
  Array(J) = Aux                                                  ! 4
end if                                                            ! 5
```

This subroutine always performs one comparison, at line 1, and it sometimes performs three moves.

Which version runs faster? The answer depends upon the relative times of comparison operations and move operations, and whether the moves are required. Let *p* be the probability that *I* and *J* are different; then the expected operation counts for the second subroutine are one comparison and 3*p* moves.

Assuming for the moment that a comparison takes the same amount of time as a move, the first subroutine performs three operations and the second performs 3*p* +1 operations. If *p* is larger than 0.67, the first subroutine is faster.

For most applications described in this text, swapping an item with itself is rare *(p* is close to 1) and the test should be omitted.

However, the relative timing of comparison and move operations can change from one application to another. Data base comparisons employ a *key* that is often a relatively small part of each item; thus the move operation takes considerably longer than the comparison. For some *indexed* data base applications, however, only pointers are moved, so the move time and comparison time are more nearly equal. For an indexed application with a long key, comparison operations can require more time than moves.

The Invariant Assertion Method

Some array techniques employ a repetitive procedure or loop that can be designed and verified with the aid of an *invariant assertion.* Consider the following example.

Suppose that you are a bunk bed salesman. Kensington Residential Academy wants to buy new bunk beds for its dormitories, which must be long enough for the tallest student at the Academy. You need to find the tallest student so that you can order beds according to his height. So you stand at the door of the dining hall as the students file in, one at a time.

How do you proceed? Imagine that you have solved a portion of the problem. Some (but not all) of the students have entered, and you have found the tallest student among those who are now in the hall. You have asked this tallest student to stand aside, at the left of the doorway.

One more student enters. What do you have to do to solve this *incremental* problem? If the next student is taller than the one standing by the door, you ask the next student to stand there instead. If the next student is not taller, you leave the previous student standing there. Now the tallest student in the slightly larger group is standing by the doorway.

An invariant assertion for an event that occurs repeatedly, such as students entering the dining hall one at a time, is a statement that is true after each repetitive occurrence. For the bunk bed problem, a suitable assertion is the following:

> "The tallest student in the dining hall is now standing by the doorway."

An invariant assertion has the following properties:

- The assertion must be true initially, before repetition begins.

  You must do something special with the first student. When he enters, you ask him to stand aside, and you start the repetitive process with the second student.

- Each occurrence of the repetitive process must maintain the validity of the assertion. That is, it can be verified that *if* the assertion is true prior to a repetitive step, *then* it remains true after that step. This is what "invariant" means.

  For the bunk bed problem, you check the height of each new student who enters and you replace the current tallest student if the new one is taller. This guarantees that the assertion remains true.

- Validity of the assertion at the end of the repetition describes the goal of the entire process.

  When all of the students have entered the hall, the process terminates, and the student standing by the doorway is the tallest of them all.

The design of a loop can often be facilitated by trying to find an invariant assertion. This is not always easy. For array applications, by analogy to the problem of finding the tallest student, it often involves imagining the situation when a typical section of the array (but not all of it) has been processed. The invariant assertion then tells what should happen when the section is enlarged by one element.

Smallest Element in an Array Section

A procedure for locating the smallest element in a section of an array **`Array(Lo: Hi)`** can be constructed by analogy to the bunk bed problem. The procedure employs a loop to examine portions of the array section, incorporating one more element at each iteration. At each step, the variable *Min_Val* records the smallest value among the elements examined so far. The *location* (subscript value) where the smallest element was found is also recorded.

An appropriate invariant assertion is:

> "The variable **`Min_Val`** records the smallest element in the current portion of the array,
> and **`Loc`** records the location (subscript value) where it was found."

The assertion is made true initially by assigning *ArrayLo* to *Min_Val* and *Lo* to *Loc.*

```
Min_Val = Array(Lo)
Loc = Lo
```

Iteration begins with the element at subscript position *Lo* + 1. To guarantee the validity of the assertion when a new item $Array_I$ is incorporated, *Min_Val* is compared with the new item and replaced if necessary.

```
do I = Lo + 1, Hi
   if (Array(I) < Min_Val) then
      Min_Val = Array(I)
      Loc = I
   end if
end do
```

At loop termination, the assertion is:

> "The variable **Min_Val** records the smallest element in the *entire array section,* and **Loc** records the location where it was found."

The array section has grown to encompass the entire array, and the current value of *Loc* is the desired result value.

Operation Counts for Minimum_Location

```
Min_Val = Array(Lo)                                    ! 1
Loc = Lo                                               ! 2
do I = Lo + 1, Hi                                      ! 3
  if (Array(I) < Min_Val) then                         ! <4
    Min_Val = Array(I)                                 ! <5
    Loc = I                                            ! <6
  end if                                               ! <7
end do                                                 ! <8
```

The number of data items processed by this function is $P = Hi + 1 - Lo$. The function includes one comparison at line 4 and data moves at lines 1 and 5. Only those steps that move an actual data item are counted. The loop body contains one comparison and one move. The comparison is executed once for each iteration of the loop, so there are $P - 1$ comparisons altogether. The expected number of moves (including the extra move at line 1) can be shown to be $\sum_{i=1}^{P}(1 / i)$; $\ln P + 0.6$ approximates this sum.[4]

Say It with Fortran

Fortran provides standard intrinsic functions **minval** and **minloc**, which return the value and location of the smallest element in an array or array section; corresponding functions **maxval** and **maxloc** are also provided. However, these intrinsic functions can be applied only to arrays of integer or real type; extension to character type is proposed for a future version of Fortran.

Furthermore, coding the operation explicitly illustrates the Fortran techniques involved. The following function locates the smallest element in the portion of an array of strings that is bounded by subscript limits given as the arguments *Lo* and *Hi*. The result variable, *Loc*, is an integer that locates the smallest element of *Array* to be found between subscript positions *Lo* and *Hi*.

When this function is used, it will *inherit* a requirement for explicit type declarations from its host. A calling program will refer to the function by the name **Minimum_Location**, but within the function the result value is called **Minimum_Location_R**.

The keyword **pure** in a function heading is recognized by Fortran 95 as an assertion that the function has no *side effects* — i.e., it has no external effects except for returning the result value. This keyword is not recognized by Fortran 90, and the electronically distributed Fortran 90 versions omit it.

[4] Paul Zeitz and Chuckson Yokota, private communications. Here, *Euler's constant* $\gamma = 0.5772 \ldots$ plus some further terms (negligible for large *P*) in the "harmonic sum" are estimated by the constant 0.6; see D. E. Knuth, *Fundamental Algorithms*, The Art of Computer Programming, vol. 1 (Reading: Addison-Wesley, 1968), 73ff.

Here $\ln P$ is the natural logarithm, base $e = 2.718 \ldots$. Natural logarithms appear rarely in this text; the most useful logarithmic base for algorithm analysis is 2. This text uses the notation $\lg P$ for the base 2 logarithm of *P*. The value of $\lg P$ is about 1.44 times the natural logarithm of *P* or 3.32 times the common (base 10) logarithm of *P*; a Fortran program can compute $\lg P$ from either of the expressions **1.44269504 * log(P)** or **3.32192809 * log10(P)**. Twenty-digit values of these constants are $\log_2 e = 1.4426950408889634074$ and $\log_2 10 = 3.3219280948873623479$ (from Mathematica®).

```
! Function to find the smallest string in an array section.
  pure function Minimum_Location( Array, Lo, Hi ) result( Minimum_Location_R )
```

`Array` is an assumed-shape rank-1 array of assumed-length strings: Array extent and character length will be taken from the actual argument. `Lo` and `Hi` are integers. The dummy arguments are declared with `intent(in)`, which means that the function must not redefine them.

```
    character (len = *), intent(in), dimension(:) :: Array
    integer, intent(in) :: Lo, Hi
    integer :: Minimum_Location_R, Loop
```

The automatic-length local character variable `Min_Val` has the same length property as `Array`.

```
    character (len = Len( Array )) :: Min_Val
! start function Minimum_Location
    Min_Val = Array(Lo)
    Minimum_Location_R = Lo
    do Loop = Lo + 1, Hi
      if (Array(Loop) < Min_Val) then
        Min_Val = Array(Loop)
        Minimum_Location_R = Loop
      end if
    end do
```

The `return` statement before `end function` or `end subroutine` is optional, as is a `stop` statement before `end program`. As a matter of programming style preference, however, these redundant statements appear consistently in the examples in this text.

```
    return
  end function Minimum_Location
```

If the function `Minimum_Location` is implemented as an internal procedure, some efficiency can be gained by passing the array by *inheritance* rather than as an argument, with the two subcript bounds as arguments.

Search in an Ordered Array

Some applications require searching an array for a specified *key*. If some array element value matches the key, the search procedure returns the location of the match; otherwise, it returns an indication that no matching key occurs in the array. For arrays that are not organized in any particular order, it may be necessary to examine every element. When the elements are known to be in ascending or descending order, however, searching can be simplified considerably.

Two methods for searching an ordered array are described in this section: *linear searching*, which can be expected to require comparison with only half of the elements in an ordered array of random values, and *binary searching*, for which the expected number of (3-way) comparisons is approximately lg N, where N is the size of the array.

Linear Search in an Ordered Array

Linear search in an array, here assumed to be in ascending order, compares the elements one at a time with a given key. The search may either succeed or fail.

During execution of the search loop, if an array element matches the key, the search is successful and no more array elements need to be compared, so the iteration terminates.

On the other hand, suppose that there is no matching element in the array. The first few array elements may be smaller than the key. When an element larger than the key is found, the search has gone beyond the point where a matching item would be if it were in the array. The search is unsuccessful and no more array elements need to be compared.

A third possibility is that the end of the array is reached without a matching element having been found; again, the search is unsuccessful.

As pointed out by Charles Zahn in 1974,[5] a program must be prepared to take quite different actions upon completion of a search procedure, depending upon whether the search is successful or unsuccessful. The procedure must return an indication of success or failure, as well as the location of the array element whose examination caused loop termination.

```
do Loop = 1, size( Array )
  if (Array(Loop) > Key) then
```

Terminate the search, returning the value of `Loop` *along with an indication that the search is unsuccessful.*

```
    :
  else if (Array(Loop) == Key) then
```

Terminate the search, returning the value of `Loop` *along with an indication that the search is successful.*

```
    :
  else
```

Continue searching. (The empty `else` *block may be omitted.)*

```
  end if
end do
```

Terminate the search, returning an indication that the search is unsuccessful because the end of the Array was reached.

A simple strategy is to record two positions, *Loc*_1 and *Loc*_2, that indicate array elements between which the *Key* value is known to lie. If the search is successful, these are given equal values; if the search is unsuccessful, they differ by one. The following procedure takes advantage of the Fortran convention that the index value is $N + 1$ if the loop is completed without execution of the **exit** statement:[6]

```
do Loop = 1, N
  if (Array(Loop) > Key) then
```

Terminate the search and `exit` *(to the end of the loop). Note that if* `Array(1)` *is larger than* `Key`*, loop* `exit` *will occur with* `Loop == 1`*; the statements that follow the loop will set* `Loc_1` *and* `Loc_2` *to* `0` *and* `1`*.*

```
    exit
  else if (Array(Loop) == Key) then
```

Terminate the search.

```
    Loc_1 = I
    Loc_2 = I
```

The fact that `Loc_1` *and* `Loc_2` *have equal values indicates that the search is successful. It is undesirable to* `exit` *(to the end of the loop) at this point — the assignment* `Loc_1 = I - 1` *must be skipped. In the Fortran procedure, a* `return` *statement provides an easy way to skip those unwanted steps.*

```
    return
```

[`else` *continue searching.]*

```
  end if
end do
```

[5] C. T. Zahn, “A Control Statement for Natural Top-Down Structured Programming,” *Proc. Colloque sur la Programmation*, Paris, April 1974.

[6] Recall that the index of a Fortran **do** loop is incremented before the test for termination is made, and the index value is preserved at normal termination.

The fact that `Loc_1` *and* `Loc_2` *have unequal values indicates that the search is unsuccessful. Note that if* `Array(N)` *is smaller than* `Key`*, the loop will terminate normally with* `Loop == N +1`*;* `Loc_1` *and* `Loc_2` *will be set to* `N` *and* `N +1`*.*

```
  Loc_1 = I - 1
  Loc_2 = I
```

The invariant assertion method can be applied to this problem; an appropriate assertion is:

$1 \le Loop \le N + 1$ and $Array_{Loop-1} \le Key < Array_{N+1}$

For this analysis, imagine that there is an extra fictitous array element at each end: $Array_0$ with a very large negative value and $Array_{N+1}$ with a very large positive value. (These fictitious elements are not actually created as part of the array, and they are never referenced by program statements. Their only role is in the invariant assertion.)

Taking into account the fictitious array elements, the assertion is true when *Loop* is initialized to 1 by loop contol processing. Because the array is in ascending order, $Array_i \le Array_j$ whenever $0 \le i \le j \le N + 1$.

The `return` statement in the `if` construct is executed only if a match is found. The `exit` statement is executed (and *Loop* is preserved) if $Array_{Loop} > Key$; normal loop termination (with $Loop = N + 1$, by Fortran convention) occurs if $Key > Array_N$. In either of these two latter cases, the statement following **end do** is reached with $1 \le Loop \le N + 1$ and $Array_{Loop-1} \le Key < Array_{Loop}$.

Say It with Fortran

The following Fortran function implements linear search for a *Key* among the elements of an array of character strings. One detail has been changed because a Fortran function can return an array but it cannot return two separate scalars. The two bracketing subscript values (named *Loc*_1 and *Loc*_2 in the foregoing discussion) are combined into a vector named *Linear_Search_R*.

```
! Linear search in an ordered array.
  pure function Linear_Search( Array, Key ) result( Linear_Search_R )
```

`Array` *is an assumed-shape rank-1 array of assumed-length strings;* `Key` *is an assumed-length string. Extent and character length of* `Array` *and character length of* `Key` *will be taken from the corresponding actual arguments.*

```
    character (len = *), intent(in), :: Array(:), Key
    integer, dimension(2) :: Linear_Search_R
! start function Linear_Search
    do Loop = 1, size( Array )
      if (Array(Loop) > Key) then
        exit
      else if (Array(Loop) == Key) then
```

The following statement assigns a scalar value to both vector elements.

```
        Linear_Search_R = Loop
        return
      end if
    end do
    Linear_Search_R(1) = Loop - 1
    Linear_Search_R(2) = Loop
    return
  end function Linear_Search
```

Binary Search in an Ordered Array

For a large ordered array, a *binary search* is much more efficient than the linear search just described. The idea of this method is to cut the search area in two at each step by finding out whether the key value is in the left half or the right half of the array. Since the array elements are in order, this determination can be made by examining just one element in the middle of the array. The selected half is again bisected, either the left half or the right half is chosen, and the process continues. The search area is ultimately reduced either to a single element that matches the key or else to two adjacent elements between which the key value lies.

Each time the search area is bisected, only one (3-way) comparison of the key with an array element is required. (As explained in the discussion of Operation Counts below, a 3-way comparison is equivalent, on the average, to 1.5 simple comparisons.) Therefore, the total number of comparisons, and the total number of repetitions of the loop, is proportional to lg N where N is the array size. A linear search in an ordered array of 10,000 elements may be expected to require some 5,000 comparisons, but a binary search never requires more than 15 three-way comparisons (or 21 simple comparisons). See also Exercise 6 at the end of this section.

The invariant assertion method can be applied to this problem. Let the variables *Loc_1* and *Loc_2* contain the index values of array elements between which the *Key* value is known to lie. It is possible, of course, that the key value is smaller or larger than all elements of the array. Again, the invariant assertion assumes fictitous elements $Array_0$ with a very large negative value and $Array_{N+1}$ with a very large positive value. An appropriate assertion is:

$$0 \le Loc\_1 \le Loc\_2 \le N + 1 \text{ and } Array_{Loc\_1} \le Key \le Array_{Loc\_2}$$

The assertion is made true initially by setting *Loc_1* to 0 and *Loc_2* to $N + 1$. The fact that the array is in ascending order implies that $Array_i \le Array_j$ whenever $0 \le i \le j \le N + 1$.

The loop is executed while the difference *Loc*_2 – *Loc*_1 is greater than 1. This difference measures the extent of the subscript range that currently encloses the *Key* value:[7]

```
Loc_1 = 0
Loc_2 = N + 1
do while (Loc_2 - Loc_1 > 1)
  Middle = (Loc_2 + Loc_1) / 2
    :
end do
```

At each iteration, the subscript range that encloses *Key* is bisected and either *Loc*_1 or *Loc*_2 is set to *Middle* to preserve the invariant assertion. However, it may happen that $Array_{Middle}$ exactly matches the search key. In this case, there is no further need to continue bisecting the array, so the loop is terminated:

```
Loc_1 = 0
Loc_2 = N + 1
do while (Loc_2 - Loc_1 > 1)
  Middle = (Loc_1 + Loc_2) / 2
  if (Key > Array(Middle)) then
    Loc_1 = Middle
  else if (Key < Array(Middle)) then
    Loc_2 = Middle
```

[7] Recall that Fortran integer division *truncates* the true quotient. If *Loc*_1 + *Loc*_2 is an even integer, the quotient is exact; if odd, the expression value is the next integer smaller than the true quotient. When *Loc*_1 and *Loc*_2 are some distance apart, a slight change in the bisection point has little effect. However, careful analysis is required when the two values are close together.

```
    else  ! Array(Middle) == Key
      Loc_1 = Middle
      Loc_2 = Middle
      exit
    end if
  end do
```

If no element of the array matches *Key*, the loop is completed without execution of the exit statement, with *Loc*_1 and *Loc*_2 pointing to the array elements next smaller and next larger than *Key*, or to 0 or *N* + 1 if *Key* is smaller or larger than all array elements. If a match occurs, both result integers point to the matching element. The loop exit conditions along with the invariant assertion give: $0 \le Loc\_1 \le Loc\_2 \le N$ and $0 \le Loc\_2 - Loc\_1 \le 1$ and $Array_{Loc\_1} \le Key \le Array_{Loc\_2}$.

Operation Counts for Binary_Search

```
  Loc_1 = 0                                            ! 1
  Loc_2 = size( Array ) + 1                            ! 2
  do while (Loc_2 - Loc_1 > 1)                         ! 3
    Middle = (Loc_1 + Loc_2) / 2                      ! < 4
    if (Key > Array(Middle)) then                     ! < 5
      Loc_1 = Middle                                  ! < 6
    else if (Key < Array(Middle)) then                ! < 7
      Loc_2 = Middle                                  ! < 8
    else  ! Array(Middle) == Key                      ! < 9
      Loc_1 = Middle                                 ! < 10
      Loc_2 = Middle                                 ! < 11
      exit                                           ! < 12
    end if                                           ! < 13
  end do                                             ! < 14
```

This function has no data move operations. (We ignore the extra assignments to *Loc_1* and *Loc_2*, and the comparison in the **do while** statement. Execution time for these is perhaps comparable to the loop overhead per iteration of a linear search procedure.)

The **if** construct has three branches. One comparison is required when the first branch is taken, which is almost half the time; a second comparison is required when the second branch is taken, which is almost all of the other half; the rarely executed third branch requires a third comparison. Thus the expected number of comparisons for the if construct is about 1.5.

In the worst case, no match is found and the loop body is executed lg(*N* +1) times, where *N* = size(*Array*), or the next lower integer if *N* is not a power of 2. The operation count for binary search in the worst case is 1.5 lg *N* comparisons.

In the best case, a match occurs at the first comparison and the total count is 1 comparison.

According to Knuth,[8] the average requires only one less iteration than the worst case, or 1.5·lg (*N* – 1) comparisons.

Say It with Fortran

The following function implements binary search for a key among the elements of an array of character strings. The function result is a vector *Binary_Search_R* of length 2, whose elements perform the roles of the scalars *Loc*_1 and *Loc*_2 in the preceding discussion. If *Key* is found in the array, both elements of the result vector are set to its array index. If *Key* is not found, the elements of the result vector indicate the two adjacent array elements between which the *Key* value lies.

[8] D. E. Knuth, *Sorting and Searching,* The Art of Computer Programming, vol. 3 [Reading: Addison-Wesley, 1973], 411.

```
! Binary search in ordered array.
  pure function Binary_Search( Array, Key ) result( Binary_Search_R )
```

Array is an assumed-shape rank-1 array of assumed-length strings; Key is an assumed-length string. Extent and character length of Array and character length of Key will be taken from the corresponding actual arguments.

```
    character (len = *), intent(in) :: Array(:), Key
    integer, dimension(2) :: Binary_Search_R, Middle
! start function Binary_Search
    Binary_Search_R(1) = 0
    Binary_Search_R(2) = size(Array) + 1
    do while (Binary_Search_R(2) - Binary_Search_R(1) > 1)
      Middle = (Binary_Search_R(1) + Binary_Search_R(2)) / 2
      if (Key > Array(Middle)) then
        Binary_Search_R(1) = Middle
      else if (Key < Array(Middle)) then
        Binary_Search_R(2) = Middle
      else ! Array(Middle) == Key
        exit
      end if
    end do
    return
  end function Binary_Search
```

Solving Systems of Linear Algebraic Equations

Perhaps the most important numerical array application is solving systems of linear algebraic equations such as the following:

$$3.0\,x + 6.0\,y - 6.0\,z = -9.0$$
$$1.0\,x + 0.0\,y + 3.0\,z = +7.0$$
$$3.0\,x + 4.0\,y + 0.0\,z = +3.0$$

The method of elimination named for Karl Friedrich Gauss (1777–1855) is a systematic way of solving such problems. As W. Kahan points out, the idea is to replace the given system of equations by another system that has the same solution but is much easier to solve. There are three kinds of transformations that do not change the solution set:

1) One of the equations may be multiplied or divided by a scalar constant;

2) A multiple of one of the equations may be added to or subtracted from another; or

3) Two of the equations may be interchanged.

Applying the Gauss method to this example, we divide the first equation by the coefficient of x, and then subtract appropriate multiples of the modified first equation from the second and third equations to eliminate x from those equations:

$$1.0\,x + 2.0\,y - 2.0\,z = -3.0$$
$$0.0\,x - 2.0\,y + 5.0\,z = +10.0$$
$$0.0\,x - 2.0\,y + 6.0\,z = +12.0$$

Next, we divide the second equation by the coefficient of y, and we subtract a multiple of the second equation from the third equation to eliminate the second variable from the third equation:

$$1.0\,x + 2.0\,y - 2.0\,z = -3.0$$
$$0.0\,x + 1.0\,y - 2.5\,z = -5.0$$
$$0.0\,x + 0.0\,y + 1.0\,z = +2.0$$

We now have a “reduced” set of equations whose solution is easily obtained by “back substitution”: The value $z = 2.0$ from the reduced third equation is substituted into the second equation to give $y = 0.0$, and these two values are substituted into the first equation to give $x = 1.0$.

Well before 1960, John von Neumann and others were already using computers to solve systems of equations. By the time George E. Forsythe and Cleve B. Moler wrote “Computer Solution of Linear Algebraic Systems” (Prentice-Hall, 1967), efficient solution and error estimation techniques were well developed. The present discussion translates, into modern Fortran syntax, the methods described by Forsythe and Moler more than 30 years ago.[9]

The usual implementation of Gauss elimination, for a system of n equations, stores the coefficients as the first n columns of an n by $n + 1$ matrix $\boldsymbol{A}$, with right side values in column $n + 1$. Thus, each row of $\boldsymbol{A}$ represents one of the equations. As the elimination proceeds, 1s appear in the diagonal positions of $\boldsymbol{A}$, representing, for each i, the coefficient of i in the ith equation. Zeros appear below the diagonal, representing the coefficient of i in equations after the ith. However, as we shall see, the program never actually refers to positions on and below the diagonal of $\boldsymbol{A}$.

A “first draft” Gauss elimination program is the following:

```
do I = 1, N
   do K = I + 1, N + 1
      A(I, K) = A(I, K) / A(I, I)
   end do
   do J = I + 1, N + 1
      do K = I + 1, N
         A(J, K) = A(J, K)- A(J, I) * A(I, K)
      end do
   end do
end do
```

Some Details of Gauss Elimination

Array sections. Fortran 90 array section notation can simplify some steps in this program. The first of the inner loops may be replaced by a single array assignment:

```
A(I, I + 1: N + 1) = A(I, I + 1: N + 1) / A(I, I)
```

Similar notation may be employed for subtracting multiples of a given row of this matrix from each of the rows below it. The doubly nested loop becomes an array section operation, with subscript ranges in both dimensions, to reduce all elements in the block `A(I + 1: N, I + 1: N + 1)`.

```
do I = 1, N
   A(I, I + 1: N + 1) = A(I, I + 1: N + 1) / A(I, I)
   A(I + 1: N, I + 1: N + 1) = A(I + 1: N, I + 1: N + 1) &
      - matmul( A(I + 1: N, I: I), A(I: I, I + 1: N + 1) )
end do
```

The call to `matmul` forms an *outer product* of parts of column i and row i of $\boldsymbol{A}$. The arguments are expressed as array sections of rank 2, with section subscript range `I: I` in one of the dimensions of each argument. It is a Fortran requirement that at least one of the arguments of `matmul` must have rank 2.

The remaining outer loop (which cannot be converted to array section syntax) applies the reduction step n times, once for each row, each time generating (“virtual”) zeros below the diagonal in the corresponding column. When row n is reached, there are no rows following it; the subscript range `(I + 1 : N)` is empty and no actual reduction occurs at this stage.

[9] See W. H. Press et al, *Numerical Recipes in Fortran 90* (Cambridge, UK: Cambridge Univ Press, 1996), p. 1014; and M. J. Maron and R. J. Lopez, *Numerical Analysis*, 3rd ed. (Belmont, Calif.: Wadsworth, 1991), algorithm 4.4B, p. 220. Example 1 in this section is based on Examples 5.15, 5.28, and 8.5 in *essential Fortran*, by Loren P. Meissner (Unicomp, 1997).

Choosing the pivotal row. We have seen how to use the *i*th row to generate zeros below the diagonal in the *i*th column. A complication arises in case the diagonal element $\boldsymbol{A}_{ii}$ happens to be zero. In this case, it is necessary to select another row below the *i*th where the element in column *i* is not zero, and to exchange that row with row *i* before proceeding with the reduction. (If all elements in column *i* below the diagonal are zeros, the system does not have a unique solution.) The element that is moved to the diagonal position is called the *pivot* element. Some pivot choices are known to result in smaller numerical error than others. The method described here, called *scaled partial pivoting,* consists of choosing the largest element in column *i,* in absolute value, relative to a scale factor $\boldsymbol{s}_i$ which is the largest coefficient in row *i* before reduction begins.

The intrinsic function `maxloc` may be employed to find the pivot element. The Fortran 90 version of this intrinsic function returns a vector of length one; a Fortran 95 variant is simpler because it returns a scalar when the optional `dim` argument is present.

```
Loc = maxloc( abs( A(I: N, I) / S(I: N) ), dim = 1 )              ! Fortran 95
```

The argument of `maxloc` is a section, with lower bound *i*, from the vector of absolute values of elementwise quotients $| \boldsymbol{A}_{ji} \ / \ \boldsymbol{s}_j \ |$, $j = i, n$. The function result is an integer value that locates the largest element relative to the beginning of the specified array section; this value must be adjusted to the top of the actual column. Within $\boldsymbol{A}$ itself, the column subscript value of the largest element is `Loc + I - 1`.

Indirect row interchange. It is not necessary to actually interchange the rows of the matrix $\boldsymbol{A}$. Instead, elements of a permutation vector $\boldsymbol{p}$ (of integer type) are interchanged, and references to rows of $\boldsymbol{A}$ apply elements of this vector as subscripts:

```
do I = 1, N
  A(P(I), I + 1: N + 1) = A(P(I), I + 1: N + 1) / A(P(I), I)
  A(P(I + 1: N), I + 1: N + 1) = A(P(I + 1: N), I + 1: N + 1) &
    - matmul( A(P(I + 1: N), I: I), A(P(I, I), I + 1: N + 1) )
end do
```

Interchange can be performed in three steps:

```
Temp = P(Loc + I - 1)
P(Loc + I - 1) = P(I)
P(I) = Temp
```

The permutation vector is initialized with the sequence of integers, 1, 2, . . . , *n*. An array constructor is suitable for this initialization:

```
P =(/ (K, K = 1, N) /)
```

Back substitution. After reduction has been completed, back substitution takes place. In our Fortran program, elements of the solution $\boldsymbol{x}$ will replace those of $\boldsymbol{b}$ in row $n + 1$ of $\boldsymbol{A}$; we continue to apply the permutation vector $\boldsymbol{p}$ to row indices. Equation *n* involves only the *n*th variable, whose coefficient in the reduced system is 1. Hence, the value of this variable is the *n*th right side element in the reduced system, and is located at $\boldsymbol{A}_{n,n+1}$. Each of the other variables in turn (working backward from $n - 1$ to 1) is computed as

$$\boldsymbol{x}_i = \boldsymbol{b}_i - \sum_{k = i + 1}^{n} \boldsymbol{A}_{ik} \, \mathbf{x}_k$$

The sum is of course a scalar product, and can be expressed with the intrinsic function `dot_product`:

```
A(P(J), N + 1) = A(P(J), N + 1) &
  - dot_product( A(P(J), J + 1: N), A(P(J + 1: N), N + 1) )
```

The first argument of `dot_product` is row $\boldsymbol{p}_j$ of $\boldsymbol{A}$; the second argument is column $n + 1$ of $\boldsymbol{A}$. The permutation vector $\boldsymbol{p}$ is applied as a row subscript to this column vector.

Say It with Fortran

A Fortran implementation of the Gauss elimination algorithm described in the foregoing paragraphs, with scaled partial pivoting and back substitution, appears as follows:

```
  subroutine Gauss( A, X, Flag )
```

A is an assumed-shape N by N + 1 matrix. At entry to the subroutine, the right side vector has been stored in column N + 1 of A; at exit, the solution vector has replaced it. The subroutine sets Flag to .false. if A is singular. A permutation vector is applied to all row subscripts to avoid physically interchanging rows. Local arrays have automatic shape. K is an array constructor implied do variable.

```
    real, dimension(:, :), intent (in out) :: A
    real, dimension(:), intent (out) :: X
    logical, intent (out) :: Flag
    real, dimension(size( A, dim = 1 )) :: S
    integer, dimension(size( A, dim = 1 )) :: P
    integer :: N, K, I, Loc, Temp
```

Start subroutine Gauss

```
    N = size( A, dim = 1 )
```

The following steps initialize the permutation vector P to a sequence of consecutive integers, and store a copy of the largest element (in absolute value) in each row in the corresponding element of S.

```
    P = (/ (K, K = 1, N) /)
    S = maxval( abs( A ), dim = 2 )
    Flag = .false.
    if (any( S <=0 )) then
      print *, " One of the row norms is zero. "
      return
    end if
```

Block reduction: For each column, the largest element below the diagonal is located; the permutation vector is modified to record this location. Then the indicated row is divided by the diagonal element, and multiples are subtracted from each of the remaining rows.

```
    do I = 1, N
      Loc = maxloc( abs( A(I: N, I) / S(I: N) ), dim = 1 )
      if (Loc <= 0) then
        print *, " A is singular."
        return
      else
        Temp = P(Loc + I - 1)
        P(Loc + I - 1) = P(I)
        P(I) = Temp
      end if
      A(P(I), I + 1: N + 1) = A(P(I), I + 1: N + 1) / A(P(I), I)
      A(P(I + 1: N), I + 1: N + 1) = A(P(I + 1: N), I + 1: N + 1) &
        - matmul( A(P(I + 1: N), I: I), A(P(I: I), I + 1: N + 1) )
    end do
```

Back substitution: The reduced right side, now stored in row N + 1 of A, is replaced by the required solution.

```
    do I = N, 1, -1
      X(I) = A(P(I), N + 1) - dot_product( A(P(I), I + 1: N), X(I + 1: N) )
    end do
    Flag = .true.
    return
  end subroutine Gauss
```

Multiple right sides. The Gauss elimination program is easily modified to process multiple right sides with the same coefficient matrix. The right sides are stored as `A(:, N + 1: N + M)`. Row operations are extended to column `N + M`. The scalar product in the back substitution step is changed to use the intrinsic function `matmul`, with the same first argument as before and the second argument changed to a matrix with column subscript `N + 1: N + M`.

Crout Factorization

In the reduced system generated during Gauss elimination, the coefficient of $\boldsymbol{x}_i$ is 1 in the *i*th equation and 0 in all subsequent equations. These values do not need to be stored explicitly, however, because the program never actually refers to them.

A variant known as Crout factorization employs these matrix positions, on and below the main diagonal of ***A*** (taking into account row interchanges), to record the multipliers that are applied when each row is subtracted from the rows below it. The computation can be rearranged so that all operations on a given element are performed in sequence. A modern optimizing Fortran compiler can preserve the common element in a register—even in an extended precision register—for higher speed and accuracy.

The effect of this Crout reduction algorithm is to replace ***A*** by a pair of triangular matrices, ***L*** and ***U***, such that $\boldsymbol{A} = \boldsymbol{L} \times \boldsymbol{U}$, where ***U*** is an upper triangular matrix and ***L*** is lower triangular. Elements of ***U*** are the same as the coefficients in the equations after Gauss elimination has been applied, and elements of ***L*** are the multipliers that are applied to perfom the elimination. The computations required for Crout factorization are the same as for Gauss elimination except that they are performed in a different sequence and the multipliers are saved.

After ***L*** and ***U*** have been computed from ***A***, the system $\boldsymbol{L}\,\boldsymbol{c} = \boldsymbol{b}$ (where ***b*** is the given right side) is easily solved for ***c***, because ***L*** is a lower triangular matrix. This solution process, called forward substitution, is described later. The solution vector ***c*** from this linear system is identical to the reduced right side obtained by “ordinary” Gauss elimination. (To see this, note that $\boldsymbol{U} = \boldsymbol{L}^{-1}\boldsymbol{A}$ and $\boldsymbol{c} = \boldsymbol{L}^{-1}\boldsymbol{b}$. The transformation by which Gauss elimination converts ***A*** to ***U*** is represented by the matrix $\boldsymbol{L}^{-1}$; the elimination process applies this same transformation $\boldsymbol{L}^{-1}$ to the right side ***b***.)

The matrices ***L*** and ***U*** share the storage space of ***A***, replacing the elements of ***A*** as factorization progresses. ***U*** is stored above the main diagonal and ***L*** is stored below (and on) the diagonal. There is no storage for the diagonal elements of ***U***; each of these represents a leading coefficient that is set to 1 at the beginning of a stage of the elimination. The program takes these values into account implicitly, and does not need to store them.

Incorporating row interchanges, the actual factorization can be represented as $\boldsymbol{P}\,\boldsymbol{A} = \boldsymbol{L}\,\boldsymbol{U}$. The permutation matrix $\boldsymbol{P}$ is defined by interchanging the rows of an identity matrix in the designated manner. (In the actual program, however, row interchanges are recorded in compact form, as a vector rather than as a matrix.) The given system $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$ becomes $\boldsymbol{P}\,\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{P}\,\boldsymbol{b}$ or (after the factorization) $\boldsymbol{L}\,\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{P}\,\boldsymbol{b}$. Here $\boldsymbol{P}\,\boldsymbol{b}$ is simply the permuted version of the given right side vector, which we may call $\boldsymbol{b}^{\sim}$. Once $\boldsymbol{L}$, $\boldsymbol{U}$, and $\boldsymbol{P}$ have been found by the factorization process, forward substitution is applied to solve the lower triangular system $\boldsymbol{L}\,\boldsymbol{c} = \boldsymbol{b}^{\sim}$. As before, back substitution is applied to solve $\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{c}$.

With this method, processing the right side may be postponed until after the factorization is completed, rather than being accomplished concurrently. The factors $\boldsymbol{L}$ and $\boldsymbol{U}$ are stored and row interchanges are recorded. After the factorization is complete, permutation is applied to the right side. Forward substitution with $\boldsymbol{L}$ followed by backward substitution with $\boldsymbol{U}$ now gives the solution $\boldsymbol{x}$.

This postponement of right side processing can be important. Some applications involve several systems of equations with the same coefficients but with different right sides. The factorization step involves only the coefficient matrix, and needs to be performed only once. Later, forward and backward substitution can be applied separately to each of the right sides. The number of computation steps required for Crout factorization (done only once) is roughly proportional to n^3, while the number of steps for forward and back substitution (repeated for each different right side) is proportional to n^2. The following are two such applications:

- For some very common data fitting calculations, $\boldsymbol{A}$ depends upon the characteristics of a measuring instrument while $\boldsymbol{b}$ is obtained from measured data values. Thus, the factorization can be performed once and applied to many sets of data over the lifetime of the instrument.
- The process of iterative refinement, which is a simple way to improve the accuracy of the solution of many linear algebraic systems and to estimate the validity of the result, is described below. This process requires solving a related system with the same matrix $\boldsymbol{A}$ and with a new right side that is not available at the time of the original reduction process, being computed as a high precision residual.

Factorization alternates between reducing a column of $\boldsymbol{L}$ (below the diagonal) and a row of $\boldsymbol{U}$ (to the right of the diagonal). A preliminary Crout factorization program that ignores row interchanges and “unrolls” all array section operations into explicit loops appears as follows:

```
do I = 1, N
   ! Reduce column I
   do J = I, N
      do K = 1, I - 1
         A(J, I) = A(J, I) - A(J, K) * A(K, I)
      end do
   end do
   ! Reduce row I
   do J = I + 1, N
      do K = 1, I - 1
         A(I, J) = A(I, J) - A(I, K) * A(K, J)
      end do
      A(I, J) = A(I, J) / A(I, I)
   end do
end do
```

Column reduction. Each element in column *i* of ***L*** is reduced by subtracting products of elements, obtained by multiplying an element in the row to the right of that element with a corresponding element in the column of ***U*** above the diagonal. (Note that there is nothing to subtract when *i* is 1).

```
do J = I, N
   do K = 1, I - 1
      A(J, I) = A(J, I) - A(J, K) * A(K, I)
   end do
end do
```

The computation in the inner loop is equivalent to subtracting a scalar product of two vectors; the range of values of the index variable *k* becomes the row subscript range for one of the vectors and the column subscript range for the other vector:

```
do J = I, N
   A(J, I) = A(J, I) - dot_product( A(J, : I - 1) * A(: I - 1, I) )
end do
```

This loop is eliminated by further use of array section notation. The row vectors are combined into a matrix that is multiplied by the same column vector as before:

```
A(I:, I) = A(I:, I) - matmul( A(I:, : I - 1) * A(: I - 1, I) )
```

A special Fortran rule permits one (but not both) of the arguments of **`matmul`** to have rank 1.

To reflect row interchanges, the permutation vector ***p*** must be applied to all row subscripts of ***A***:

```
A(P(I:), I) = A(P(I:), I) &
      - matmul( A(P(I:), : I - 1) * A(P(: I - 1), I) )
```

Row reduction. Each element in the row of ***L*** is similarly reduced. Note that when *i* = 1 the inner loop collapses and the only effect is to divide the row by its diagonal element; also, the outer loop collapses when *i* = *n*.

```
do J = I + 1, N
   do K = 1, I - 1
      A(I, J) = A(I, J) - A(I, K) * A(K, J)
   end do
   A(I, J) = A(I, J) / A(I, I)
end do
```

As before, the loops can be converted to array section and matrix multiplication operations. Row interchanges are applied, and division by the diagonal element is incorporated into the assignment operation:

```
A(P(I), I + 1: ) = (A(P(I), I + 1:) &
   - matmul( A(P(I), : I - 1), A(P(: I - 1), I + 1:) )) / A(P(I), I)
```

The column reduction loop and the row reduction loop have each been reduced to a single array assignment statement. Only the outer loop remains.

Say It with Fortran

In the following Fortran implementation, the subroutine Factor computes the factors ***L*** and ***U*** (stored in ***A***) and the permutation vector ***p***.

```
! Crout Factorization with scaled partial pivoting.
  subroutine Factor( Flag )
```

A, P, and N are inherited from a containing program unit. A is an N by N matrix; P is an integer vector of length N; At entry to the subroutine, the coefficient matrix is stored in A. Upon completion, the factors of A have replaced A and the permutation is recorded in P. The local array S has automatic shape. K is an array constructor implied do variable.

```
    logical, intent( out ) :: Flag
    real, dimension(size( A, dim = 1 )) :: S
    integer :: K, I, Loc, Temp
! start subroutine Factor
    Flag = .false.
```

The following steps initialize the permutation vector P to a sequence of consecutive integers, and store a copy of the largest element (in absolute value) in each row in the corresponding element of S.

```
    P = (/ (K, K = 1, N) /)
    S = maxval( abs( A ), dim = 2 )
    if (any( S <=0 )) then
      print *, " One of the row norms is zero. "
      return
    end if
```

Column reduction and row reduction are performed alternately.

```
    do I = 1, N
```

Reduce column I.

```
      A(P(I:), I) = A(P(I:), I) &
        - matmul( A(P(I:), : I - 1), A(P(:I - 1), I))
```

Find the largest element (in absolute value) in the reduced column.

```
      if (all( A(P(I:), I) == 0 )) then
        print *, " All pivot candidates are zero. "
        return
      else
        Loc = maxloc( abs( A(P(I:), I) ) / S(P(I:)), dim = 1 )
        Temp = P(Loc + I - 1)
        P(Loc + I - 1) = P(I)
        P(I) = Temp
      end if
```

Reduce row I.

```
      A(P(I), I + 1:) = (A(P(I), I + 1:) &
        - matmul( A(P(I), : I - 1), A(P(: I - 1), I + 1:) )) / A(P(I), I)
    end do
    Flag = .true.
    return
  end subroutine Factor
```

A separate subroutine applies the result of Crout factorization to a right side vector. This subroutine could easily be modified to process multiple right sides. The arguments ***B*** and ***X*** and the local array ***C*** would all be changed to *n* by *m* matrices; scalar products in the forward and back substitution steps would be changed to matrix multiplication.

```
  subroutine For_Bak( B, X )
```

A, P, and N are inherited from a containing program unit. A previous call to Factor has replaced A with its LU factorization, and has recorded the permutation in P. The vectors B and X have length N.

```
    real, dimension(:), intent( in ) :: B
    real, dimension(:), intent( out ) :: X
    real, dimension(N) :: C
    integer :: I
```

Start subroutine For_Bak

Forward substitution.

```
    do I = 1, N
      C(I) = (B(P(I)) - dot_product( A(P(I), : I - 1), C(: I - 1) )) / A(P(I), I)
    end do
```

Back substitution.

```
    do I = N, 1, -1
      X(I) = C(I) - dot_product( A(P(I), I + 1:), X(I + 1:) )
    end do
    return
  end subroutine For_Bak
```

Iterative Refinement

Once upon a time, a linear system $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$ was considered difficult if the *determinant* of its coefficient matrix ***A*** was small. It is now understood that a much more significant criterion is the *condition number* of the coefficient matrix. This number, cond (***A***), is the product of the norms of ***A*** and of its inverse. Multiplying an *n* by *n* matrix by a scalar *k* has no effect on the condition number, but multiplies the determinant by k^n. It is possible to obtain a fairly accurate and rather inexpensive estimate of cond (***A***) as a byproduct of solving the linear system.

Forsythe and Moler (page 20) describe cond (***A***) as a measure of the maximum distortion that the linear transformation with matrix ***A*** makes on the unit sphere, which is a bound for the ratio of the relative uncertainty of the solution ***x*** to that of the given right side ***b***. The value of cond (***A***) is always 1 or greater; if its order of magnitude is 10^n, the solution can contain approximately *n* fewer correct significant decimal digits than the data. Thus, in single precision on typical IEEE hardware the data is represented with about 6 decimals, and a condition number as large as 10^6 can indicate that the solution is worthless.

Small matrices as “ill conditioned” as this do not appear every day, but they are not extremely rare, either: As an example, the 2 by 2 matrix ***A*** with $a_{ij} = n + i + j$, where *n* is large, has determinant –1 and (depending on the norm) condition number approximately $4n^2$: The condition number of the matrix

$$\begin{pmatrix} 499 & 500 \\ 500 & 501 \end{pmatrix}$$

is about 10^6.

The accuracy of a computed solution $\boldsymbol{x}_c$ can be checked by calculating the residual vector $\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\,\boldsymbol{x}_c$ which would be zero if there were no numerical errors. In practice (as Wilkinson discovered early in the days of computing), any well constructed Gauss elimination or Crout factorization program produces a solution with an acceptably small residual, so practically nothing is learned by simply calculating the residual. However, solving the system $\boldsymbol{A}\,\boldsymbol{e} = \boldsymbol{r}$ gives an estimate of $(\boldsymbol{x} - \boldsymbol{x}_c)$, the *error* in $\boldsymbol{x}$:

$$\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\,\boldsymbol{x}_c = \boldsymbol{A}\,\boldsymbol{x} - \boldsymbol{A}\,\boldsymbol{x}_c = \boldsymbol{A}\,(\boldsymbol{x} - \boldsymbol{x}_c)$$

The solution $\boldsymbol{e}$ can be used as an error estimate or can be added to $\boldsymbol{x}_c$ to refine the solution. For the latter purpose, the residual must be calculated with high precision.

If the data is represented with 6 digits and the *relative error* norm($\boldsymbol{e}$) / norm($\boldsymbol{x}_c$) is 10^{-2}, we say that the solution contains 4 fewer significant digits than the data, and we may estimate cond($\boldsymbol{A}$) as 10^4. Loosely speaking, with 6-decimal hardware we might have expected the relative error to be as small as10^{-6} but we find it to be 10^4 times as large as we expect; the factor 10^4 is attributable to the large condition number. We may add $\boldsymbol{e}$ to $\boldsymbol{x}_c$ to obtain a refined solution.

If we iterate this process, we find that the relative error decreases by about the same amount each time: in this example, the relative error should be about 10^{-4} after the first refinement and about 10^{-6} (as good as can be obtained with 6-digit arithmetic) after the second. For further details, see Chapter 13 of the book by Forsythe and Moler. The electronically distributed examples include program D01C which applies the Crout method without iterative refinement, and D01 with refinement. The first set of example data is an ill-conditioned problem with a known solution; the Crout solution (and the first step of iterative refinement) contains two or three correct decimal digits; after the third iteration, the solution is correct to IEEE hardware precision.

Iterative refinement costs very little (see Exercise 7 below), especially in view of the valuable information that it provides. As pointed out earlier, most of the computational effort of the Crout method is in the factorization. If the factors are saved, little extra work is required for solving the related system $\boldsymbol{A}\,\boldsymbol{e} = \boldsymbol{r}$. Each step of iterative refinement computes a new residual and applies forward and back substitution to obtain a new estimate of the error.

Example 1. The following program performs Crout factorization with partial pivoting, indirect row interchange, and iterative refinement. It processes multiple right sides, as described earlier. (If there is only one right side, it must be formatted as an *n* by 1 array and not as a vector.) Working storage employs private allocatable arrays at the module level. These remain allocated so that new right sides may be processed.

```
! Example 1. Linear Algebraic Equations by Crout Factorization
! with Iterative Refinement
module D01_M
```

Specification part

```
  implicit none
  public :: Solve, Iterate
  private :: Factor, For_Bak, Residual
  integer, parameter, private :: HI = kind( 1.0d0 )
  integer, save, private :: N
  real, dimension(:, :), allocatable, save, private :: LU
  real(kind = HI), dimension(:, :), allocatable, save, private :: Save_A
  integer, dimension(:), allocatable, save, private :: P
  logical, save, private :: Saved, Exist = .false.
  integer, private :: I
```

Procedure part

```
contains
```

```
  subroutine Solve( A, B, X, Rel_Err, Flag )
```

This subroutine solves the system of simultaneous linear algebraic equations A X = B, where A is an N by N matrix and X and B are N by M matrices. A and B are assumed-shape arrays supplied by the calling program. X, Rel_Err, and Flag are computed and returned by Factor. Solve does not change A or B. On return from Solve, X contains the solution and Rel_Err contains an estimate of the relative error in X. However, if Flag is false, the contents of X and Rel_Err are unpredictable, since the algorithm has short-circuited. The problem size N, a copy of A, and the LU decomposition matrix (with permutation vector P) are saved as private module-level variables, and are not changed except when Solve is called.

DUMMY ARGUMENTS and LOCAL DATA (K is an array constructor implied do variable.)

```
    real, dimension(:, :), intent (in) :: A, B
    real, dimension(:, :), intent (out) :: X
    real, intent (out) :: Rel_Err
    logical, intent (out) :: Flag
    integer :: K
```

Start subroutine Solve. Determine problem size; initialize private arrays

```
    Saved = .false.
    Flag = .false.
    N = size( A, dim = 1 )
    if (size( A, dim = 2 ) /= N &
      .or. size( B, dim = 1 ) /= N &
      .or. any( shape( X ) /= shape( B ) )) then
      print *, " SOLVE argument shape incompatibility."
      return
    end if
```

Allocate working arrays. Exist is a logical variable at the module level that is true when the necessary arrays have been allocated. Save a high-precision copy of A (without row interchanges) for the residual calculation. Store row norms in S.

```
    if (Exist) deallocate( Save_A, LU, P )
    if (N == 0) then
      Exist = .false.
      return
    end if
    allocate( Save_A(N, N), LU(N, N), P(N) )
    Exist = .true.
    Save_A = real( A, kind = HI )
    LU = A
    P = (/ (K, K = 1, N) /)
    call Factor( )
```

Saved is a logical variable at the module level that is true when a Crout factorization has been performed and the necessary arrays have been saved so that a solution can be calculated from any given right side.

```
    if (Flag) then
      Saved = .true.
      call For_Bak( B, X )
      call Iterate ( B, X, Rel_Err )
      if (Rel_Err > 0.5 )) then
        print *, " Relative Error > 0.5.", Rel_Err
        Flag = .false.
      end if
    end if
    return
```

```
  contains
```

*Internal procedure to perform factorization A = L * U with scaled partial pivoting. Column reduction and row reduction are performed alternately.*

```
    subroutine Factor( )
```

LOCAL DATA

```
      real, dimension(N) :: S
      integer :: I, Loc, Temp
```

Start subroutine Factor

```
      Flag = .false.
      S = maxval( abs( LU ), dim = 2 )
      if (any( S <= 0 )) then
        print *, " Row norms: ", S
        print *, " One of the row norms is zero. "
        return
      end if
      do I = 1, N
```

Reduce column I.

```
        LU(P(I:), I) = LU(P(I:), I) &
          - matmul( LU(P(I:), : I - 1), LU(P(:I - 1), I) )
```

Find the largest element (in absolute value) in the reduced column; record row interchange in P.

```
        if (all( LU(P(I:), I) == 0 )) then
          print *, " All pivot candidates are zero. "
          return
        else
          Loc = maxloc( abs( LU(P(I:), I) ) / S(P(I:)), dim = 1 ) + I - 1
          Temp = P(Loc)
          P(Loc) = P(I)
          P(I) = Temp
        end if
```

Reduce row I.

```
        LU(P(I), I + 1:) = (LU(P(I), I + 1:) &
          - matmul( LU(P(I), : I - 1), LU(P(: I - 1), I + 1:) )) &
          / LU(P(I), I)
      end do

      Flag = .true.
      return
    end subroutine Factor

  end subroutine Solve
  subroutine Iterate (B, X, Rel_Err)
```

DUMMY ARGUMENTS and LOCAL DATA

```
    real, dimension(:, :), intent (in) :: B
    real, dimension(:, :), intent (out) :: X
    real, intent (out) :: Rel_Err
    real, dimension(size( B, dim = 1 ), size( B, dim = 2 )) :: R, E
```

Start subroutine Iterate

```
    if (.not. Saved &
      .or. size( B, dim = 1 ) /= N &
      .or. any( shape( X ) /= shape( B ) )) then
      print *, " ITERATE argument shape incompatibility."
      return
    end if
```

Calculate high-precision residual for right side B and solution X, using Save_A from latest call to Factor. For each right side column, calculate norm of the residual; find largest such norm among all right sides.

```
    R = real( real( B, kind = HI ) - matmul( Save_A, real( X, kind = HI ) ) )
    print *, " Residual: ", maxval( sqrt( sum( R ** 2, dim = 1 ) ) )
```

Use the calculated residual to “refine” X. For each right side, divide norm of the error estimate by norm of the solution; find largest such ratio among all right sides. Reference to `tiny` *guarantees no division by zero.*

```
    call For_Bak( R, E )
    X = X + E
    Rel_Err = maxval( sqrt( sum( E ** 2, dim = 1 ) ) &
      / max( sqrt( sum( X ** 2, dim = 1 ) ), 8 * tiny( 1.0 ) ) )
    return
  end subroutine Iterate
```

The subroutine For_Bak performs forward and back substitution, using LU and P stored at the latest call to Factor. B is M right side vectors. The result will be returned in X.

```
  subroutine For_Bak( B, X )
```

DUMMY ARGUMENTS and LOCAL DATA

```
    real, dimension(:, :), intent (in) :: B
    real, dimension(:, :), intent (out) :: X
    integer :: I
    real, dimension(size( B, dim = 1), size( B, dim = 2)) :: C
```

Start subroutine For_Bak

```
    do I = 1, N
      C(I, :) = (B(P(I), :) &
        - matmul( LU(P(I), : I - 1), C(: I - 1, :) )) / LU(P(I), I)
    end do
    do I = N, 1, -1
      X(I, :) = C(I, :) - matmul( LU(P(I), I + 1: ), X(I + 1: , :) )
    end do
    return
  end subroutine For_Bak

end module D01_M
```

As in the following test driver, the main program must provide space for data arrays ***A*** and ***B*** as well as for the result array ***X***. Here, these are allocated after the array size has been read. A call to **Solve** computes an approximate solution and performs one step of iterative refinement to estimate the relative error. The program calls **Iterate** as necessary to reduce the relative error to an acceptable value. Finally, the arrays allocated at the main program level are deallocated.

```
program D01
```

Example driver program for Crout factorization with iterative refinement.

```
  use D01_M
  implicit none
  integer :: EoF, I, M, N, Loop
  real, dimension(:, :), allocatable :: A, B, X
  real :: Rel_Err
  logical :: Flag
```

Start program. Connect input file and read N, the number of equations, from the first record.

```
  open (unit = 1, file = "gaudata.txt", &
    status = "old", action = "read", position = "rewind")
  read (unit = 1, fmt = *, iostat = EoF) N
  if (EoF /= 0) then
    print *, " Data error at start of file. "
  end if
```

Allocate A and read values for A, by rows. Echo print A.

```
  allocate( A(N, N) )
  do I = 1, N
    read (unit = 1, fmt = *) A(I, :)
    if (EoF /= 0) then
      print *, " Insufficient data for A. "
    end if
    print *, " Matrix A, Row ", I, A(I, :)
  end do
```

Read M, the number of right sides. Allocate arrays for B and for results. Read B by rows and echo print it.

```
  read (unit = 1, fmt = *, iostat = EoF) M
  if (EoF /= 0) then
    print *, " Insufficient data for M. "
  end if
  allocate( B(N, M), X(N, M) )
  do I = 1, N
    read (unit = 1, fmt = *) B(I, :)
    if (EoF /= 0) then
      print *, " Insufficient data for B. "
    end if
    print *, " Matrix B, Row ", I, B(I, :)
  end do
```

Solve for X in A X = B. Print initial error estimate.

```
  call Solve( A, B, X, Rel_Err, Flag )
  if (.not. Flag) then
    print *, " Factor cannot solve this one."
    stop
  else
    print *, 0, " Relative error: ", Rel_Err
  end if
```

(Optional) Iterative refinement. Stop when relative error is small or after 10 iterations; print the relative error estimate for each iteration.

```
  do Loop = 1, 10
    if (Rel_Err < 1.0e-7) exit
    call Iterate(B, X, Rel_Err)
    print *, Loop, " Relative error: ", Rel_Err
  end do
```

Print the final result.

```
  do I = 1, M
    print *, " Matrix X, Column ", I, X(:, I)
  end do
  stop
end program D01
```

Another driver is distributed electronically as example D01X. This driver generates a rather large ill-conditioned matrix, inverts it, and then re-inverts the inverse; the driver also estimates the time required for the computation.

Section 1.2 Exercises

1. If the next student is taller than the one standing by the door, you ask the next student to stand there instead. If the next student is not taller, you leave the previous student standing there. Explain how this repeated step preserves the invariant assertion, “The tallest student in the dining hall is now standing at the left of the doorway.”

2. For the function **Minimum_Location**, show that executing an iteration of the loop preserves the invariant assertion.

   a) Is the procedure correct when **Loc_1** and **Loc_2** have the same value?

   b) Does the procedure work correctly for an array of size zero (e.g., when **Loc_1** is 1 and **Loc_2** is zero)? If not, what changes should be made?

3. For the function **Linear_Search**, show that executing an iteration of the loop preserves the invariant assertion.

   a) If the procedure terminates because the key matches an array element, show that the assertion is true.

   b) Show that the invariant assertion is always preserved during every iteration of the loop.

   c) In case the loop exit is taken, the invariant assertion is true and $1 \le i \le N$. Show that the key value lies between $Array_{i-1}$ and $Array_i$ even if i is 1.

   d) In case the loop exit is not taken, the invariant assertion is true and the value of i is $N + 1$. Show that the key value lies between $Array_{i-1}$ and $Array_i$.

   e) What will happen if the given array has zero length (i.e., if **size(Array)** is zero)?

4. Study the function **`Binary_Search`**.

   a) Show that **`Middle`** is always between 1 and N inclusive: i.e., **`Array(Middle)`** is always an element within the designated array section and is never one of the fictitious elements **`Array(0)`** or **`Array(N + 1).`**

   b) Show that the integer division step preserves the relation $Loc\_1 \le Middle \le Loc\_2$.

   c) Show that if **`Loc_1`** and **`Loc_2`** differ by exactly two at the beginning of an iteration, they differ by exactly one at the end of the same iteration. (Consider all possible combinations of odd and even values.)

   d) Show that the invariant assertion is always preserved during every iteration of the loop; show that it would still be preserved without the exact match shortcut.

   e) In case the key matches an array element, at loop termination the invariant assertion is true and the **`while`** condition is also true. Since the key cannot match a fictitious element, **`Loc_1`** is at least **`1`** and **`Loc_2`** is at most N. Show that the key value lies between **`Array(Loc_1)`** and **`Array(Loc_2)`**.

   f) In case the key does not match any **`Array`** element, at loop termination the invariant assertion is true and the **`while`** condition is false. Show that the key value lies between **`Array(Loc_1)`** and **`Array(Loc_2)`**, even if **`Loc_1`** is zero or **`Loc_2`** is $N + 1$.

   g) What happens when the given array has one element? Consider the case in which the key matches the array element, as well as the case in which it does not match.

   h) What happens when the size of the given array is zero?

5. Rewrite **`Binary_Search`** to use recursion instead of iteration.

6. The three-way comparison in **`Binary_Search`** is more efficient than a simple two-way comparison if the search key actually appears in the array. Quantify the expected improvement in terms of p, the probability that the key is present in the array.

7. For the Crout algorithm with iterative refinement, matrix factorization requires on the order of n^3 operations. Forward substitution, back substitution, and calclulating the residual each require on the order of n^2 operations. Give arguments to support the following conjectures.

   a) If $n \ge 10$, the amount of computation required for iterative refinement is insignificant.

   b) If $n < 10$, the amount of computation required for iterative refinement is insignificant.

   Compare B.W. Kernighan and P.J. Plauger, “The Elements of Programming Style” (McGraw-Hill, 1974), p. 9.

8. Run the program of Example 1 with the electronically distributed file **`gaudata.txt`**, and estimate the condition number of each (nonsingular) matrix in the data set.

1.3. POINTERS

The Pointer Attribute

A variable of any data type may be declared to have the **`pointer`** attribute. The value of such a variable is stored in the form of a *pointer* to a *target object* of the specified type:

```
  real, pointer :: Root, Temp                               ! type declaration
```

The type declaration creates (reserves space for) pointers as local objects in automatic or static storage.

Association Status

A pointer that is currently associated with a target has a defined value that indicates the particular target.

The *association status* of a pointer is "associated" if the pointer is currently associated with a target, and it is "disassociated" if the pointer is not currently associated with a target. When a pointer has no target, its value is undefined and the pointer is said to be *null*.

There are four ways to give a pointer a defined association status:

1. Pointer assignment with the intrinsic function reference **`null( )`**, as in the following type declaration, sets the association status to disassociated. This is the only way to nullify a pointer initially:

   ```
   real, pointer :: Root => null( ), Temp => null( )
   ```

   As a matter of good programming practice, all pointers should be initially nullified in this way. In Fig. 1.2, the symbol ∅ indicates that the association status is disassociated.

FIGURE 1.2. A null pointer has no target

2. Executing a **`nullify`** statement sets the association status of a pointer to disassociated, indicating that the pointer does not currently have a target:

   ```
   nullify( Root, Temp )
   ```

3. Executing an **`allocate`** statement for a pointer creates (reserves space for) a new target object in heap storage, sets the pointer value to indicate that the pointer is associated with the newly created object, and sets the association status to associated:

   ```
   allocate( Root )
   ```

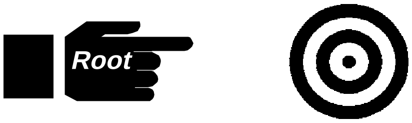


FIGURE 1.3. An allocate statement creates a new target for the pointer

After execution of the **allocate** statement, the pointer has a value that indicates or “points to” the new target. In Fig. 1.3, the “target” symbol indicates that the association status is associated. (The allocate statement may be used with allocatable arrays as well as pointers: See Examples 6, 7, 19, 21, and 25.)

4. Executing a pointer assignment statement can associate the pointer with an existing target object:

```
 Pointer_1 => Pointer_2
```

The assignment sequence is from right to left, as usual, even though the direction of the arrow might seem to indicate otherwise. The effect of such a pointer assignment is to “copy” **Pointer_2** to **Pointer_1**. That is, the existing association status and target (if any) of **Pointer_2** now also become the association status and the target, respectively, of **Pointer_1**. If **Pointer_2** is null, the same will be true of **Pointer_1** after the pointer assignment has been executed.

For example, executing the following statement will set **Temp** to point to the same target (if any) as **Root**:

```
 Temp => Root                                              ! Pointer assignment
```

The current target (if any) of the pointer named **Root** is now also the target of the pointer named **Temp**. The pointer assignment may be read as follows: “Assign the target of **Root** as the (new) target of **Temp**.” Executing a later statement that changes **Root** (by means of a **nullify** statement, an **allocate** statement, or a pointer assignment statement) will not change the association status or the target of **Temp**. (See Fig. 1.4.)

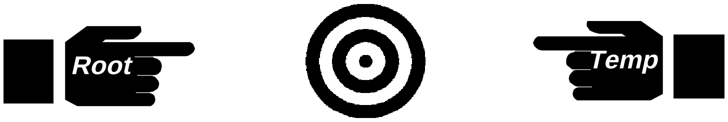


FIGURE 1.4. Executing the pointer assignment statement gives Temp the same target as Root

Automatic Dereferencing

Fortran does not give a separate name to the target of a pointer. The target has the same name as its pointer. When a variable has the **pointer** attribute, Fortran is able to determine from the context whether an occurrence of the name is intended to designate the target or the pointer itself. A name designates the *target* when it appears in an expression, when it appears on the left side of an assignment statement, or when it appears in an **allocate** or **deallocate** statement. It designates the *pointer* when it appears in a **nullify** statement or when it appears in a pointer assignment statement.

The only way to detect that a pointer has been nullified is by means of the intrinsic function reference **associated(Temp)**, which examines the association status of the pointer.

```
associated( Temp )                              ! intrinsic function reference
```

The result value is true if *Temp* is currently associated with a target so that its association status is associated. The function result is false if *Temp* has been nullified so that its association status is disassociated.

The deallocate Statement

Executing the statement

```
deallocate( Root )
```

where *Root* is a pointer whose target has been created by execution of an **allocate** statement, releases the space occupied by the target object. If the target had a defined value prior to deallocation, that value is lost. Thus the association between the pointer and the target is destroyed, and the pointer is nullified. (See Fig. 1.5.)

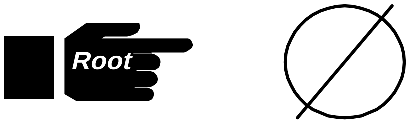


FIGURE 1.5. Executing the statement deallocate(Root) releases the space occupied by the target object and nullifies the pointer

Deallocation is permited only if the current association status of the pointer is associated (that is, if the pointer is currently associated with a target) and if the target is an object that was created by execution of an **allocate** statement. After the **deallocate** statement has been executed, the association status of the designated pointer becomes defined as disassociated. The pointer value becomes undefined because the pointer no longer has a target.

Storage for Pointers and Allocated Targets

Recall that a type declaration creates (reserves space for) an object of the declared type in automatic storage (or in static storage if the object has the **save** attribute) at the beginning of execution of the main program or procedure in which the declaration appears. The same is true when the declared object is a structure (of a derived type). If a declared object has the **pointer** attribute, the pointer is created (space is reserved for it) in static or automatic storage, but initially no target is created.

Also recall that executing the statement **allocate(Root)** (where **Root** is an existing pointer that may or may not have been previously allocated or nullified) has two effects:

1. It creates (reserves space for) a new target object of the type specified in the declaration for **Root**.
2. It associates the pointer **Root** with the new target.

Storage for allocated pointer targets is obtained from a “heap” of free space that is administered by a sophisticated storage management system. Storage for allocatable arrays is allocated from this same heap.

Management of Allocated Targets

Executing an **`allocate`** statement for a pointer causes space from the heap to be reserved for the target, and gives the pointer a value that permits Fortran to gain access to the target via the pointer. At this point, Fortran has no other way of obtaining access to the target — that is, to the area of heap space that has just been allocated.

Some care is required here to avoid storage management problems. If the pointer value is destroyed (by nullification, reallocation, or pointer assignment) but the target is not deallocated, the heap space becomes "garbage" — that is, it is still reserved by the storage management system but it is inaccessible to the program for which it was reserved. To ensure that the target space will be returned to the heap for possible further use when the pointer is nullified, a **`deallocate`** statement should be employed.

After a pointer assignment with a pointer on the right is executed, on the other hand, there is more than one pointer with the same target. So long as at least one of these pointers remains associated with the target, the others may be nullified.

But another problem can arise in this case. When two or more pointers have the same target, deallocating one of the pointers deletes the target object (and releases heap storage space) without affecting the other pointers. The other pointers are now said to be "dangling references" — pointers to heap space that is no longer reserved.

Programs that manipulate pointers should strictly observe the following important rules:

1. If there is *only one* pointer currently pointing to a particular target object, do not change the value of (**`nullify`**, reallocate, or assign to) the pointer without first deallocating it.

2. If there is *more than one* pointer currently pointing to a particular target object, do not deallocate any of these pointers.

Some processors provide little assistance for diagnosing allocation errors such as heap overflow. Fortran provides a second (optional) clause in the **`allocate`** statement, of the form **`stat =`** *Status variable*. During execution, the *Status variable* will be set to zero if the allocation is successful, or to a positive value in case of an allocation error such as insufficient heap storage space:

```
allocate( Temp_NP, stat = Err )
if (Err > 0 ) then
   :
```

Pointers as Derived Type Components

A component of a derived type may have the **`pointer`** attribute. Note the following points:

- The type specified for each component in a derived type definition, *except* for components that have the pointer attribute, must be an intrinsic type or a previously defined derived type.

- A derived type may have a component that is a pointer to the same type. Such components most frequently occur in derived types that are intended for linked list applications.

- Initial nullification may be specified for pointer components. (This feature was introduced in Fortran 95 and is not available with Fortran 90. See the electronically distributed examples for alternative programming strategies.)

- Any pointer component that has the dimension attribute must have deferred shape — its actual subscript bounds are specified when the target array is allocated rather than in the type definition.

```
! Pointer as a derived type component.
  program Finger
    implicit none
    type :: I_Type                                 ! Derived type definition
      integer :: Nuc_Count = 0
      real :: Abundance = 0.0
    end type I_Type
    type :: Chem_El_Type                           ! Derived type definition
      character (len = 16) :: El_Name = ""
      character (len = 2) :: Symbol = ""
      real :: Atomic_Num = 0.0, Atomic_Mass = 0.0
      type (I_Type) :: Prin                  ! Previously defined derived type
      type (Chem_El_Type), pointer :: Next_P => Null( )
    end type Chem_El_Type
    type (Chem_El_Type) :: Carbon_12                       ! Type declarations
    type (Chem_El_Type), pointer :: Root_P => Null( )

! start program Finger
    Carbon_12 % Prin % Nuc_Count = 5             ! Component of substructure Prin
    allocate( Carbon_12 % Next_P )
    Carbon_12 % Next_P % Symbol = "He"
      :
    allocate( Root_P )
  end program Finger
```

The derived type named **Chem_El_Type** has a component that is a structure of the previously defined derived type **I_Type**. An additional component of **Chem_El_Type** is a pointer to another structure of the same type.

Carbon_12 is declared to be a structure of type **Chem_El_Type**. The type declaration creates a structure of this type in automatic storage, with six components named **El_Name**, **Symbol**, **Atomic_Num**, **Atomic_Mass**, **Prin**, and **Next_P**. The first four of these are ordinary scalars, Prin is a substructure of type **I_Type**, and **Next** is a pointer. The type declaration for **Root_P** creates a disassociated pointer. See Fig. 1.6.

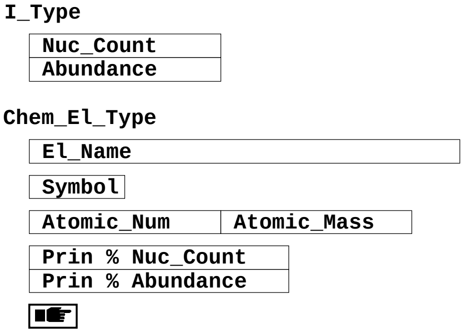


FIGURE 1.6. Components of the derived type Chem_El_Type

The assignment statement

```
Carbon_12 % Prin % Nuc_Count = 5
```

changes the value of the component *Nuc_Count* of the substructure **Carbon_12 % Prin** from its initial zero value to 5. The statement

```
allocate( Carbon_12 % Next_P )
```

creates a target structure named **Carbon_12 % Next_P** in heap storage. The assignment statement

```
Carbon_12 % Next_P % Symbol = "He"
```

assigns the string **"He"** to the component *Symbol* in the structure **Carbon_12 % Next.**

Note carefully the difference between two deceptively similar assignment statements.

```
type :: I_Type                                        ! Derived type definition
  integer :: Nuc_Count = 0
  real :: Abundance = 0.0
end type I_Type
type :: Chem_El_Type                                  ! Derived type definition
  character (len = 16) :: El_Name = ""
  character (len = 2) :: Symbol = ""
  real :: Atomic_Num = 0.0, Atomic_Mass = 0.0
  type (I_Type) :: Prin                      ! Previously defined derived type
  type (Chem_El_Type), pointer :: Next_P => Null( )
end type Chem_El_Type
type (Chem_El_Type) :: Carbon_12                            ! Type declarations
  :
Carbon_12 % Prin % Nuc_Count = 5
Carbon_12 % Next_P % Symbol = "He"
```

The variable name **Carbon_12 % Prin % Nuc_Count** consists of the name of a declared (automatic storage) structure, the name of a substructure, and the name of a component of the substructure. On the other hand, in the reference to the variable **Carbon_12 % Next_P % Symbol**, the component named *Next_P* has the **pointer** attribute, so **Carbon_12 % Next_P** refers to the structure (in heap storage) that is the target of the pointer, and *Symbol* is a component of that target structure.

A pointer variable can be created in automatic storage as an independent object that is not part of a structure. The type declaration creates **Root_P** as a pointer to type **Chem_El_Type**. Executing the **allocate** statement creates a structure named **Root_P**.

Pointers with Arrays

Fortran does not provide arrays of pointers. (A variable with **pointer** and **dimension** attributes is a pointer to an array, not an array of pointers.) However, it is possible to define a structure with a single component that is a pointer, and then to create an array of these structures. This feature is illustrated in Examples 24 and 25 (in Chapter 7).

Chapter 2 Introduction to Sorting

Your mail has just arrived. Your bank has sent you a statement with last month's cancelled checks enclosed. There are only three checks, which need to be arranged in numerical order and stored away for future reference.

You don't have to undertake an elaborate research project to decide how to put three checks in order. Here is a simple method:

1. Lay the three checks down side by side. Compare the checks that are in the first and second positions, and interchange them if they are in the wrong order.
2. Compare the checks that are now in the first and third positions, and interchange them if they are in the wrong order.
3. Compare the checks that are now in the second and third positions, and interchange them if they are in the wrong order.

The comparison depends on a *sort key*. Here we assume that the key is a check number that appears on each check. (The sort key might instead be the date or the amount.) Objects can be sorted into either increasing or decreasing order, depending upon how the comparison is made. At first, it will be assumed that all of the objects have *different* key values. Duplicate keys cause no real difficulty, but they introduce some minor complications that will be considered later in this chapter.

Computer Sorting

Many computer applications, from maintaining and updating simple arrays to data base indexing, require sorting of data. It may be that the elements are simply numbers or character strings to be arranged by numerical value, or they may be structures that can be viewed as rows of a table. For example, the table of California cities mentioned earlier might be sorted with respect to any of three keys: alphabetically by the name of the city, or numerically by latitude or by longitude.

Inside the computer, data to be sorted is usually stored in an array. The sorting procedure converts an array of unsorted elements into an array of sorted elements. For most applications, large quantities of extra space are not available — a sorting method that requires as much additional space as the array to be sorted would usually be considered unacceptable. The sorted data should end up in the same array originally occupied by the unsorted data.[10] Initially, the unsorted data occupies the entire array, and there is no sorted data.

For example, numbers to be sorted by the three-item sorting method just considered would be stored in an array of length three:

[10] This is not true of certain methods such as merge sort that are used mainly for sorting data from external files.

```
 subroutine Sort_3( Array )
   real, intent(in), dimension(3) :: Array
! start subroutine Sort_3
   if (Array(1) > Array(2)) call Swap( 1, 2 )
   if (Array(1) > Array(3)) call Swap( 1, 3 )
   if (Array(2) > Array(3)) call Swap( 2, 3 )
   return
 end subroutine Sort_3
```

Some computer sorting methods are simple and easy to understand and are adequate for sorting a few (up to perhaps 10,000) data items. As we shall see, these simple methods are impossibly inefficient for large quantities of data.

- Selection sorting is probably the easiest of all known methods to understand and to implement.
- Insertion sorting is faster than selection for “random” data, and is only slightly more complicated. Some variations can considerably increase the speed of this method.

The remainder of this chapter is devoted to sorting by the two simplest methods, selection and insertion.[11] Two more sophisticated methods that are related to insertion, Shell sort and heapsort, are also described here. Quicksort, a method that is usually implemented recursively, is discussed in Chapter 3.

Operation Counts for Sort_3

```
if (Array(I) > Array(J)) call Swap( 1, 2 )                             ! 1
if (Array(I) > Array(K)) call Swap( 1, 3 )                             ! 2
if (Array(J) > Array(K)) call Swap( 2, 3 )                             ! 3
```

There are six possibilities, which are equally likely for random data.

```
A B C
A C B                 → A B C
B A C → A B C
B C A         → A C B → A B C
C A B → A C B         → A B C
C B A → B C A → A C B → A B C
```

The first of these situations requires no swaps, the next two require one swap, the next two require two swaps, and the last one requires three swaps. Thus the expected number of calls to **Swap** for random data is 1.5. Each call to **Swap** performs three move operations. The subroutine therefore requires 3 comparisons and 4.5 moves (for random data). In practice, however, these basic operations are completely dominated by procedure call overhead.

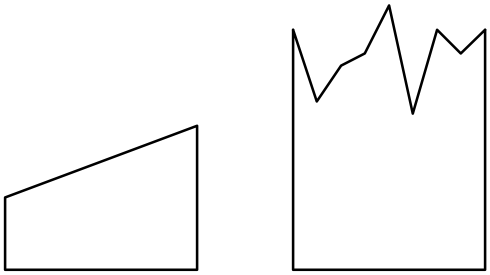
[11] Another well-known simple method, bubble sorting, is not discussed in this text.“The bubble sort seems to have nothing to recommend it, except a catchy name and the fact that it leads to some interesting theoretical problems”: Knuth, *Sorting and Searching*, 111. “If you know what bubble sort is, wipe it from your mind; if you don’t know, make a point of never finding out!”: Press, et al, *Numerical Recipes in Fortran*, Second Ed. (Cambridge: Cambridge Univ. Press, 1992), 321.

2.1 SORTING BY SELECTION

Selection is probably the easiest sorting method to understand, although it is far from the fastest. Beginning with a set of unsorted data items, this method constructs a set of sorted items by moving one item at a time from the unsorted set to the sorted set. The method proceeds in the following way:

1. Find the data item that belongs at the *first* position in the sorted sequence; this is the smallest unsorted item. Remove it from the unsorted sequence and place it as the first sorted item.
2. Find the data item that belongs at the *second* position in the sorted sequence; this is now the smallest unsorted item. Remove it from the unsorted sequence and place it as the next sorted item.
3. Repeat this process, each time finding the smallest unsorted item and moving it into place as the next sorted item, until all items have been moved from the unsorted sequence to the sorted sequence.

The sorted and unsorted data items share an array. The set of sorted data items (initially empty) occupies the low-numbered subscript positions, and the set of unsorted items occupies the high-numbered end of the array. Note that at each stage all of the sorted items are smaller than all of the unsorted items. Rawlins[12] illustrates this situation as follows:



A selection sort procedure employs an indexed loop construct. The loop index, *I*, varies from from 1 up to *N*, the number of data items. Subscript positions *1* to *I* – 1 contain sorted data; positions beginning at position *I* contain unsorted data. When *I* is 1, the sorted portion is empty.

For each value of *I*, one data item is moved from the unsorted portion to the sorted portion. The following steps are performed:

1. Examine all of the unsorted items to find the one with the smallest key.
2. Move this smallest unsorted item to position *I*. But wait — position *I* is already occupied by an unsorted data item that must be moved out of the way. A good maneuver is to *swap* the smallest unsorted item with the one in position *I*.
3. The item in position *I* has been appended to the sorted data, which is now located at subscript positions *1* to *I*. These items will never be moved again, nor even examined, during remaining iterations of the selection sort loop.

Fig. 2.1 shows the sequence of steps for sorting, by selection, an array containing the characters QUICKLYSELECT.

[12] G.J.E. Rawlins, *Compared to What? An Introduction to the Analysis of Algorithms.* [New York: Computer Science Press, 1991].

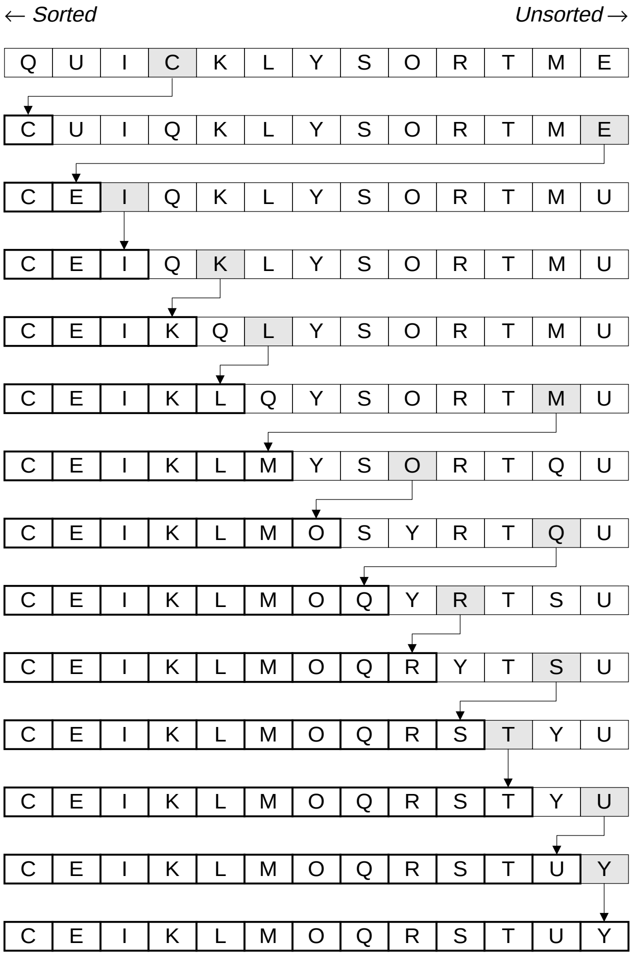

← Sorted
Unsorted →
Q U I C K L Y S O R T M E
C U I Q K L Y S O R T M E
C E I Q K L Y S O R T M U
C E I Q K L Y S O R T M U
C E I K Q L Y S O R T M U
C E I K L Q Y S O R T M U
C E I K L M Y S O R T Q U
C E I K L M O S Y R T Q U
C E I K L M O Q Y R T S U
C E I K L M O Q R Y T S U
C E I K L M O Q R S T Y U
C E I K L M O Q R S T Y U
C E I K L M O Q R S T U Y
C E I K L M O Q R S T U Y

FIGURE 2.1. Example of sorting by selection

When *I* is 1, the unsorted data items occupy all 13 positions in the array. The smallest item is C; this item is moved to position 1 where it becomes the first sorted item, and the J that was formerly in that position moves to the place vacated by C.

When *I* is 2, there are 12 unsorted data items as shown on the second line in Fig. 2.1. The smallest is C, which is swapped with the element U in position 2. There are now two sorted items, both C, which will never again be examined or moved.

The process continues until *I* reaches 12 and all items except Y have been moved to the sorted portion.

The final iteration of the loop, with $I = N$, is supposed to search among the unsorted items to find the largest, and move it to position *N*. Since there is only one item in the portion to be searched, and it is already in position *N*, this final iteration accomplishes nothing and can be omitted. Thus, the upper loop bound should be $N - 1$, where *N* is the size of the array.

```
N = size( Array )
do I = 1, N - 1
   Location = Minimum_Location( I, N )
   call Swap( I, Location )
end do
```

The function **Minimum_Location** is implemented as an internal procedure that inherits *Array* from the host program, so only the two subcript bounds are passed as arguments. The subroutine **Swap** also inherits *Array*; subscript values for the items to be exchanged are passed as dummy arguments.

Operation Counts for Selection Sort

```
 N = size( Array )                                          ! 1
   do I = 1, N - 1                                          ! 2
     Location = Minimum_Location( I, N )                    ! < 3
     call Swap( I, Location )                               ! < 4
   end do                                                   ! < 5
```

Each **Swap** call requires 3 move operations, as stated earlier. For random data, each reference to the function **Minimum_Location(I, N)** requires $N - I + 1$ comparisons and $0.7 \cdot \lg (N - I) + 0.6$ moves. Thus, the loop body (lines 3 and 4) performs $N - I + 1$ comparisons and $4.6 + 0.7 \cdot \lg (N - I)$ moves. These formulas are to be summed over all $N - 1$ iterations of the loop.

- Terms independent of I are multiplied by $N - 1$:
  $N + 1$ comparisons times $N - 1 = N^2 - 1$; 4.6 moves times $N - 1 = 4.6 \cdot N - 4.6$
- Terms in I:
  Sum of $- I$ comparisons for $I = 1$ to $(N - 1)$ is $- 0.5 \cdot N^2 + 0.5 \cdot N$
- Terms logarithmic in I:
  A sum of logarithmic terms can be estimated by analogy to the integral $\int \ln z = z(\ln z - 1)$;
  noting that $\lg k$ is about $1.4 \ln k$, the sum from a to b of $\lg k$ is approximately
  $b \lg b - a \lg a - 1.4\,(b - a)$.
  Let $k = N - I$; the loop is executed with $k = N - 1$ to 1 so the sum is
  $(N - 1) \lg(N - 1) - 1 \cdot \lg 1 - 1.4\,(N - 2)$

Total comparisons: $0.5 \cdot N^2 + 0.5 \cdot N - 1$

Total moves: $0.7 \cdot N \lg(N - 1) + 5.6 \cdot N - 0.7 \cdot \lg(N - 1) - 6.6$

A benchmark, run with a 50 MHz 486DX computer, sorted 20,000 random real numbers by selection in 350 seconds.

Say It with Fortran

Example 2. This version sorts an array of strings. The subroutine **Se_Sort** contains two internal procedures, the function **Minimum_Location** and the subroutine **Swap**. The subroutine **Se_Sort** is contained in the module **D02_M** along with a subroutine to print the aray. A main program to test the module is shown as well.

```
! Example 2. Sorting an array of strings by selection.
module D02_M
  implicit none
  public :: Se_Sort

contains

  subroutine Se_Sort( Array )                          ! Module subprogram
```

The dummy argument **Array** *has assumed shape (with rank 1), character type, and assumed length. (The array size and the length of the strings in the array will be taken from the actual argument.) Its* **intent** *attribute is* **in out***, which means that the corresponding actual argument array must be definable (for example, it must not be an array-valued expression that contains operators). Its elements must be defined before they are used: here it is assumed that they have defined values at entry to the subroutine.*

```
    character (len = *), intent(in out), dimension(:) :: Array
    integer :: N, I, Location
! start subroutine Se_Sort
    N = size( Array )
    do I = 1, N - 1
      Location = Minimum_Location( I, N )
      call Swap( I, Location )
    end do
    return
  contains

    pure function Minimum_Location( Lo, Hi ) result( Minimum_Location_R )
      :
    end function Minimum_Location

    subroutine Swap( I, J )
      integer, intent(in) :: I, J
```

Exchanging the values of the two array elements requires an auxiliary or temporary variable of the same type. The character length is derived from that of the assumed-length dummy argument **`Array`**.

```
      character (len = len(Array)) :: Aux
        :
    end subroutine Swap

  end subroutine Se_Sort

end module D02_M
```

The following main program creates an array and calls Sort.

```
  program D02
```

The following statement incorporates the sorting module into the main program.

```
    use D02_M
    implicit none
    integer, parameter :: L = 13
    character (len = 1), dimension(L) :: Array
! start program D02
```

The right side is an array constructor.

```
    Array = (/ "Q", "U", "I", "C", "K", "L", "Y", &
      "S", "E", "L", "E", "C", "T" /)
    call Se_Sort( Array )
    write (*, "(13 A2)") Array
    stop
  end program D02
```

Sorting an Array of Structures

Example 3. The following example illustrates the modifications necessary for sorting data of a different type — in this case, an array of structures that contain the name, latititude, and longitude of California cities. Any sorting method can be adapted in this way; this example shows a variant of the selection sort method.

Note that comparison operations are applied only to the sort key (the city name in this case) while move operations (in the subroutine **`Swap`**) involve whole structures.

```
! Example 3. Sorting an array of structures by selection.
module D03_M
  implicit none
  public :: Se_Sort
  integer, parameter, private :: NAME_LEN = 20
```

Derived type definition. The data to be sorted is an array of structures of this type. The `use` *statement in the main program imports the type definition for* `City_Data_Type` *as well as the procedures* `Sort` *and* `Print_Array`*.*

```
  type, public :: City_Data_Type
    character (len = NAME_LEN) :: City_Name
    integer :: Latitude, Longitude
  end type City_Data_Type

contains

  subroutine Se_Sort( Array )
```

The data to be sorted is a rank-1 assumed shape array of structures of the new derived type.

```
    type (City_Data_Type), intent(in out), dimension(:) :: Array
    integer :: N, I, Location
! start subroutine Se_Sort
    N = size( Array )
    do I = 1, N - 1
```

Locate the structure with the smallest key value, in the array of structurs.

```
      Location = Minimum_Location( I, N )
      call Swap( I, Location )
    end do
    return
  contains

    pure function Minimum_Location( Lo, Hi ) result( Minimum_Location_R )
      integer, intent(in) :: Lo, Hi
      integer :: Minimum_Location_R, I
```

Min_Val must have the same type as the key component.

```
      character (len = NAME_LEN) :: Min_Val
  ! start function Minimum_Location
```

The array is inherited from the host subroutine. Array references must include the key component selector. (See another variant, below.)

```
      Min_Val = Array(Lo) % City_Name
      Minimum_Location_R = Lo
      do Loop = Lo + 1, Hi
        if (Array(Loop) % City_Name < Min_Val) then
          Min_Val = Array(Loop) % City_Name
          Minimum_Location_R = Loop
        end if
      end do
      return
    end function Minimum_Location
    subroutine Swap( I, J )
      integer, intent(in) :: I, J
```

Exchanging the values of the two array elements requires an auxiliary or temporary variable of the same type.

```
      type (City_Data_Type) :: Aux
  ! start subroutine Swap
      Aux = Array(I)
      Array(I) = Array(J)
      Array(J) = Aux
      return
    end subroutine Swap

  end subroutine Se_Sort

  subroutine Print_Array( Array )
    type (City_Data_Type), intent(in), dimension(:) :: Array
      :
  end subroutine Print_Array

end module D03_M
```

Example 3A. An alternative is to pass the array of keys — here, the array of *City_Name structure components* — as an argument to **`Minimum_Location`**. This slightly complicates the function reference but simplifies the internal workings of the function. Experiments indicate that this variant runs faster on many Fortran processors.

```
! Example 3A. Selection Sort with Array Argument
      :
    Location = Minimum_Location( Array % City_Name, I, N )
      :
  pure function Minimum_Location( A, Lo, Hi ) result( Minimum_Location_R )
    character (len = *), dimension(:), intent(in) :: A
    integer, intent(in) :: Lo, Hi
    integer :: Minimum_Location_R, Loop
```

The local variable `Min_Val` *must have the same properties (except dimension) as the argument array.*

```
    character (len = Len( A )) :: Min_Val
! start function Minimum_Location
    Min_Val = A(Lo)
    Minimum_Location_R = Lo
    do Loop = Lo + 1, Hi
      if (A(Loop) < Min_Val) then
        Min_Val = A(Loop)
        Minimum_Location_R = Loop
      end if
    end do
    return
  end function Minimum_Location
```

Selection during Output

In some applications, the sorted data is immediately written to an external file and is put to no further internal use. The sorting and output operations can be combined, as shown in this example. The selection method is especially well suited for sorting during output. Furthermore, for some applications the total time required may be dominated by the output phase so that the comparison operations cost nothing.

Say It with Fortran

Example 4.

```
! Example 4. Sorting integers by selection during output.
  subroutine Se_Sort_And_Write( Array )
    integer, intent(in out), dimension(:) :: Array
    integer :: N, I, Location
! start subroutine Se_Sort_And_Write
    N = size( Array )
    do I = 1, N
      Location = minloc( Array(I: ), 1 ) + I - 1
      print *, Array(Location)
```

There is no need to perform a complete **`Swap`** *operation, since* **`Array(I)`** *will never be referenced again.*

```
      Array(Location) = Array(I)
    end do
    return
  end subroutine Se_Sort_And_Write
```

The actual argument to **`minloc`** is an array section, so the intrinsic function returns the location relative to the beginning of the section; $I - 1$ must be added to adjust for the lower bound offset. The offset can be eliminated by reversing the sort, keeping unsorted items at the left end of the array, so that the lower bound of the array section is always 1:

```
do I = N, 1, -1
  Location = minloc( Array(: I), 1 )
  print *, Array(Location)
  Array(Location) = Array(I)
end do
```

Duplicate Keys

Suppose that two or more data items in an array to be sorted have the same key. Two different cities (in different states, presumably) might have the same name but different latitude and longitude coordinates. The foregoing sorting programs will process such data without difficulty; only the comparison operations are affected.

Recall that selection sort employs the function **`Minimum_Location`** to find the smallest item in a designated portion of the array:

```
Min_Val = Array(Lo)
do Loop = Lo + 1, Hi
  if (Array(Loop) < Min_Val) then
    Min_Val = Array(Loop)
    Minimum_Location_R = Loop
  end if
end do
```

If the smallest key value appears more than once, its *first* occurrence will be recorded as the value of *Location*; subsequent occurrences of the same key value will not change this result. However, if the condition *Array(Loop)* < *Min_Val* is changed to *Array(Loop)* ≤ *Min_Val*, *Location* is replaced whenever a duplicate of the smallest key is found, and its final value records the *last* occurrence.

Selection Sort is not Stable.

A *stable* sorting method maintains the relative positions of data items that have duplicate keys. For example, transactions may be entered chronologically and then sorted by a customer identification number. It is often required that the transactions for a given customer be maintained in chronological order, even after data for the various customers has been separated. For such applications, a stable method is required. As we shall see, this requirement is not satisfied by the selection sort procedure.

The two following displays illustrate the effect on selection sorting when the condition in **`Minimum_Location`** is changed. Here the data array contains four occurrences of the letter E and two each of L, O, N, and T. In these displays, subscripts have been appended to the duplicate letters for identification, but are assumed to be ignored by the comparison operations. (This example was actually constructed by sorting an array of structures, each consisting of a character key along with an integer that is different for each occurrence of a repeated character.)

The final results are, of course, the same with regard to the key values. However, the sequemce of occurrences of duplicated characters in the final arrays are often different for the two strategies. Intermediate values differ especially toward the right side of the display — for example, compare the two displays with regard to the columns headed by E_3, P, and E_4.

Both versions of the selection sort are obviously unstable. The sequence of swaps introduces an erratic behavior that is difficult to predict — some sets of duplicate items end up in their original order, some are reversed, and some (such as the Es in the first display) are permuted in other ways.

Choosing the first occurrence of a duplicate key:

#S_1	E_1	L_1	E_2	C	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	A	M	P	L_2	E_4
A	#E_1	L_1	E_2	C	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	E_4
A	C	#L_1	E_2	E_1	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	E_4
A	C	E_2	#L_1	E_1	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	E_4
A	C	E_2	E_1	#L_1	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	E_4
A	C	E_2	E_1	E_3	#T_1	I	O_1	N	S_2	O_2	R	T_2	L_1	X	S_1	M	P	L_2	E_4
A	C	E_2	E_1	E_3	E_4	#I	O_1	N	S_2	O_2	R	T_2	L_1	X	S_1	M	P	L_2	T_1
A	C	E_2	E_1	E_3	E_4	I	#O_1	N	S_2	O_2	R	T_2	L_1	X	S_1	M	P	L_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	#N	S_2	O_2	R	T_2	O_1	X	S_1	M	P	L_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	#S_2	O_2	R	T_2	O_1	X	S_1	M	P	N	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	#O_2	R	T_2	O_1	X	S_1	S_2	P	N	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	#R	T_2	O_1	X	S_1	S_2	P	O_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	#T_2	R	X	S_1	S_2	P	O_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	#R	X	S_1	S_2	P	T_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	P	#X	S_1	S_2	R	T_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	P	R	#S_1	S_2	X	T_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	P	R	S_1	#S_2	X	T_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	P	R	S_1	S_2	#X	T_2	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	P	R	S_1	S_2	T_2	#X	T_1
A	C	E_2	E_1	E_3	E_4	I	L_1	L_2	M	N	O_1	O_2	P	R	S_1	S_2	T_2	T_1	#X

Choosing the last occurrence of a duplicate key:

#S_1	E_1	L_1	E_2	C	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	A	M	P	L_2	E_4
A	#E_1	L_1	E_2	C	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	E_4
A	C	#L_1	E_2	E_1	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	E_4
A	C	E_4	#E_2	E_1	T_1	I	O_1	N	S_2	O_2	R	T_2	E_3	X	S_1	M	P	L_2	L_1
A	C	E_4	E_3	#E_1	T_1	I	O_1	N	S_2	O_2	R	T_2	E_2	X	S_1	M	P	L_2	L_1
A	C	E_4	E_3	E_2	#T_1	I	O_1	N	S_2	O_2	R	T_2	E_1	X	S_1	M	P	L_2	L_1
A	C	E_4	E_3	E_2	E_1	#I	O_1	N	S_2	O_2	R	T_2	T_1	X	S_1	M	P	L_2	L_1
A	C	E_4	E_3	E_2	E_1	I	#O_1	N	S_2	O_2	R	T_2	T_1	X	S_1	M	P	L_2	L_1
A	C	E_4	E_3	E_2	E_1	I	L_1	#N	S_2	O_2	R	T_2	T_1	X	S_1	M	P	L_2	O_1
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	#S_2	O_2	R	T_2	T_1	X	S_1	M	P	N	O_1
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	#O_2	R	T_2	T_1	X	S_1	S_2	P	N	O_1
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	#R	T_2	T_1	X	S_1	S_2	P	O_2	O_1
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	#T_2	T_1	X	S_1	S_2	P	O_2	R
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	#T_1	X	S_1	S_2	P	T_2	R
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	P	#X	S_1	S_2	T_1	T_2	R
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	P	R	#S_1	S_2	T_1	T_2	X
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	P	R	S_2	#S_1	T_1	T_2	X
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	P	R	S_2	S_1	#T_1	T_2	X
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	P	R	S_2	S_1	T_2	#T_1	X
A	C	E_4	E_3	E_2	E_1	I	L_1	L_2	M	N	O_1	O_2	P	R	S_2	S_1	T_2	T_1	#X

Section 2.1 Exercises

1. Modify Example 1 to sort an array of 12 real numbers.

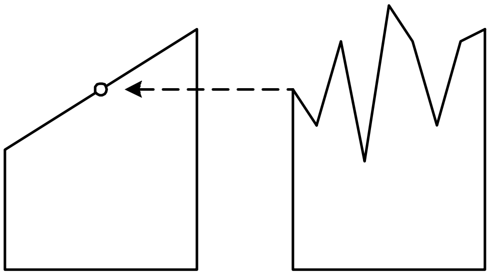
2. Modify Example 2 to sort the same array by latitude instead of by city name.

2.2 SORTING BY INSERTION

It is said that every flock of chickens has a *pecking order* — a social hierarchy in which each bird knows its rank. A bird pecks another lower in the scale without fear of retaliation and submits to pecking by one of higher rank. When a new bird is added to the flock, a certain amount of random pecking occurs at first, but then the new bird establishes its rank and settles into the hierarchy accordingly.

The idea of sorting by insertion is to introduce new chickens (unsorted data items) into the flock one at a time, systematically placing each new bird in its correct position before bringing in the next. Initially, the flock consists of just one chicken and the pecking order is correct by definition. The second chicken is then compared with the first chicken, which either remains at the bottom of the pecking order or rises above the new bird. Each new bird is compared with those already in the flock to establish its rank.

Insertion sorting may be illustrated as follows:



Computer sorting is rarely applied to chickens; more commonly, data items to be sorted are numbers or character strings in an array. Assume that the data is to be sorted into ascending order. Initially, the sorted portion of the array consists only of the item in the first subscript position; the remaining items are unsorted. After some items have been sorted, smaller items are at the left end of the array and larger items are at the right end. Fig. 2.2 shows the sequence of steps for sorting, by insertion, an array containing the characters QUICKLYSORTME.

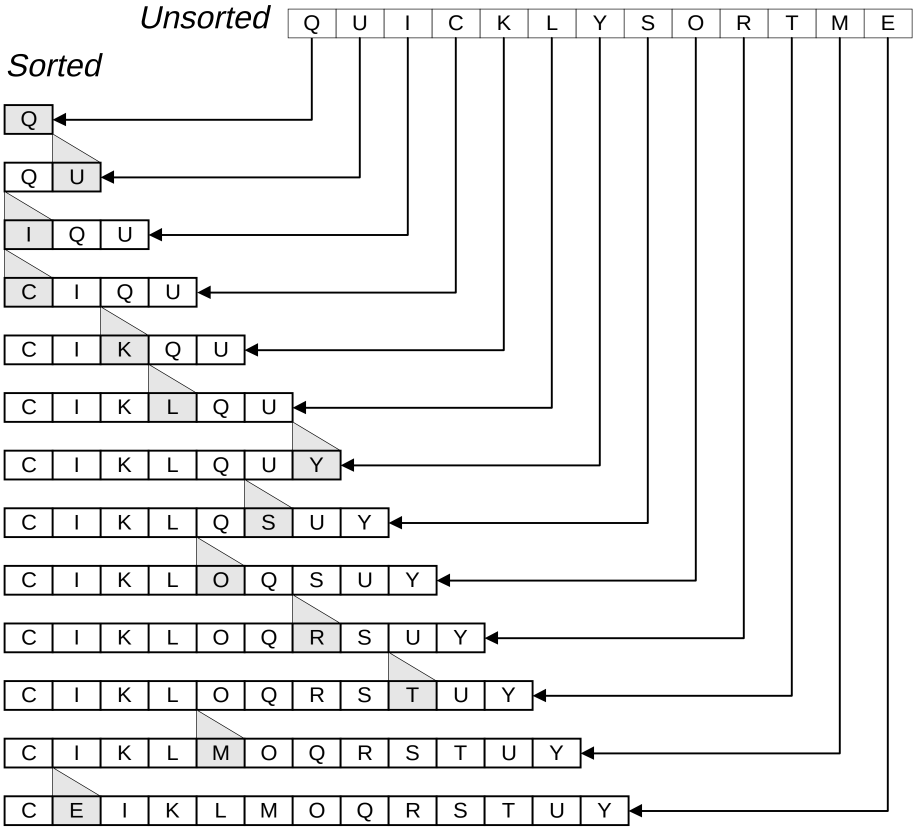


FIGURE 2.2. Example of sorting by insertion

Straight Insertion

At the beginning of each pecking episode, the flock is arranged by increasing rank in *Array*$_1$ to *Array*$_I$, where *I* is initially 1. The new bird to be introduced to the flock is taken from the first position in the unsorted portion of the array, that is, from *Array*$_{I+1}$.

The new bird is removed from the flock — copied to the auxiliary variable *Next* — and is then compared with those already in the flock, beginning with the highest ranking bird and tentatively pecking its way down until it finds a bird that it can dominate. At that point, the pecking stops and the new bird takes its place in the hierarchy. The program accomplishes this by comparing the auxiliary variable *Next* with data items in the sorted portion of the *Array*, beginning at the right and scanning toward the left until an item smaller than *Next* is found.

Note that the pecking process — search for the correct position and insertion into that position — has a slightly specialized form in the straight insertion procedure. The new bird does not challenge other birds at random. It is as though the existing flock were lined up with the highest ranking bird closest to the entrance, so that the new bird must proceed in order of decreasing rank until it finds its correct position. When the new bird arrives, a space is made available next to the entrance, ahead of the currently highest ranking bird. The new bird challenges the current leader; if the challenge is unsuccessful, the leader moves up into the new space next to the entrance and remains as the highest ranking bird. This vacates the space formerly occupied by the leader. The new bird then challenges the other birds in turn, moving along in order of decreasing rank. Whenever a challenge is unsuccessful, the challenged bird moves up, vacating its former space. When the challenge is successful, the new bird slips into the vacant space just above the bird that lost the challenge.

Each complete pecking episode increases the size of the sorted portion of the array from *J* to *J* + 1. Space at position $Array_{J+1}$ is made available when the first unsorted item is copied to *Next*. During the scan, *Next* is compared with $Array_I$, where *I* begins at *J* and decreases. Note that $Array_{I+1}$ is "vacant" — its value is no longer needed — at the time *Next* is compared with $Array_I$. If *Next* is less than $Array_I$, that array element is moved right by one position, into the vacant space; otherwise $Array_I$ remains in place and *Next* is inserted at $Array_{I+1}$, completing the scan. It may happen that all of the previously sorted items are larger than *Next*, so that they are all moved and *Next* is inserted at $Array_1$. Or it may happen that *Next* is the new dominant item, in which case the scan terminates immediately and *Next* is simply stored back in $Array_{J+1}$.

The pecking operation is repeated for values of *J* from 1 to size(*Array*) – 1.

```
do J = 1, size( Array ) - 1
```

The first `J` *items are sorted. Copy the first unsorted item,* `Array(J +1)`*, to* `Next`*; call* `Peck` *to move this new item to its correct position.*

```
    Next = Array(J + 1)
    call Peck( 1, J, Next )
end do
      :
    subroutine Peck( L, R, Next)
```

Working from right to left in the sorted portion, `Array(L: R)`*, the subroutine* `Peck` *moves larger items to the right and inserts* `Next` *as a new sorted item.*

```
      do I = R, L, -1
```

Exit (to the end of the loop) if `Next` *is smaller than an item in the sorted portion.*

```
        if (Array(I) <= Next) exit
        Array(I + 1) = Array(I)
      end do
```

The loop terminates normally if all items in the sorted portion are larger than `Next`*.*

```
      Array(I + 1) = Next
      return
```

Operation Counts for Straight Insertion

```
do J = 1, size( Array ) - 1                                     ! 1
    Next = Array(J + 1)                                        ! < 2
    call Peck( 1, J, Next )                                    ! < 3
end do                                                         ! < 4
```

```
subroutine Peck( L, R, Next )
  do I = R, L, -1                                      ! < 5
    if (Array(I) <= Next) exit                         ! << 6
    Array(I + 1) = Array(I)                            ! << 7
  end do                                               ! << 8
  Array(I + 1) = Next                                  ! < 9
  return                                               ! < 10
```

Each iteration of the loop in the subroutine (lines 6 to 8) requires one comparison. If the exit does not occur, the move operation at line 7 is executed.

In the "worst case," when the given data is presented in reverse order, the early exit never occurs so lines 5 to 8 perform J comparisons and J moves. There are two additional move operations, at lines 2 and 9. These J comparisons and $J + 2$ moves are repeated for $J = 1$ to $N - 1$, where N is the size of *Array*. Thus the total in the worst case is $0.5 \cdot N\ (N - 1) = 0.5 \cdot N^2 - 0.5 \cdot N$ comparisons and $0.5 \cdot N\ (N - 1) + 2 \cdot (N - 1) = 0.5 \cdot N^2 + 1.5 \cdot N - 2$ moves.

For the "average case" (random data), the loop at lines 6 to 8 will be iterated $J\ /\ 2$ times before exit occurs, so lines 3 to 8 perform $0.5 \cdot J$ comparisons and $0.5 \cdot J - 1$ moves; adding the moves at lines 2 and 9 gives $0.5 \cdot J + 1$ moves for the body of the outer loop, lines 2 to 4. Repeating these for $J = 1$ to $N - 1$, the average case total is $0.25 \cdot N^2 - 0.25 \cdot N$ comparisons and $0.25 \cdot N^2 + 0.5 \cdot N - 1$ moves.

Note that insertion sorting requires about half the number of comparisons and moves required by selection. This is because insertion searches a *sorted* array section, and thus requires only an expected $0.5 \cdot J$ comparisons, terminating when the insertion point is found. Selection, on the other hand, searches an *unsorted* array section and must examine every item.

In the "best case," when the given data is already in the correct order, exit occurs at the first iteration of the inner loop so the total count for lines 3 to 8 is one comparison and no moves (independent of J); lines 2 to 4 require one comparison and two moves. The entire procedure requires $N - 1$ comparisons and $2 \cdot N - 2$ moves in the best case.

Initially Ordered Data

Straight insertion is an excellent method for large amounts of data that is already almost in order. In the extreme case of data already completely in order, each item is compared with only one other and no move operations are required. Otherwise, the number of comparisons and moves for an item depends only upon the distance between its original and final positions. Benchmark time for 1 million real numbers already in order, on a 50 MHz 486DX computer, was found to be 4 seconds.

Straight Insertion Is Stable

For straight insertion sorting, each unsorted item is compared only with items that preceded it in the original unsorted array. The comparison relation causes termination of the insertion loop when a smaller or equal item is encountered. When an equal item is found, that item remains in place and the new item is inserted on its right. (To continue searching for a strictly smaller item would exactly reverse all duplicate items, besides being inefficient.) Thus it can be seen that the insertion sort method, if implemented with a bit of care, is stable.

I_1 #N_1 S_1 E1 R1 T1 I_2 O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
I1 N1 #S1 E1 R1 T1 I_2 O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
I1 N1 S1 #E1 R1 T1 I_2 O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 N1 S1 #R1 T1 I_2 O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 N1 R1 S1 #T1 I_2 O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 N1 R1 S1 T1 #I_2 O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 R1 S1 T1 #O N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 O R1 S1 T1 #N_2 S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 N_2 O R1 S1 T1 #S_2 O R_2 T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 N_2 O R1 S1 S_2 T1 #O R_2 T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 N_2 O O R1 S1 S_2 T1 #R_2 T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 N_2 O O R1 R_2 S1 S_2 T1 #T_2 E_2 X A M P L E_3
E1 I1 I_2 N1 N_2 O O R1 R_2 S1 S_2 T1 T_2 #E_2 X A M P L E_3
E1 E_2 I1 I_2 N1 N_2 O O R1 R_2 S1 S_2 T1 T_2 #X A M P L E_3
E1 E_2 I1 I_2 N1 N_2 O O R1 R_2 S1 S_2 T1 T_2 X #A M P L E_3
A E1 E_2 I1 I_2 N1 N_2 O O R1 R_2 S1 S_2 T1 T_2 X #M P L E_3
A E1 E_2 I1 I_2 M N1 N_2 O O R1 R_2 S1 S_2 T1 T_2 X #P L E_3
A E1 E_2 I1 I_2 M N1 N_2 O O P R1 R_2 S1 S_2 T1 T_2 X #L E_3
A E1 E_2 I1 I_2 L M N1 N_2 O O P R1 R_2 S1 S_2 T1 T_2 X #E_3
A E1 E_2 E_3 I1 I_2 L M N1 N_2 O O P R1 R_2 S1 S_2 T1 T_2 X

Say It with Fortran

For small amounts of data, or for data that is already nearly in order, insertion sorting is very suitable for Fortran (why?)

Example 5. Here, subroutine **Peck** has been moved in-line for efficiency. The subroutine **Print_Array** and the main program to test the module are the same as for Example 1 (except for the **use** statement in the main program).

```
! Example 5. Sorting an array of strings by straight insertion.
  subroutine In_Sort( Array )
    character (len = *), intent(in out), dimension(:) :: Array
```

The dummy argument **Array** *has assumed shape (with rank 1), character type, and assumed length. (The array size and the length of the strings in the array will be taken from the actual argument.) Its* **intent** *attribute is* **in out***, which means that the corresponding actual argument array must be definable (for example, it must not be an array-valued expression that contains operators), and all of its elements must have defined values at entry to the subroutine.*

```
    character (len = len( Array )) :: Next
    integer :: I, J
! start subroutine In_Sort
    do J = 1, size( Array ) - 1
      Next = Array(J + 1)
      do I = J, 1, - 1
```

The value of **J** *will be retained if an* **exit** *occurs.*

```
        if (Array(I) <= Next) exit
        Array(I + 1) = Array(I)
      end do
```

If the loop terminates normally, the value of **`I`** *is* **`0`** *and* **`Next`** *is inserted at position* **`1`**.

```
      Array(I + 1) = Next
    end do
    return
  end subroutine In_Sort
```

Insertion Sort with Pointers

Suppose that the structures in an array are very large. Would it be possible to sort them without moving them? This example shows how to move a corresponding array of *pointers* until the first pointer points to the item with the smallest key, etc. For purposes of illustration, in this example each data item consists of a string (*City_Name*), two scalar integers (*Latitude* and *Longitude*), and an array of 1,000 integers (*Stuff*). (In the following example, all elements of *Stuff* are zero. In practice, the data to be sorted would be generated by means that are not of concern here.)

In database terminology, the sorted array of pointers is an *index* to the data array. Pointer techniques can be applied with any of the sorting methods, but it is particulary advantageous for insertion since (as we have seen) much of the effort of this method occurs in moving the data elements.

The steps in this **`Sort`** subroutine parallel those of Example 5. The only changes are to move the pointers instead of the array elements.

Say It with Fortran

Example 6. Fortran does not provide arrays of pointers. (A variable with **`pointer`** and **`dimension`** attributes is a pointer to an array, not an array of pointers.) However, it is possible to define a structure having a single component that is a pointer, and then to create an array of these structures. (See the data type **`BOX`** in the following example.) Further examples of this technique are shown in Chapter 5.

```
! Example 6. Sort an array of structures by straight insertion with pointers.
  program D06
    implicit none
    integer, parameter :: NAME_LEN = 20
    type :: City_Data_Type
      character (len = NAME_LEN) :: City_Name
      integer :: Latitude, Longitude
      integer, dimension(1000) :: Stuff = 0
    end type City_Data_Type
    type :: BOX
      type (City_Data_Type), pointer :: DP
    end type BOX
    integer :: Array_Size, Loop
    type (City_Data_Type) Array
    type (City_Data_Type), dimension(:), allocatable, target :: Array
```

`X(I) % DP` *is a pointer to* **`City_Data_Type`**.

```
    type (BOX), dimension(:), allocatable :: X
```

```
! start program D06
    open (1, file = "jacumba.dat", status = "old", action = "read", &
      position = "rewind" )
    read (1, *) Array_Size
    allocate( Array(Array_Size), X(Array_Size) )
```

Load sample data into **`Array`**.

```
  do Loop = 1, Array_Size
    read (unit = 1, fmt = "(a, 2i)" ) Array(Loop) % City_Name, &
      Array(Loop) % Latitude, Array(Loop) % Longitude
  end do
  call In_Sort( )
  call Print_Array( )
  deallocate( Array, X)
  stop
contains
```

Array, which contains the data to be sorted, is an intent(in) argument; it will not be changed during execution of Sort. The intent(out) argument X is an array of type BOX; its pointer components will be set so that the first pointer points to the item with the smallest key, etc..

```
  subroutine In_Sort( )
    type (City_Data_Type), Pointer :: Next
    integer :: I, J
! start subroutine In_Sort
```

Array(1) becomes the target of the first pointer.

```
    X(1) % DP => Array(1)
    do J = 1, size( Array ) - 1
```

The first **`I`** *items are sorted. The next unsorted item becomes the target of* **`Next`**.

```
      Next => Array(J + 1)
      do I = J, 1, - 1
```

Compare the target of **`Next`** *with the target of an already sorted pointer.*

```
        if (X(I) % DP % City_Name <= Next % City_Name) exit
```

Move a pointer. (Note that elements of **`Array`** *never move.)*

```
        X(I + 1) % DP => X(I) % DP
      end do
```

Copy **`Next`** *to insert it among the sorted pointers.*

```
      X(I + 1) % DP => Next
    end do
    return
  end subroutine In_Sort

  subroutine Print_Array( X )
    integer :: I
! start subroutine Print_Array
    do I = 1, size( X )
```

Print components of the target of **`X(I) % DP`**, *including an arbitrary component of the array* **`Stuff`**

```
    print *, I, ': "', X(I) % DP % City_Name, '" ', &
      X(I) % DP % Latitude, X(I) % DP % Longitude, X(I) % DP % Stuff(17)
    end do
    return
  end subroutine Print_Array

end program D06
```

Insertion during Input

Some applications read data from an external file and sort it. The two operations can be combined, as shown in this example. For sorting during input, the insertion method is especially well suited, because it considers the unsorted items one at a time. Furthermore, for some applications the total time required may be dominated by the input phase so that the comparison and move operations cost nothing.

Expanding array.

The structure *Elastic* in this program illustrates use of an expanding array to hold a variable amount of data. The maximum amount of data that can be processed is limited by the size of the array, which is fixed at the time the array is created. It is convenient to enclose an expanding array in a structure along with an integer that holds the current length — i.e., the current number of array elements to which actual data has been assigned. The (maximum) array size is also recorded in the structure.

Say It with Fortran

Example 7.

```
! Example 7. Sort structures by straight insertion during input.
  program D07
    implicit none
    integer, parameter :: NAME_LEN = 20
    type :: City_Data_Type
      character (len = NAME_LEN) :: City_Name
      integer :: Latitude, Longitude
      integer, dimension(1000) :: Stuff = 0
    end type City_Data_Type
```

The derived type **`Elastic`** *holds the expanding array of structures along with an integer,* **`Current_Length`***, that records the current number of array elements to which actual data has been assigned. The (maximum) array size is also recorded in the structure for convenience.*[13]

```
    type :: Elastic
      type (City_Data_Type), dimension (:), pointer :: Array
```

Initialize **`Current_Length`** *to zero .*

```
      integer :: Current_Length = 0, Maximum_Length
    end type Elastic
    type (Elastic) :: A
! start program D07
    open (1, file = "jacumba.dat", status = "old", action = "read" &
      position = "rewind" )
    read (1, *) A % Maximum_Length
    allocate( A % Array(A % Maximum_Length) )
    call Read_And_Sort( )
```

[13] It should be noted that a standard Technical Report on Enhanced Derived Type Facilities supports allocatable arrays as derived type components; with Fortran versions that do not implement this report, pointers may be employed instead.

Component initialization in a derived type definition is a Fortran 95 enhancement; for versions that do not implement this feature, the declared initialization must be replaced by assignment statements in the main program.

```
  call Print_Array( )
  deallocate( A % Array )
  stop
contains
  subroutine Read_And_Sort( )
    type (City_Data_Type) :: Next
    integer :: I, J, EoF
! start subroutine Read_And_Sort
    do J = 0, A % Maximum_Length - 1
      read (1, "(a, i3, i4)", iostat = EoF) Next % City_Name, &
        Next % Latitude, Next % Longitude
      if (EoF < 0) exit
      do I = J, 1, - 1
```

Compare and move operations involve the array **`Array`**, *which is a component of the structure* **`A`** *of type* **`Elastic`**.

```
          if (A % Array(I) % City_Name <= Next) exit
        A % Array(I + 1) = A % Array(I)
      end do
      A % Array(I + 1) = Next
      A % Current_Length = J + 1
    end do
    return
  end subroutine Read_And_Sort
  subroutine Print_Array( )
    integer :: I
! start subroutine Print_Array
    do I = 1, A % Current_Length
      print *, I, ": ", A % Array(I) % City_Name, &
        A % Array(I) % Latitude, A % Array(I) % Longitude, &
        A % Array(I) % Stuff(17)
    end do
    return
  end subroutine Print_Array
end program D07
```

Binary Insertion

Any of the insertion methods that have been described, when applied to random data, compare the *J*th new item with about *J/2* sorted items. The expected number of comparisons can be reduced to lg *J* with binary searching. (Knuth notes that the idea of binary insertion was described by Mauchly as early as 1946 in a paper on nonnumerical computing.)

The steps must be reorganized a bit to separate the search process from the move operation. Instead moving up the sorted items one by one as they are found to exceed the new item, they are all moved up together after the insertion point has been located.

The binary search function (displayed earlier) is applied to the array of items that are already sorted, to obtain a 2-element vector. The second element of the result vector locates the smallest previously sorted item (or possibly a rather arbitrary one of two or more equal smallest items) that is at least as large as the new unsorted item to be inserted.

```
  do J = 1, size( Array ) - 1
```

Array(1: J) contains previously sorted data.

```
    Next = Array(J + 1)
```

Use binary search to locate `Next` *in the array section* `Array(1: J)`*. The insertion point, returned as Location(2), is between* `1` *and* `J +1`*, inclusive.*

```
    Location = Binary_Search( Array(: J), Next )
```

Move all items between `Array(Location(2))` *and* `Array(J)` *one position to the right; insert* `Next` *at* `Array(Location)`*. Note that nothing is moved if* `Location(2)` *is* `J +1`*.*

```
    Array(Location(2) + 1: J + 1) = Array(Location(2) : J)
    Array(Location(2)) = Next
  end do
```

Example 8.

The program examples distributed electronically include an expanded implementation of binary insertion during input. This algorithm will later be compared with linked list and tree algorithms for the same application.

Binary Insertion Is Not Stable

A disadvantage for some applications is that this method is not stable for duplicate items.

Operation Counts for Binary Insertion

```
  do J = 1, size( Array ) - 1                                        ! 1
    Next = Array(J + 1)                                              ! < 2
    Location = Binary_Search( 1, J, Next )                           ! < 3
    Array(Location(2) + 1: J + 1) = Array(Location(2) : J)           ! < 4
    Array(Location(2)) = Next                                        ! < 5
  end do                                                             ! < 6
```

In the average case, with arguments `( 1, J, Next )`, $1.5\cdot(\lg(J +1) -1)$ compares and no moves are required; the array section assignment performs $0.5\cdot I$ moves. The loop body (lines 2 – 6) performs $1.5\cdot(\lg(J +1) - 1)$ compares and $0.5\cdot I +2$ moves. This must be summed for J from 1 to $N - 1$, where N is the array size.

Let $k = J + 1$; the loop is executed with $k = 2$ to N, so the sum is

$N \lg N - 2\cdot\lg 2 - 1.4\cdot(N - 2) = N \lg N - 1.4\cdot N + 0.8$

Comparisons: $1.5\cdot N \lg N - 2.1\cdot N - 0.3$

Moves: $0.25\ N\ (N - 1) +2.0\ (N - 1) = 0.25\ N^2 +1.75\cdot N - 2$

The search scheme employed here is efficient — about $1.5\ N \lg N$ total comparisons — but it requires slightly more move operations, $0.25\cdot N^2 +1.75\cdot N - 2$, than straight insertion. However, modern pipeline and parallel processors can move contiguous array sections at high speed.

In the worst case, when the data is in reverse order, the array section assignment makes twice as many moves as straight insertion, in total $0.5\cdot N^2 +1.5\cdot N - 2$. In the best case, when the data is already in order, the array section assignment moves nothing so the total move count is $2.0\ N - 2.0$. For sorting a large amount of data that is almost in order, the $1.5\ N \lg N$ comparison count makes binary insertion inferior to straight insertion.

A benchmark, run with a 50 MHz 486DX computer, sorted 20,000 random real numbers in 65 seconds.

2.3 SHELL SORT

Donald Shell in 1959 proposed a “diminishing increment” sort method. As Sedgwick explains, “Insertion sort is slow because it exchanges only adjacent elements. For example, if the smallest element happens to be at the end of the array, N steps are needed to get it where it belongs. Shell sort is a simple extension of insertion sort which gains speed by allowing exchanges of elements that are far apart.”[14]

Shell sort consists of a sequence of insertion sorts applied to nonconsecutive sections of the given array. At first, widely spaced elements are sorted by insertion. The spacing is then diminished until the final stage, which is a straight insertion sort of the entire array. The effect of the earlier stages is to guarantee that the array is almost in order before the final sort is applied.

Various increment sequences are possible. A popular sequence employs integers of the form floor($3^p / 2$), beginning with the largest such value that does not exceed the array size. For example, if the array size is more than 29,524 but less than 88,573 the sequence is 29,524, 9,841, 3,280, 1,093, 364, 121, 40, 13, 4, 1. Note that 3^p is odd for any positive integer p, so floor($3^p / 2$) = $(3^p - 1) / 2$. The initial increment can be calculated as $p_{max} = \log_3(2 \cdot N + 1) = \log_3(e) \cdot \ln(2 \cdot N + 1)$:

```
P_Max = int( LOG3_OF_E * log( 2.0 * N + 1.0 ) )
do P = P_Max, 1, -1
  H = (3 ** P) / 2
  do J = 1, N - H
    Next = Array(J + H)
    do I = J, 1, -H
      if (Array(I) <= Next) exit
      Array(I + H) = Array(I)
    end do
    Array(I + H) = Next
  end do
end do
```

Suppose that $13 \le N < 40$ (for example, $N = 28$) so that the increment sequence is 13, 4, 1; and consider the second stage, when the increment is 4. This stage begins by comparing position 5 with position 1; later on, position 9 is compared with the sorted sequence in positions (5, 1); position 13 is compared with the “chain” of sorted data at positions (9, 5, 1); position 17 is compared with the chain (13, 9, 5, 1); position 21 is compared with the chain (17, 13, 9, 5, 1); and finally position 25 is compared with the chain (21, 17, 13, 9, 5, 1). The effect is a straight insertion sort of the chain (25, 21, 17, 13, 9, 5, 1).

The straight insertion sorts (for a given increment) are are interleaved. For example, elements in positions between 21 and 25 are examined as they naturally occur. Immediately after element 21 is inserted into the chain (17, 13, 9, 5, 1), the next step is to insert element 22 into the chain (18, 14, 10, 6, 2), then to insert element 23 into the chain (19, 15, 11, 7, 3), and so on.

Shell sort is not a stable sorting method.

Operation Counts for Shell Sort

The running time for Shell sort is very difficult to predict, and is known to depend heavily upon the increment sequence. Sedgewick states that $N^{1.5}$ is a provable upper bound on the number of comparisons for a wide variety of sequences including the one given here; for other carefully chosen increment sequences the bound $N^{4/3}$ can be proved and $N^{7/6}$ is conjectured empirically.

A benchmark, run with a 50 MHz 486DX computer, sorted 1 million random real numbers in 201 seconds. This timing is consistent with an estimate of $1.2 \cdot N^{1.3}$ comparison operations and the same number of move operations.

[14] R. Sedgewick, *Algorithms,* Second Ed. [Reading: Addison-Wesley, 1988], 107.

Shell Sort with Array Sections

Example 9. It is possible to subdivide the outer **do** construct so that each chain is separately completely ordered:

```
do K = 1, min( H, N - H )
  do J = K, N - H, H
    Next = Array(J + H)
    do I = J, 1, -H
      if (Array(I) <= Next) exit
      Array(I + H) = Array(I)
    end do
    Array(I + H) = Next
  end do
end do
```

The two inner loops can now be replaced by a call to **In_Sort** with a noncontiguous array section argument. **In_Sort** is the normal straight insertion sort procedure (as in Example 5) with an assumed shape array dummy argument. From the viewpoint of **In_Sort**, the dummy argument is a contiguous array object; the loop increment value inside the procedure **In_Sort** is one.

Say It with Fortran

When the increment value is *H*, the following modified Shell sort procedure makes *H* calls to **In_Sort** with different array sections that all have *stride H*:

```
! Example 9. Shell Sort with array Sections
  subroutine Sh_Sort( Array )
    real, intent(in out), dimension(:) :: Array
    integer :: N, P_Max, P, H, K
    real, parameter :: LOG3_OF_E = 0.9102392227
! start subroutine Sh_Sort
    N = size( Array )
    P_Max = LOG3_OF_E * log( 2.0 * N + 1.0 )
    do P = P_Max, 1, -1
      H = (3 ** P) / 2
      do K = 1, min( H, N - H )
```

Call straight insertion sort procedure. The actual argument is an array section whose stride is the current Shell sort increment. See the discussion of Explicit Interface, below.

```
      call In_Sort( Array(K: N : H) ) ! Array section
      end do
    end do
    return
  end subroutine Sh_Sort
```

Explicit Interface

Under certain conditions, reference to a procedure requires that interface information for the procedure be *explicit* at the point of reference (see any complete Fortran 90 or 95 handbook or textbook; for example, Appendix D.6 in *Fortran 90* by Meissner). One such condition is the appearance of a dummy argument that is an assumed shape array, like **In_Sort** in this example. Other conditions that require explicit interface information are pointer arguments, optional or keyword arguments, and function results whose properties are established during execution.

We recommend making *all* procedure interfaces explicit. This can be accomplished by entirely avoiding external procedures; the recommended alternatives are internal procedures and module procedures, whose interfaces are automatically explicit. In the electronic versions of Example 9, **`In_Sort`** is implemented either as an internal procedure contained in **`Sh_Sort`** or else as a module procedure in the same module. If an external procedure is unavoidable for some reason, an *interface block* may be provided in the referencing program unit or module.

2.4 HEAPSORT

Heapsort, like insertion sort, compares unsorted items against a chain of items that are already in order.[15] A “peck” operation compares a new item to items in the chain, beginning with the largest, promoting each item that is larger and inserting the new item just above the first one that is smaller or equal. As with Shell sort, a chain does not consist of consecutive array elements; however, instead of being evenly spaced, heapsort chains “fan out”: the subscript value approximately doubles at each step as the chain is traversed.

Binary Trees (Array Representation) and Heaps

A *binary tree* is a set of *nodes* (data items) with a *root node.* As many as two “child” nodes may be connected to each node in the tree; thus the tree is divided into *layers* according to the distance of nodes from the root. If a node in the *k*th layer has any children, they are in the k + 1st layer. Each layer may potentially contain twice as many nodes as the previous layer.

A binary tree can be constructed within an array by interpreting array subscript values in a special way. (Unlike the trees described in Chapter 7, this representation does not employ pointers.) Each layer occupies a set of *consecutive* array elements. The root, layer 0, is stored at $Array_1$. Space for nodes in the first layer is reserved at array element positions 2 and 3; for the second layer at positions 4, 5, 6, and 7; etc. In general, the *k*th layer is stored at positions 2^k through $2^{k+1} - 1$. Array elements form the binary tree as follows:

- Element $Array_1$ is the root node in the tree.
- An element $Array_J$ has zero, one, or two *children*. If there is one child, it is at $Array_{2J}$; if there are two, the second is at $Array_{2J+1}$.
- Unless the element $Array_J$ is the root, its *parent* is at $Array_{\mathrm{floor}(J/2)}$. (In a Fortran program, the subscript for a parent can be computed by integer division.)

A *heap*[16] is a binary tree represented in an array (in the manner just described), with the following two additional properties:

1. A heap has a structure property called *completeness*: each layer is filled from left to right. Since each layer is stored consecutively, this means that there are no “holes” (unoccupied elements) in the array. A tree with N nodes, where N is at least 2^p but is less than 2^{p+1}, has layers 0, ..., p. In all layers except the last two, every node must have two children. In layer $p - 1$, any nodes with two children must be at the left end of the layer, followed by at most one node with a single child, and then by any nodes with no children. Items in layer p have no children.

   Elements in the right half of the array (all of layer p and possibly the left end of layer $p - 1$) have no children, because a child must have a subscript at least twice that of its parent. The following can be verified by closer examination: For odd N, all elements at positions up to $(N - 1)/2$ have two chil-

[15] If data items are not simply numbers, ordering is of course based on a sort key.

[16] This use of the term *heap* has no relation to dynamic storage. It was applied to the storage scheme used in this sorting algorithm in 1964 by the discoverers, J.W.J. Williams and R.W. Floyd. (Knuth, *Sorting and Searching*, 145).

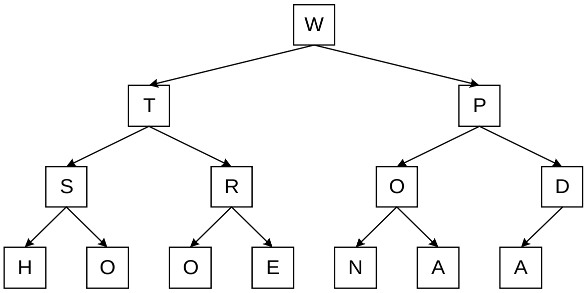
dren and all elements beginning with $(N+1)/2$ have no children. For even N, element $N/2$ has one child; all preceding elements have two children and all following elements have no children.

Thus nodes with a single child are rare: there is exactly one such a node when the number of nodes is even, and there is no such node when the number of nodes is odd. This means, as we shall see later, that the single-child case has little effect on timing estimates.

2. A heap has a rather loose *order* property: In terms of key value, any node must always be larger than each of its children, if it has any. If there are two children, either one of them may be the larger. Note that the root, at layer 0, will always be the largest in the entire heap. The second-largest node may be either child of the root, at layer 1; the third-largest may be (at layer 1) the other child of the root, or it may be (at layer 2) either child of the second-largest node.

Note that removing one or more elements from the end of the array does not destroy the completeness property nor the heap order property.

For example, the following heap has 14 elements in layers 0, 1, 2, and 3. Layer 3 is not full. The three largest nodes are W, T, and S.



W	T	P	S	R	O	D	H	O	O	E	N	A	A

1

The Procedure Peck

Heapsort consists of two phases. First, a heap is constructed from data items already stored in the array. Second, the largest item in the heap is repeatedly selected and removed to a sorted region. Each phase employs a “pecking order” procedure.

```
  subroutine He_Sort( Array )
    real, dimension(:) :: Array
    integer :: N, J

! start subroutine He_Sort
    N = size( Array )
    do J = N / 2, 1, -1
      call Peck( J, N )
    end do
    do J = N, 2, -1
      call Swap( 1, J )
      call Peck( 1, J - 1 )
    end do
    return
  end subroutine He_Sort
```

The procedure **Peck** is applied to subtrees that have the heap order property except at the root. This procedure orders the entire subtree by moving the root item down a chain that chooses the *larger* child at each branch.

Except for the fact that the chain elements are not equally spaced in the array, and that the scan moves toward the right rather than toward the left, this procedure closely resembles the pecking order procedure of insertion sort or of Shell sort. The root item is set aside — copied to an auxiliary variable — and it is then compared with data items in the chain, beginning with the larger child of the root element and scanning down until it dominates some element in the chain. At that point, the scan terminates and the former root item takes its place in the chain. For random data, the expected insertion point is about half way down the chain. The following steps may be compared with the insertion sort procedure:

```
subroutine Peck( L, R )
  Next = Array(L)
  I = 2 * L
  do while (I <= R)
```

Choose larger child at each branch. If the number of elements is even, the last element has no sibling.

```
    if (I < R) then
      if (Array(I) < Array(I + 1)) I = I + 1
    end if
    if (Array(I) <= Next) exit
```

Use integer division to find the new position **Array(I / 2)**.

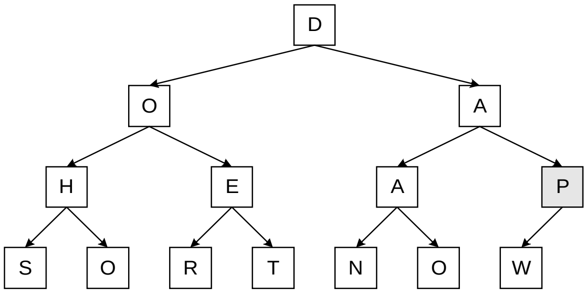
```
    Array(I / 2) = Array(I)
    I = 2 * I
  end do
  Array(I / 2) = Next
```

Note the importance of choosing the *larger* child at each branch of the chain: When a data item is moved upward in the chain, it becomes the parent of its former sibling; the order property is preserved because the new parent is larger than the former sibling that becomes its child.

Building the Heap by Chain Insertion

The first phase of heapsort constructs a heap from data that is already stored in the array. Note that the element at position floor(N / 2) is the rightmost array element that has a child. The procedure **Peck** is applied to the array elements in turn, beginning at position floor(N / 2) and moving to the left. The effect is to construct small heap-ordered trees and merge them into larger trees. Thus, when **Peck** moves an item into position its children (if any) are already in their correct positions.

As an example, consider the following initially unordered data set:

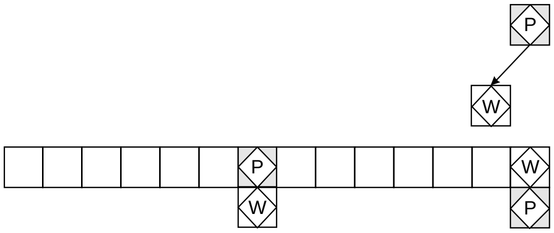


D	O	A	H	E	A	P	S	O	R	T	N	O	W

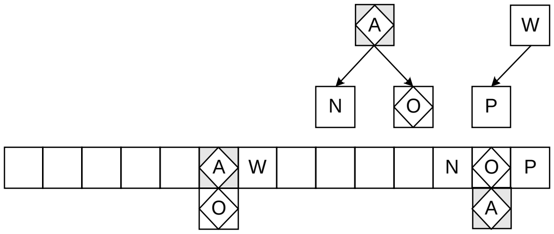
2

Here, the size of the data set, *N*, is 14. Heap construction begins with the rightmost element that has a child, which is P in subscript position *N* / 2 at the right end of layer 2. The procedure **Peck** is applied to the chain that begins with this element.

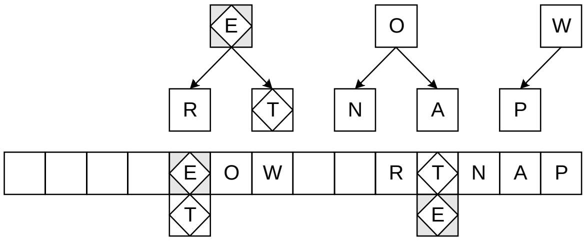
In the following diagrams, items in the current chain are enclosed in diamond shapes, and the element to be inserted is shown with a shaded background.



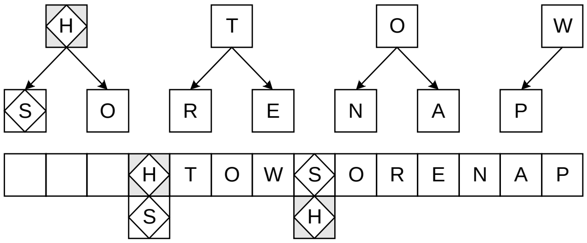
3



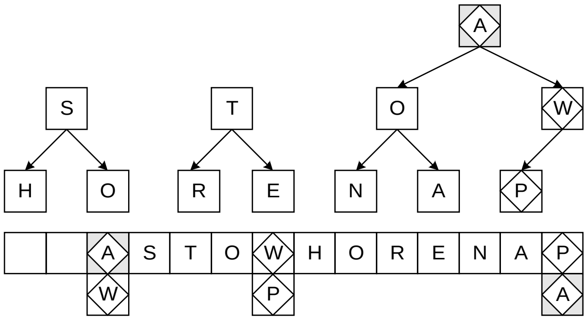
4



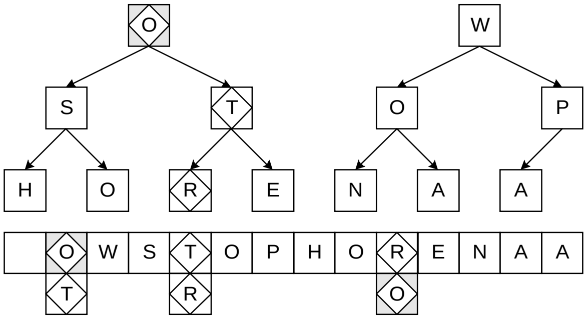
5



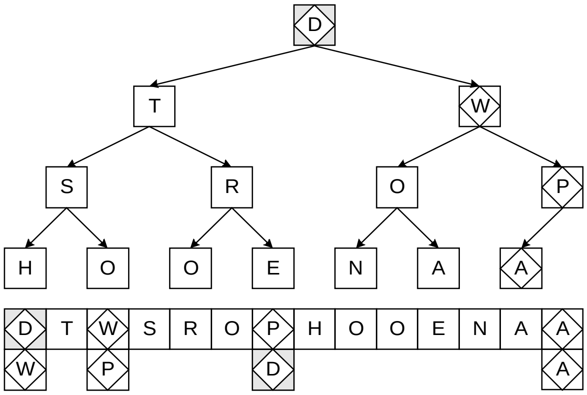
6


A
S
T
O
W
H
O
R
E
N
A
P
A S T O W H O R E N A P
W P A

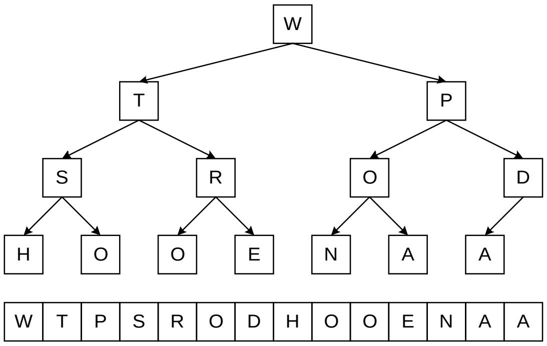
7


O
W
S
T
O
P
H
O
R
E
N
A
A
O W S T O P H O R E N A A
T R O

8


D
T
W
S
R
O
P
H
O
O
E
N
A
A
D T W S R O P H O O E N A A
W P D A

9


W
T
P
S
R
O
D
H
O
O
E
N
A
A
W T P S R O D H O O E N A A

10

It may be verified that the result is a heap with the required structure and loose order properties.

Sorting the Heap by Selection

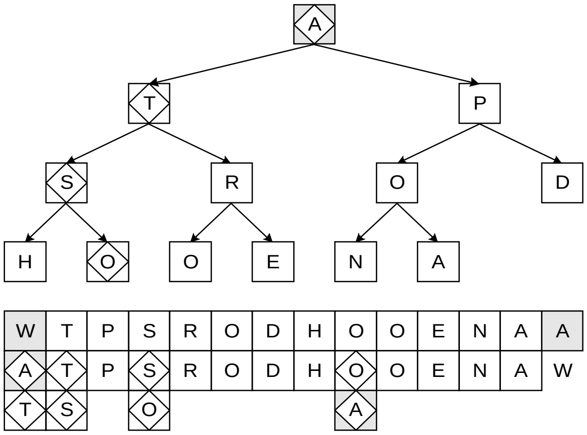
After the heap has been constructed, the second phase begins. As mentioned earlier, because of the heap order property the largest item is now the root element, *Array*$_1$.

This phase resembles selection sort in that it repeatedly finds the largest item in the (unsorted) heap, removes it from the heap, and stores it as the smallest sorted item. Because of the loose order property of the heap, a chain of only lg *J* elements must be traversed to reorder the heap so that the largest of *J* items is in the root position.

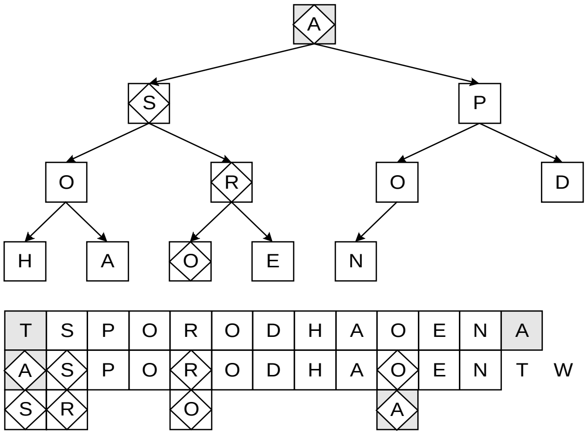
A sorted section is constructed, beginning at the right end of the array. For each value of *J* from *N* down to 2, the largest remaining item, at *Array*$_1$, is removed from the heap and is added to the sorted section at *Array*$_J$. The operation actually performed is to swap *Array*$_J$ with *Array*$_1$. This removes *Array*$_J$ from the heap and decreases the size of the heap by one item while maintaining the heap structure property.

The swap operation does not reorder any of the items in the heap except the one just moved to *Array*$_1$. Applying the procedure **Peck** to the chain beginning at *Array*$_1$ restores heap order and again guarantees that the largest unsorted item is at the root.

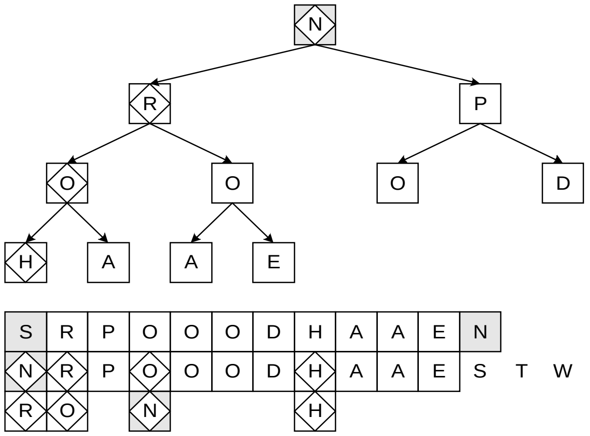
So long as *J* (the number of items in the heap) is two or more, *J* is decreased by one and the process is repeated. In the following diagrams, the first two rows at the bottom show the heap before the swap and the entire array after the swap. As before, diamonds indicate the pecking chain, and the item enclosed in a diamond with a shaded background is the one that is to be inserted.



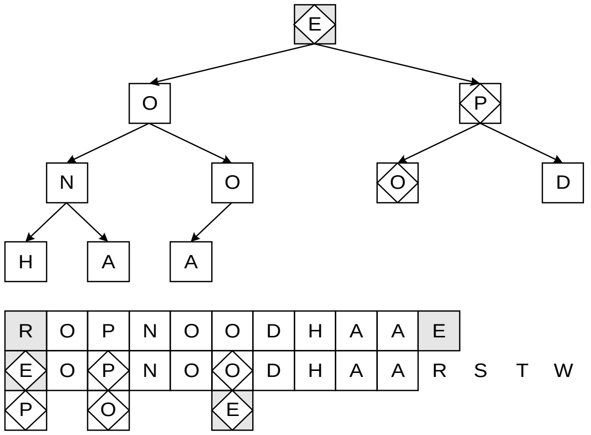
11



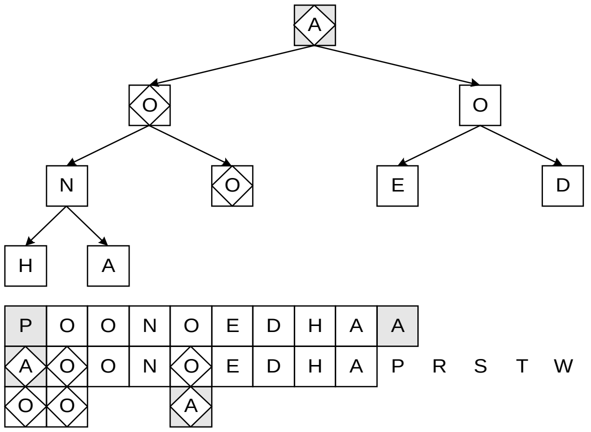
12


N
R
P
O
O
O
D
H
A
A
E
S R P O O O D H A A E N
N R P O O O D H A A E S T W
R O N H

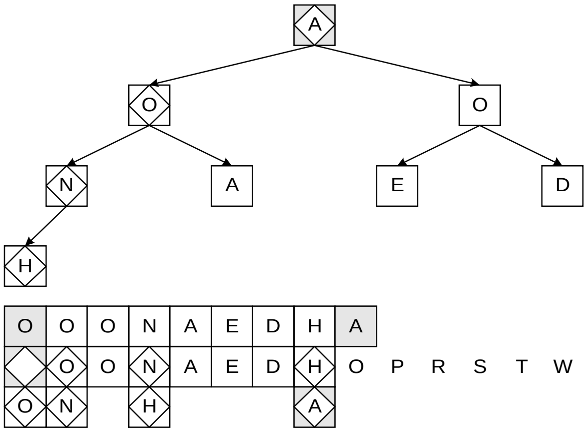
13


E
O
P
N
O
O
D
H
A
A
R O P N O O D H A A E
E O P N O O D H A A R S T W
P O E

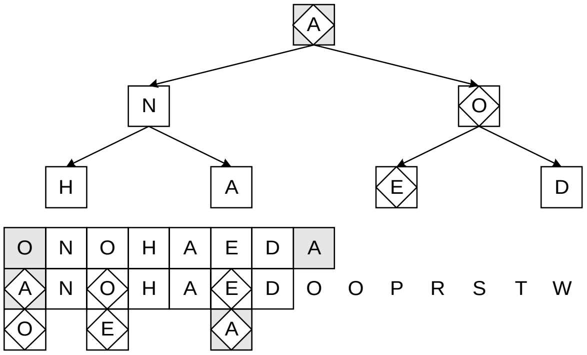
14


A
O
O
N
O
E
D
H
A
P O O N O E D H A A
A O O N O E D H A P R S T W
O O A

15


A
O
O
N
A
E
D
H
O O O N A E D H A
O O N A E D H O P R S T W
O N H A

16


A
N
O
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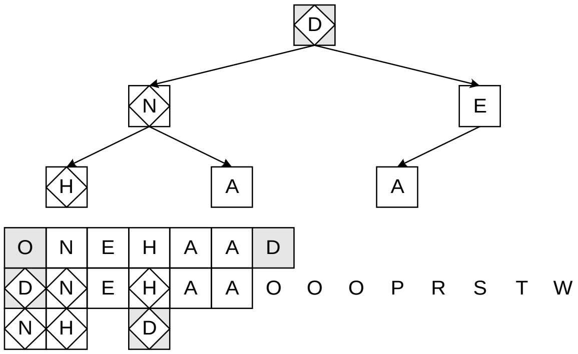
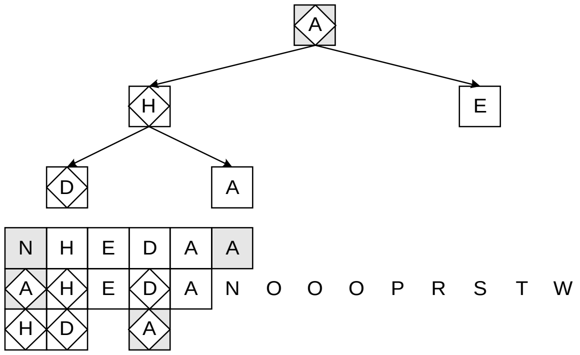
A
E
D
O N O H A E D A
A N O H A E D O O P R S T W
O E A

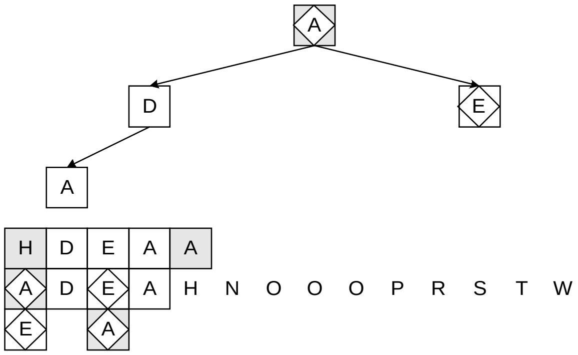
17


D
N
E
H
A
A
O N E H A A D
D N E H A A O O O P R S T W
N H D

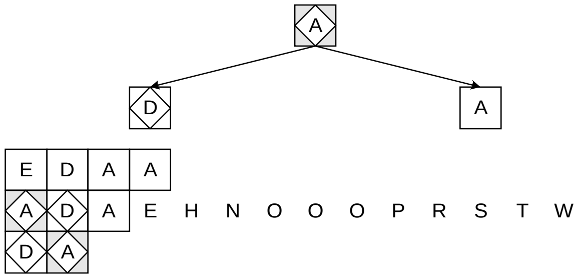
18


A
H
E
D
A
N H E D A A
A H E D A N O O O P R S T W
H D A

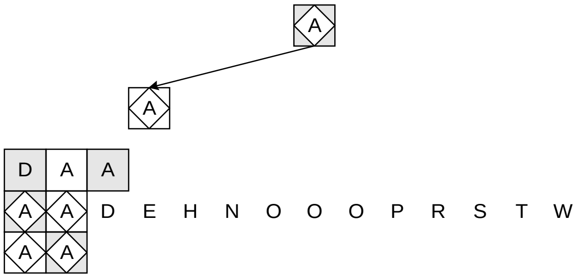
19


A
D
E
A
H D E A A
A D E A H N O O O P R S T W
E A

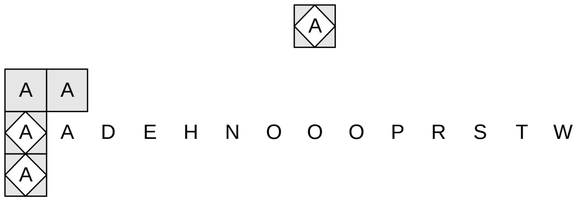
20


A
D
A
E D A A
A D A E H N O O O P R S T W
D A

21


A
A
D A A
A A D E H N O O O P R S T W
A A

22



23

During this second selection phase, insertion of items into the chain is definitely not random — in this example, A occurs as the item to be inserted on 10 of the 13 occasions. The item to be inserted has just been swapped into the root position from the last layer of the tree, so it is likely to be much smaller than average and insertion is unlikely to occur until almost the end of the chain.

Operation Counts for Heapsort

```
N = size( Array )                                        ! 1
do J = N / 2, 1, -1                                      ! 2
  call Peck( J, N )                                      ! 3
end do                                                   ! 4
do J = N, 2, -1                                          ! 5
  call Swap( 1, J )                                      ! 6
  call Peck( 1, J -1 )                                   ! 7
end do                                                   ! 8

subroutine Peck( L, R )
Next = Array(L)                                          ! 9
I = 2 * L                                               ! 10
do while (I <= R)                                       ! 11
  if (I < R) then                                       ! 12
    if (Array(I) < Array(I + 1)) I = I + 1              ! 13
  end if                                                ! 14
  if (Array(I) <= Next) exit                            ! 15
  Array(I / 2) = Array(I)                               ! 16
  I = 2 * I                                             ! 17
end do                                                  ! 18
Array(I / 2) = Next                                     ! 19
```

At line 13, the two siblings $Array_I$ and $Array_{I+1}$ are compared unless $Array_I$ has no sibling (a case that is rare enough to have no significant effect upon timing, as noted earlier).

The loop at lines 11 – 18 processes a chain of approximate length (lg R – lg L), but may exit before reaching the end of the chain. Each iteration requires two data item comparisons and one move, except for the last iteration in case of early exit.

As described earlier, by analogy to the integral the sum of logarithms $\sum_{i=a}^{b}$ lg i can be estimated as b lg b – a lg a – 1.4·(b – a).

- First phase, building the heap by insertion, lines 1 – 4: $\sum_{i=N/2}^{1} Peck_{i,N}$

For random data, exit during the first phase is expected at the midpoint of each chain. Thus the operation count for **`Peck`** consists of one move (line 9), plus two comparisons and one move for each iteration of lines 11 – 18. The number of iterations is

$$\begin{aligned}
&\textstyle\sum_{i=N/2}^{1} 0.5\cdot(\lg N - \lg i)\\
&\quad = 0.5\cdot\textstyle\sum_{i=N/2}^{1} \lg N - 0.5\cdot\sum_{i=N/2}^{1} \lg i\\
&\quad = 0.25\cdot N \lg N - 0.5\cdot(0.5\cdot N\ (\lg N - \lg 2)) - \lg 1 - 1.4\cdot(0.5\cdot N) + 1.4)\\
&\quad = 0.25\cdot N + 0.35\cdot N - 0.7 \text{ (Note that the terms in } N \lg N \text{ cancel.)}\\
&\quad = 0.6\cdot N - 0.7
\end{aligned}$$

The number of comparisons (two per iteration) is $1.2 \cdot N - 1.4$; the number of moves (one per iteration) is $0.6 \cdot N + 0.3$

- Second phase, sorting the heap by selection, lines 5 – 8: Three moves plus $\sum_{i=N/2}^{1} Peck_{1,i-1}$
  As noted earlier, exit is likely to occur near the end of the chain. For the worst case (exit at the end), the number of iterations is

  $$\begin{aligned} \sum_{i=2}^{N} \lg(\, i - 1\,) &= \sum_{k=1}^{N-1} \lg k \\ &= (N - 1) \lg(\, N - 1\,) - 1.4 \cdot (N - 2) \\ &= N \lg(\, N - 1\,) - \lg(\, N - 1\,) - 1.4 \cdot N + 2.8; \text{ approximating } \lg(N - 1) \text{ by } \lg N\text{:} \\ &= N \lg N - \lg N - 1.4 \cdot N + 2.8 \end{aligned}$$

  The estimated number of comparisons is $2 \cdot N \lg N - 2 \cdot \lg N - 2.8 \cdot N + 5.6$ and the number of moves is $N \lg N - \lg N - 1.4 \cdot N + \cdot 5.8$

- Total for lines 1 – 8:
  Comparisons: $2 \cdot N \lg N - 2 \lg N - 1.6\, N + 4.2$
  Moves: $N \lg N - \lg N - 0.8\, N + 4.5$

A heapsort benchmark, run with a 50 MHz 486DX computer, sorted one million random real numbers in 117 seconds. Inlining Peck and Swap (as in the following Fortran procedure) reduces the time to 108 seconds. (As wil be seen later, quicksort under the same conditions sorted one million random numbers in 56 seconds.) Knuth[17] shows that the worst case behavior for heapsort is only about ten percent slower than the average case; thus heapsort is the only internal sorting method with *guaranteed* $N \lg N$ behavior.

Say It with Fortran

Example 10. To reduce procedure call overhead, two copies of **Peck** are incorporated as in-line code; benchmarks show that this moderately decreases running time (by about 10%). Since the two **Peck** operations are written as separate statement sequences, it is possible to slightly simplify the swap operation at the beginning of the second phase: the item to be inserted into a chain is not actually stored at $Array_1$ but instead is moved to *Next*.

```
! Example 10. Heapsort [L P Meissner, 12 Nov 1995]
  subroutine He_Sort( Array )

    real, dimension(:), intent(in out) :: Array
    integer :: N, I, J
    real :: Next

! start subroutine He_Sort

    N = size( Array )
```

Build the heap. Start by “pecking” with the last element that has a child.

```
    do I = N / 2, 1, - 1
      Next = Array(J)
      J = I + I
      do while (J <= N)
        if (J < N) then
          if (Array(J) < Array(J + 1)) J = J + 1
        end if
```

[17] *Sorting and Searching*, 149

```
        if (Array(I) <= Next) exit
        Array(J / 2) = Array(J)
        J = J + I
      end do
      Array(J / 2) = Next
    end do
```

Now sort by selection. Move `Array(1)` *to the sorted portion, then restore the heap order property.*

```
    do I = N, 2, - 1
      Next = Array(I)
      Array(I) = Array(1)
      J = 2
      do while (J < I)
        if (J < I - 1) then
          if (Array(J) < Array(J + 1)) J = J + 1
        end if
        if (Array(J) <= Next) exit
        Array(J / 2) = Array(J)
        J = J + I
      end do
      Array(J / 2) = Next
    end do
    return
  end subroutine He_Sort
```

2.5 OPERATION COUNTS FOR SORTING: SUMMARY

`Swap`

Comparisons: 0
Moves: 3

`Swap` with test; *p* is the probability that the items to be exchanged are actually different.

Comparisons: 1
Moves: $3p$

`Min_Location`

Comparisons: $N - 1$
Moves: = $0.7 \cdot \lg N + 0.6$

`Binary_Search`

Comparisons: $1.5 \cdot \lg N - 1.5$
Moves: 0

`Sort_3`

Comparisons: 3
Moves: 4.5

Sorting Methods Described So Far (Slower to Faster)

Benchmark results are consistent with about ½ million compares or 1½ million moves per second on a 50 MHz 486DX. These numbers include the accompanying overhead.

`Se_Sort` (selection)
    Comparisons: $0.5 \cdot N^2 + 0.5 \cdot N - 1$
    Moves: $0.7 \cdot N \lg (N - 1) + 5.6 \cdot N - 0.7 \cdot \lg (N - 1) - 6.6$
    Benchmark time for 20,000 random real numbers: 350 seconds

`In_Sort` (straight insertion)
    Timing is strongly data-dependent.
    Average Case (random data):
        Comparisons: $0.25 \cdot N^2 - 0.25 \cdot N$
        Moves: $0.25 \cdot N^2 + 0.5 \cdot N - 1$
        Benchmark time for 20,000 random real numbers: 291 seconds.
    Best Case (data in order)
        Comparisons: $N - 1$
        Moves: $2 \cdot N - 2$
    Benchmark time for 1 million real numbers already in order: 4 seconds
    Worst Case (data in reverse order)
        Comparisons: $0.5 \cdot N^2 - 0.5 \cdot N$
        Moves: $0.5 \cdot N^2 + 1.5 \cdot N - 2$

Binary Insertion with block move.
    Timing is strongly data-dependent.
    Average Case (random data):
        Comparisons: $1.5 \cdot N \lg N - 2.1 \cdot N - 0.3$
        Moves: $0.25 \cdot N^2 + 1.75 \cdot N - 2$
        Benchmark time for 20,000 random real numbers: 65 seconds.
    Best Case (data in order)
        Comparisons: $1.5 \cdot N \lg N - 2.1 \cdot N - 0.3$
        Moves: $2 \cdot N - 2$
    Worst Case (data in reverse order)
        Comparisons: $1.5 \cdot N \lg N - 2.1 \cdot N - 0.3$
        Moves: $0.5 \cdot N^2 + 1.5 \cdot N - 2$

`Sh_Sort` (Shell sort) with array sections. Conjectured operation counts are based on benchmark.
    Timing is dependent on choice of intervals.
    Comparisons: $1.2 \cdot N^{1.3}$
    Moves: $1.2 \cdot N^{1.3}$
    Benchmark time for 1 million random real numbers: 201 seconds

`He_Sort` (heapsort)
    Comparisons: $2 \cdot N \lg N - 1.6 \cdot N - 2 \cdot \lg N + 4.2$
    Moves: $N \lg N - 0.8 \cdot N - \lg N + 4.5$
    Benchmark time for 1 million random real numbers: 104 seconds

Chapter 3 Recursion and Quicksort

The sorting methods descibed up to this point employ *iteration* to cycle through the data. A completely different approach to repetition is *recursion*, as illustrated in Fig 3.1. Quicksort, the fastest known sorting method, is most naturally implemented with recursion.

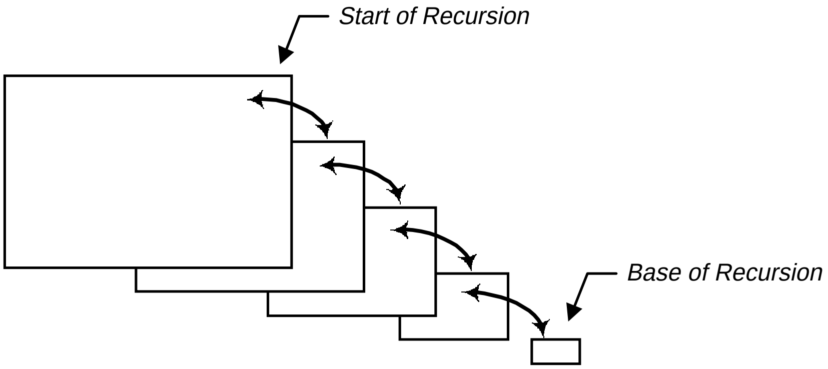


FIGURE 3.1. Recursion

This form of repetition starts with a call to a procedure that performs the set of steps to be repeated. The procedure continues the repetition by calling another *instance* of itself, unless no further repetitions are needed. In that case — called the *base* of the recursion — the recursion begins to unwind by terminating execution of all the recursive procedure calls, beginning with the last called instance.

3.1 RECURSION

Discussion of recursive sorting is here preceded by an overall description of the application and implementation of recursion. The implementation concept most crucial for making recursion work is that the system allocates a separate block of local storage for each instance of the recursive procedure when it is called.

Consider a recursive method for printing a list of data items in reverse order:

> To reverse-print a list of integers:
> If the list is empty, do nothing.
> Otherwise, reverse-print a smaller list that consists of all except the first integer, and then print the first integer.

Some features of this description are common to many recursive problems:

1. The method for performing a *sequence of tasks* (“reverse-print a list of integers”) is described quite differently from the method for performing a *component task* (“print an integer”).
2. The way to perform a *component task* (“print an integer”) is supposed to be already known or to be defined elsewhere.
3. The way to perform a *sequence of tasks* (“reverse-print a list”) is never completely specified; it is described only incrementally — the procedure itself is composed from a *derivative sequence of tasks* (“reverse-print a smaller list”) and a *component task* (“print an integer”).
4. However, the performance of a certain *base sequence* (“reverse-print an empty list”) is described completely.

Recursive procedures should be created with some care. It is especially necessary to be sure that the sequence of derivations generated at step 3 will eventually lead to the base. A very common class of recursive procedures involves an integer argument that decreases with each recursive call; with a small integer base, such as 1 or 0, eventual termination is assured.

The print application employs a slightly different strategy: It employs a list that grows shorter at each derivation, with an empty list as the base. Suppose that the input file holds three integers, 101, 201, 301, and 0, in this order. The zero is a “sentinel” value that is not considered part of the list; it merely terminates the list and is not to be printed.

```
Reverse-print “101, 202, 303” by doing the following:
        Reverse-print “202, 303” by doing the following:
            Reverse-print “303” by doing the following:
                    Reverse-print “” (an empty list) by doing nothing;
                    Print “303”.
            Print “202”.
        Print “101”.
    Stop.
```

Example 11. The following recursive procedure reads a data item and tests whether it is zero; if not, it calls itself recursively to read and process another item:

```
! Example 11. Reverse-print a list of integers.
  program D11
    implicit none
! start program D11
    call Reverse_Print( )
    stop
  contains
    recursive subroutine Reverse_Print( )
      integer :: A
  ! start subroutine Reverse_Print
      read *, A
```

Skip the recursive call when zero is read (the base case).

```
      if (A /= 0) then
        call Reverse_Print( )
        print *, A
      end if
      return
    end subroutine Reverse_Print

  end program D11
```

The program declares only one variable, *A*, and yet it could apparently process an arbitrarily large number of data items. What happens to the earlier data items while later items are being read and printed? As mentioned earlier, the crucial idea in the implementation of recursion is to give each instance of a recursive procedure its own *activation record,* which is a block of storage that contains an instance of each local variable declared in the procedure.[18] This block also contains procedure arguments (if any — in the form of values or references) for the current procedure instance, as well as information needed for returning to the reference point.

Let us examine the execution sequence for **`Reverse_Print`** in detail.

- The main program calls **`Reverse_Print`**. Since there will be several instances of **`Reverse_Print`**, let us call the first one **RP**$_1$.
- **RP**$_1$ reads the integer 101 and assigns it to the variable **A** in the activation record for **RP**$_1$, which we designate as "**RP**$_1$'s **A**". Since **A** is not zero, it calls **`Reverse_Print`** — i.e., **RP**$_2$.
- **RP**$_2$ reads 202 and assigns it to the variable **A**, this time designated as "**RP**$_2$'s **A**". Again **A** is not zero so it calls **`Reverse_Print`** — i.e., **RP**$_3$.
- **RP**$_3$ reads 303 and assigns it to the variable "**RP**$_3$'s **A**". Again **A** is not zero so it calls **RP**$_4$.
- **RP**$_4$ reads 0 and assigns it to the variable "**RP**$_4$'s **A**". This time **A** is the sentinel which is not to be processed. **RP**$_4$ makes no further procedure call and exits, thus returning control to **RP**$_3$ at the point just after the call to **RP**$_4$.
- **RP**$_3$ continues by printing its copy of the variable **A**, namely "**RP**$_3$'s **A**" which is 303. This is the first number that has been printed during program execution up to this point. After the print step, **RP**$_3$ returns control to **RP**$_2$ at the point just after the call to **RP**$_3$.
- **RP**$_2$ prints "**RP**$_2$'s **A**", which is 202, then returns control to **RP**$_1$.
- **RP**$_1$ prints "**RP**$_1$'s **A**", which is 101, then returns control to the main program and stops.

Recursion Compared with Iteration

Some problems can be described more naturally as recursive processes than as iterative processes. If you normally think of a factorial as an integer times a smaller factorial, you can translate that problem description directly into a recursive program. On the other hand, recursion usually entails some loss in efficiency, including extra procedure-call overhead and hidden storage requirements.

This text recommends that program comprehension be viewed as the primary objective, giving somewhat less importance to efficiency of execution. In the 1970s, emphasis on "structured programming" awakened computer users to the fact that small gains in efficiency can easily be lost due to errors introduced by failure to understand a problem.

- Some applications can be viewed with almost equal ease either iteratively or recursively. Iteration is *always* somewhat more efficient — it requires less overhead and less space — so iteration is preferable when there is no special reason to choose recursion.
- Some problems are very naturally understood with recursion and exceedingly awkward in iterative form. Tree structures (see Chapter 7) are processed naturally by means of recursion, because a tree consists of subtrees that have essentially the same structure as the tree itself. Quicksort (to be explained next) depends naturally on recursion. Even in Fortran, such applications should not be forced into an unsuitable iterative form. Effort may be directed toward making the recursive version as efficient as possible.
- Some applications require a more difficult choice between a recursive version that is a bit easier to understand and an iterative version that runs a bit faster or uses less storage. If efficiency is truly the dominant factor, iteration should be chosen. Otherwise, the recursive approach should be adopted

[18] The activation record does not include variables with the **`save`** or **`allocatable`** attributes.

if it seems more natural: a program that is more natural or easier to understand may justify some moderate loss of efficiency.

Another example is linked list insertion (see Section 5.2). The recursive method is significantly more elegant than iteration, but can be very wasteful of space if the list is very long. Algorithms (such as recursive linked list insertion) for which the depth of recursion is close to *N* (the amount of data) are useful only for small quantities of data.

- It has been shown that iteration is equivalent to a special form of recursion called *tail recursion*, which may be recognized by the fact that a recursive call is executed as the last step of the recursive process. In principle, therefore, iteration can invariably be converted to recursion, but the converse is not always true.[19] Some modern optimizing compilers detect tail recursion and translate it automatically to iteration. Thus, it is sometimes possible to maximize comprehensibility without sacrificing efficiency.

A Good Example of Recursion: Towers of Hanoi

A puzzle known as *The Towers of Hanoi* lends itself well to a recursive solution. The puzzle consists of three pegs, one of which holds a pile of discs of different sizes arranged in order with the largest disc on the bottom and the smallest disc on top. Typical versions of the puzzle have between three and six discs. The pile of discs is to be moved to one of the empty pegs; at each step only one disc is to be moved, and a larger disc must never be placed on top of a smaller disc. The pegs may be numbered 0, 1, and 2, with the discs on peg 0 at the beginning and on peg 2 at the end.

Suppose, for the moment, that a method were known for moving the pile of discs *except the largest one* from one peg to another. This smaller pile could be moved from peg 0 to peg 1; then a simple move would transfer the large disc from peg 0 to peg 2; and finally the hypothetical method would move the smaller pile from peg 1 to peg 2, thus moving the entire original pile from 0 to 2 as required.

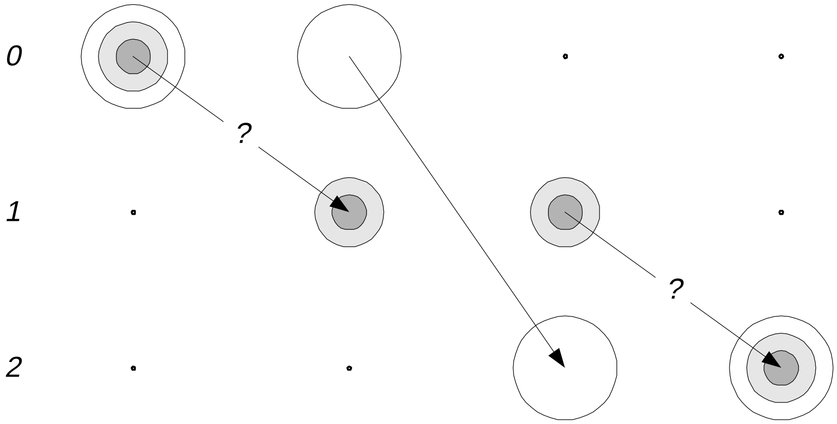


FIGURE 3.2. Solution to 3-disc Hanoi puzzle

[19] For an excellent discussion of iteration versus (linear) recursion, see H. Abelson and G. J. Sussman, *Structure and Interpretation of Computer Programs* (Cambridge, Mass.: MIT Press, 1985), 30–34. As noted in Section 5.2, some tail-recursive linked list processing techniques are apparently not directly convertible to Fortran iterative syntax. See also T. W. Pratt, *Pascal, A New Introduction to Computer Science* (Englewood Cliffs, N.J.: Prentice Hall,1990), Section 12.7.

Like the reverse-print procedure, the foregoing paragraph never completely tells how to “move a pile of discs”; it describes only a similar but simpler task (“move all of the discs except the largest one”) and a component task (“transfer the largest disc”):

To move *n* discs from peg *i* to peg *j*:

- If *n* is 1, simply transfer the single disc from peg *i* to peg *j*;
- Otherwise, move *n* – 1 discs (all except the largest) from peg *i* to peg *k* (the peg that is neither *i* nor *j*), transfer the largest disc from peg *i* to peg *j*, and move *n* – 1 discs from peg *k* to peg *j*.

For a more complicated iterative solution, place the pegs at the vertices of an equilateral triangle and alternate between moving the smallest disc clockwise and moving the only other available disc counterclockwise.

The number of moves for *n* discs is $2^n - 1$. As we shall see in the following chapter, this algorithm is unfeasible if *n* is large. However, an algorithm that simulates each of the individual moves will unavoidably require an amount of calculation approximately proportional to 2^n. The size of the task is inherent in the problem, and not in the method of solution. The recursive solution seems to give more insight into the problem than the iterative version.

A Bad Example of Recursion: The Fibonacci Sequence

About 800 years ago Leonard of Pisa, surnamed Fibonacci, posed the following problem: “A certain man put a pair of rabbits in a place surrounded by a wall. How many pairs of rabbits can be produced from that pair in a year, if it is supposed that every month each pair begets a new pair which from the second month on becomes productive?” The number of pairs each month is given by the *Fibonacci sequence* 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, . . ., in which each number after the first two is the sum of the two previous numbers:

```
   pure recursive function Fibonacci( N ) result( Fibonacci_R )
     integer, intent(in) :: N
     integer :: Fibonacci_R
 ! start function Fibonacci
     if (N <= 2) then
       Fibonacci_R = 1
     else
       Fibonacci_R = Fibonacci( N - 1) + Fibonacci(N - 2 )
     end if
     return
   end function Fibonacci
```

This recursive function produces the correct result so long as *N* is small enough. For the result to be representable as a 4-byte IEEE integer, *N* must not exceed 46; however, the procedure is intolerably slow for values of *N* near the upper end of this range. Each call to the function with $N > 2$ generates two more calls to the same function; the total number of recursive function calls is the same as the result being calculated: approximately 1.6^N calls, or more than 10^7 (46 seconds on our benchmark machine) for $N = 36$, 10^8 (almost nine minutes) for $N = 41$, and 10^9 function calls (more than 1.5 hours) for $N = 46$.

Much simpler methods are available. Fibonacci numbers can be calculated iteratively by a method whose running time is linear in *N*. The following steps begin with the first two Fibonacci numbers, both of which are 1. The two previous values are saved at each step.

```
Fibonacci_R = 1
if( N > 2) then
  Prev_1 = 1
  do Loop = 3, N
    Prev_2 = Prev_1
    Prev_1 = Fibonacci_R
    Fibonacci_R = Prev_1 + Prev_2
  end do
end if
```

Still more simply (and with constant running time, *independent* of N), the Nth Fibonacci number can be calculated directly from the formula $(\alpha^N - \beta^N) / (\alpha - \beta)$, where α and β are roots of the quadratic equation $x^2 - x - 1 = 0$; namely, $(1 \pm \sqrt{5}) \ / \ 2$, i.e., 1.618033989 and –0.618033989 . With IEEE eight-byte real representation, this formula gives correct results (to the nearest integer) for $N \leq 46$.

```
! Fibonacci numbers by direct calculation from formula
  program Fibonacci
    integer, parameter :: SRK9 = selected_real_kind( 9 )
    real(kind = SRK9), parameter :: ALFA = 1.618033988749895_SRK9, &
      BETA = - 0.618033988749895_SRK9, &
        DELTA = 2.23606797749978969641_SRK9
    integer :: N
! start program Fibonacci
    do
      print *, " Please enter an integer between 0 and 46"
      print *, " Enter an integer larger than 46 to stop."
      read *, N
      if ((N < 0) .or. (N > 46)) stop
      write (*, "( t2, i4, f20.0 )") N, (ALFA ** N - BETA ** N) / DELTA
    end do
    stop
  end program Fibonacci
```

Since β is smaller than 1, it turns out that β^N can be ignored if the “nearest integer” function is applied:

```
      write (*, "( t2, i4, i24.0 )") N, nint( ALFA ** N / DELTA )
```

Application: Adaptive Quadrature (Numerical Integration)

Example 12. A numerical application that employs recursion is adaptive quadrature. A one-step Simpson Rule calculation is applied to the whole interval (A, B); the result is compared with the sum of one-step calculations applied separately to the left and right halves of the interval. If these are nearly equal, the sum is accepted as the final answer; otherwise, adaptive quadrature is applied recursively to each half interval. The effect is to apply smaller step sizes where the integrand has greater functional variation. It has been pointed out that this technique is successful for most problems because each subdivision typically decreases the approximation error by a factor of 15 but tightens the accuracy requirement by only a factor of two.[20] (For Fortran 95 versions, which declare **Quad** as a **pure** function, the integrand **Func** must also be a **pure** function. See also the electronic examples, in which the integrand is implemented as a dummy procedure.)

[20] R. L. Burden and J. D. Faires, *Numerical Analysis*, 5th ed. (Boston: PWS Publishing, 1993)

```
! Example 12. Adaptive Quadrature (Numerical Integration)
    :
  integer, parameter, public :: HI = selected_real_kind( 12 )
  type, public :: Result_Type
    real(kind = HI) :: X, Err_Loc
    logical :: Error
  end type Result_Type
    :
  recursive pure function Quad(A, B, I, Tol, M_Int ) result( Quad_R )
    real(kind = HI), intent (in) :: A, B, I, Tol, M_Int
    type(Result_Type) :: Quad_R
    type(Result_Type) :: R1, R2
    real(kind = HI) :: Y, Z, M

! start function Quad
    M = (A + B) / 2.0_HI
    Y = Simpson( A, M )
    Z = Simpson( M, B )
    if (abs( Y + Z - I ) > Tol) then
      if (abs( B - A ) < M_Int) then             ! Not OK but interval is too small
        Quad_R = Result_Type( I, M, .true. )
      else                                     ! Not OK: Subdivide interval again
        R1 = Quad( A, M, Y, Tol / 2.0_HI, M_Int )
        R2 = Quad( M, B, Z, Tol / 2.0_HI, M_Int )
        Quad_R % X = R1 % X + R2 % X
        Quad_R % Error = R1 % Error .or. R2 % Error
        if (Quad_R % Error) then
          Quad_R % Err_Loc = merge(R1 % Err_Loc, R2 % Err_Loc, R1 % Error)
        end if
      end if
    else                                               ! OK: Accept current value.
      Quad_R = Result_Type( Y + Z, M, .false. )
    end if
    return
  end function Quad

  pure function Simpson( A, B ) result( Simpson_R )
    real (kind = HI), intent(in) :: A, B
    real (kind = HI) :: Simpson_R
    real (kind = HI) :: M
! start function Simpson
    M = (A + B) / 2.0_HI
    Simpson_R = (B - A) * (Func( A ) + 4.0_HI * Func( M ) + Func( B )) / 6.0_HI
    return
  end function Simpson
```

Application: Recursive Selection Sort

The selection sort method is easy to describe as a recursive algorithm: If there is more than one item to sort, find the largest item, swap it with the last item, and then apply the selection sort algorithm to everything else.

```
module Recursive_Select
  use Swap_Reals_M
  implicit none
  private
  public :: Selection_Sort
contains
  recursive subroutine Selection_Sort( Unsorted )      ! Module subprogram
    real, dimension(:), intent (in out) :: Unsorted
    integer :: N
    integer, dimension(1) :: Loc
! start subroutine Selection_Sort
    N = Size( Unsorted )
    if (N > 1) then             ! End recursion if only one element remains.
      Loc = maxlLoc( Unsorted )               ! Location of largest element
      call Swap( Unsorted(N), Unsorted(Loc(1)) )
      call Selection_Sort( Unsorted(1: N - 1) )                 ! Recursion
    end if
    return
  end subroutine Selection_Sort
end module Recursive_Select
```

Tail Recursion vs Iteration

Printing a List Forward

Consider a recursive method for printing a list of data items in forward order:
To forward-print a list of integers:
If the list is empty, do nothing.

Otherwise, print the first integer, and then forward-print the remainder of the list (consisting of the original list except for the first integer).

```
  recursive subroutine Forward_Print( )
    integer :: A
! start subroutine Forward_Print
    read *, A
```

Skip the recursive call when zero is read (the base case).

```
    if (A /= 0) then
      print *, A
      call Forward_Print( )
    end if
    return
  end subroutine Forward_Print
```

This recursive algorithm has the special form mentioned earlier (a recursive call is executed as its last step) so it can be converted to an iterative procedure. The recursive call can simply be changed to a **go to** statement, as follows:

```
1   read *, A
    if (A /= 0) then
      print *, A
      go to 1
    end if
```

Better programming style would be the equivalent **do** construct:

```
  subroutine Forward_Print( )                   ! iterative, with do construct
    integer :: A
! start subroutine Forward_Print
    do
      read *, A
      if (A == 0) then
        exit
      else
        print *, A
      end if
    end do
    return
  end subroutine Forward_Print
```

Factorial

Viewed recursively, the *factorial* of a nonnegative integer *n* is *n* times the factorial of *n* – 1; the factorial of zero is 1:

```
  pure recursive function Factorial( N ) result( Factorial_R )
    integer :: Factorial_R
! start function Factorial
    if (N < 1) then
      Factorial_R = 1
    else
      Factorial_R = N * Factorial( N - 1 )
    end if
    return
  end function Factorial
```

The procedure call overhead of this tail-recursive implementation makes it terribly inefficient, as compared to iteration (except with optimizers that perform the conversion automatically). See Exercise 2 below. However, if you view the recursive definition as more natural, and if efficiency is not especially important, you might still prefer this version. Anyway, on typical hardware the factorial function is representable as an ordinary integer only for quite small values of *N*: for example, the factorial of 13 is too large to be represented as an IEEE 4-byte integer.

Section 3.1 Exercises

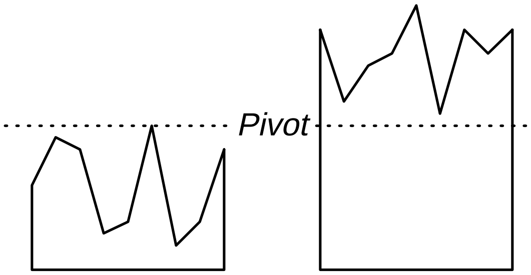
1. Write a recursive subroutine that simulates the moves in a Towers of Hanoi puzzle, and prints each move. Subroutine dummy arguments are *n*, *i*, and *j*. (Hint: set *k* to 3 – (*i* + *j*).) Write a main program that calls the subroutine with *n* = 4, *i* = 0, *j* = 1.

2. Write an iterative factorial function with a **do** construct.

3.2 QUICKSORT

Recursive Partitioning

Quicksort is a partition sort method (sometimes called split sorting). The idea is to partition (i.e., to split) the data into two sets, with smaller items in one set and larger items in the other. This is done by choosing a *pivot* and then moving the data so that items on the left are at least as small as the pivot and items on the right are at least as large as the pivot, as in the following sketch based on Rawlins' diagram:



The partitioning operation is then applied recursively to each of the two sets; recursion terminates when a set to be partitioned contains only one item.

Ideally, each recursive partitioning step would divide the data set into two equal subsets. To make this work, it would be necessary to choose the median of the data items as the pivot at each step; however, finding the median of a large number of items is not easy. A recommended alternative is to apply a 3-item sort to the elements at the left end, middle, and right end of of the array, and to choose the resulting middle item for the pivot. This pivoting strategy (called median-of-3) will be discussed later and will be compared to other strategies.

Once a pivot has been selected, partitioning proceeds by moving data items that are on the wrong side of the pivot. A significant feature of Quicksort is its pair of very fast inner loops that scan inward from opposite ends of the data array until they meet. For maximum efficiency, it is crucial that nonessential operations be avoided in these inner loops. The necessary steps include modifying an index variable and comparing the corresponding array element with the pivot; it is possible, and highly preferable, to avoid additional comparison steps involving the index value itself. These loops lend themselves well to optimization since they compare a sequence of adjacent array elements to a fixed pivot value.

Suppose that **`Array(L: R)`** is to be partitioned, and suppose that the pivot has been selected by the median-of-3 strategy.

Initialize **`I`** *to* **`L`** *and* **`J`** *to* **`R`***. The invariant assertion is: "All items to the left of* **`Array(I)`** *are at least as small as* **`Pivot`***, and all items to the right of* **`Array(J)`** *are at least as large as* **`Pivot`***."*

```
  I = L
  J = R
```

Make separate searches, scanning to the right with **`I`** *until a large data item (***`Array(I) >= Pivot`***) is found, and then scanning to the left with* **`J`** *until a small data item (***`Array(I) <= Pivot`***) is found. (It has been shown that testing for >= and <= works better than testing for > and < in case there are many equal key values.)*

```
do
  do
    I = I + 1
    if (Array(I) >= Pivot) exit
  end do
  do
    J = J - 1
    if (Array(J) <= Pivot) exit
  end do
```

If the two scans have met or crossed, this partition is complete. Otherwise, swap the large and small data items and continue scanning to the right with **I** *and to the left with* **J***.*

```
  if (I >= J) exit
  call Swap( I, J )
end do
call Recursive_QS( L, J )
call Recursive_QS( J + 1, R )
```

Here is an example.

```
S  O  R  T  M  E  Q  U  I  C  K  L  Y
```

A 3-item sort is applied to S, Q, and Y, thus changing S Q Y to Q S Y, and S (the median of these three items) is chosen as the *Pivot*. The scans begin moving inward from each end.

```
Q> O  R  T  M  E  S  U  I  C  K  L  <Y
```

Starting from the left end and moving toward the right, T is the first item that is at least as large as S; starting from the right end and moving toward the left, L is the first item that is at least as small as S. These two items are swapped; then the inward scans continue, comparing the items that remain between the two that were swapped.

```
Q  O  R  L> M  E  S  U  I  C  K  <T Y
```

Moving right, S is at least as large as S; moving left, K is at least as small as S. Therefore, S and K are swapped, and the scans continue.

```
Q  O  R  L  M  E  K> U  I  C  <S T  Y
```

Moving right, U is at least as large as than S; moving left, C is at least as small as S. After U and C are swapped, the scans continue.

```
Q  O  R  L  M  E  K  C> I  <U S  T  Y
```

Moving right, U is again at least as large as S; moving left, I is at least as small as S. The scans have now crossed, so no swap occurs.

```
Q  O  R  L  M  E  K  C  <I U> S  T  Y
```

This partition is now complete. The first nine items are at least as small as S, and the last four items are at least as large as S. Note that the pivot does not necessarily end up adjacent to the partition.

```
Q  O  R  L  M  E  K  C  I# U  S  T  Y
```

Recursively, each of the two groups is now partitioned. Consider the first group of nine items. The scans begin after Q, M, and I have been sorted and M has been chosen as the *Pivot*.

```
I> O  R  L  M  E  K  C  <Q
```

Moving right, O is at least as large as M; moving left, C is at least as small as M. These two items are swapped and the scans continue.

```
I  C> R  L  M  E  K  <O Q
```

Moving right, R is at least as large as M; moving left, K is at least as small as M. These two items are swapped and the scans continue.

```
I  C  K> L  M  E  <R O  Q
```

Moving right, M is at least as large as M; moving left, E is at least as small as M, so M and E are swapped and the scans continue.

I C K L E> <M R O Q

Moving right, M is at least as large as M; moving left, E is at least as small as M. The scans have now crossed, so no swap occurs.

I C K L <E M> R O Q

The first five items are at least as small as M, and the last four items are at least as large as E.

I C K L E# M R O Q

Quicksort continues, recursively partitioning each of these two groups.

Quicksort is Unstable for Duplicates

It is easy to see that quicksort is unstable for duplicate items. (Here, subscripts are shown only for identification and are not part of the key.) The pivot for the first partition is E_1:

A_1 B_1 C_1 D_1 E_1 A_2 B_2 C_2 D_2 E_2

A_1> B_1 C_1 D_1 E_1 A_2 B_2 C_2 D_2 <E_2

A_1 B_1 C_1 D_1 D_2> A_2 B_2 C_2 <E_1 E_2

A_1 B_1 C_1 D_1 D_2 A_2 B_2 <C_2 E_1> E_2

A_1 B_1 C_1 D_1 D_2 A_2 B_2 C_2# E_1 E_2

For positions 1 to 8, the pivot is C_2:

A_1 B_1 C_1 D_1 D_2 A_2 B_2 C_2

A_1> B_1 C_1 C_2 D_2 A_2 B_2 <D_1

A_1 B_1 B_2> C_2 D_2 A_2 <C_1 D_1

A_1 B_1 B_2 A_2> D_2 <C_2 C_1 D_1

A_1 B_1 B_2 <A_2 D_2> C_2 C_1 D_1

A_1 B_1 B_2 A_2# D_2 C_2 C_1 D_1

For positions 1 to 4, the pivot is A_2:

A_1 B_1 B_2 A_2

A_1> A_2 B_2 <B_1

A_1 <A_2> B_2 B_1

A_1 A_2# B_2 B_1

For positions 1 to 2, the pivot is A_1:

A_1 A_2

A_1> <A_2

<A_1 A_2>

A_1# A_2

For positions 3 to 4, the pivot is B_2:

B_2 B_1

B_2> <B_1

<B_2 B_1>

B_2# B_1

For positions 5 to 8, the pivot is D_2:

$$\begin{array}{lllll}
D_2 & C_2 & C_1 & D_1 & \\
C_2> & & D_2 & C_1 & <D_1 \\
C_2 & C_1> & & <D_2 & D_1 \\
C_2 & <C_1 & D_2> & & D_1 \\
C_2 & C_1\# & & D_2 & D_1
\end{array}$$

For positions 5 to 6, the pivot is C_2:

$$\begin{array}{ll}
C_2 & C_1 \\
C_2> & <C_1 \\
<C_2 & C_1> \\
C_2\# & C_1
\end{array}$$

For positions 7 to 8, the pivot is D_2:

$$\begin{array}{ll}
D_2 & D_1 \\
D_2> & <D_1 \\
<D_2 & D_1> \\
D_2\# & D_1
\end{array}$$

For positions 9 to 10, the pivot is E_1:

$$\begin{array}{lll}
E_1 & E_2 & \\
E_1> & & <E_2 \\
<E_1 & E_2> & \\
E_1\# & & E_2
\end{array}$$

The final sorted array appears as follows:

$$\begin{array}{cccccccccc}
A_1 & A_2 & B_2 & B_1 & C_2 & C_1 & D_2 & D_1 & E_1 & E_2
\end{array}$$

Choosing the Pivot

Properly implemented, quicksort is the fastest known sorting algorithm. However, as Sedgewick[21] points out, the algorithm is “fragile”: small changes in some of the program steps can destroy the efficiency of the method or can lead to undesirable and unexpected effects for some inputs.

> “Once a version has been developed and seems free of such effects, this is likely to be the program to use for a library sort or for a serious sorting application. But [one must be] willing to invest the effort to be sure that a quicksort implementation is not flawed. . . .”

One change that can have dramatic effects relates to the choice of a pivot element for each partition. As stated earlier, the ideal pivot would be the median of the data items, so that the partitioning process would produce equal subgroups. However, the extra time required to find the true median would destroy the fast performance of quicksort.

Some published quicksort algorithms choose a specific array element, such as $Array_L$ or $Array_{L+R/2}$, as the pivot. Others generate a random subscript value between L and R.

Warnock[22] suggests using the median-of-3 pivot strategy mentioned earler, based on the first and last items and an item between them chosen at random. A random array element can be selected with the intrinsic subroutine **`random_number`**:

```
call random_number( X )
C = L + int( X * real( R - L ) )
call Sort_3( L, C, R )
Pivot = Array(C)
```

[21] Sedgewick, *Algorithms*, 116.

[22] Private communication

Use of the actual median of a tiny sample of the data tends to equalize the partitions somewhat.[23] It has the additional advantage that a bit of the sorting is done along with the pivot choice, so the scan can omit the item at each end — for most other strategies, the elements at each end are not examined before the scans begin, so I must be initialized to $L - 1$ and and J to $R + 1$. Furthermore, median-of-3 pivoting guarantees that both inner loops will exit without running off the ends of the array; other strategies may require extra steps to avoid disaster. (The index values could be tested in the inner loop, of course, but this would dramatically increase the total sort time.)

The Cutoff

One variation of quicksort can significantly improve the performance of the algorithm. Quicksort is very effective for large amounts of data but is not especially fast for sorting fewer than a dozen items. Furthermore, sorting small groups of items by quicksort requires several recursive calls and thus introduces a disproportionate amount of overhead.

A quicksort implementation may specify a *cutoff* value to avoid recursively processing small sets, i.e., sets for which the difference between right end and left end subscripts does not exceed the cutoff. In the algorithms presented here, small sets are left *unsorted* and a final pass is made over the whole array with straight insertion, taking advantage of the efficiency of this latter method for data that is nearly in order.[24]

The optimum cutoff value depends somewhat on hardware characteristics. Some experimentation usually reveals a very shallow minimum, with any cutoff from about 5 to 20 giving an improvement between 5% and 15%, even after taking into account the extra time required for the final insertion sort.

Testing a Quicksort Implementation

At least three tests should be made to improve confidence in an implementation of quicksort.

1. *Sequence check.* It goes without saying that the data should be in order after it has been processed by quicksort.

2. *Timing comparison with insertion sort.* Many implementations of quicksort end with a straight insertion pass, so a quicksort procedure that is not working at all will produce a correct data sequence if the insertion sort is implemeted correctly. For about 10,000 random data items, a correct quicksort procedure is at least 100 times as fast as insertion. If your procedure is only slightly faster than insertion, most of the work is being done during the final insertion pass.

3. *Asymptotic running time.* Quicksort should be applied to several large sets of random data of different sizes — for example, 100,000 items and one million items. The elapsed time ratio should verify the N lg N asymptotic behavior that is characteristic of quicksort: One million items should take between 10 and 15 times as long as 100,000 items.

[23] According to Moret and Shapiro (B. M. E. Moret and H. D. Shapiro, *Algorithms from P to NP,* Redwood City CA: Benjamin / Cummings, 1990, 516), consistently choosing any specific element as the pivot (or choosing the pivot at random) results in an expected split of 25:75; the median-of-3 strategy gives an expected split close to 33:67 and reduces the probability of a 25:75 or worse split to about 0.3.

A strategy sometimes suggested is simply to use the leftmost data array element as the pivot. However, if this method is applied to a set of data that happens to be in order (or in reverse order) already, each group of k items will be partitioned into a single item and a group of $k - 1$ items. The method is nearly as bad for data that is *almost* in order: quicksort becomes merely an inefficient recursive version of selection sort. Since sorting algorithms are often applied to data that is nearly in order, the effect of this bad pivot choice is “quite embarrassing,” to quote Knuth.

[24] In a paged environment, it may be preferable to sort the small sets by insertion or selection as they are created, as Moret and Shapiro note: “This strategy preserves the excellent locality of quicksort, whereas the final sweep of a single insertion sort pass would trigger another series of page faults.”

Storage Space Considerations

When a procedure with an array argument calls itself recursively, does each instance of the procedure store another copy of the array? Probably not — array arguments are almost invariably passed by *reference*, so each instance stores only an address. For Fortran assumed-shape arrays this is a reference to the array descriptor.

It is not difficult to entirely eliminate the array argument from a recursive procedure. A nonrecursive "wrapper" procedure with an array argument is constructed, with the recursive procedure as an internal procedure inside it. The recursive procedure *inherits* the original array from the wrapper and has only two integer scalar arguments, the left and right end index values. A less flexible alternative that eliminates the wrapper (and, perhaps surprisingly, seems to run almost twice as fast on some systems) declares a **`public`** data array in the module where the recursive sort is defined. (The F subset does not support internal procedures; the nonrecursive wrapper and the recursive procedure are module procedures at the same level, so the recursive procedure can inherit only from the specification part of the module. A **`public`** array may be employed as just described, or the array may be passed as an argument to the wrapper and then copied to a **`private`** array declared at the module level.)

For ideal partitioning (and with zero cutoff), the maximum depth of recursion would be lg *N*. Experiments with random data and with the median-of-3 pivot strategy find a maximum recursive depth only slightly greater than lg *N*, but it can be 2 to 3 times this large — in one test with a million items (*lg N* = 20) and cutoff 16, the maximum depth reached 52 levels of recursion. However, the extra recursive levels do not consume much space because the activation record for each instance needs to store only two scalar integer arguments (the endpoint index values *L* and *R*), a local variable for the partition point *J*, and a few items of system information — a few hundred extra bytes altogether for a million data items. The following implementation employs three additional local variables, *I*, *C*, and *Pivot*; to minimize local storage space in the recursive procedure, these three variables may be moved to the wrapper subroutine or to the specification part of the containing module.[25]

Say It with Fortran

Example 13.

```
! Example 13. Quicksort
```

Nonrecursive "wrapper"

```
  subroutine Qu_Sort( Array )
      real, dimension(:), intent(in out) :: Array
      integer :: N
! start subroutine Qu_Sort
      N = size( Array )
      call Recursive_QS( 1, N )
      if (CUT_OFF > 0) call In_Sort( )
      return

  contains
```

[25] If very deep recursion occurs due to unusual data characteristics, the endpoints of the larger partition may be pushed on a user-defined stack and the smaller partition processed iteratively. As Moret and Shapiro note (p. 516), this technique insures that the stack does not contain more than lg *N* entries. Sedgewick (p. 122) gives a Pascal implementation of this iterative (pseudo-recursive) version.

Recursive Quicksort procedure, with Median-of-3 pivot strategy

```
  recursive subroutine Recursive_QS( L, R )
    integer, intent(in) :: L, R
    integer, parameter :: CUT_OFF = 12
    integer :: J, I, C
    real :: Pivot
! start subroutine Recursive_QS
    if (L + CUT_OFF < R) then
      call random_number( X )
      C = L + int( X * real( R - L ) )
      call Sort_3( L, C, R )
      Pivot = Array(C)
      I = L
      J = R
      do
        do
          I = I + 1
          if (Array(I) >= Pivot) exit
        end do
        do
          J = J - 1
          if (Array(J) <= Pivot) exit
        end do
        if (I >= J) exit
        call Swap( I, J )
      end do
      call Recursive_QS( L, J )
      call Recursive_QS( J + 1, R )
    end if
    return
  end subroutine Recursive_QS
end subroutine Qu_Sort
```

Quicksort Operation Counts

```
N = size( Array )                                                  ! 1
call Recursive_QS( 1, N )                                          ! 2
if (CUT_OFF > 0) call Insertion_Sort( )                            ! 3
return                                                             ! 4

recursive subroutine Recursive_QS( L, R )                          ! 5
  if (L + CUT_OFF < R) then                                        ! 6
    call random_number( X )                                        ! 7
    C = L + int( X * real( R - L ) )                               ! 8
    call Sort_3( L, C, R )                                         ! 9
    Pivot = Array(C)                                              ! 10
    I = L                                                         ! 11
    J = R                                                         ! 12
```

```
      do                                              ! 13
        do                                            ! < 14
          I = I + 1                                   ! << 15
          if (Array(I) >= Pivot) exit                 ! << 16
        end do                                        ! << 17
        do                                            ! < 18
          J = J - 1                                   ! << 19
          if (Array(J) <= Pivot) exit                 ! << 20
        end do                                        ! << 21
        if (I >= J) exit                              ! < 22
        call Swap( I, J )                             ! 23
      end do                                          ! 24
      call Recursive_QS( L, J )                       ! 25
      call Recursive_QS( J + 1, R )                   ! 26
    end if                                            ! 27
```

Sort_3 uses 3 comparisons and 4.5 moves (but sorting the three items by insertion can decrease these counts slightly). An estimate for the outer loop (lines 13 – 24) is $0.25 \cdot N$ iterations, with each inner loop iterating twice. Each iteration of the outer loop body performs 4 data item comparisons (2 in each inner loop) and one swap (3 move operations) almost always. Thus lines 13 – 24 require N comparisons and $0.75 \cdot N$ moves; the total for lines 1– 24 (ignoring the call to **random_number**) is $N + 3$ comparisons and $0.75 \cdot N + 4.5$ moves.

For a recursive procedure, the operation count formula for a given number of items often depends upon the same formula applied to a smaller number of items — that is, it must be expressed as a *recurrence* relation. The operation count for lines 25 and 26 has the form $T_N = A + B \cdot N + T_{J+1-L} + T_{R-J}$, where T is either the number of comparisons or the number of moves. For the case of ideal partitioning, T_{J+1-L} and T_{R-J} are nearly equal so that $T_N = A + B \cdot N + 2\ T_{N/2}$. Moret and Shapiro[26] show how to solve such recurrence relations, by difference equation methods that are similar to well-known methods for initial value problems in differential equations, to obtain a closed-form formula for T_N. In this case, if N is a power of 2 the solution with $T(1) = 0$ is $T_N = B \cdot N \lg N + A \cdot (N - 1)$. Although the solution of recurrences is beyond the scope of this text, Section 4.3 shows how to use mathematical induction to show consistency between a recurrence relation and the derived closed-form formula.

For comparison operations, A is 3 and B is 1 giving $C_N = N \lg N + 3 \cdot N - 3$; for move operations, A is 4.5 and B is 0.75 giving $M_N = 0.75 \cdot N \lg N + 4.5 \cdot N - 4.5$

A benchmark, run with a 50 MHz 486DX computer, sorted one million random real numbers in 56 seconds, with median-of-3 pivot strategy and cutoff 12.

- Quicksort
  The worst-case operation count is proportional to N^2, but median-of-3 pivot strategy with the middle element chosen at random makes the worst case extremely unlikely. A “cutoff” value between 5 and 20 is recommended, with a final straight insertion sort.
  Comparisons: $N \lg N + 3 \cdot N - 3$
  Moves: $0.75\ N \lg N + 4.5 \cdot N - 4.5$
  Benchmark time for 1 million random real numbers: 56 seconds

[26] *Algorithms from P to NP*, 61-81. The substitution $K = \lg N$ converts the recurrence to $S(K) = A + B \cdot 2K + 2 \cdot S(K - 1)$; $S(0) = 0$. See also Sedgewick, *Algorithms*, 77.

Chapter 4 Algorithm Analysis

4.1 WHAT IS AN ALGORITHM?

The sorting methods described in Chapter 2 are examples of algorithms — each is a sequence of steps for accomplishing a specific task. There is an important difference between an algorithm and a computer program: The algorithm describes the general *method* for performing a task, without regard to the details of its implementation. In principle, a given algorithm should be capable of implementation in any of several computer languages, or even by some other means without using a computer at all. An example of an algorithm that would usually be implemented without a computer is a recipe for baking apple pie, which is a description of the sequence of steps that are required to perform this specific task.

To constitute an algorithm, a sequence of steps should have the following properties:

1. The steps in an algorithm must not be too big nor too small. The size of an appropriate step depends upon the *executor* of the algorithm, which could be a machine, a person, a trained chimpanzee, or whatever. Each step should be the right size for the executor to perceive as a single unit of work.

   An apple pie recipe in an old-fashioned cookbook consists of instructions appropriate for someone with a reasonable amount of experience as a baker of pies. A cookbook for a sixth grade cooking class would be much more detailed, while a baker with many years' experience might require only one or two notes.

2. An algorithm must be finite: the list of steps must be finite in length, and its execution sequence must eventually terminate. If some of the steps will be repeated (iteratively or recursively), the repetition must be guaranteed to terminate and not to continue forever. For some algorithms, progress toward completion can be measured by an integer — for example, the selection sort algorithm removes one item from the unsorted sequence at each step, so the number of unsorted items will eventually reach zero.

3. Each step of an algorithm must be definite. That is, the executor must know precisely what to do at each point. The steps are not strictly required to be *deterministic;* some algorithms, such as one for counting "heads" in a sequence of coin tosses, may incorporate random elements. But the executor must know precisely how to proceed in any possible situation; for example, how to toss the coin, how to decide whether it is "heads," and how to accumulate the count value.

Most useful algorithms have some degree of generality — they are adaptable for solving any one task from a class of related tasks. For example, a general sorting algorithm can be applied to any number of items.

Computer Algorithms

When an algorithm is to be executed by a computer, it must be expressed in steps each of which can be undertaken as a unit. An algorithm may be written initially in *pseudocode*, i.e., as a list human-readable statements that cannot be interpreted directly by the computer but can easily be transformed into any of several programming langauges such as Fortran, C++, or Pascal.

Some of the pseudocode steps — for example, “add a given item to the end of the sorted sequence” — will correspond to a single statement in Fortran. Others, such as “find the smallest unsorted item,” may become a procedure that consists of several Fortran statements.

Ultimately, the actual computer hardware executes the algorithm as a sequence of machine-language instructions that the compiler generates from the program statements.

4.2 WHAT MAKES A GOOD ALGORITHM?

For most applications that are implemented with Fortran, speed of execution is a primary objective. Fortran compilers perform many extensive and sophisticated optimizations, such as detecting program statements that can be moved out of a loop. For example, suppose that the selection sort procedure were written as follows:

```
do I = 1, size( Array ) - 1
   Location = Minimum_Location( I, size( Array ) )
   call Swap( I, Location )
end do
```

An optimizing compiler might recognize that the statements as written call for repeated execution of the intrinsic function reference

```
size( Array )
```

(in the actual argument list for **Minimum_Location**) at every iteration of the loop, even though the same result value is returned at every reference. This expression can be evaluated once before the loop begins, instead of once for every iteration of the loop; moving this statement would save a total of $N - 2$ calls to the intrinsic function **size**. (Bill Long observes that no reasonable compiler would need to make an actual procedure reference to determine the size of an array — even one that is dynamically allocated. Nevertheless, we proceed with the example for purposes of hypothetical illustration.)

For sorting 1,000 items by selection, the optimization saves almost 1,000 intrinsic function calls. The 50 MHz processor of our estimates performs the sort in about 1 second; the optimization saves perhaps 200 microseconds or less than 0.2%. On the other hand, sorting the same 1,000 items by binary insertion takes about 0.19 second and thus saves about 80%; quicksort takes 0.03 second and saves 97%.

Moral: There may be more gain from choosing a suitable algorithm than from cleverly optimizing an unsuitable one. Choice of a suitable algorithm can have an even greater effect for larger amounts of data.

Relative speed is not the only criterion for judging algorithms, however.

Another traditional criterion is the storage space required. Although this factor seems less important in a typical modern computing environment, there are some scientific applications (such as hydrodynamics calculations involved in weather research or in simulations of the effects of explosives) for which space availability significantly affects the precision of the results. Modern utility software such as operating systems, word processors, spreadsheets, and database systems is often space limited, so space economy is an important criterion for the sorting, searching, and similar algorithms that are imbedded in this software.

Other criteria that are harder to measure can be at least as important in the long run. In a choice between two algorithms, one of them might be easier to understand, to code, to debug, and to maintain; or one might be less dependent on properties of a particular operating environment and hence more portable; or one might be more *robust* — i.e., less likely to have difficulty in the face of unexpected circumstances such as improper input data. Differences like these should often be weighted ahead of *slight* improvements (say 10 percent) in speed.

Sorting is a good introductory subject for the study of algorithm efficiency, both because the subject has been extensively studied and because it has many practical applications. This text covers several of the best-known and most useful sorting algorithms.

For any computer application that is to be applied to large amounts of data, it is important to obtain good advice concerning various algorithms that are available. A few selected applications are described in this text.

From Thousands to Millions of Data Items

If you write a selection sorting program, prepare 1,000 data items to be sorted, and type "**`sort`**" or whatever command is required to begin execution, the results will be available one second later — almost as soon as you finish entering the command. The same task requires 0.2 second by binary insertion and 0.03 second by quicksort.

For realistic modern computer applications, the time required for searching or sorting operations with 1,000 items is nearly insignificant unless the sorting process is to be executed many times as a part of a larger application. Data sets that contain several million items are not uncommon.

- A good example is the Automatic Teller Machine at your local bank. You insert your ATM card and punch in your "PIN number." If your bank is part of a large chain, you are using a terminal that is connected to perhaps 10 million accounts. Yet, you wait only a second or two for the response.
- The word processor file for a textbook such as this one contains a few million characters of text. Searching a million characters for a specific string with a 50 MHz computer takes less than 2 seconds.

To search for a given key in an *unordered* array of N items, in case there is in fact no matching item, every element must be examined. One million items requires a million comparisons and takes perhaps 2 seconds.

In an *ordered* array of one million items, binary search takes only about 60 microseconds. Would it be better to sort the million unordered items with quicksort and then do a binary search? For a single search, the answer is no. As shown in the table below, quicksort for a million items requires about a minute, much longer than the unordered search.

Operation Counts for Sorting

With comparison operations weighted as 3 and move operations as 1, an estimate of 1.5 million weighted operations per second is reasonably consistent with times actually measured on the 50 MHz computer used for benchmark testing. Times measured on a 200 MHz Pentium Pro are faster by about a factor of 20 than those listed here. The following formulas, except the last, assume random data.

- Selection Sort: $1.5 \cdot N^2 + 0.7 \cdot N \lg N + 3.5 \cdot N - 0.7 \cdot \lg N - 3$
- Insertion Sort, straight insertion: $N^2 - 0.25 \cdot N - 1$
- Binary Insertion Sort: $0.25 \cdot N^2 + 4.5 \cdot N \lg N - 4.8 \cdot N - 2.9$
- Shell sort (conjectured): $4.8 \cdot N^{1.3}$
- Heapsort: $7 \cdot N \lg N - 5.6 \cdot N - 7 \cdot \lg N + 17.1$
- Quicksort: $3.75 \cdot N \lg N + 13.5 \cdot N - 13.5$
- Straight insertion sort (data known to be already nearly in order): $5 \cdot N - 5$

Here are some values calculated from these formulas for the 50 MHz benchmark computer:

Algorithm	1,000 items	20,000 items	1 million items
SLOW ALGORITHMS			
Selection	1.01 sec	350 sec	6.9 days
Straight insertion	0.67 sec	291 sec	4.6 days
Binary insertion	0.19 sec	65 sec	28 hrs
FAST ALGORITHMS			
Shell sort	0.03 sec	1.31 sec	201 sec
Heapsort	0.04 sec	1.26 sec	104 sec
Quicksort	0.03 sec	0.89 sec	59 sec

If you prepare and sort 1,000 data items, the time actually spent in sorting, even with one of the slow algorithms, is negligible in comparison to other parts of the task (unless the sorting process is to be executed many times as a part of a larger application). If you have 20,000 items and no program for any of the fast algorithms is immediately available, you could start a slow sort algorithm and take a 5 minute coffee break; when you come back, the sort will be finished. For a million items, the fast algorithms take a minute or so; to tie up your computer for hours or days with a slow algorithm would be ridiculous.

Quicksort is 1.5 to 2 times as fast as heapsort for random data, but it has two disadvantages. First, quicksort requires some extra stack space (proportional to lg *N*) for recursion; and second, quicksort has bad “worst case” behavior — in rare cases, it can be as slow as selection sort. To sort a million integers on the benchmark computer used here, heapsort will *always* take less than two minutes (no more than 10% above its average time, as noted earlier); quicksort will *almost always* take less than one minute, but certain rare data sets could require almost a week.

Shell sort is difficult to analyze. Sedgewick asserts that its asymptotic behavior is between $O(N^{1.2})$ and $O(N^{1.5})$ for various “good” interval sequences. Experiments (using array sections and the interval sequence described earlier) are consistent with the formula $4.8 \cdot N^{1.3}$. For a million items, Shell sort takes about twice as long as heapsort and 3 to 4 times as long as quicksort.

4.3 ASYMPTOTIC ANALYSIS

Some parts of an operation count formula have very little effect on the result. The tabulated values for selection sort and for binary insertion sort would not change significantly if the formulas were simplified to $1.5 \cdot N^2$ and $0.25 \cdot N^2$, respectively. The following table compares counts (3·C + M) computed from the complete formulas with those computed by ignoring all terms except the first.

	Selection Sort		Binary Insertion Sort	
N	All Terms	First Term	All Terms	First Term
50	4.12·103	3.75·103	1.66·103	0.63·102
1,000	1.51·106	1.50·106	2.90·105	2.50·105
20,000	6.00·108	6.00·108	1.01·108	1.00·108

For 50 items, the first term in the selection sort formula accounts for about 90% of the total; the first term for binary insertion sort accounts for only about 38%. For 20,000 items, the first term values are within 1% of the total.

How can one decide which parts of such a formula to ignore? The sort formulas include combinations of terms in N^2, *N*, lg *N*, and *N*·lg *N*. Which of these terms are most significant, and which can be ignored?

We have noted that the execution times for most algorithms are negligible when *N* is small (say, up to a few thousand data items) in comparison to other parts of the task such as data acquisition and preparation. The important criterion is *asymptotic* behavior of the execution time — its limit as *N* “tends toward infinity.” The relative significance of various terms in an operation count formula is determined by the *limiting* behavior of each term.

Although terms in N^2, *N*, lg *N*, or *N*·lg *N* all have infinite limits, some of these have a faster growth rate than others. It is easy to compare *N* with N^2 or lg *N* with *N·lg N*, but other comparisons such as N^2 vs lg *N* are a bit more difficult. If simple algebra fails, the limiting ratio of two functions when both are unbounded can be evaluated by L’Hospital’s Rule,[27] i.e., by comparing their growth rates (derivatives with respect to *N*) in the limit.

[27] See, for example, G. B. Thomas, Jr. and R. L. Finney, *Calculus and Analytic Geometry,* Ninth Edition (Reading MA: Addison Wesley, 1996). **[Get page ref for L’Hospital in 9th edition]**

Function	Derivative
lg N	1 / N
N	1
N lg N	lg N + 1
N2	2·N

Among these four functions, only the last two have unbounded derivatives; to compare these two, it is necessary to apply L'Hospital's rule more than once. A comparison of these four functions and some others that will arise during analysis of some of the algorithms in this text produces a hierarchy of functional forms. In the following list, the limiting ratio of any function to another that is farther down the list is zero.

The second and third formulas in the list are $(\lg N)^k$ and N^α. The parameters k and α in these formulas are supposed to be constants, with $k > 1$ and $0 < \alpha < 1$. In the limit as N tends to infinity, it can be shown (see Exercise 4 at the end of this section) that $(\lg N)^k$ for any large fixed $k > 1$ is less than N^α for any small fixed α between 0 and 1. Two algorithms being compared may both have the same one of these forms, but with different values of k or α.

Hierarchy of Functional Forms:

1
$\lg N$
$(\lg N)^k$ for $k > 1$
N^α for $0 < \alpha < 1$
N
$N \lg N$
$N (\lg N)^k$ for $k > 1$
$N^{1+\alpha}$ for $0 < \alpha < 1$
N^2
. . .
N^3
. . .
$(1 + \alpha)^N$ for $0 < \alpha < 1$
2^N

Functions commonly encountered in algorithm analysis include products of (integer and fractional) powers of N and of $\lg N$, where N is a measure of the amount of data. Algorithms whose execution time formula has N as an exponent, such as $(1 + \alpha)^N$ or 2^N, are impractical in general — that is, they are impractical except for special applications that involve very small amounts of data — because execution time ultimately grows faster than any fixed power of N. Other "impractical" functions that sometimes occur are the factorial $N!$ and other exponential forms such as N^N. (According to Stirling's formula, $N!$ grows slightly faster than N^N).

The Role of Constants

It happens to be true that the limiting ratio for any pair of (different) functions in the hierarchy listed above is either zero or infinity. Multiplying any of these functions by a constant (or changing from one logarithmic base to another; for example, $\lg N = 1.44...\cdot\ln N$.) does not change this limiting behavior.

Not all functions have this behavior.[28] For example, $\tan^{-1} N$ (the principal value) approaches the constant $\pi/2$ as $N \to \infty$. The asymptotic behavior of any rational function (ratio of two polynomials) in N is determined by the degrees and leading coefficients of the numerator and denominator polynomials.

[28] Some functions of N have no limit as $N \to \infty$. Obvious examples are simple periodic functions such as $\sin N$ or $\cos N$. Such functions are of no value for asymptotic analysis, and we will not consider them further.

Consider the two rational functions ($a\ N^5 + ...$) / ($N^2 + ...$) and ($b\ N^5 + ...$) / ($N^2 + ...$) where the omitted parts are polynomials of lower degree that may be different for the two functions. The functions have asymptotic behavior $a\ N^3$ and $b\ N^3$ respectively; the limiting ratio of the two rational functions is a / b.

The Complexity of an Algorithm: Big Oh

Asymptotic analysis employs a notation that reduces a formula to its most significant terms, ignoring terms that are insignificant in the limit. The asymptotic *order* of a function is found as follows:

Express the function as a sum of terms.

In principle, it is necessary to compare each term with all of the others. If the limiting ratio of any two terms F and G is zero, F may be deleted from the sum.

All of the terms that remain have the same asymptotic behavior. Any such term, with constant factors deleted, may be said to be the asymptotic behavior of the function.

Consider the formula $f(N) = N^2\ (3 + 4 \tan^{-1} N) + \lg N$. Expressed as a sum of terms, this formula becomes $3N^2 + 4 \cdot N^2 \tan^{-1} N + \lg N$. The logarithm is not significant in the limit, so it is deleted and two terms remain. The asymptotic behavior of $f(N)$ can be said to be either N^2 or $N^2 \tan^{-1} N$ — the simpler form would ordinarily be preferred.

We say that $f(N)$ is $O(N^2)$ or is $O(N^2 \tan^{-1} N)$; again, the simpler form is preferred. Orally, one would say that $f(N)$ is "big oh" N^2 or that it has "big oh" N^2 asymptotic behavior. This means that some constant multiple of N^2 is an upper bound for $f(N)$ as N grows large. If $f(N)$ is an estimate for the running time of some algorithm, it can be said that the "complexity" of the algorithm is N^2.

It is not always easy to find such an upper bound for the running time of an algorithm, in terms of the amount of data. If such bounds can be obtained for different algorithms that might be applied to the same application, they can be used to compare the algorithms with regard to asymptotic running time or complexity.

Asymptotic upper bounds do not give the whole story, of course. Average behavior estimates can also be valuable; lower bounds are sometimes useful as well. The quicksort operation count formula $3.75 \cdot N \lg N + 13.5 \cdot N - 13.5$ is an estimate of average behavior. The worst case for this algorithm (if each pivot happens to be the largest or smallest data item) is $O(N^2)$, but careful implementation of the algorithm can ensure that this case occurs rarely. The best case (lower bound) for straight insertion sorting (but not for binary insertion) is proportional to N, which is achieved when the data is already in order, because the inner loop always exits after the first comparison in that case.

When two algorithms have the same complexity, it may be desirable to compare them further, taking into account constants that appear in the bounds or estimates, and perhaps other considerations as well:

- The formula $1.5 \cdot N^2 + 0.7 \cdot N \lg N + 3.5 \cdot N - 0.7 \cdot \lg N - 3$ for selection sorting is an upper bound, but it differs only slightly from the estimated average and from the lower bound. The binary insertion formula $0.25 \cdot N^2 + 4.5 \cdot N \lg N - 4.8 \cdot N - 2.9$ is again an estimated average; the worst case for this algorithm is $0.5 \cdot N^2 + 4.5 \cdot N \lg N - 4.8 \cdot N - 2.9$ and its best case is $4.5 \cdot N \cdot \lg \mathrm{N} - 4.3 \cdot N - 2.9$. For sorting a large amount of data that is almost in order, the term in $N \lg N$ makes binary insertion inferior to straight insertion.

- For random data, both Quicksort and Heapsort have complexity $O(N \lg N)$, but the constant factor in the leading term for Heapsort is about twice that of Quicksort. However, the complexity of Quicksort in the worst case is $O(N^2)$ while the worst case for Heapsort remains $O(N \lg N)$.

Complexity of Sorting Methods

- Selection: O(N^2)
- Insertion (straight insertion): O(N^2)
- Binary insertion: O(N^2)
- Shell sort, conjectured: O($N^{1.3}$)
- Heapsort: O(N lg N)
- Quicksort: O(N lg N)
- Straight insertion with ordered data: O(N)

Selection and insertion (except for insertion with ordered data) are O(N^2) algorithms; quicksort and heapsort are O(N lg N) algorithms.

Section 4.2 Exercises

1. In the "Hierarchy of Functional Forms" on page 78, compare each function on the list with the one that immediately follows it. For each pair of functions, show that the limiting ratio is zero as $N \to \infty$. Apply L'Hospital's rule one or more times, if necessary.

2. Consider the formulas N^{100} and 2^N. Use the approximation $2^{10} = 10^3$.

   a) Show that for $N = 100$, the first formula is about 10^{200} while the second is about 10^{30}.

   b) Show that for $N = 1{,}000$, both formulas are approximately 10^{300}.

   c) Show that for $N = 10{,}000$, the first is about 10^{400} while the second is about 10^{3000}.

   d) Which of the two formulas is asymptotically larger?

3. Suppose that two functions each have the form $(\lg N)^k$ with different values of k. Show that the limiting ratio (with the smaller k value in the numerator) is zero. Do the same for two functions of the form N^α with different values of α.

4. The preceding discussion states that $(\lg N)^k$ (for any fixed k such that $k > 1$) is less than N^α (for any fixed α such that $0 < \alpha < 1$) in the limit as $N \to \infty$. Compare $(\lg N)^3$ with $N^{0.2}$. For large N, it is easier to compare logarithms: substitute L for lg N and compare $3 \cdot \lg L$ to $0.2 \cdot L$. When N is about one million, observe that L is about 20 and lg L is between 4 and 5, so the first formula is larger than the second. Show that the "crossover point," beyond which the second formula is larger than the first, occurs between $L = 99$ and $L = 100$ (N is about 10^{30}). You may use the following table of base-2 logarithms:

L	lg L
95	6.570
96	6.585
97	6.600
98	6.615
99	6.630
100	6.644
101	6.658
102	6.673
103	6.687
104	6.701
105	6.714

4.4 MATHEMATICAL INDUCTION

According to Section 3.3, the forumula $t_n = b\cdot n \lg n + a\cdot(n-1)$ satisfies the recurrence relation $t_1 = 0$, $t_n = a + b\cdot n + 2\cdot t_{n/2}$ when n is a power of 2. The present section shows how to use the method of *mathematical induction* to verify this formula, and how to apply the method to other similar problems.

The method depends upon the *Induction Principle*, which states that a function of an integer argument is valid for all nonnegative values of its argument, provided that both of the following can be shown:

1. The function is valid for the argument value 0; and
2. Validity of the function for any nonnegative argument value m implies validity for $m + 1$.

In this particular application, the substitution $n = 2^{k+1}$ gives a new independent variable k that takes on nonnegative integer values. With $s_{k+1} = t_n$; $s_k = \mathrm{t}_{n/2}$, it is to be shown that the function $s_k = b\cdot k\cdot 2^k + a\cdot(2^k - 1)$ satisfies the recurrence relation $s_{k+1} = a + b\cdot 2^{k+1} + 2\cdot s_k$ with $s_0 = 0$.

Step one of the method requires that the proposed function be *verified* for $k = 0$:

$s_0 = b\cdot 0\cdot 2^0 + a(2^0 - 1) = 0$

Step two *assumes* that the proposed function is correct for an arbitrary (nonnegative) value $k = m$:

$s(m) = b\cdot m\cdot 2^m + a\cdot 2^m - a$

and then uses this assumption to compute the function value for $k = m + 1$ from the given recurrence relation:

$s_{m+1} = a + b\cdot 2^{m+1} + 2\cdot(b\cdot m\cdot 2^m + a\cdot 2^m - a) = b\cdot(m+1)\cdot 2^{m+1} + a\cdot 2^{m+1} - a$

This calculation shows that the assumption for $k = m$ *implies* that the proposed function is correct for the *next* value $k = m + 1$.

Thus both requirements of the Induction Principle are satisfied and the proposed function is correct for all nonnegative values of k. The original formula in n is therefore valid whenever n is a power of 2 with a positive integer exponent.

Section 4.4 Exercises

1. Fibonacci numbers: Use mathematical induction to prove that the recurrence $F_0 = 0$, $F_1 = 1$, $F_{m+2} = F_{m+1} + F_m$ is satisfied by the formula $\mathrm{F}_N = (\alpha^N - \beta^N) / (\alpha - \beta)$. First, show that the formula gives the correct result when N is zero or 1. Then, assuming that the formula is correct for $N = m$ and for $N = m + 1$, write out $F_{m+1} + F_m$. Show algebraically that this sum is equal to $(\alpha^{m+2} - \beta^{m+2}) / (\alpha - \beta)$, using the fact that α and β are roots of the equation $x^2 - x - 1 = 0$.
2. Shell sort interval sequence: Use mathematical induction to prove that the recurrence $h_0 = 1$, $h_{k+1} = 3\cdot h_k + 1$ is satisfied by the formula $h_k = (3\cdot k - 1) / 2$.

Chapter 5 Linked Lists

Although arrays can be accessed very rapidly and efficiently, they have one major shortcoming: An array has a fixed size that cannot be changed after data has been stored in it. On the other hand, a linked list is stored dynamically and becomes larger or smaller when data is added or removed. Data can be inserted or deleted at the beginning or end of a linked list or at a specific position in the middle.

A linked list is a sequence of *nodes* connected with pointers. Each node is a structure, and one of its components is a pointer to the remainder of the list. For example:

```
type :: Node_Type
  type (Info_Type) :: Info
  type (Node_Type), pointer :: Next_NP
end type Node_Type
```

The pointer in the last node of a linked list is null because the remainder of the list is empty.

A linked list is accessed through a *root* pointer whose target is the first node — unless the list is empty, in which case the root pointer is null. The root is declared as a variable with the pointer attribute, of the data type that has been defined for the node structures.

```
type (Node_Type), pointer :: Root_NP => null( )
```

The root is declared as a pointer variable in a main program, a subprogram, or a module. The root pointer itself is usually not a dynamically allocated object, but its target node is allocated in dynamic storage during program execution, by the following statement:

```
allocate( Root_NP )
```

Each additional node in the list is allocated dynamically as required, as the target of the pointer component in a previously allocated node.

5.1 LINKED LIST NODE OPERATIONS

Let the nodes of a linked list be structures of type **Node_Type**, with a data component named *Info* and a pointer component named *Next_NP*:

```
type :: Node_Type
  type (Info_Type) :: Info
  type (Node_Type), pointer :: Next_NP => null( )
end type Node_Type
```

The declared (target) type of the pointer component is **Node_Type**; this pointer provides access to the remainder of the linked list beyond the node in which it appears. Nodes are initialized with a null pointer component; thus a new node has no target until steps are taken to incorporate it into the linked list.

The data component, *Info*, occupies a structure of type **Info_Type**; for simplicity, let this structure consist of a character string component named *Key* and an integer vector component named *Data*. The type definition for **Info_Type** specifies default initialization for the character and integer components.

```
type :: Info_Type
  character (len = S_LEN) :: Key = " "
  integer :: Data(2) = 0
end type Info_Type
```

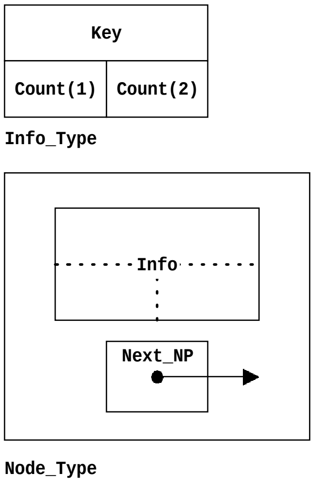


FIGURE 5.1. Derived types for linked list nodes

The forward pointer in each node and the root pointer may be viewed as pointers to the remainder of the list, not merely to the next node. Unless the remainder of the list is empty, it is a node that contains an information component and a pointer to the (further) remainder.[29]

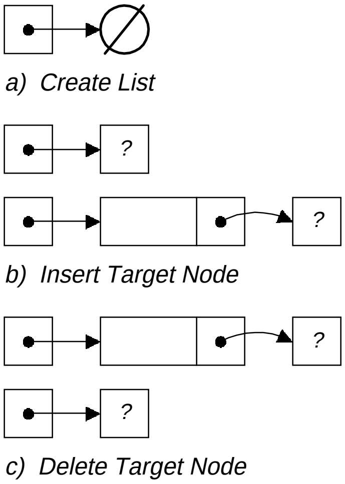
Create List

A linked list is created by a type declaration for the root pointer. Initially, there are no nodes in the list; the root pointer has no target (see Fig. 5.2a). The derived type definition specifies initial nullification for the root pointer.[30]

```
type (Node_Type), pointer :: Root_NP => null( )
```

[29] This point of view is explored further by Brainerd, et al in *Programmer's Guide to F* (Albuquerque: Unicomp, 1996), 280

[30] Default initiallization of structure components as shown here, including initial nullification of pointers, is possible with Fortran 95. Fortran 90 requires assignment statements to initialize data components and **nullify( )** statements for pointers. Electronically distributed examples include alternative Fortran 90 versions.



a) *Create List*

b) *Insert Target Node*

c) *Delete Target Node*

FIGURE 5.2. Operations to Create, Insert, and Delete a linked list node

Insert Target Node

A simple operation on a linked list is the insertion of a new node as the target of a given pointer (see Fig. 5.2b). For example, a node may be added to an empty list by inserting it as the target of *Root_NP*; or a node may be added as the target of the forward pointer in an existing node. An information structure to be assigned as the *Info* component of the new node may be passed as an argument to an insertion procedure. The operation **`Insert_Target( Arg_NP, Item )`** has two parts:

1. Allocate a new node as the target of a temporary pointer, **`Temp_NP`**. Give values to all components of the new node. Copy **`Arg_NP`** (by pointer assignment) to the forward component of the new node, **`Temp_NP % Next_NP`**, thus linking the remainder of the list to the newly allocated node.

   `Arg_NP` *must* be copied before it is changed; otherwise, changing **`Arg_NP`** would remove the only pointer to the remainder (if any) of the linked list, and the remainder of the list would be lost.

2. Copy **`Temp_NP`** (by pointer assignment) to **`Arg_NP`**, thus linking the remainder of the list (including the new node) to **`Arg_NP`**.

```
   subroutine Insert_Target( Arg_NP, Item )
     type (Node_Type), pointer :: Arg_NP, Temp_NP
     type (Info_Type), intent(in) :: Item
 ! start subroutine Insert_Target
     allocate( Temp_NP )
     Temp_NP % Info = Item
     Temp_NP % Next_NP => Arg_NP
     Arg_NP => Temp_NP
     return
   end subroutine Insert_Target
```

As shown below, a linked list can be generated by calling this procedure repeatedly with the root pointer *Root_NP* as the argument. Each call will allocate a new node and insert it as the target of *Root_NP*. Thus, after each call the new node will be the first node in the linked list and the sequence of nodes that previously comprised the linked list will follow the new node.

Delete Target Node

The procedure **Delete_Node(Arg_NP)** deletes the linked list node that is the target of *Arg_NP*, as illustrated in Fig. 5.2c. The successor of the deleted node becomes the target of *Arg_NP* (unless the deleted node was the last node in the linked list, in which case the null successor pointer is copied to *Arg_NP*). Here, the procedure is implemented as a function whose result value is a copy of the *Info* component of the deleted node. The procedure consists of the following steps:

1. Copy **Arg_NP** (by pointer assignment) to **Temp_NP**. This *must* be done before **Arg_NP** is changed (at step 3); otherwise, there would be no way to delete the node that is the target **Arg_NP**. If **Arg_NP** has a target, continue with the remaining steps; otherwise, skip them. (In the latter case, the function result variable retains its default initialization value).

2. Assign the **Info** component, in the node that will be deleted, to the function result variable.

3. Change **Arg_NP** so that its target is the successor (if any) of the node to be deleted — that is, the **Next_NP** component of the node to be deleted is copied (by pointer assignment) to **Arg_NP**. If the deleted node has no successor, its **Next_NP** component is a null pointer and copying it has the effect of nullifying **Arg_NP**.

4. Deallocate **Temp_NP**, which is now the only pointer whose target is the node to be deleted; thus, deallocating **Temp_NP** deletes the node. This deallocation must take place *after* **Next_NP** has been copied to **Arg_NP** (at step 3).

```
  function Delete_Target( Arg_NP ) result( Item )
    type (Node_Type), pointer :: Arg_NP, Temp
    type (Info_Type) :: Item
! start function Delete_Target
    Temp => Arg_NP
    Item = Arg_NP % Info
    Arg_NP => Arg_NP % Next_NP
    deallocate( Temp )
    return
  end function Delete_Target
```

Print Target Node

The procedure **Print_Target(Arg_NP)** prints components of the target of *Arg_NP*. Fortran does not permit pointers in input or output lists; only the nonpointer component **Arg_NP % Info** is printed.

```
  subroutine Print_Target( Arg_NP )
    type (Node_Type), pointer :: Arg_NP
! start subroutine Print_Target
    print *, " Print: ", Arg_NP % Info
    return
  end subroutine Print_Target
```

Modify Target Node

The procedure **Modify_Target(Arg_NP)** performs a predetermined modification upon the node that is the target of *Arg_NP*. In our examples, we increment **Arg_NP % Info % Data(2)**. This element thus contains a count of the number of occurrences of the corresponding key, if it was given the value 1 when the node was inserted.

```
    subroutine Modify_Target( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine Modify_Target
      Arg_NP % Info % Data(2) = Arg_NP % Info % Data(2) + 1
      return
    end subroutine Modify_Target
```

5.2 OPERATIONS ON WHOLE LINKED LISTS

Making a Linked List by Insertion at the Root

The subroutine **Insert_Target** can be called repeatedly with *Root_NP* as its argument. A loop such as the following will read data and insert it at the root until the end of input is detected.

```
  type (Node_Type), pointer :: Root_NP
    :
  do
    read (1, *, iostat = EoF) Temp_NP % Key
    if (EoF < 0) exit
    Temp_NP % Data(1) = Loop
    Temp_NP % Data(2) = 1
    call Insert_Target( Root_NP, Temp_NP )
  end do
```

The read statement accepts data for a node of the linked list and inserts the node as the target of *Root_NP*. The data that was read first will be at the end of the linked list, and the data that was read most recently will be in the node that is the final target of *Root_NP*.

Print List

Very common in linked list applications is the use of a declared “traveling node pointer,” here called *Trav_NP*, that points to the current node and then advances to the next node.

The first execution step copies *Root_NP* to *Trav_NP*. Just before the end of each iteration, the forward pointer component of the current node, **Trav_NP % Next_NP**, is copied to *Trav_NP*. When the end of the list is reached, *Trav_NP* is null. The subroutine **Print_List** prints data from the current node and then advances to the next node to print the remainder of the list. The entire list will be printed in order, beginning with the root and proceeding to the tail.

```
   type (Node_Type), pointer :: Root_NP
     :
   subroutine Print_List( )
     type (Node_Type), pointer :: Trav_NP
 ! start subroutine Print_List
     Trav_NP => Root_NP
     do while (associated( Trav_NP ))
       call Print_Target( Trav_NP )
       Trav_NP => Trav_NP % Next_NP                   ! Advance to next node
     end do
     return
   end subroutine Print_List
```

Delete List

A traveling pointer is not needed for repeatedly deleting the first node (the target of the root pointer) until the list is empty:

```
 type (Node_Type), pointer :: Root_NP
   :
 do while (associated( Root_NP ))
   print *, " Deleted: ", Delete_Target( Root_NP )
 end do
```

Searching in a Linked List

A linked list search can easily be implemented with a traveling pointer. The following example shows how to perform a linear search in a list, beginning at *Root_NP*, for a node wherein **Info % Key** matches the *Key* component of the input *Item*. When a match is found, a message is printed and data in the target node is modified. If the end of the list is reached, the message **" Not Found."** is printed.

```
   type (Node_Type), pointer :: Root_NP
     :
   subroutine Search_List( Item )
     type (Info_Type), intent(in) :: Item
     type (Node_Type), pointer :: Trav_NP
 ! start subroutine Search_List
     Trav_NP => Root_NP
     do
       if (associated( Trav_NP )) then
         if (Item % Key == Trav_NP % Info % Key) then
           print *, Item % Key, " Found."
           call Modify_Target( Trav_NP, Item % Data(1) )
           return
         end if
       else
         print *, Item % Key, " Not Found."
         return
       end if
       Trav_NP => Trav_NP % Next_NP                       ! Keep searching.
     end do
   end subroutine Search_List
```

The situation is not quite so simple, however, if the *linkage* is to be modified when a particular key is found in the middle of a linked list. Procedures such as **`Insert_Target`** and **`Delete_Target`** (described earlier) link remaining nodes of the list only to *Trav_NP* which is a copy of the an actual list link; they do not correctly modify the linkage of the actual list. This situation is discussed in more detail in the following paragraphs.

Maintaining a Large Ordered List

Suppose that a linked list is ordered according to a key, and a new item is to be inserted. A linear search for the new key, beginning at the root of the linked list, has three possible outcomes.

1. An item in the linked list with a *matching* key may be found. In this case no new item is to be inserted. In our examples, the matching item is modified. When the search terminates, the target of **`Trav_NP`** is the node with a matching key.

2. If all items in the list have keys *smaller* than the new one, the end of the linked list will be reached. In this case, **`Trav_NP`** is null when the search terminates. The new item is to be inserted at the end, as the new successor of the previous target of **`Trav_NP`**.

3. Otherwise, the search terminates when an item with a *larger* key is found. The node with the larger key is the target of **`Trav_NP`**, and the new item is to be inserted as the new successor of the previous target of **`Trav_NP`**.

There is a difficulty in either case 2 or case 3, because *Trav_NP* has already moved *beyond* the insertion point when the search terminates and a larger key or a null pointer has been encountered. It would be easy to insert a new item as the successor of the *Trav_NP* target node: it is only necessary to call **`Insert_Target`** with **`Trav_NP % Next_NP`** as the argument. But the forward node pointer in the *preceding* node is no longer accessible.

A similar problem arises when an item that matches a given key is to be deleted from a linked list. With the linked list search procedure described earlier, *Trav_NP* has again moved beyond the deletion point when the search terminates, and the pointer whose target is to be deleted from the linked list is no longer accessible.

The heart of the difficulty lies in the fact that *Trav_NP* is a *copy* of the pointer *Next_NP* in the predecessor node; therefore, deleting the target of *Trav_NP* or creating a new target for *Trav_NP* does not change the actual linkage of the linked list.

The obvious solution to this difficulty, described by many authors, is very inelegant and wasteful: A travelling pointer points to the *predecessor* of the node that is currently being examined. This requires extra steps at the beginning of a search (or other traversal of the linked list). One method declares the root as a separate pointer; this requires that a different sequence of statements be executed to examine the root target node. An alternative method creates the list with an otherwise unused “header node” as the target of the root pointer.

Two strategies that avoid these complications are discussed in Sections 5.3 and 5.4:

1. The search may be performed *recursively*, with the forward node pointer as the argument at each recursive call; or

2. The forward node pointer — or, in Fortran, a **`BOX`** containing the forward node pointer — may be assigned as the target of the traveling pointer. With a **`BOX`** that performs the role of the predecessor node, the Fortran syntax is still somewhat complicated. However, this method does not require a separate statement sequence nor a separate header node with wasted space for nonpointer node components (which, in some applications, can be significant).

5.3 PROCESSING LINKED LISTS RECURSIVELY

The actual argument to a recursive linked list procedure is a pointer to the remainder of a list (initially *Root_NP*, the pointer to the entire list). The procedure processes the current node and then calls itself recursively to process the remainder (unless the remainder is empty). While processing the current node, the procedure may modify the dummy argument pointer. Such modifications affect the actual linkage of the list, and not merely a copy of the argument pointer.

The following example shows how to insert a new item into an ordered linked list. Arguments in the initial call to the recursive subroutine are *Root_NP* and the data to be inserted.

The outer **`if`** construct tests whether the current node pointer is associated (i.e., whether it has an actual target).

- If the current node pointer is not null, the inner **`if`** construct compares the **`Key`** in the current node, referred to as **`Arg_NP % Info % Key`**, with the **`Key`** component of the given item. This comparison has three possible outcomes:

  1. If the keys match, information in the current node is to be modified.
  2. If **`Arg_NP % Info % Key`** is larger, no matching key will be found — the search has passed the point where a match would have occurred — so the given item is inserted ahead of the given node. The procedure **`Insert_Target`** discussed earlier performs this operation and correctly modifies the current input pointer.
  3. Otherwise, **`Arg_NP % Info % Key`** is smaller than the search key, so the procedure is called recursively to search the remainder of the list.

- If the current node pointer is null, the **`else`** block of the outer **`if`** construct is executed and the given item is inserted at the end of the list.

```
 recursive subroutine Look_Up( Arg_NP, Item )
   type (Node_Type), pointer :: Arg_NP
   type (Info_Type), intent(in) :: Item
! start subroutine Look_Up
   if (associated( Arg_NP )) then
     if (Item % Key == Arg_NP % Info % Key) then
       call Modify_Target( Arg_NP, Item )
     else if (Arg_NP % Info % Key > Item % Key) then
       call Insert_Target( Arg_NP, Item )        ! Insert before next node.
     else
       call Look_Up( Arg_NP % Next_NP )                  ! Keep looking.
     end if
   else
     call Insert_Target( Arg_NP, Item )    ! Insert at end of linked list.
   end if
   return
 end subroutine Look_Up
```

This recursive approach is very elegant, but the time and space overhead imposed by recursion leave some scholars unconvinced of its merits. A new activation record (see Section 3.1) is created at each recursive call — that is, for each node encountered by the linked list operation. For a very long linked list, the amount of extra storage occupied by these activation records may be intolerable. On the other hand, a long list will itself necessarily occupy a great deal of storage unless the amount of data in each node is trivial.

Nevertheless, for long lists it is well to minimize the space occupied by each activation record. In particular, the procedure **Look_Up** has an argument *Item* that might be a large data structure in an actual application; it would be well to avoid storing redundant copies of this *Item*. A solution is to construct the subroutine **Look_Up** as a nonrecursive “wrapper.” The application program calls **Look_Up**, which in turn calls a recursive internal procedure **R_Look_Up** that inherits *Item* from the wrapper. The argument *Item* is stored only in the activation record for the wrapper; the activation record for **R_Look_Up** is now quite small because there are no local variables and the only argument is a pointer.

Say It with Fortran

Example 14

```
! Example 14. Linked List with Recursion
module D14_M
  implicit none
  public :: Look_Up, Print_List, Delete_List
  integer, parameter, public :: S_LEN = 20
  type, public :: Info_Type
    character (len = S_LEN) :: Key
    integer, dimension(2) :: Data = (/ 0, 1 /)
  end type Info_Type
  type, private :: Node_Type
    type (Info_Type) :: Info
    type (Node_Type), pointer :: Next_NP => Null( )
  end type Node_Type
  type (Node_Type), pointer, private :: Root_NP => Null( )
contains

  subroutine Look_Up( Item )
    type (Info_Type), intent(in out) :: Item
! start subroutine Look_Up
    call R_Look_Up( Root_NP )
    return
  contains

    recursive subroutine R_Look_Up( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine R_Look_Up
      if (associated ( Arg_NP )) then
        if (Item % Key == Arg_NP % Info % Key) then
          call Modify_Target( Arg_NP, Item )
        else if (Arg_NP % Info % Key > Item % Key) then
          call Insert_Target( Arg_NP, Item )   ! Insert ahead of next node.
        else
          call R_Look_Up( Arg_NP % Next_NP )                ! Keep looking.
        end if
      else
        call Insert_Target( Arg_NP, Item )  ! Insert at end of linked list.
      end if
      return
    end subroutine R_Look_Up
    subroutine Modify_Target( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine Modify_Target
      Arg_NP % Info % Data(2) = Arg_NP % Info % Data(2) + 1
      return
    end subroutine Modify_Target

    subroutine Insert_Target( Arg_NP, Item )
      type (Node_Type), pointer :: Arg_NP, Temp_NP
      type (Info_Type), intent(in) :: Item
  ! start subroutine Insert_Target
      allocate( Temp_NP )
      Temp_NP % Info = Item
      Temp_NP % Next_NP => Arg_NP
      Arg_NP => Temp_NP
      return
    end subroutine Insert_Target

  end subroutine Look_Up

  subroutine Print_List( )
! start subroutine Print_List
    call R_Print_List( Root_NP )
    return
  contains

    subroutine R_Print_List( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine R_Print_List
      if (associated ( Trav_NP )) then
        call Print_Target( Trav_NP )
        call R_Print_List( Arg_NP % Next_NP )          ! Advance to next node
      end if
      return
    end subroutine R_Print_List

    subroutine Print_Target( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine Print_Target
      print *, " Print: ", Arg_NP % Info
      return
    end subroutine Print_Target

  end subroutine Print_List

  subroutine Delete_List( )
! start subroutine Delete_List
    call R_Delete_List( Root_NP )
    return
  contains
```

```
    subroutine R_Delete_List( )
  ! start subroutine R_Delete_List
    if (associated( Root_NP )) then
      print *, " Deleted: ", Delete_Target( Root_NP )
```

Delete at root: Next call deletes at the same point.

```
      call R_Delete_List( )
    end if
    return
    end subroutine R_Delete_List

    function Delete_Target( Arg_NP ) result(Item)
      type (Node_Type), pointer :: Arg_NP, Temp
      type (Info_Type) :: Item
  ! start function Delete_Target
      Temp_NP => Arg_NP
      Item = Arg_NP % Info
      Arg_NP => Arg_NP % BOX % Next_NP
      deallocate( Temp_NP )
    end function Delete_Target

  end subroutine Delete_List

end module D14_M
```

```
  program D14
    use D14_M
    implicit none
    integer :: EoF
    type (Info_Type) :: Item

! start program D14
    open (1, file = "dxf.txt", status = "old", action = "read", &
      position = "rewind")
    do
      read (1, *, iostat = EoF) Temp_NP % Key
      if (EoF < 0) exit
      Item % Data(1) = Item % Data(1) + 1
      call Look_Up( Item )
    end do
    call Print_List( )
    call Delete_List( )
    stop
  end program D14
```

As mentioned earlier, a linked list may be viewed as a recursive data structure: Each node contains data as well as a pointer to the remainder of the list. Besides its philosophical elegance, recursive linked list processing fortuitously circumvents a syntactic shortcoming of Fortran and of some other programming languages. The recursive technique passes the pointer argument (at each recursive call) *by reference*: what is actually transmitted is a *pointer* to the argument pointer. Pointers to pointers are needed, and recursion provides this facility in a (syntactically) simple manner. This philosophical elegance and syntactic simplicity are achieved at the expense of extra space and time overhead imposed by the mechanism of recursion, although with some care the space overhead can be minimized. Converting the tail recursion in this program to iteration without introducing significant syntactic complication seems impossible.

5.4 LINKED LISTS WITH POINTERS TO POINTERS

Some programming languages support pointers to pointers. Fortran does not permit a pointer whose target is a pointer, but it permits a pointer to a structure whose only component is a pointer. (Compare arrays of pointers, described in Chap. 2). Such a structure is here called a **BOX**: its type is **BOX_Type** and its only component is a node pointer named *Next_NP*, as shown in Fig. 5.3. A pointer to a **BOX** provides a Fortran substitute for a pointer to the node pointer inside the **BOX**. This permits iterative linked list search with insertion and deletion of nodes.

Here each linked list node has two components, one of which holds data, as before. The second component is now a **BOX** whose node pointer component *Next_NP* designates the remainder of the list: The target of *Next_NP* is the linked list successor node, if there is one; otherwise, *Next_NP* is null. The root of the linked list is a **BOX** named *Root*; if the linked list is empty, the node pointer component of *Root*, designated as **Root % Next_NP**, is null.

```
type, private :: BOX_Type
  type (Node_Type), pointer :: Next_NP => Null( )
end type BOX_Type
type, private :: Node_Type
  type (Info_Type) :: Info
  type (BOX_Type) :: BOX
end type Node_Type
type (BOX_Type), pointer, private :: Trav_BP      ! "traveling" BOX pointer
type (BOX_Type), target, private, save :: Root
```

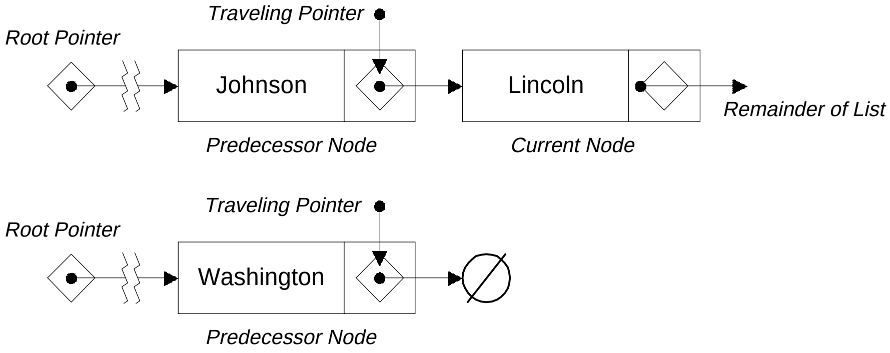


FIGURE 5.3. Fortran Pointer-to-Pointer technique

The traveling **BOX** pointer *Trav_BP* points to a **BOX** in the predecessor node; the node pointer in this **BOX** is **Trav_BP % Next_NP**, the forward pointer to the current node. If **Trav_BP % Next_NP** is null, no current node is the “target of the target” of *Trav_BP*. Otherwise (with Fortran’s automatic dereferencing), the components of the current node are referred to as **Trav_BP % Next_NP % Info** and **Trav_BP % Next_NP % BOX**. The latter is a **BOX** that contains a pointer to the remainder of the linked list; **Trav_BP** advances when this **BOX** is assigned as its new target: **Trav_BP** => **Trav_BP % Next_NP % BOX**.

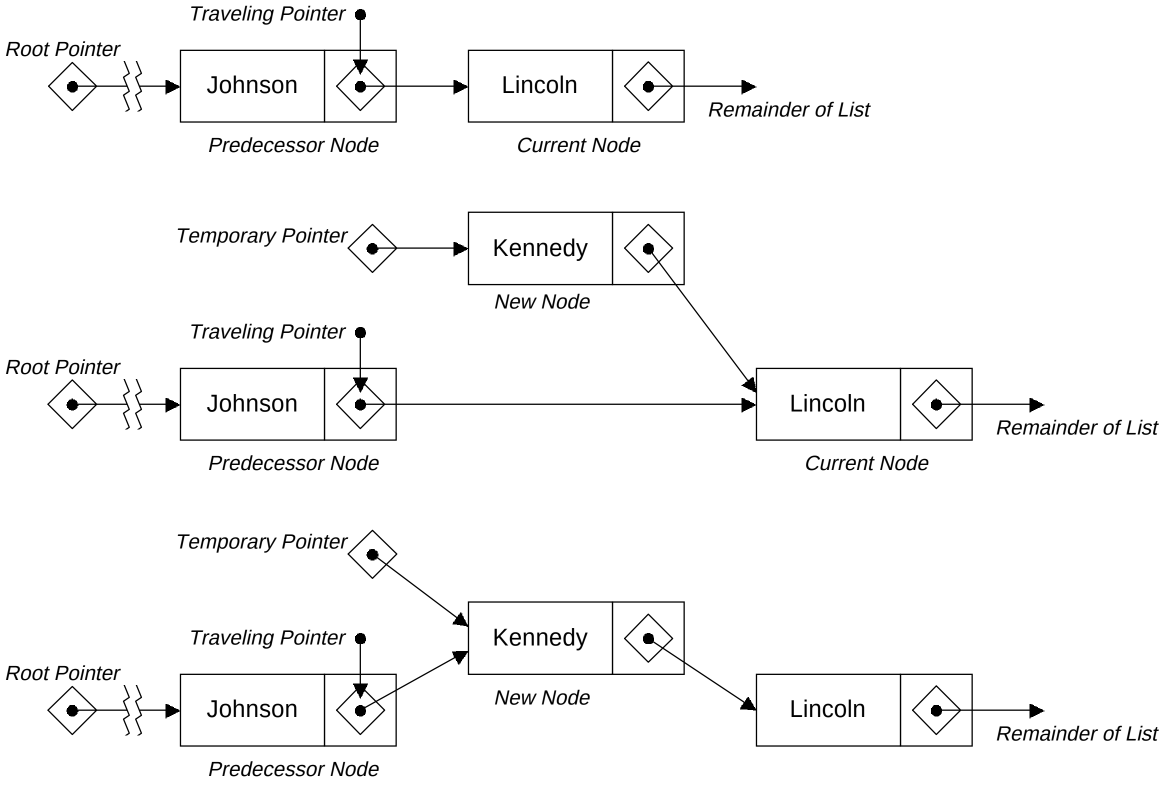


FIGURE 5.4. Inserting a new node ahead of the current node

Fig. 5.4 illustrates insertion of a new node ahead of the current node. The subroutine **Insert_Target** is called with argument **Trav_BP % Next_NP** to insert the new node as the target of the forward node pointer in the predecessor node. The only change from the version shown at the beginning of this chapter appears in the pointer assignment **Temp_NP % BOX % Next_NP => Arg_NP** that links the current target of **Arg_NP** to the forward pointer **Temp_NP % BOX % Next_NP** in the new node.

```
  subroutine Insert_Target( Arg_NP, Item )
    type (Node_Type), pointer :: Arg_NP
    type (Info_Type), intent(in) :: Item
    type (Node_Type), pointer :: Temp_NP
! start subroutine Insert_Target
    allocate( Temp_NP )
    Temp_NP % Info = Item
    Temp_NP % BOX % Next_NP => Arg_NP
    Arg_NP => Temp_NP
    return
  end subroutine Insert_Target
```

Fig. 5.5 illustrates the procedure **Delete_Target**, which is called with the actual argument **Trav_BP % Next_NP**, the forward node pointer in the predecessor node. The only change from the earlier version appears in the pointer assignment **Arg_NP => Arg_NP % BOX % Next_NP**.

```
  function Delete_Target( Arg_NP ) result( Item )
    type (Node_Type), pointer :: Arg_NP
    type (Info_Type) :: Item
    type (Node_Type), pointer :: Temp_NP
! start function Delete_Target
    Temp_NP => Arg_NP
```

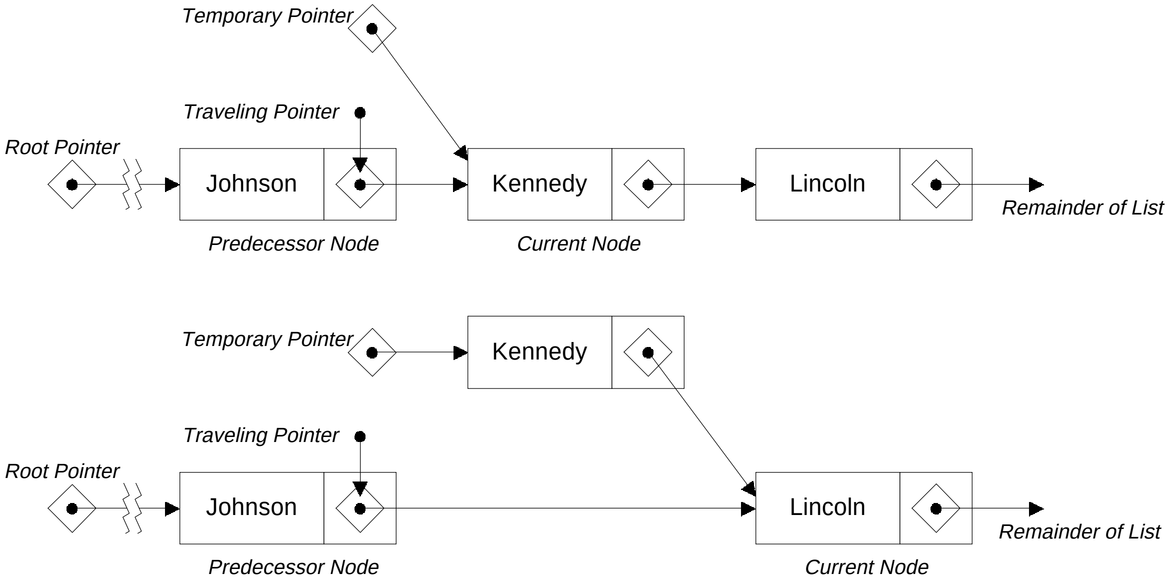


FIGURE 5.5. Deleting the current node

```
    Item = Arg_NP % Info
    Arg_NP => Arg_NP % BOX % Next_NP
    deallocate( Temp_NP )
    return
  end function Delete_Target
```

The first step of the procedure **Look_Up** assigns *Root* (which has been declared in the module **Linked_List_Ops**) as the initial target of *Trav_BP*.

```
  type (BOX_Type), target :: Root
    :
  subroutine Look_Up( Item )
    type (Info_Type), intent(in) :: Item
! start subroutine Look_Up
    Trav_BP => Root                          ! Make Root the target of Trav_BP
    do
      if (associated( Trav_BP % Next_NP )) then
        if (Item % Key == Trav_BP % Next_NP % Info % Key) then
          call Modify_Target( Trav_BP % Next_NP )
        else if (Item % Key < Trav_BP % Next_NP % Info % Key) then
          call Insert_Target( Trav_BP % Next_NP, Item )
        else
          Trav_BP => Trav_BP % Next_NP % BOX          ! Move to successor node.
          cycle                                               ! Keep looking.
        end if
      else
        call Insert_Target( Trav_BP % Next_NP, Item )         ! Insert at end.
      end if
      return
    end do
  end subroutine Look_Up
```

This iterative procedure is equivalent to the earlier recursive version, modified by tail recursion removal and with the introduction of pointers to pointers.

Example 15. Shown here is a slightly modified version of the subroutine **Look_Up** for the Pointer to Pointer technique, along with a main program. The **BOX** named *Root* is declared in module. Procedures that operate at the target level are the same as with recursion.

```
! Example 15. Linked list with pointers to pointers.
module D15_M
  implicit none
  public :: Look_Up, Print_List, Delete_List
  integer, parameter :: S_LEN = 20
  type, public :: Info_Type
    character (len = S_LEN) :: Key
    integer, dimension(2) :: Data = (/ 0, 1 /)
  end type Info_Type
  type, private :: BOX_Type
    type (Node_Type), pointer :: Next_NP => Null( )
  end type BOX_Type
  type, private :: Node_Type
    type (Info_Type) :: Info
    type (BOX_Type) :: BOX
  end type Node_Type
  type (BOX_Type), pointer, private :: Trav_BP  !"traveling" BOX pointer
  type (BOX_Type), target, private, save :: Root

contains

  subroutine Look_Up( Item )
    type (Info_Type), intent(in) :: Item
! start subroutine Look_Up
    Trav_BP => Root                     ! Make Root the target of Trav_BP
```

The **if** *constructs have been rearranged to agree with the recursive Fortran program shown earlier. Note that the* **end do** *statement is never reached except from the* **cycle** *statement, which transfers control to the top of the* **do** *block.*

```
    do
      if (associated ( Trav_BP % Next_NP )) then
        if (Item % Key == Trav_BP % Next_NP % Info % Key) then
          call Modify_Target( Trav_BP % Next_NP )
        else if ( Item % Key < Trav_BP % Next_NP % Info % Key) then
          call Insert_Target( Trav_BP % Next_NP, Item )
        else
          Trav_BP => Trav_BP % Next_NP % BOX  ! Move to successor node.
          cycle                                         ! Keep looking.
        end if
      else
        call Insert_Target( Trav_BP % Next_NP, Item )  ! Insert at end.
      end if
      return
    end do
  contains

    subroutine Modify_Target( Arg_NP )
      :
    end subroutine Modify_Target
    subroutine Insert_Target( Arg_NP, Item )
      :
    end subroutine Insert_Target

  end subroutine Look_Up

  subroutine Print_List( )
! start subroutine Print_List
    Trav_BP => Root
    do while (associated ( Trav_BP % Next_NP ))
      call Print_Target( Trav_BP )
      Trav_BP => Trav_BP % Next_NP % BOX                ! Advance to next node
    end do
    return
  contains

    subroutine Print_Target( Arg_BP )
      :
    end subroutine Print_Target

  end subroutine Print_List

  subroutine Delete_List( )
! start subroutine Delete_List
    do while (associated ( Root % Next_NP ))
      print *, " Deleted: ", Delete_Target( Root )
    end do
    return
  contains

    function Delete_Target( Arg_NP ) result(Item)
      :
    end function Delete_Target

  end subroutine Delete_List

end module D15_M
```

Section 5.4 Exercises

1. Write a recursive subroutine **Print_List** that prints information from the nodes of a linked list in reverse order: If the argument pointer is not null, call **Print_List** with the forward pointer (i.e., the remainder of the list) as its actual argument and then call Print_Target to print the current node. Calling **Print_List** with the root node as the actual argument will print the entire list in reverse order.

2. Write a recursive subroutine **Delete_List** that deletes nodes from a linked list in reverse order: If the argument pointer is not null, call **Delete_List** with the forward pointer (i.e., the remainder of the list) as its actual argument and then call **Delete_Target** to delete the current node. (Print the **Info** component of each node as it is deleted.) Because the remainder of the list has already been deleted, the current node is the *last* node at the time it is deleted, and its deletion nullifies the argument pointer. Calling **Delete_List** with the root node as the actual argument will delete the entire list in reverse order.

4. Implement the operation **Look_Up** with the data structure **Item** declared as a module variable; modify the module procedures to inherit **Item** and modify the main program to import it.

5.5. APPLICATIONS WITH SEVERAL LINKED LISTS

The foregoing examples provide a single linked list whose root is declared in the list definition module. However, for many applications it is preferable to permit the consumer to create more than one list and to designate a specific list for each linked list operation. A root for each separate list is declared in the application program and can be passed to any of the linked list procedures. In the Pointer to Pointer version shown here, each separate list is declared as a **BOX**, which becomes the initial target of *Trav_BP* in subroutine **Look_Up**.

```
      type :: BOX_Type
        type (Node_Type), pointer :: Next_NP => Null( )
      end type BOX_Type
      type :: Node_Type
        type (Info_Type) :: Info
        type (BOX_Type) :: BOX
      end type Node_Type
        :
      subroutine Look_Up( Arg_B, Item )
        type (BOX_Type), intent(in) :: Arg_B
        type (Info_Type), intent(in) :: Item
    ! start subroutine Look_Up
        Trav_BP => Arg_B
        :
    ! Main program
        :
      type (BOX_Type), target :: List1, List2, . . .
        :
      call Look_Up( List1, Item )
        :
```

An array of linked lists may be required for some applications:

```
    ! Main program
        :
      type (BOX_Type), target, dimension(17) :: List
        :
      call Look_Up( List(I), Item )
        :
```

Multiply Linked Lists

Some lists have more than one pointer in each node.

In a *doubly-linked list,* each node has both a forward pointer (to the successor node) and a backward pointer (to the predecessor node). All of the node-level procedures are essentially unchanged except for the extra overhead of modifying both pointer nodes during insertion or deletion. In a *circular list*, the last node points back to the first (i.e., in most implementations, to the successor of the root). These ways of organizing the list are especially useful for certain applications, where it is necessary to access to the predecessor of a given node or for data with a circular structure that has no natural beginning and end.

A *threaded list* consists of a single set of data that can be accessed according to any of several sequences (threads). For example, it might be desirable to order a mailing list so that it could be printed sequentially by name or by postal ZIP code. Each node in a threaded list contains a pointer for each different key sequence that is to be applied; to facilitate insertions and deletions, each thread may be linked both forward and backward.

5.6 LINKED LISTS VS. ARRAYS

A great many data processing applications store a collection of data items each of which contains a key identifying a unique item in the collection. For some applications the key is expanded to include a secondary key that distinguishes different items with the same primary key; in other cases a collection with unique keys merely serves as an index to the actual data — for example, a collection of pointers to sets of items that share a given key.

The two principal operations to be performed upon such a collection are:

- Insert a new item into the collection if the key is not matched by that of any current item, or modify the existing item (in some predetermined manner) if the key is matched.
- Search and delete an item with a given key.

Each of these operations begins with a search to determine whether or not the the key is matched by that of any item that is currently in the collection. For insertion, either outcome may be expected and appropriate actions are specified for either case. For deletion, however, an unmatched search key is considered an error.

Either an array or a linked list could be employed to hold such a collection. In either case, the data items may be stored either in key order or in some other manner unrelated to the key values. The following paragraphs discuss the advantages and disadvantages of these four possibilities. For the most part, it is assumed that the set of different keys in the collection at any given time is random and that keys presented for insertion or deletion are random. However, some timing assumptions can have considerable effect — for example, some applications insert almost all items into the collection before making any deletions, so the current size of the collection at the time of a deletion is always nearly its maximum size. In any case, it is assumed here that the modification phase of the insertion operation is straightforward and does not require any significant further effort when the key is matched; also, the effort of processing a deletion error is ignored. The most significant disadvantage of arrays, that the maximum size of the collection must be known in advance, is not discussed at this point — it is assumed here that sufficient array space is provided.

Array Implementation

Unordered Array

The search phase requires a linear search through the entire collection. If the search key is matched, the expected number of comparisons is one-half the current size of the collection; if not, a comparison is required for every item currently in the collection.

If the search key is not matched, insertion is trivial: the new item is merely appended at the next higher subscript position beyond the current last item in the collection.

Deletion can occur at any point. Deleting an item requires that all items on its right be moved to the left so that no gaps will remain between data items in the array. The expected number of items to be moved as a result of the deletion is one-half the current size of the collection.

Ordered Array

Search in an ordered array can employ the binary search algorithm. Whether or not the search key is matched, the expected number of comparisons is lg N where N is the current size of the collection.

If there is no match, the search locates the point at which the new item must be inserted. All items to the right of the insertion point must be moved farther to the right (to a higher subscript position in the array) to make room for the new item. The expected number of items to be moved is one-half the current size of the collection.

After the search phase, deletion is the same as for an unordered array: All items to the right of the deletion point, estimated as one-half the current size of the collection, must be moved.

Linked List Implementation

Unordered Linked List

As in the array implementation, the search phase requires a linear search through the entire collection. If the item is present, the expected number of comparisons is one-half the current size of the collection; otherwise, a comparison is required for every item currently in the collection.

If the search key is not matched, insertion is trivial: the new item is merely inserted at the root of the linked list.

After the search phase, deletion of an item at any point in a linked list (properly implemtented) is also trivial.

Ordered Linked List

Binary search in a linked list is not possible; however, algorithms more or less equivalent to binary search may be implemented with trees or with skip lists (see Chapter 7). A linear search terminates (with or without a match) when an item with a larger or equal key is encountered; thus the expected number of comparisons is one-half the current size of the collection. Perhaps surprisingly, ordering a linked list gives no advantage in the matching case.

Insertion and deletion are trivial, as for an unordered linked list.

Summary

Aside from the requirement that the size of an array must be known in advance, the most efficient implementation for *searching* is an ordered array, because of the applicability of binary search; however, algorithms more or less equivalent to binary search may be implemented with trees or with skip lists (see Chapter 7).

For *insertions* and *deletions*, linked lists are clearly superior to arrays because there is no need to move large amounts of data, and keeping the list in order gives a slight advantage. For insertions, the number of comparisons with an unordered linked list implementation is no better than with an unordered array.

The relative cost of comparisons and moves is also sometimes a factor. Comparison is expensive for long keys. Moving is expensive when the data items are large, but in such cases the implementation can be designed so that the data remains in place and only a pointer moves.

For many applications, neither a linked list application nor an array application is ideal.

Almost all transactions at a bank's Automated Teller Machine are modifications that update an existing account balance. Opening and closing accounts (insertion and deletion) is handled separately and with much less severe time constraints. Thus an ordered array would be appropriate; however, a balanced tree or a skip list is even better, as we shall see (Chapter 7).

Mailing list maintenance consists mainly of insertions and deletions; modifying the address of an existing customer is much more rare. An ordered linked list would be preferable to an array in this case.

Chapter 6 Abstract Data Structures

6.1 STACKS

Applications of Stacks

Depth-First Search in a Graph

In Greek mythology, we read of the hero Theseus who killed a monster called a Minotaur to win the hand of the maiden Ariadne. Ariadne helped him find his way to the Minotaur, which was kept in a labyrinth; she gave him a ball of thread to unwind as he searched through the corridors of the labyrinth, while she held one end of the thread firmly in her hand. After killing the monster, Theseus returned to claim the maiden by rewinding the thread. The labyrinth can be simulated with a program that follows Theseus as he searches for the Minotaur, finds and kills it if it is in an accessible part of the labyrinth, and returns to Ariadne.

The solution presented here employs a *depth-first search* of the undirected graph whose nodes are the N rooms in the labyrinth and whose arcs are the corridors. For purposes of the program, the rooms are numbered with consecutive integers. An $N \times N$ matrix of logical type, called the *adjacency matrix*, is true in position (i, j) if there is a corridor leading from room i to room j. A list which (as we shall see) is implemented as a stack) represents the thread — it gives, in order, the numbers of the rooms through which the thread currently passes. Whenever Theseus leaves a room, he records its number on the thread list as he “unwinds the thread.”

The myth neglects to mention that Theseus also carries a piece of chalk, with which he marks each room that he visits.[31] A logical array stores the chalk marks (initially false) for all rooms in the labyrinth.

The search proceeds as follows:

- If the Minotaur is in the current room, Theseus kills it and returns to his lover by rewinding the thread.
- Otherwise, Theseus marks the current room with his chalk so that he will not visit it again. Then he selects the next corridor in order from the adjacency list for his current position, and looks down that corridor to see whether there is a chalk mark in the room at the far end. If he sees a chalk mark in the new room, he ignores that corridor and makes another selection from the adjacency list. When he finds a corridor leading to an unmarked room, he records the current room number on the thread list, unwinding the thread as he moves to the room at the far end of the selected corridor.
- After all of the corridors on the adjacency list for the current room have been explored, Theseus looks at the thread list to find the number of the room from whence he traveled to the current room. He rewinds the thread as he moves to that room, deleting its room number from the list. However,

[31] It is not strictly necessary to mark each room as it is visited, provided that the corridors from a given room are traversed in order (for example, according to the adjacency list sequence). However, the marking technique considerably improves the efficiency of the algorithm.

if Theseus finds that the thread list is empty, this means that he has returned to Ariadne without finding the Minotaur — the beast is in a part of the labyrinth that cannot be reached from the given initial position.

As an example, consider the labyrinth in Fig. 6.1. Suppose that Theseus and Ariadne are initially in room 8 and the Minotaur is in room 6. The thread list is initialized with Room 8. Theseus unwinds the thread as he searches rooms 7, 4, 2, and 1, choosing the lowest-numbered adjacent corridor from each room and marking each room as he visits it. When he reaches room 1, the rooms on the thread are 8, 7, 4, and 2.

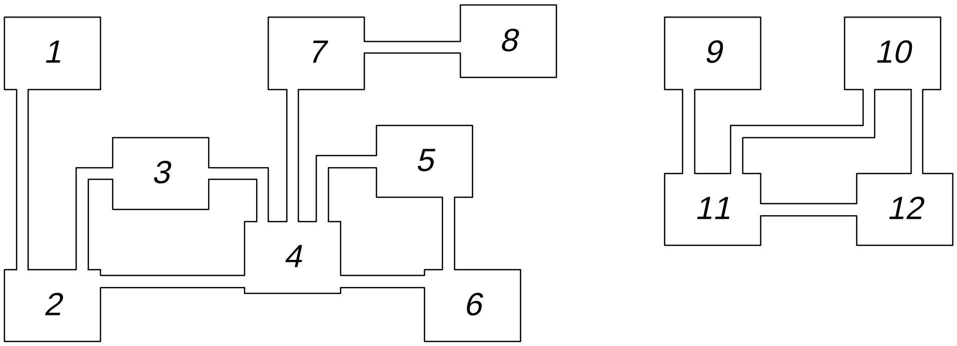


FIGURE 6.1. A labyrinth

From room 1 Theseus first looks down the corridor leading to room 2, but he sees a chalk mark indicating that this room has already been visited. There are no more adjacent rooms that have not been visited, so he rewinds the thread to room 2. He selects the next room from the adjacency list for room 2 and moves to room 3, unwinding the thread. Rooms on the thread at this point are 8, 7, 4, and 2.

The only rooms adjacent to room 3 are rooms 2 and 4, both of which have been visited, so Theseus again rewinds to room 2. All rooms adjacent to room 2 have now been visited, so he rewinds the thread and returns to room 4. The rooms now on the thread are 8 and 7.

Rooms adjacent to room 4 are 2, 3, 5, 6, and 7. On his previous visit to room 4, Theseus selected the corridor leading to room 2 and to the adventures just described. He now looks down the next corridor on the adjacency list, but it leads to room 3 which he visited earlier, so he selects another corridor and moves to room 5. Rooms 8, 7, and 4 are on the thread.

From room 5, Theseus looks down the corridor leading to room 4; has previously visited that room so he tries again, this time selecting room 6. Here he finds the Minotaur, kills it, rewinds the thread via rooms 5, 4, and 7, and returns in triumph to Ariadne who still waits paitently in room 8 for her heroic lover.

A suitable data structure to represent the thread is a *stack* of integers: the operation **Pop** will return the integer most recently placed on the stack by a **Push** operation. Theseus unwinds the thread by pushing the current room number onto the stack as he moves to the next room. He rewinds the thread by popping a room number from the top of the stack and returning to the indicated room, where he resumes his search.

```
logical, dimension(20, 20) :: Adjacent
logical, dimension(20) :: Mark = .false.
integer :: Tried(20)                ! Number of adjacent nodes already tried
  :
read *, Maid, Goal
Here = Maid
print *, Here, " Start."
```

```
Node: do
  if (Here /= Goal) then
    Mark(Here) = .true.                              ! Mark the current node.
    do Next = Tried(Here) + 1, Many           ! Find next adjacent node, if any.
      Tried(Here) = Next
      if (Adjacent(Here, Next) then
        print *, Here, Next, " Look down corridor."
        if (Mark(Next)) then
          print *, Here, Next, " Already visited."
        else
          call Push( Here )                                ! Move to next node.
          print *, Here, Next, " Unwind thread."
          Here = Next
          cycle Node                                 ! Continue from new node.
        end if
      end do
      print *, Here, " Dead end."
      if (Is_Empty( )) exit Node
      call Pop( Here )
      print *, Here, " Resuming."
    else
      print *, Here, " Minotaur is dead."
      do
        if (Is_Empty( )) exit
        call Pop( Here )
        print *, Here, Next, " Going home in triumph."
      end do
    end if
    stop
  end if
end do Node
print *, Here, " Minotaur is inaccessible. "
```

Stack Operations

The mechanism of a stack is "last in, first out" or LIFO. Stacks are also called *pushdown* structures by analogy to a stack of physical objects (saucers in a cafeteria are often suggested) stored in a hole and supported by a spring with only the top item visible. A **Push** operation pushes previous items farther down into the hole and gives the stack a new *Top* item; a **Pop** operation removes the current *Top* item and exposes the item below it as the new *Top*.

Several different operations are required for manipulating a stack:

- **Push(Here)** appends the value of the variable **Here** to the stack as a new item (which becomes the new Top).
- **Pop(Here)** removes the *most recently appended* item (the current Top) from the stack and returns it as the value of the variable **Here**.
- **Is_Empty( )** returns **.true.** if the stack is currently empty.

Two additional stack operations are often useful:

- **Peek(Here)** returns the most recently appended item (the current Top) as the value of the variable **Here**, but does not remove it from the stack.
- **Is_Full( )** returns **.true.** if the stack is currently full — that is, if the implementation does not permit any further items to be appended to the stack.

These stack operations do not permit access to any part of the stack except the current Top item — i.e., the stack item that was most recently appended. An item lower in the stack can be retrieved only by a sequence of **Pop** operations that remove all items above it.

Although a **Pop** operation is not permitted when a stack is empty and a **Push** operation is not permitted when it is full, the inverse operations are quite legal. In particular, the stack may become empty at one or more points during execution of an application, after which **Push** operations may again activate the stack. In the labyrinth example, the search does not fail when Theseus returns to Ariadne without killing the Minotaur *unless* all corridors from Ariadne's room have been explored and a rewind (**Pop**) is attempted while the stack is empty. (In Fig. 6.1, consider the case in which Ariadne is in room 4 and the Minotaur is in room 8.)

Fig. 6.2 shows the contents of the array at each step of a successful search in the labyrinth of Fig. 6.1. Ariadne is in room 8 and the Minotaur is in room 6.

8				
8	7			
8	7	4		
8	7	4	2	
8	7	4	2	1
8	7	4	2	
8	7	4	2	3
8	7	4	2	
8	7	4		
8	7	4	5	
8	7	4	5	6
8	7	4	5	
8	7	4		
8	7			
8				

FIGURE 6.2 Push and Pop operations during Labyrinth search

Evaluating a Postfix Expression

Stacks are suitable for many different applications. For example, some hand-held calculators employ a stack for evaluating expressions entered in *postfix* form, which means that an operator such as + or ∗ must follow the numbers or expressions that are its operands. For example, $2 * (3 + 4)$ is entered as $2\ 3\ 4 + *$ and $(2 + 3) * 4$ is entered as $2\ 3 + 4\ *$. One advantage of postfix notation is that no parentheses are required, provided that each operator has a known number of operands.

Whenever a number is entered, it is pushed on the stack. When an operator is entered, its operands are popped from the stack, the operation is performed, and the result is pushed on the stack. The calculator display shows the top of the stack at any point. For example, the two postfix expressions $2\ 3\ 4 + *$ and $2\ 3 + 4\ *$ are evaluated in the following manner:

Entry	Stack (Top, ...)		
2	2		
3	3	2	
4	4	3	2
+	7	2	
∗	14		

2	2	
3	3	2
+	5	
4	4	5
*	20	

Stacks and Recursion

We have noted earlier that the activation record for a procedure contains space for local variables (except those for which space is reserved statically and those that are explicitly allocated in dynamic storage), for dummy argument values or their locations, for function result values, and for a few bytes of information that are needed for returning execution control to the point from which the procedure was referenced. In the absence of recursion, only one copy of the activation record for each procedure is required, and some processors set aside space for all of these before execution of the main program begins.

On the other hand, a procedure that calls itself recursively needs to save a copy of its activation record for each recursive call, so that the previous instance can be restored at exit. The usual implementation of recursion employs a stack of activation records, sometimes called the *central stack*. The activation record for each procedure (also called a *stack frame*) is pushed onto this stack at the time of procedure entry and is popped from the stack at procedure exit. While stack storage of activation records is also possible for nonrecursive procedure calls, stack storage (or some other form of dynamic storage) is absolutely essential for recursion because the depth of recursion and hence the number of activation records required cannot be predicted in advance.

The stack model is appropriate for activation record storage because procedure entry and exit always conforms to a Last-In-First-Out (LIFO) discipline. However, the activation record stack fails in one respect to conform to the usual definition of a stack, which permits access only to the top element. In cases such as inheritance by an internal procedure of a variable from its host, the currently executing procedure makes reference to a local variable in a procedure whose activation record is not at the top of the stack.

Recursive Depth-First Search

The following recursive procedure corresponds to a part of the iterative program presented earlier. Here the central stack performs the role of the programmed stack in the earlier example.

```
   recursive subroutine Depth_First( Here )
   integer, intent (in) :: Here
     integer :: Next
 ! start subroutine Depth_First
     Mark(Here) = .true.                            ! Mark the current node.
     if (Here /= Goal) then
       !.. Find next unmarked adjacent node, if any.
       do Next = 1, Many
         if (Adjacent(Here, Next) .and. .not. Mark(Next)) then
           call Depth_First( Next )                 ! Move to new node.
           if (Found) return
         end if
       end do
     else
       Found = .true.
       return
     end if
     return
   end subroutine Labyrinth
```

Reversing a List

How does a railroad train turn around?

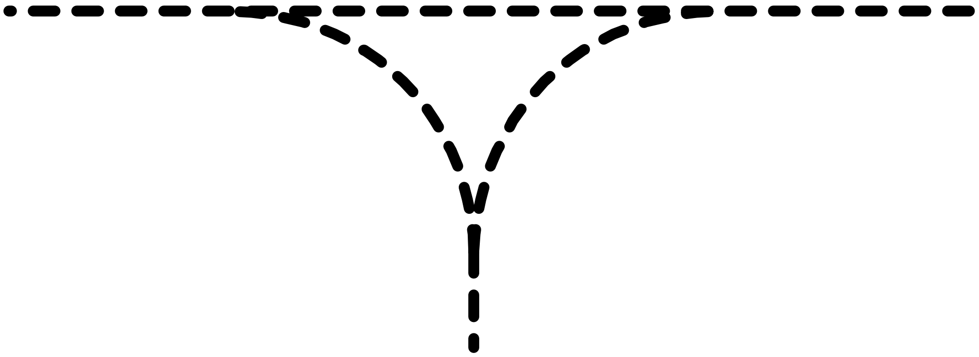


FIGURE 6.3. Using a stack to reverse a list

All of the cars are pushed onto a side track, which plays the role of a stack, and they are then popped onto the main line in the opposite direction, as indicated in Fig. 6.3. Similarly, a stack whose elements are single characters (strings of length one) can be used to reverse the characters of a string:

```
do I = 1, String_Length
  Push ( String(I: I) )
end do
do I = 1, String_Length
  Pop ( String(I: I) )
end do
```

Previous examples have illustrated the use of a recursion to reverse a list. For example, a procedure to print a string in reverse order would appear as follows:

```
call Print_Remainder( Whole_String )
  :
subroutine Print_Remainder( String )
  call Print_Remainder( String(2: ) )
  print *, String(1:1)
  return
end subroutine Remainder
```

A curious affinity can be observed among the concepts of stacks, recursion, and list reversal.

Abstraction, Encapsulation, and Information Hiding

Notice that nothing has been said up to this point about how a program should implement a stack. It is quite possible to understand the concept of a stack, and how it can be applied in a problem such as depth-first search in an unordered graph, without knowing how stack information is stored and manipulated in the computer. Creating an application program requires only *interface* specifications for stack operations such as those just described.

In this sense, the stack concept is an abstraction. A stack has certain *structural* characteristics and must *behave* in certain defined ways, regardless of its actual programming language implementation. The structural part of the stack abstraction is fixed by the requirement that it must be able to hold data items of a certain type — for example, it may be a stack of integers, a stack of character strings of a specific length, or a stack of structures of a particular derived type. The behavioral part is determined by a list of stack operations, with a precise description of the way in which each operation affects (or is affected by) the stack.

Data abstraction — definition of the structure and behavior of an object, independent from its implementaion (as exemplified by the stack concept) — is a technique that has been shown to permit significant improvements in program design and reliability. Data abstraction and two other techniques, *object encapsulation*, and *information hiding*, are important principles in object design methodology.

Object encapsulation combines the structural and behavioral aspects of an object into a self-contained set of program statements. For encapsulation, Fortran provides modules that contain the data type definitions and variable declarations for an abstract object, along with procedures that define each of the required operations.

Information hiding protects the implementation from inadvertent modification by a consumer program. Some of the derived types and variables in the module are accessible to the consumer. The consumer also has access to interface information for the procedures that perform each of the required operations. But derived types or their components, as well as the inner details of module procedures, can be made inaccessible from outside the module. The most important Fortran feature for information hiding is the **`private`** declaration, which may appear in the specification part of a module with a list of names that are not to be imported when a **`use`** statement for the module appears in the main program or in a consumer module. Internal procedures within module subprograms are also automatically inaccessible outside the module.

Consequently, a programming team can be organized so that consumers of an abstract object such as a stack are insulated from the producers. The producers create a module to implement the **`Stack`** abstraction and they make it available (perhaps only in the form of compiled machine instructions) to consumers along with written information concerning the external interface. Consumer programs call upon the module **`Stack`** to create objects and to perform operations on them but cannot modify or even examine **`Stack`** data except through the operations provided.

In a less formal environment, there may be only one programmer who wears two hats, sometimes acting as producer and sometimes as consumer. Nevertheless, a programmer can wear only one hat at a time and, while in the consumer role, must simulate information hiding by pretending to know only the external interface.

Stack as an Object

A **`Stack`** can be implemented in any of several ways; the two most obvious implementations employ an array or a linked list. The necessary type definitions, variable declarations, and procedure definitions are encapsulated in a module that is imported to an application by a **`use`** statement.

The two following program examples present an array implementation module and a linked list implementation module for the same **`Stack`** abstraction, along with a single main program that can use either module. This demonstrates the possibility of constructing a **`Stack`** module so that a consumer without access to the source program cannot tell whether it employs an array or a linked list (except perhaps by some trick that might reveal the limited capacity of the former).

These two examples, and the other stack examples that follow, show the stack operations **`Push`**, **`Pop`**, and **`Peek`** implemented as *functions* of logical type, omitting **`Is_Empty`** and **`Is_Full`**. **`Push`** returns **`.true.`** unless the stack is full (which, in the linked list versions, we assume cannot occur). **`Pop`** and **`Peek`** return **`.true.`** unless the stack is empty; the top item is returned as an **`intent(out)`** argument. **`Push`**, **`Pop`**, and **`Peek`** are not **`pure`** functions because they modify nonlocal data. In the examples distributed electronically, the subset versions implement these operations as subroutines (and include separate **`Is_Empty`** and **`Is_Full`** procedures), because neither subset permits **`intent(out)`** function arguments.

Array Implementation of Stack

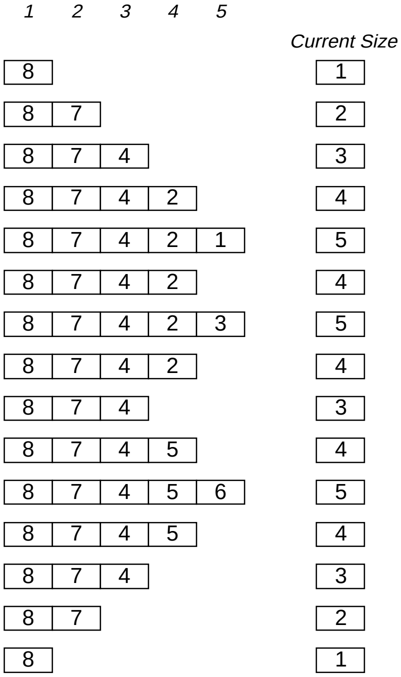
A stack of integers may be implemented as a one-dimensional array, along with an integer scalar that stores the *Current_Size* of the stack. Unlike the saucer analogy, the most convenient array implementation is analogous to a stack of bricks or other physical objects that sit on a fixed base so that the top of the stack moves up (to a larger array subscript value) with each **`Push`** operation and down (to a smaller subscript value) with each **`Pop`**. See Fig. 6.4.

Initially, the stack is empty and *Current_Size* is zero. A **`Push`** operation increases *Current_Size* to 1 and stores the new item at position 1; if this is followed by another **`Push`** operation, *Current_Size* is increased to 2 and the new item is stored at position 2, and so on. A **`Pop`** operation, when the current stack size is *N*, returns the element at position *N* and decreases the *Current_Size* to *N* – 1. Thus the current stack size becomes the subscript value during push and pop operations.

`MAXIMUM_SIZE` of the stack, which is the size of the array, is declared as a named constant. The stack is full if *Current_Size* is equal to **`MAXIMUM_SIZE`**.

```
integer, parameter, private :: MAXIMUM_SIZE = 100
integer, private :: Current_Size = 0
integer, dimension(MAXIMUM_SIZE), private :: Space
```

Here *Space* is the array where the data will be stored. The keyword **`private`** in declarations in a module means that a consumer of the module does not have access to the declared object, except by calling one of the procedures defined in the module.



1	2	3	4	5	Current Size
8					1
8	7				2
8	7	4			3
8	7	4	2		4
8	7	4	2	1	5
8	7	4	2		4
8	7	4	2	3	5
8	7	4	2		4
8	7	4			3
8	7	4	5		4
8	7	4	5	6	5
8	7	4	5		4
8	7	4			3
8	7				2
8					1

FIGURE 6.4. Array implementation of stack for Labyrinth search

Say it with Fortran

Example 16. The operation **Push(Item)** increases *Current_Size* by one and copies the given item to the data array using *Current_Size* as the subscript value, unless the stack is full; **Pop(Item)** copies an element of the data array to *Item*, using *Current_Size* as the subscript value, and then decreases *Current_Size* by one, unless the stack is empty. **Peek(Item)** is the same as **Pop** except that it does not decrease *Current_Size*. The logical function **Is_Empty( )** returns **.true.** if *Current_Size* is zero; **Is_Full( )** returns **.true.** if *Current_Size* is equal to **MAXIMUM_SIZE**.

```
! Example 16. Array implementation of STACK
module D16_M
  implicit none
  public :: Push, Pop, Peek
  integer, parameter, private :: MAXIMUM_SIZE = 100
  integer, save, private :: Current_Size = 0
  integer, dimension(MAXIMUM_SIZE), private :: Space
contains

  function Push( Item ) result( Push_R ) ! not a pure function
    integer, intent(in) :: Item
    logical :: Push_R
! start function Push
    Push_R = Current_Size < MAXIMUM_SIZE
    if (Push_R) then
      Current_Size = Current_Size + 1
      Space(Current_Size) = Item
    end if
    return
  end function Push
  function Pop( Item ) result( Pop_R )                 ! not a pure function
    integer, intent(out) :: Item
    logical :: Pop_R
! start function Pop
    Pop_R = Peek( Item )
    if (Pop_R) then
      Current_Size = Current_Size - 1
    end if
    return
  end function Pop
  function Peek( Item ) result( Peek_R )               ! not a pure function
    integer, intent(out) :: Item
    logical :: Peek_R
! start function Peek
    Peek_R = Current_Size > 0
    if (Peek_R) then
      Item = Space(Current_Size)
    else
      Item = 0
    end if
    return
  end function Peek
end module D16_M
```

```
program D16
  use D16_M
  implicit none
  integer :: op
  integer :: Item
! start program D16
  open (1, file = "intstack.dat", status = "old", action = "read", &
   position = "rewind" )
  do
   print *, " Please enter operation: "
   print *, " 0 to quit; 1 to push; 2 to pop, 3 to peek."
   read (1, *) op
   select case (op)
   case (0)
    print *, " operation 0 means quit."
    do while (Pop (Item) )
     print *, Item, " Left on stack. "
    end do
    exit
   case (1)
    print *, " Please enter an integer to push."
    read (1, *) Item
    if (Push( Item )) then
     print *, " Pushed: ", Item
    else
     print *, " Can't push. Stack is full."
    end if
   case (2)
    if (Pop( Item )) then
     print *, " Popped: ", Item
    else
     print *, " Can't pop. Stack is empty."
    end if
   case (3)
    if (Peek( Item )) then
     print *, " Peeked: ", Item
    else
     print *, " Can't peek. Stack is empty."
    end if
   case default
    print *, op, " is not a valid operation."
   end select
  end do
  stop
 end program D16
```

Linked List Implementation of Stack

The most convenient linked-list implementation of a stack reverts to the pushdown model with the top of the stack at the root of the linked list. Because all insertions and deletions take place at the root, a simple nonrecursive linked list implementation is adequate.

Is_Empty( ) returns **.true.** if *Root_NP* is currently null. In this example, **Is_Full( )** always returns **.false.**; a more robust implementation might employ look-ahead node allocation and return **.true.** when the **stat** variable in the allocate statement indicates an allocation error.

Fig. 6.5 shows the contents of the linked list at each step of a successful search in the labyrinth of Fig. 6.1. Ariadne is in room 8 and the Minotaur is in room 6.

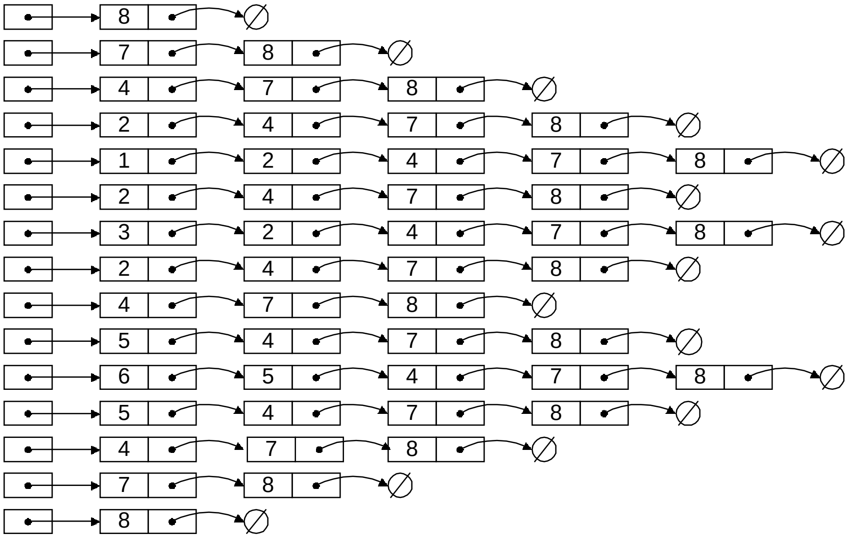


FIGURE 6.5. Linked list implementation of Stack

Say it with Fortran

Example 17. Note that the *same* main program shown for the array implementation can also be used with the following linked list implementation; the only change required is in the module name in the **use** statement at the beginning of the main program. All stack operations in this module have the same interfaces as before, although their internal actions are quite different.

A program that inherits the module cannot refer to module variables with the **private** attribute. As noted earlier, without access to the source program a consumer cannot even tell whether the module employs an array implementation or a linked list implementation, except by some trick that might reveal the limited capacity of the former.

```
! Example 17. Linked List implementation of STACK
module D17_M
  implicit none
  public :: Push, Pop, Peek
  type, private :: Node_Type
    integer :: Info
    type (Node_Type), pointer :: Next_NP
  end type Node_Type
  type (Node_Type), pointer, private :: Root_NP => null( )
contains
```

```
  function Push( Item ) result( Push_R )                ! not a pure function
    integer, intent(in) :: Item
    logical :: Push_R
    type (Node_Type), pointer :: Temp_NP
! start function Push
    Push_R = .true.
    allocate( Temp_NP )
    Temp_NP % Info = Item
    Temp_NP % Next_NP => Root_NP                       ! Copy Root to new node
    Root_NP => Temp_NP
    return
  end function Push
  function Pop( Item ) result( Pop_R )                  ! not a pure function
    integer, intent(out) :: Item
    logical :: Pop_R
    type (Node_Type), pointer :: Temp_NP
! start function Pop
    Pop_R = Peek( Item )
    if (Pop_R) then
      Temp_NP => Root_NP
      Root_NP => Root_NP % Next_NP
      deallocate(Temp_NP)
    end if
    return
  end function Pop
  function Peek( Item ) result( Peek_R )                ! not a pure function
    integer, intent(out) :: Item
    logical :: Peek_R
! start function Peek
    Peek_R = associated( Root_NP )
    if (Peek_R) then
      Item = Root_NP % Info
    else
      Item = 0
    end if
    return
  end function Peek
end module D17_M
```

A Stack of What?

In the foregoing examples, each data item on the stack is an integer. Few changes are needed to implement a stack of some other data type — a stack of strings that each contain 12 characters, for example, or a stack of items of some derived type. The most important change is in the data type declaration for the data component *Info* in the derived type definition for **Node_Type**; a few changes are needed in other places in the module and in the main program.

Generic Stack Module

A *generic* stack module can also constructed, which is capable of manipulating several stacks with different predetermined types. Each stack operation is called by the same name as before, which is now its generic name; separate procedures with different *specific* names are defined for manipulating stacks of each different data type; an interface block for each operation relates the generic name to the specific names for the separate data types. For example, when the application program refers to **`Push`** by its generic name, the data type of the actual argument determines which specific **`Push`** operation will be selected for execution.

Say it with Fortran

Example 18. Some highlights are shown here for a linked list implementation of a generic stack that accommodates three specific data types; the complete module is distributed electronically. A generic stack could, of course, be implemented with an array instead of a linked list. A Fortran language manual or textbook should be consulted for further details about implementing generic procedures in a module.

```
! Linked Stack implementation of GENERIC STACK
  module D18_M
    implicit none
    public :: Push, Pop, Peek
    private :: Push1, Push2, Push3, Pop1, Pop2, Pop3, Peek1, Peek2, Peek3
    type, private :: Node_Type1
      character (len = 12) :: Info
      type (Node_Type1), pointer :: Next_NP
    end type Node_Type1
    type, private :: Node_Type2
      integer :: Info
      type (Node_Type2), pointer :: Next_NP
    end type Node_Type2
    type, public :: Info_Type
      integer :: I
      character (len = 12) :: S
    end type Info_Type
    type, private :: Node_Type3
      type (Info_Type) :: Info
      type (Node_Type3), pointer :: Next_NP
    end type Node_Type3
    interface Push
      module procedure Push1, Push2, Push3
    end interface Push
      :
    type (Node_Type1), pointer, private, save :: Root1 => null( )
    type (Node_Type2), pointer, private, save :: Root2 => null( )
    type (Node_Type3), pointer, private, save :: Root3 => null( )
  contains

    function Push1( Item ) result( Push1_R )             ! not a pure function
      character (len = *), intent(in) :: Item
        :
    end function Push1
  end module D18_M
  program D18
    use D18_M
    implicit none
    character (len = 12) :: Item1
    integer :: Item2
    type (Info_Type) :: Item3
! start program E18
    if (Push( "ABCDEFGHIJKL" )) print *, " Push: ABCDEFGHIJKL"
    if (Push( 11111 )) print *, " Push: 11111"
    if (Push( Info_Type( 11, "Hello world.") )) print *, " Push: 11 Hello world."
      :
```

Here three stacks are defined with different node types, each having a different *Info* component data type. Based on the node type of the actual argument data item in each call to the generic procedures **Push**, **Pop**, or **Peek**, the module *resolves* the generic reference and selects one of the specific procedures.

Push and **Pop** operations with items of different data types can be intermixed; each operation will automatically select the specific stack appropriate to the data type of the actual argument item. A **Pop** operation will return the latest pushed item from the corresponding stack, even though items of other types may have been pushed on the other stacks in the meantime.

Stack Objects

In the foregoing examples a single stack (or in the generic example a single stack for each supported data type) is declared in the module. The main program does not specify a particular stack that is to be operated upon.

For some applications, it may be preferable to permit the application program to create more than one stack and to designate a specific stack at each reference to an operation. Deferring, for the moment, discussion of generic stacks, we now assume a fixed node type with a data component of type **Info_Type**.

The main program for an array implementation could include declarations such as

```
integer, parameter :: MAXIMUM_SIZE1 = 100
integer :: Current_Size1 = 0
integer, dimension(MAXIMUM_SIZE1) :: Space1 = 0
```

while the main program for a linked list implementation would declare a root pointer such as

```
type (Node_Type), pointer :: Root_NP1 => Null( )
```

STOP! Whatever happened to information hiding?

This approach clearly violates the principles of data abstraction. Although stack *operations* are still combined in a module, the *data structure* is no longer encapsulated — it is declared in the main program where it is fully accessible and can be changed in ways that might violate the integrity of the module procedures.

[32] Versions prior to Fortran 95 nullify the root pointer.

Instead, the module should declare a **Stack_Type**, whose inner details will vary according to the implementation. For an array implementation:

```
integer, parameter, private :: M = 100
type, public :: Stack_Type
  private
  integer, private :: Maximum_Size = M, Current_Size = 0
  character (len = 12), pointer, dimension(:) :: Space
end type Stack_Type
```

and for a linked list implementation:

```
type, public :: Stack_Type
  private
  type (Node_Type), pointer :: Root_NP => Null( )
end type Stack_Type
```

For each different stack, a declaration in the application program creates an object of **Stack_Type** according to the derived type definition in the module, whose components are inaccessible because of the **private** specification. This declared object can be passed as an actual argument to any of the stack operations defined in the module. A module procedure **Create_Stack**, with a dummy argument of type **Stack_Type**, allocates the *Space* array for an array implementation but does essentially nothing for a linked list implementation.[32] **Delete_Stack** terminates the lifetime of a particular stack and deallocates any space that was allocated for the stack by **Create_Stack**.

```
! Array implementation
  subroutine Create_Stack( Arg_S )
    type (Stack_Type), intent(in out) :: Arg_S
! start subroutine Create_Stack
    allocate( Arg_S % Space(100))
    Arg_S % Space = " "
    return
  end subroutine Create_Stack

! Linked list implementation
  subroutine Create_Stack( Arg_S )
    type (Stack_Type), intent(in out) :: Arg_S
! start subroutine Create_Stack
    return
  end subroutine Create_Stack

! MAIN PROGRAM
  type (Info_Type) :: Item
  type (Stack_Type) :: Stack
    :
  call Create_Stack( Stack )
  Item = Info_Type( "ABCDEFGHIJKL" )
  if (Push( Stack, Item )) print *, Item
    :
  call Destroy_Stack( Stack )
```

The consumer will need to be aware of the structure of Info_Type so that items to be pushed onto the stack can be generated properly.

Example 19. The main program contains declarations for objects of two different types: a stack object of type **Stack_Type** and a data item of type **Info_Type**. The create and destroy operations are not shown here.

```
! Linked Stack implementation of STACK OBJECT
module D19_M
  implicit none
  public :: Push, Pop, Peek
  type, public :: Info_Type
    character (len = 12) :: S
  end type Info-Type
  type, private :: Node_Type
    type (Info-Type) :: Info
    type (Node_Type), pointer :: Next_NP
  end type Node_Type
  type, public :: Stack_Type
    private
    type (Node_Type), pointer :: Root_NP
  end type Stack_Type
contains

  function Push( Arg_SP, Item ) result( Push_R ) ! not a pure function
    type (Stack_Type), intent(in out) :: Arg_SP
    type (Info_Type), intent(in) :: Item
    logical :: Push_R
    type (Node_Type), pointer :: Temp_NP
! start function Push
    Push_R = .true.
    allocate( Temp_NP )
    Temp_NP % Info = Item
    Temp_NP % Next_NP => Arg_SP % Root_NP                ! Copy Root to new node
    Arg_SP % Root_NP => Temp_NP
    return
  end function Push
  function Pop( Arg_SP, Item ) result( Pop_R )             ! not a pure function
    type (Stack_Type), intent(in out) :: Arg_SP
    type (Info-Type), intent(out) :: Item
    logical :: Pop_R
    type (Node_Type), pointer :: Temp_NP
! start function Pop
    Pop_R = Peek( Arg_SP, Item )
    if (Pop_R) then
      Temp_NP => Arg_SP % Root_NP
      Arg_SP % Root_NP => Arg_SP % Root_NP % Next_NP
      deallocate( Temp_NP )
    end if
    return
  end function Pop
  function Peek( Arg_SP, Item ) result( Peek_R )          ! not a pure function
    type (Stack_Type), intent(in) :: Arg_SP
    logical :: Peek_R
    type (Info-Type), intent(out) :: Item
! start function Peek
    Peek_R = associated( Arg_SP % Root_NP )
    if (Peek_R) then
      Item = Arg_SP % Root_NP % Info
    else
      Item = Info_Type( "" )
    end if
    return
  end function Peek
end module D19_M
```

Extension to a generic module for stack objects requires a separate stack type for each stack data item type, along with a separate set of specific stack procedures for each stack type (as before). The consumer declares objects of various specific stack types as required and calls stack operation procedures by their generic names such as **Create_Stack**, **Push**, and **Pop**.

6.2 QUEUES

Queue is a French word meaning tail. The word in English is applied to waiting lines, which are supposed to resemble a tail. A familiar queue is the checkout line in a supermarket where customers with their shopping carts wait to pay for their groceries.

A queue is a list that operates according to a first-in, first-out (FIFO) discipline. Items (such as customers) enter the queue at one end and exit at the other end — in contrast to a LIFO stack where items enter and exit at the same end. The queue operations **Enqueue** (for entering the queue) and **Dequeue** (for leaving the queue) correspond to the stack operations **Push** and **Pop**. As in a waiting line, items leave (**Dequeue**) at the *front* of a queue and they enter (**Enqueue**) at the *rear*.

Six queue operations are considered here, corresponding to the seven stack operations with the omission of **Peek**.

- **Create_Queue( )** allocates space for the queue and marks it as empty.
- **Delete_Queue( )** removes any remaining items from the queue and releases the space that was allocated for it.
- **Enqueue(Item)** appends **Item** to the contents of the queue.
- **Dequeue(Item)** removes the *least recently appended* integer from the queue and returns it as the value of **Item**.
- **Is_Empty( )** returns **.true.** if the queue is currently empty.
- **Is_Full( )** returns **.true.** if the queue is currently full — that is, if the implementation does not permit any further items to be appended to the queue.

Dequeue operations are not permitted when a queue is empty and **Enqueue** operations are not permitted when it is full, but the inverse operations are quite legal. In particular, the queue may become empty at one or more points during execution of an application, after which **Enqueue** operations may again produce a nonempty queue.

Queue Objects

A queue can be implemented with an array or with a linked list. In either case, the necessary type definitions, variable declarations, and procedure definitions are encapsulated in a module that is imported to an application by a **use** statement. Queues in the following examples hold character strings of length 12; queues for data of other intrinsic or derived types, as well as generic queues and allocated queues, are of course also possible.

The following program examples present both an array implementation and a linked list implementation for the same queue abstraction. Thus they show that it is possible to construct a queue module so that a consumer without access to the source program cannot tell (except by trickery) whether it employs a linked list or an array.

Linked List Implementation of Queue

A queue may be implemented as a linked list, with one end of the queue at the root and the other end at the tail. Which end of the queue should be at the root of the linked list?

An operation for repeatedly deleting the tail node from a linked list would be difficult to implement (without some enhancement such as the bidirectional pointers of a *doubly-linked* list; see Sec. 5.4), for the following reason: To avoid searching through the entire list at each deletion, an extra pointer to the tail node is required. Deleting the current tail node from a linked list moves the tail pointer to the predecessor node, but there is no straightforward way to find the predecessor of the current target of a node pointer in a singly-linked list. Therefore, the *tail* of the linked list should correspond to the *rear* of the queue where insertions (**Enqueue** operations) occur; it follows that the *root* of the linked list should correspond to the *front* of the queue where deletions (**Dequeue** operations) occur.

A bit of complication is still required for the **Enqueue** operation — that is, for inserting a new node at the tail of a linked list and updating the queue rear pointer. In the obvious implementation, the target of the queue rear pointer should always be the current tail node in the linked list, but there is no such node when the linked list is empty.

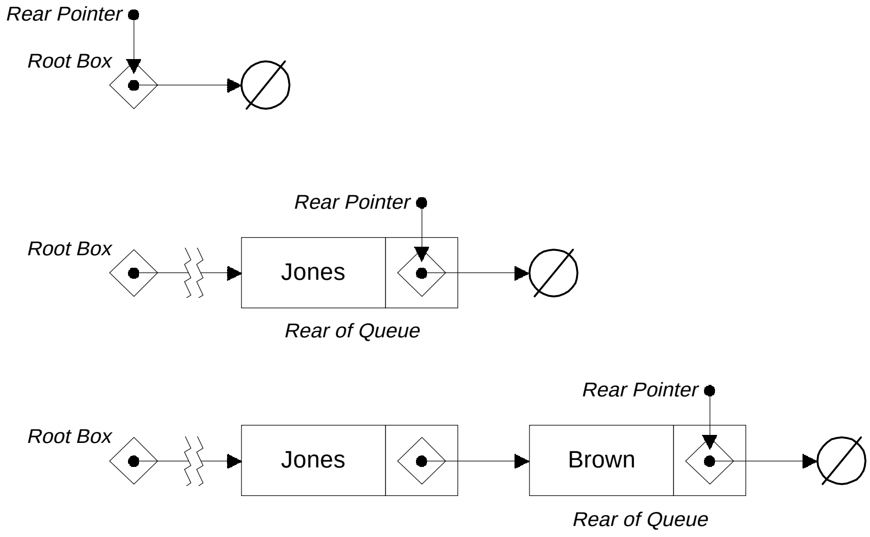


FIGURE 6.6. Pointer to Pointer implementation of Enqueue

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Example 20. The implementation given here employs the Pointer to Pointer strategy mentioned earlier: each node pointer (that is, the *Root* pointer as well as the *Next_NP* component in each node) is replaced by a *pointer to* this node pointer, implemented in Fortran as a pointer to a **BOX** structure whose only component is the node pointer. In this implementation the queue rear is a **BOX** pointer whose target is either the **BOX** component of the tail node in the linked list or (if the linked list is empty) the root **BOX**, as shown in Fig. 6.6.

A **Dequeue** operation deletes the current root node, which is the target of **Root % Next_NP**. This is the usual **Delete_Node** linked list operation except when there is only one item in the queue; in that case, deleting the root node also deletes the tail node so the **Dequeue** operation must modify the queue rear pointer *Tail_BP* as well as *Root*.

Create_Queue nullifies the node pointer component of *Root* and makes *Root* the target of *Tail_BP*.

```
! Example 20. Linked List (Pointer to Pointer) implementation of QUEUE OBJECT
module D20_M
  implicit none
  public :: Create_Queue, Destroy_Queue, Enqueue, Dequeue, &
    Is_Empty, Is_Full

  type, private :: BOX_Type
    type (Node_Type), pointer :: Next_NP => Null( )
  end type BOX_Type

  type, private :: Node_Type
    character (len = 12) :: Info
    type (BOX_Type) :: BOX
  end type Node_Type

  type, public :: Queue_Type
    private
  type (BOX_Type) :: Root
  type (BOX_Type), pointer :: Tail_BP => null( )
  end type Queue_Type

contains

  subroutine Create_Queue( Arg_Q )
    type (Queue_Type), target, intent(in out) :: Arg_Q
! start subroutine Create_Queue
    Arg_Q % Tail_BP => Arg_Q % Root
    return
  end subroutine Create_Queue

  subroutine Destroy_Queue( Arg_Q )
    type (Queue_Type), intent(in out) :: Arg_Q
    character (len = 12) :: Info
! start subroutine Destroy_Queue
    do while (.not. Is_Empty( Arg_Q ))
      call Dequeue( Arg_Q, Info )
      print *, " Left on Queue: ", Info
    end do
    return
  end subroutine Destroy_Queue
  subroutine Enqueue( Arg_Q, Item )
    type (Queue_Type), intent(in out) :: Arg_Q
    character (len = 12), intent(in) :: Item
    type (Node_Type), pointer :: Temp_NP
! start subroutine Enqueue
    allocate( Temp_NP )
    Temp_NP % Info = Item
    Arg_Q % Tail_BP % Next_NP => Temp_NP         ! Link new node into list.
    Arg_Q % Tail_BP => Temp_NP % BOX           ! New node becomes new tail.
  ! nullify( Temp_NP )
    return
  end subroutine Enqueue

  subroutine Dequeue( Arg_Q, Item )
    type (Queue_Type), target, intent(in out) :: Arg_Q
    character (len = *), intent(out) :: Item
    type (Node_Type), pointer :: Temp_NP
! start subroutine Dequeue
    if (Is_Empty( Arg_Q )) then
      print *, " Attempt to pop from empty stack. "
      Item = " "
    else
      Temp_NP => Arg_Q % Root % Next_NP
      Item = Temp_NP % Info
      Arg_Q % Root = Temp_NP % BOX
      deallocate( Temp_NP )
      if (Is_Empty( Arg_Q )) Arg_Q % Tail_BP => Arg_Q % Root
    end if
    return
  end subroutine Dequeue

  pure function Is_Empty( Arg_Q ) result( X )
    type (Queue_Type), intent(in out) :: Arg_Q
    logical :: X
! start function Is_Empty
    X = (.not. associated (Arg_Q % Root % Next_NP))
    return
  end function Is_Empty

  pure function Is_Full( Arg_Q ) result( X )
    type (Queue_Type), intent(in out) :: Arg_Q
    logical :: X
! start function Is_Full
    X = .false.
    return
  end function Is_Full

end module D20_M
```

```
  program D20
    use D20_M
    implicit none
    integer :: Op
    character (len = 12) :: Item = " "
    type(Queue_Type) :: Queue
! start program D20
```

```
    call Create_Queue ( Queue )
    do
      print *, " Please enter Operation: "
      print *, " 0 to quit; 1 to enqueue; 2 to dequeue."
      read *, Op
      select case (Op)
      case (0)
        print *, " Operation 0 means quit."
        exit
      case (1)
        if (Is_Full( Queue )) then
          print *, " Can't enqueue. Queue is full. "
        else
          print *, " Please enter an item to enqueue."
          read *, Item
          call Enqueue( Queue, Item )
          print *, " Enqueued: ", Item
        end if
      case (2)
        if (Is_Empty( Queue )) then
          print *, " Can't dequeue. Queue is empty. "
        else
          call Dequeue( Queue, Item )
          print *, " Dequeued: ", Item
        end if
      case default
        print *, Op, " is not a valid operation."
      end select
    end do
    call Destroy_Queue( Queue )
    stop
  end program D20
```

Array Implementation of Queue

An important queue application in computer systems is input and output buffering, motivated by the slow execution speed of external data transmission. When an input file is opened, data is transmitted from the file and is enqueued in an *input buffer*, to be dequeued during execution of a read statement. Write statements enqueue data in an *output buffer*, from which it is written to the file as a separate operation while program execution proceeds. For maximum efficiency, these buffers are traditionally implemented as one-dimensional arrays.

Although the customers in a supermarket queue move toward the front of the queue each time a **Dequeue** operation occurs, queues implemented as arrays avoid the inefficiency that such moves would entail. Each data item remains in a fixed position during queue operations, while front and rear queue position marker values change. The rear position is incremented when an item is enqueued; the front position is incremented when an item is dequeued.

In a typical queue, only a few items are stored at one time, while the total number of items that pass through the queue during an interval is many times larger. Someone long ago discovered how to maintain a queue with an array just big enough to hold the maximum number of *concurrently* stored items. It is not necessary to allocate separate space for all the items that pass through the queue — array space is not needed for items that have not yet been enqueued or for those that have already been dequeued.

Queues used for input or output are traditionally described as *circular buffers*, because their array subscripts are kept within bounds by applying a circular transformation — that is, by reducing the subscript *modulo* the declared maximum array size — although the front and rear queue positions grow indefinitely. Declaring the array with bounds **`(0: Maximum_Size – 1)`** simplifies this calculation slightly. The relation **`Rear == modulo( Front + Current_Size, Maximum_Size )`** is always true. The *Current_Size* of the queue is initially 0 and the *Front* and the *Rear* are both initially at position 0.

An **`Enqueue`** operation stores a new item at *Rear*, increments *Rear* with the circular transformation, and increments *Current_Size*. As an example (obviously unrealistically small for an actual application), if *Maximum_Size* is 6 the first six items will be enqueued at positions 0, 1, 2, 3, 4, and 5, respectively; the seventh item reverts to position 0. Similarly, a **`Dequeue`** operation retrieves an item from *Front*, increments *Front* with the circular transformation, and decrements *Current_Size*.

Fig. 6.7 illustrates the following sequence of operations: enqueue a; enqueue b; enqueue c; enqueue d; dequeue a; enqueue e; enqueue f; dequeue b; dequeue c; enqueue g; enqueue h; dequeue d; dequeue e; dequeue f; dequeue g; dequeue h.

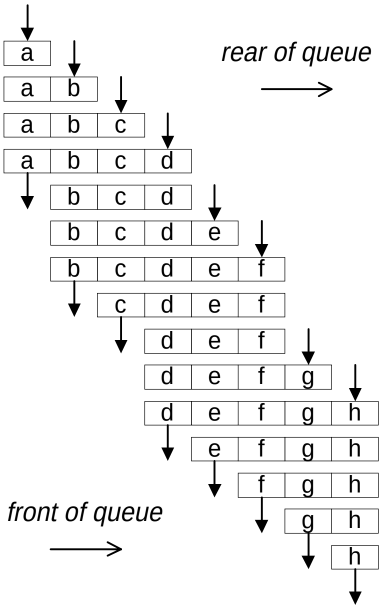

FIGURE 6.7. Array implementation of Queue

In the following table, these operations are mapped circularly into an array of size 6 with declared bounds **`(0: 5)`**. The values of *Front*, *Rear*, and *Current_Size* *after* each operation are shown.

	Rear (mod 6)	Front (mod 6)	Current Size	Contents
(Start)	0	0	0	_ _ _ _ _ _
Enqueue a	1	0	1	a _ _ _ _ _
Enqueue b	2	0	2	a b _ _ _ _
Enqueue c	3	0	3	a b c _ _ _
Enqueue d	4	0	4	a b c d _ _
Dequeue a	4	1	3	_ b c d _ _
Enqueue e	5	1	4	_ b c d e _
Enqueue f	0	1	5	_ b c d e f
Dequeue b	0	2	4	_ _ c d e f
Dequeue c	0	3	3	_ _ _ d e f
Enqueue g	1	3	4	g _ _ d e f
Enqueue h	2	3	5	g h _ d e f
Dequeue d	2	4	4	g h _ _ e f
Dequeue e	2	5	3	g h _ _ _ f
Dequeue f	2	0	2	g h _ _ _ _
Dequeue g	2	1	1	_ h _ _ _ _
Dequeue h	2	2	0	_ _ _ _ _ _

Say it with Fortran

Example 21. The following Fortran program saves the actual *Current_Size* and the *Front* position value, and applies the circular transformation each time *Front* is incremented. This program does not store the *Rear* position but computes it in the **Enqueue** procedure from *Front* and *Current_Size*.

```
! Example 21. Array implementation of QUEUE OBJECT
module D21_M
  implicit none
  public :: Create_Queue, Destroy_Queue, Enqueue, Dequeue, &
    Is_Empty, Is_Full
  integer, parameter, private :: M = 6
  type, public :: Queue_Type
    private
  integer :: Maximum_Size = M, Current_Size = 0, Front = 0
  character (len = 12), pointer, dimension(:) :: Space_P
  end type :: Queue_Type
contains

  subroutine Create_Queue( Arg_Q )
    type (Queue_Type), intent(in out) :: Arg_Q
! start subroutine Create_Queue
    allocate( Arg_Q % Space_P(0: M - 1) )
    Arg_Q % Space_P = " "
    return
  end subroutine Create_Queue

  subroutine Destroy_Queue( Arg_Q )
    type (Queue_Type), intent(in out) :: Arg_Q
    character (len = *) :: Info
! start subroutine Destroy_Queue
    do while (.not. Is_Empty( Arg_Q ))
      call Dequeue( Arg_Q, Info )
      print *, " Left on Queue: ", Info
    end do
    deallocate( Arg_Q % Space_P )
    return
  end subroutine Destroy_Queue

  subroutine Enqueue( Arg_Q, Item )
    type (Queue_Type), intent(in out) :: Arg_Q
    character (len = *), intent(in) :: Item
! start subroutine Enqueue
    if (Is_Full( Arg_Q )) then
      print *, " Attempt to enqueue when queue is full. "
    else
      Arg_Q % Space_P(modulo( Arg_Q % Front + Arg_Q % Current_Size, &
        Arg_Q % Maximum_Size )) = Item
      Arg_Q % Current_Size = Arg_Q % Current_Size + 1
    end if
    return
  end subroutine Enqueue
  subroutine Dequeue( Arg_Q, Item )
    type (Queue_Type), intent(in out) :: Arg_Q
    character (len = *), intent(out) :: Item
! start subroutine Dequeue
    if (Is_Empty( Arg_Q )) then
      print *, " Attempt to dequeue when queue is empty. "
      Item = " "
    else
      Item = Arg_Q % Space_P(Arg_Q % Front)
      Arg_Q % Front = modulo (Arg_Q % Front + 1, Arg_Q % Maximum_Size)
      Arg_Q % Current_Size = Arg_Q % Current_Size - 1
    end if
    return
  end subroutine Dequeue

  pure function Is_Empty( Arg_Q ) result( X )
    type (Queue_Type), intent(in out) :: Arg_Q
    logical :: X
! start function Is_Empty
    X = (Arg_Q % Current_Size <= 0)
    return
  end function Is_Empty

  pure function Is_Full( Arg_Q ) result( X )
    type (Queue_Type), intent(in out) :: Arg_Q
    logical :: X
! start function Is_Full
    X = (Arg_Q % Current_Size >= Arg_Q % Maximum_Size)
    return
  end function Is_Full

end module D21_M
```

Special Considerations for High Efficiency

For maximum efficiency, traditional input and output buffer queues avoid the *modulo* function which, according to mathematics, requires a divide operation. Instead, a simple circular transformation is combined with each increment step; for example:

```
  Rear = Rear + 1
  if (Rear == MAXIMUM_SIZE) Rear = 0
```

Only the *Front* and *Rear* positions are actually needed for **Enqueue** and **Dequeue** operations; however, the two positions are equal both when the queue is full and when it is empty. Some common highly optimized implementations still manage to avoid calculating *Current_Size* at each operation, by making the maximum queue size smaller by one than the array size. A **Dequeue** request is refused if *Front* and *Rear* are equal; an **Enqueue** request is refused if the circularly transformed *Rear* + 1 is equal to *Front*. (The circular transformation is based on array size and not on maximum queue size.)

Chapter 7 Trees

A *tree* may be defined recursively as a node with zero or more descendants, each of which is a tree. A tree with no descendants is a *leaf*. A node has at most one *ancestor*; a node that has no ancestor is a *root*. A tree has exactly one root. A tree has the further property that there is exactly one *path* from the root to each node. Because of the natural representation of a tree as a recursive structure, tree operations are most easily implemented with recursive procedures.

We have noted that arrays are relatively inflexible: the size cannot be changed after data is stored, and inserting a new element in the middle requires moving all elements to the right of the insertion point. Trees, like linked lists, do not have these disadvantages, since they are constructed with pointers whose target nodes can be allocated dynamically. A tree can provide logarithmic access time to an arbitrary node, as compared to the linear time requirement for a linked list.

The operation of deleting a particular node from a tree is often rather complicated, however. Some suggestions are given below. Weiss suggests, "... If the number of deletions is expected to be small, then a popular strategy is lazy deletion. . ."[33] This means that the node is not actually deleted, but is left in the tree and marked as "inactive"; the tree is then occasionally reconstructed, deleting all inactive nodes at once.

7.1 BINARY SEARCH TREES

A *binary tree* is one in which each node has at most two descendants, called the *left subtree* and the *right subtree*. Either subtree, or both, may be absent. A *binary search tree* is a binary tree with a form that makes it especially suitable for storing and retrieving data. (It is a binary tree and it is a search tree; the name is unrelated to binary search.) Each node of a binary search tree has a *search key*, and presumably also some data or a pointer to data, at each node. For simplicity, it will be assumed unless stated otherwise that the keys at all nodes in the tree are distinct.

A binary search tree also has an order property at each node: the key at a given node is greater than any key in the left subtree and is smaller than any key in the right subtree.

A typical binary search tree implementation has a declared pointer whose target is the root node; initially this pointer is null. As each data item is read, a node is allocated, with null pointers to the left and right subtrees, and the key (and other information) in the new node is generated from data just read.

The first node (the root node) becomes the target of the root pointer. More generally, a search begins by comparing the new key with the key at the root; the search continues with the left subtree if the new key is smaller, or with the right subtree if the new key is larger. The search terminates when the indicated subtree is absent; i.e., the pointer to it is null. The newly allocated node is then inserted as the new target of the null pointer. It is important to note that an unsuccessful search always terminates at a leaf — i.e, at a null pointer.

[33] *Data Structures and Algorithm Analysis*, 104

```
subroutine Look_Up( Search_Key )
    :
  call R_Look_Up( Root_NP, Search_Key )
    :
contains
  recursive subroutine R_Look_Up( Arg_NP )
      :
    if (associated( Arg_NP )) then
      if (Search_Key < Arg_NP % Key) then
        R_Look_Up( Arg_NP % Left, Search_Key)
      else  if (Search_Key > Arg_NP % Key) then
        R_Look_Up( Arg_NP % Right, Search_Key)
    else
      call Insert_Target( Arg_NP )
    end if
      :
```

Note that the tree search is implemented recursively. Recursion is natural for tree structures, and it is not inordinately wasteful because the depth of recursion depends only upon the distance of the current node from the root, which is expected to be much smaller than the total number of nodes in the tree (but see Section 7.2).

The tree print operation is also implemented recursively. When the following subroutine is called with the root pointer as its actual argument, the left subtree will be printed, then the current node, and finally the right subtree. Thus the entire tree will be printed in key order:

```
  recursive subroutine R_Print_Tree( Arg_NP )
  type(Node_Type), pointer :: Arg_NP
! start subroutine R_Print_Tree
  if (associated( Arg_NP )) then
    call R_Print_Tree( Arg_NP % Left_NP )
    print *, Arg_NP % Info % Data, Arg_NP % Info % Key
    call R_Print_Tree( Arg_NP % Right_NP )
  end if
  return
  end subroutine R_Print_Tree
```

A search without insertion is possible, of course. One application is to locate the largest or smallest key in a tree by searching with an “infinitely large” or “infinitely small” search key. A search for the largest key, for example, aways goes to the right until a node with a null right pointer is encountered; the key at this node is the maximum.

Deleting a node is not difficult unless the both subtrees are present. If both are absent, the node is deleted by deallocating a pointer in the predecessor node. If one subtree is present, the pointer in the predecessor node is changed so that its target is the subtree.

Weiss describes the more difficult process of deleting a node with two subtrees:[34] The strategy is to replace the key of this node with the smallest key in its right subtree, which is easily found by the method just described, and recursively delete that node. (Remember that in any tree the node with the smallest key has an empty right subtree.)

Say it with Fortran

Example 22. The following module implements **`Look_Up`** and **`Print_Tree`** operations for a binary search tree.

[34] *Data Structures and Algorithm Analysis,* 103

```
! Example 22. Binary Search Tree
module D22_M
  implicit none
  public :: Look_Up, Print_Tree
  integer, parameter, private :: KEY_LEN = 16
  type, public :: Info_Type
    character(len = KEY_LEN) :: Key
    integer, dimension(2) :: Data = (/ 0, 0 /)
  end type Info_Type
  type, private :: Node_Type
    type(Info_Type) :: Info
    type (Node_Type), pointer :: Left_NP
    type (Node_Type), pointer :: Right_NP
  end type Node_Type
  type (Node_Type), pointer, private :: Root_NP = null( )
contains

  subroutine Look_Up( Item )
! start subroutine Look_Up
    call R_Look_Up( Root_NP )
    return
  contains
    recursive subroutine R_Look_Up( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine R_Look_Up
      if (associated( Arg_NP )) then
        if (Item % Key < Arg_NP % Info % Key) then
          call R_Look_Up Arg_NP % Left_NP )           ! Search the left subtree
        else if (Item % Key > Arg_NP % Info % Key) then
          call R_Look_Up( Arg_NP % Right_NP )        ! Search the right subtree
        else
```

Modify the target node if a matching key is found.

```
          call Modify_Target( Arg_NP )
        end if
      else
        call Insert_Target( Arg_NP, Item )
      end if
      return
    end subroutine R_Look_Up

    subroutine Insert_Target( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine Insert_Target
```

Insertion always occurs at a leaf, so there is no need to move pointers as with a linked list.

```
      allocate( Arg_NP )
      Arg_NP % Info = Item
      return
    end subroutine Insert_Target
    subroutine Modify_Target( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine Modify_Target
      Arg_NP % Info % Data(2) = Arg_NP % Info % Data(2) + 1
      return
    end subroutine Modify_Target

  end subroutine Look_Up

  subroutine Print_Tree( )
! start subroutine Print_Tree
    call R_Print_Tree( Root_NP )
    return
  end subroutine Print_Tree

  recursive subroutine R_Print_Tree( Arg_NP )
  type(Node_Type), pointer :: Arg_NP
  character (len = 20) :: Line
! start subroutine R_Print_Tree
  if (associated( Arg_NP )) then
    call R_Print_Tree( Arg_NP % Left_NP )
    print *, Arg_NP % Info
    call R_Print_Tree( Arg_NP % Right_NP )
  end if
  return
  end subroutine R_Print_Tree

end module D22_M
```

```
  program D22
    use D22_M
    implicit none
    type (Info_Type) :: Item
    integer :: EoF
! start program D22

    Item % Data(2) = 1
    Item % Data(1) = 0
    open (1, file = "dxf.txt", status = "old", action = "read", &
      position = "rewind")
    do
      Item % Data(1) = Item % Data(1) + 1
      read (1, *, iostat = EoF) Item % Key
      if (EoF < 0) exit
      call Look_Up( Item )
    end do
    call Print_Tree( )
    stop
  end program D22
```

The Balance Problem

The *depth* of a node in a tree is its distance from the root node — i.e., the number of steps required to move from the root to the given node along a search path. The *height* of a tree (or subtree) is the maximum depth of any of its nodes.

For a binary search tree created at random, there should be about two nodes with depth one, four with depth two, etc.; the expected search time for an arbitrary key is O(lg *N*). However, most trees encountered in actual applications are far from random. As an extreme case, suppose that a binary search tree is created from data already in (increasing) order. Each data item will be inserted into the right subtree of the previously created node; all left subtrees will be empty. In this case, the binary search tree becomes a linked list with extra unused left pointers. In practice, most data sets posses some structure, which almost always causes the corresponding binary search tree to be somewhat *unbalanced* — i.e., to have some nodes whose left and right subtrees differ considerably in height.

We next consider two different ways to keep a tree from becoming badly unbalanced. Section 7.4 describes a different approach based on an augmented linked list instead of a tree.

7.2 AVL TREES

An AVL tree is a binary search tree that is continually adjusted to keep it almost balanced.[35] The heights of the left and right subtrees *at each node* are not permitted to differ by more than one. Each node now contains an integer that records the height of the (sub)tree for which that node is the root. Whenever a node is inserted, a test is made to determine whether the tree is still almost balanced.

We begin by creating a simple tool to avoid repeated testing for empty subtrees: a separate function that returns the height of the subtree for which the argument node is the root. This function returns –1 for a null argument node.

```
  pure function Height( Arg_NP ) result ( Height_R )
    type (Node_Type), pointer :: Arg_NP
    integer :: Height_R
! start function Height
    if (associated( Arg_NP )) then
      Height_R = Arg_NP % Node_Height
    else
      Height_R = -1
    end if
    return
  end function Height
```

Rotating a Subtree

A recursive call to **`R_Look_Up`** will have resulted in an insertion at some lower level of the tree (except in case of a match), and may have caused the tree to become unbalanced.

Assuming that the tree was almost balanced before the latest insertion, either it is still almost balanced (i.e., the maximum height difference is still 0 or 1) or the height difference just above the insertion point has increased from 1 to 2.

[35] G.M. Adelson-Velskii and E.M. Landis, “An Algorithm for the Organization of Information,” *Soviet Math. Doklady* 3 (1962), 1259-1263. An extensive discussion with detailed examples may be found in Weiss, *Data Structures and Algorithms*, 107–119. The description here follows Weiss.

In the following diagram (Fig. 7.1), triangles represent subtrees. The short triangles all represent trees of equal height, and the tall triangle represents a tree whose height is greater by 1. Suppose that a new node has just been inserted into one of the subtrees of node E, creating a height difference of 2 at S.

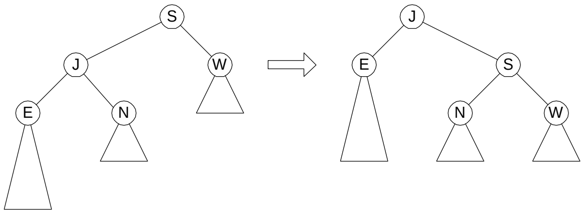

FIGURE 7.1. Left rotation at S to correct unbalanced AVL tree

A “left rotation” is applied to correct this imbalance, as follows:

- Node J is copied to a temporary node.
- The right subtree of J replaces J as the left subtree of the unbalanced node S.
- Node S is moved to the right subtree of J in the temporary node.
- Finally, the temporary node replaces S.

```
Temp_NP => Arg_NP % Left_NP
Arg_NP % Left_NP => Temp_NP % Right_NP
Temp_NP % Right_NP => Arg_NP
Arg_NP => Temp_NP
```

A left rotation corrects imbalance caused by insertion into the right subtree of the right subtree. An entirely analogous right rotation corrects imbalance caused by insertion into the left subtree of the left subtree. A slightly more complicated case occurs when the fault occurs at the right subtree of the left subtree, or vice versa.

When a node, such as S in Figure 7.2, is found to be unbalanced to the left, a test made to determine whether or not current item was inserted in the left or right subtree of the left subtree. In the mixed case, shown here, a right rotation is applied to the left subtree at J, followed by a left rotation at S. The same operations are performed in the two cases shown, where the insertion has occurred either at L or at P.

The balance condition is checked immediately after return from the recursive call at each level up to the root. However, no further unbalance can occur above the level at which balance has been restored.

```
call R_Look_Up( Arg_NP % Left_NP )
if (Height( Arg_NP % Left_NP ) == Height( Arg_NP % Right_NP ) + 2) then
  if (Item % Key > Arg_NP % Left_NP % Info % Key) &
    call Rotate_Right( Arg_NP % Left_NP )
  call Rotate_Left( Arg_NP )
end if
  :
```

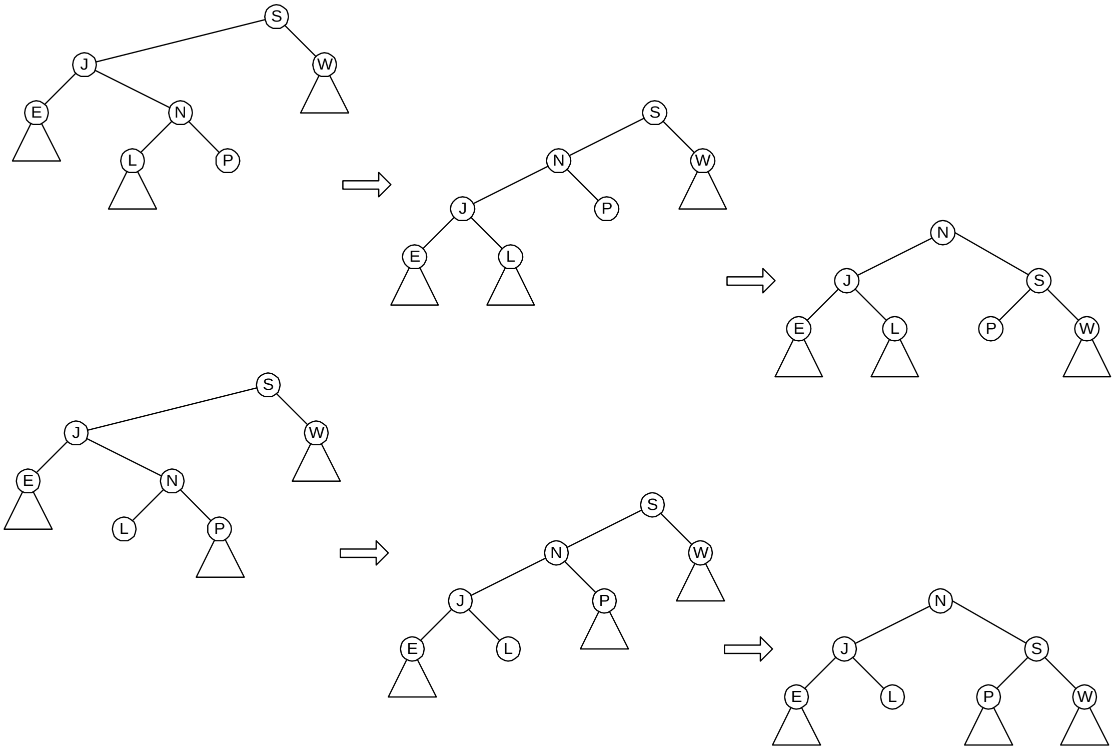

FIGURE 7.2. Right rotation at subtree J followed by left rotation at S (two cases)

Say it with Fortran

Example 23

```
! Example 23. AVL (Adelson-Velskii & Landis) Tree
module D23_M
  implicit none
  public :: Print_Tree, Look_Up, Initialize
  type, public :: Info_Type
    character(len = 15) :: Key = " "
    integer, dimension(2) :: Data = (/ 0, 1 /)
  end type Info_Type
  type, private :: Node_Type
    type(Info_Type) :: Info
    type (Node_Type), pointer :: Left_NP = null( ), Right_NP = null( )
    integer :: Node_Height = 0
  end type Node_Type
  type (Node_Type), pointer, private :: Root_NP = null( )
contains

  subroutine Look_Up( Item )
    type (Info_Type), intent(in) :: Item
! start subroutine Look_Up
    call R_Look_Up( Root_NP )
    return
  contains
```

```
    recursive subroutine R_Look_Up( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
  ! start subroutine R_Look_Up
      if (associated( Arg_NP )) then
        if (Item % Key < Arg_NP % Info % Key) then
          call R_Look_Up( Arg_NP % Left_NP )
```

Check whether the tree is still in balance.

```
          if (Height( Arg_NP % Left_NP ) &
                == Height( Arg_NP % Right_NP ) + 2) then
            if (Item % Key > Arg_NP % Left_NP % Info % Key) &
              call Rotate_Right( Arg_NP % Left_NP )
            call Rotate_Left( Arg_NP )
          else
            Arg_NP % Node_Height = 1 + max( Height( Arg_NP % Left_NP ), &
              Height( Arg_NP % Right_NP ) )
          end if
        else if (Item % Key > Arg_NP % Info % Key) then
```

Same as the previous case, except that **Right** *and* **Left** *are interchanged.*

```
          :
        else                           ! Item % Key == Arg_NP % Info % Key
          call Modify_Target( Arg_NP )
        end if
      else
        call Insert_Target( Arg_NP )
      end if
      return
  contains

    subroutine Rotate_Left( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
      type (Node_Type), pointer :: Temp_NP
  ! start subroutine Rotate_Left
      Temp_NP => Arg_NP % Left_NP
      Arg_NP % Left_NP => Temp_NP % Right_NP
      Temp_NP % Right_NP => Arg_NP
      Arg_NP % Node_Height = 1 + &
        max( Height( Arg_NP % Left_NP ), Height( Arg_NP % Right_NP ) )
      Temp_NP % Node_Height = 1 + &
        max( Height( Temp_NP % Left_NP ), Arg_NP % Node_Height )
      Arg_NP => Temp_NP
      return
    end subroutine Rotate_Left

    subroutine Rotate_Right( Arg_NP )
      :
    end subroutine Rotate_Right

    pure function Height( Arg_NP ) result ( Height_R )
      :
    end function Height
```

Subroutines **Modify_Target**, **Insert_Target**, *and* **Print_Tree** *go here*

```
  end subroutine Look_Up

end module D23_M
```

7.3 B-TREES

A B-tree is a more general search tree that is not necessarily binary. Each node has room for *M* pointers and *M* – 1 keys, where *M* is an integer called the *order* of the B-tree. A B-tree of order 2 is a (rather inefficient) binary search tree; however, the most important application is for maintaining a large data bases on an external device. The search requires only about $\log_M N$ external access operations, so for this application large values of *M* (typically, 256) are common.

Each node in the B-tree is a data structure that includes an integer, an array of structures to hold the keys and other data, and an array of pointers to nodes at the next lower level. (Since Fortran does not permit arrays of pointers, this component of the node is implemented as an array structures of type **BOX**, each holding a pointer.

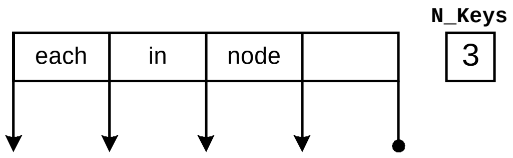

Figure 7.3. In a B-tree of order 5, each node has room for 5 pointers and 4 keys

The integer *N_Keys* gives the number of elements of the array that are currently occupied by data. Fig. 7.3 shows a node of a B-tree of order 5, with three keys currently active.

A search begins by examining all of the keys at the root node. A binary search, in the ordered array of data keys at the current node, locates two adjacent keys between which the search key value lies (unless a match occurs, in which case the search terminates immediately and the data item is modified as required). There is a downward pointer corresponding to each possible binary search result, including 0 (for the case in which the search key is less than the smallest data key) and *N_Keys* (for the case in which the search key is larger than the largest data key). The search continues recursively with the indicated downward pointer unless this pointer is null, in which case a new data item is inserted into the current node.

```
call Binary_Search( Arg_NP % Info(1: Arg_NP % N_Keys) % Key, &
  Carrier % Info % Key, Loc )
if (Loc(2) == Loc(1)) then          ! Search key matches a key at current node
  call Modify_Target( Arg_NP, Loc(1) )
else if (associated( Arg_NP % BOX(Loc(1)) % Next_NP )) then
  call R_Look_Up( Arg_NP % BOX(Loc(1)) % Next_NP )          ! Recursive call
else
  call Insert_Target( Arg_NP, Loc(1) )
end if
```

A complication occurs if insertion is required at a node with no room to store another data item. If this *overflow* occurs, the node is split into two nodes; one of these replaces the current node and the other (here called *Carrier*) is propagated upward for insertion at the next higher level of the B-tree. This may cause the next higher level to overflow as well; if overflow propagates all the way to the root, the root itself is split — this is the only operation that increases the height of the tree.

The insertion procedure is thus rather intricate. The present implementation simplifies it a bit by by providing extra space in each node, so that insertion can be accomplished before the test for oveflow: each node has room for *M* keys instead of *M* – 1, and for *M* + 1 pointers instead of *M*. It would be possible to avoid this extra space by testing for overflow before insertion, copying a full node to a slightly larger temporary storage space, performing the insertion, spliting the temporary node, and finally copying the temporary node back to its original position. However, a simple B-tree algorithm already wastes a fair amount of space, which can be reduced only by more sophisticated procedures.

Upward propagation of overflow gives a nice illustration of recursion. At the upper level, a search has located the position of the search key among the data keys in the node. A recursive call with the corresponding downward key has resulted in insertion at some lower level. In case the recursive call returns to the upper level with an indication of overflow propagation, the earlier search result will have been retained in the local environment and will still be available for inserting the data item that has propagated upward to this level.

Say it with Fortran

Example 24.

```
! Example 24. B Tree
module D24_M
  implicit none
  public :: Look_Up, Print_Tree
  integer, private, parameter :: M = 4
  integer, parameter, public :: KEY_LEN = 16
  type, public :: Info_Type
    character(len = KEY_LEN) :: Key = " "
    integer, dimension(2) :: Data = (/ 0, 1 /)
  end type Info_Type
  type, private :: BOX_Type
    type (Node_Type), pointer :: Next_NP = null( )
  end type BOX_Type
  type, private :: Node_Type
    integer :: N_Keys = 0
    type(Info_Type), dimension(M) :: Info
    type(BOX_Type), dimension(0: M) :: BOX                ! Array of pointers
  end type Node_Type
  type, private :: Van_Type
    type (Info_Type) :: Info
    type (Node_Type), pointer :: Next_NP = null( )
  end type Van_Type
  type (Node_Type), pointer, private :: Root_NP
contains

  subroutine Look_Up( Arg_Info )                             ! Start from Root
    type (Info_Type), intent(in) :: Arg_Info
    type (Node_Type), pointer :: Temp_NP
    type (Van_Type) :: Carrier
! start subroutine Look_Up
    Carrier % Info = Arg_Info
    call R_Look_Up( Root_NP )
    if (associated( Carrier % Next_NP )) then
```

Split has propagated all the way up to the root. Make a new Root node.

```
      Temp_NP % BOX(0) % Next_NP => Root_NP
      Root_NP => Temp_NP
      nullify( Temp_NP )
      call Insert( Root_NP, 0 )
    end if
    return
  contains
    recursive subroutine R_Look_Up( Arg_NP )
      type (Node_Type), pointer :: Arg_NP
      integer, dimension(2) :: Loc
  ! start subroutine R_Look_Up
```

Locate the search key among the keys at the current node.

```
    Loc = Binary_Search( Arg_NP % Info(1: Arg_NP % N_Keys) % Key, &
      Carrier % Info % Key )
    if (Loc(2) == Loc(1)) then
      call Modify_Target( Arg_NP, Loc(1) )
    else if (associated( Arg_NP % BOX(Loc(1)) % Next_NP )) then
      call R_Look_Up( Arg_NP % BOX(Loc(1)) % Next_NP )
```

If **`Carrier % Next_P`** *is not null on return from the recursive call, a split at the lower level has overflowed and propagated up to the current level. During the recursive call,* **`Loc(2)`** *has retained the value that was previously set for the current instance.*

```
      if (associated( Carrier % Next_NP )) &
        call Insert_Target( Arg_NP, Loc(1) )
    else
```

A null pointer signals the base of recursion: Insert a new node with the new key into the current leaf.

```
      call Insert_Target( Arg_NP, Loc(1) )
    end if
    return
  end subroutine R_Look_Up

  subroutine Modify_Target( Arg_NP, Loc_1 )
    :
  end subroutine Modify_Target

  subroutine Insert_Target( Arg_NP, Loc_1 )
```

Insert a new item in the middle of a node.

```
    type (Node_Type), pointer :: Arg_NP
    integer, intent(in) :: Loc_1
    integer :: Loop, A_Keys, C_Keys
! start subroutine Insert_Target
```

Insert, ignoring overflow until later: There is one extra space in the node for temporary use. Move up **`Info`** *from {***`Loc_1 + 1: N_Keys`***} to {***`Loc_1 + 2: N_Keys + 1`***}; insert at* **`Loc_1 + 1`**

```
    Arg_NP % Info(Loc_1 + 2: Arg_NP % N_Keys + 1) = &
      Arg_NP % Info(Loc_1 + 1: Arg_NP % N_Keys)
    Arg_NP % Info(Loc_1 + 1) = Carrier % Info
```

*Move up pointers from {***`Loc_1 + 1: N_Keys`***} to {***`Loc_1 + 2: N_Keys + 1`***}; insert at* **`Loc_1 + 1`**

```
    do Loop = Arg_NP % N_Keys, Loc_1 + 1, -1
      Arg_NP % BOX(Loop + 1) % Next_NP => Arg_NP % BOX(Loop) % Next_NP
    end do
    Arg_NP % BOX(Loc_1 + 1) % Next_NP => Carrier % Next_NP
    Arg_NP % N_Keys = Arg_NP % N_Keys + 1
    nullify( Carrier % Next_NP )
```

Insertion is complete. Now check for oveflow.; if there is overflow, split the current node. Otherwise, **`Carrier % Next_NP`** *remains null as a signal to the next higher level that there is no pending upward propagation.*

```
      if (Arg_NP % N_Keys >= M) then
        allocate( Carrier % Next_NP )
        A_Keys = (M - 1) / 2
        C_Keys = M - A_Keys - 1
```

The first **`A_Keys`** *items remain in the current node, the item at* **`A_Keys + 1`** *moves to* **`Carrier`** *for upward propagation, and the remaining* **`C_Keys`** *items are copied to the new successor of* **`Carrier`**.

```
        Carrier % Info = Arg_NP % Info(A_Keys + 1)
        Carrier % Next_NP % Info(1: C_Keys) = Arg_NP % Info(A_Keys + 2: M)
        do Loop = 0, C_Keys
          Carrier % Next_NP % BOX(Loop) % Next_NP => &
            Arg_NP % BOX(Loop + A_Keys + 1) % Next_NP
        end do
        Arg_NP % N_Keys = A_Keys
        Carrier % Next_NP % N_Keys = C_Keys
      end if
      return
    end subroutine Insert_Target

    pure function Binary_Search( Array, Key) result( Location )
      :
    end function Binary_Search

  end subroutine Look_Up

  subroutine Print_Tree( )
    integer :: Total
! start subroutine Print_Tree
    call R_Print_Tree( Root_NP )
    return
  end subroutine Print_Tree

  recursive subroutine R_Print_Tree( Arg_NP )
    type(Node_Type), pointer :: Arg_NP
    integer :: Loop
! start subroutine R_Print_Tree
    if (associated( Arg_NP )) then
      do Loop = 0, Arg_NP % N_Keys
        call R_Print_Tree( Arg_NP % BOX(Loop) % Next_NP )
        if (Loop < Arg_NP % N_Keys) print *, Arg_NP % Info(Loop + 1)
      end do
    end if
    return
  end subroutine R_Print_Tree

end module D24_M
```

7.4 SKIP LISTS

Can an ordered linked list be organized in some special way to make binary searching possible? With an extra pointer to the middle of the linked list, a single key comparison would cut the linear search time in half. Additional pointers to the midpoints of each of the halves would further reduce linear search time.

A *skip list* extends this idea, reducing search time from O(n) to O(lg n).[36] In a growing list, the midpoint and the other subdivision points change continually; instead of maintaining fixed subdivisions, a skip list inserts random subdivision points that *approximate* the comparison points of the binary search algorithm for arrays.

The maximum number of pointers at each node (the *order* of the skip list) should be an overestimate of the base-2 logarithm of the number of nodes that will be in the list. If the order is too small, the efficiency of the algorithm will suffer somewhat; if the order is too large, the storage space for extra pointers at each node will be wasted, but no extra search time is required. However, as shown later, Fortran permits postponed space allocation, which eliminates wasted space and makes it unnecessary to specify a fixed order in advance.

Each pointer at a node is designated by a *pointer level* between 1 and the order of the skip list. The *node level* is the number of pointers at a node; i.e., the maximum pointer level for the node. The order of the skip list is the largest node level in the skip list. For each node to be inserted, a random node level is generated. Approximately one-half of the nodes have level 1, with one pointer at level 1; one-fourth of the nodes have level 2, with pointers at levels 1 and 2; one-eighth of the nodes have level 3, with pointers at levels 1, 2, and 3; etc. Integers with this distribution can be generated as –lg R, where R is obtained from a uniform distribution on the real interval (0.0, 1.0). Optimum performance requires a good random distribution.

```
do
   call random_number( R )
   L = ceiling( - LG_OF_E * log( R ) )
end do
```

For example, in the following sequence of 16 random numbers, eight are between 0.5 and 1.0, at level 1; four are between 0.25 and 0.5, at level 2; three are between 0.125 and 0.25, at level 3; and one is between 0.0625 and 0.125, at level 4:

R	**L**	**R**	**L**
0.131546	3	0.613989	1
0.887143	1	0.318195	2
0.214255	3	0.902918	1
0.991417	1	0.350382	2
0.751726	1	0.865537	1
0.266004	2	0.088034	4
0.725909	1	0.583162	1
0.358161	2	0.200850	3

When a node is inserted at level L, its Ith pointer (for $I = 1$ to L) is adjusted to point to the next node whose level is I or greater.

Let us suppose that the following sixteen items are to be inserted: for; a; large; ordered; array; binary; search; is; much; more; efficient; than; the; linear; just; described. With the random level sequence of the previous example, the skip list appears as shown in Fig. 7.4 after insertion of the first fifteen of these items.

[36] Skip lists are described by W. Pugh, “Skip Lists: A Probabilistic Alternative to Balanced Trees,” *Communications of the ACM* 33 (1990), 668-676. Skip lists, as well as some alternatives, are explained by M.A. Weiss in *Data Structures and Algorithm Analysis*, second edition, Benjamin / Cummings, 1995.

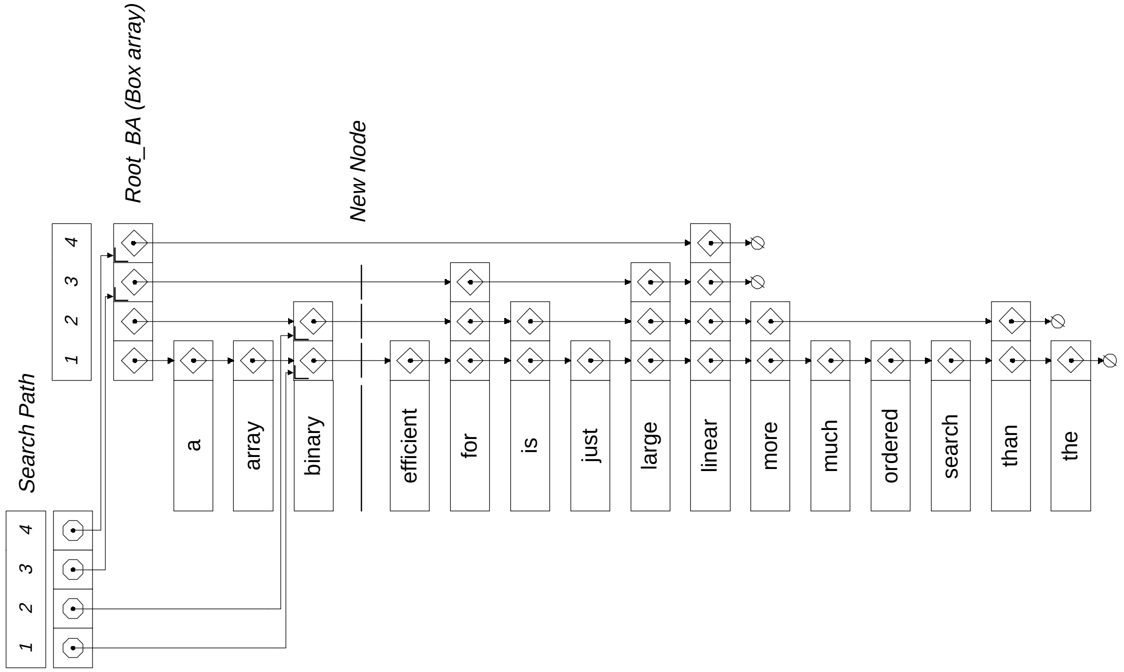

FIGURE 7.4. Skip list before insertion of “described”

The sequence of nodes at a given level is, in effect, an ordinary linked list that begins with the root pointer at the given level and terminates with a null pointer. At level 1, the list consists of the entire sequence of nodes. The level 2 sequence consists of the nodes with keys binary, for, is, large, linear, more, and than. At level 3, the keys are for, large, and linear. There is only one node at level 4, with the key linear.

The highest node level that actually occurs in the skip list at any time is recorded as *Max_Level*. The root consists of an array of pointers; for each level from 1 through *Max_Level*, the root pointer points to the first node at that level — i.e., to a at level 1, to binary at level 2, to for at level 3, and to linear at level 4. Another array, called the *search path*, is used during a search to store a pointer for each level. Fortran syntax does not actually permit arrays of pointers; a variable with both pointer and dimension attributes is a pointer to an array. However, an array with elements of **BOX_Type** (a derived type with a single component that is a pointer) is suitable.

Searching in a skip list starts from the root pointer at the maximum level, and continues at the same level until the current pointer at this level is null or its target node has a key larger than the search key. The search does not terminate at this point; instead, the current status is recorded (by making the current pointer — i.e, its **BOX** — the target of the *Path* array element at this level) and the search continues with the current pointer, but at the next lower level. When the search at the lowest level terminates, the search process is complete.

Let us trace the search with the sixteenth key, described, as the search key.

The search starts at the current maximum level 4, The linked list at this level is **Root_BA(4)** → linear → *null*. Starting with the level 4 pointer in the root as the current pointer, the search key is compared with linear. This key is too large, so the level 4 root pointer (**BOX**) is made the target of the *Path* array element at level 4.

The linked list at level 3 is **Root_BA(3)** → for → large → linear → *null*. The level 4 search did not move away from the root, so the level 3 search continues from the level 3 root pointer. The first comparison is with for, which is again too large, so the level 3 root pointer (**BOX**) is made the target of the level 3 *Path* element.

As before, the level 2 search continues from the level 2 root pointer; the linked list at this level is **Root_BA(2)** → binary → for → is → large → linear → more → than → *null*. The key binary is smaller than the search key but for is larger, so level 2 ends. The pointer (**BOX**) in the node whose key is binary is made the target of the *Path* element at level 2.

The final search starts with the pointer at level 1 in the node whose key is binary. Its target at this level is efficient, which is larger, so level 1 terminates and the current pointer (i.e., the **BOX** in node binary) is made the target of the level 1 *Path* element. The path is shown at the lower left in Fig. 7.4. The path pointer targets at levels 4 and 3 are **BOX**es in the root array; the path pointer targets at levels 2 and 1 are **BOX**es in the node with key "binary".

The new node, described, is to be inserted after the current node position at level 1. A level for the node is generated — this time, 3, so described is inserted with level 3, following the node binary.

After insertion of described, the skip list appears as shown in Fig. 7.5.

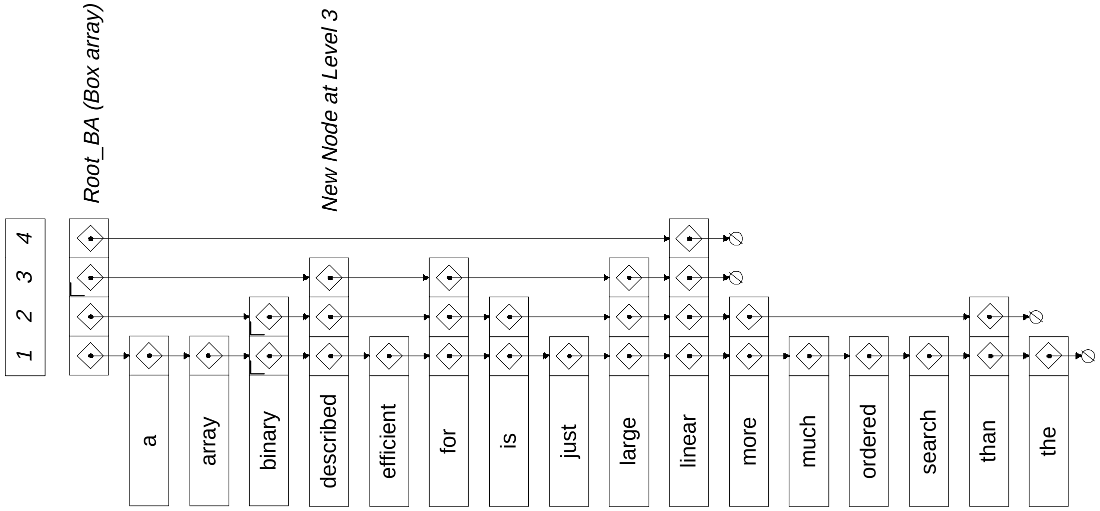

FIGURE 7.5. Skip list after insertion of "described"

Insertion of a new node requires the following steps:

1. Generate the **Level** for the new node.
2. Allocate a new node with a full set of pointers.[37]
3. At each level up to the new node level, insert the new node:

```
New_NP % BOX_Array(Level) = Path(Level) % BP          ! Copy target
Path(Level) % BP % Next_NP => New_NP                  ! Copy pointer
```

An interesting feature of this implementation is allocation of a new root whenever the maximum level increases. Initially, the maximum level is zero and the *Root* and *Path* arrays are not allocated. At the first call to **Look_Up**, the outer search loop is skipped and **Insert_Target** is called. This procedure generates a level for the new node to be inserted, which will be nonzero and is therefore certain to be larger than the current maximum level (initially zero). This increase in the maximum level triggers a call to the procedure **New_Root**, which allocates *Root* and *Path* arrays with enough space for the new maximum level.

[37] The expected number of pointers is N at level 1, $N/2$ at level 2, $N/4$ at level 3, etc.; thus, only about two pointers per node are actually required.

```
    subroutine New_Root( New_NP, L )
      type (Node_Type), pointer :: New_NP
      integer, intent(in) :: L
      type (BOX_Type), dimension(:), pointer :: Temp_BAP        ! To BOX array
      integer :: Level
  ! start subroutine New_Root
```

L *is the new maximum level. Allocate* **Temp_BAP** *which will become the new root. Copy the old items and pointers from* **Root_BAP** *to* **Temp_BAP***; link the new root at higher levels to the node just inserted, which is the first node that has been created with these higher levels.*

```
      allocate( Temp_BAP(L) )
      do Level = 1, Max_Level
        Temp_BAP(Level) = Root_BAP(Level)        ! Target of Temp_BAP(Level)
      end do
      do Level = Max_Level + 1, L
        Temp_BAP(Level) % Next_NP => New_NP
      end do
```

Clean up: deallocate old root and path, set new root pointer, increase maximum level, and reallocate **Path** *with room for the new maximum level.*

```
      if (Max_Level > 0 ) then
        deallocate( Root_BAP )
        deallocate( Path )
      end if
      Root_BAP => Temp_BAP
      Max_Level = L
      allocate( Path(Max_Level) )
      return
    end subroutine New_Root
```

Say it with Fortran

Example 25. A Fortran program for skip lists closely resembles a linked list program that employs the pointer to pointer technique. However the target type for *Root_BAP* and for the traveling pointer is now an *array* of **BOX_Type** (with the pointer in each **BOX** initially nullified); also, each node now consists of an *Info* component and an *array* of **BOX_Type**. The traveling pointer is initialized with a copy of *Root_BAP*, and can advance to the **BOX** array component of a successor node.

The *Path*, as described earlier, is an array of pointers to nodes, but the actual Fortran program is based on a slightly different description. First, node pointers do not have to be stored: what is needed for insertion at each level is a pointer to a **BOX** — namely, to the element of the **BOX** array that is the current target of the traveling pointer. Second, as just noted, Fortran does not support arrays of pointers, so the *Path* is an array of *structures*, each containing a **BOX** pointer.

```
! Example 25. Skip list
module D25_M
  implicit none
  public :: Look_Up, Print_List
  integer, parameter, private :: S_LEN = 20
  type, public :: Info_Type                               ! Also used in main program
    character (len = S_LEN) :: Key
    integer, dimension(3) :: Data = (/ 0, 1, 999 /)
  end type Info_Type
  type, private :: BOX_Type
    type (Node_Type), pointer :: Next_NP => null( )
  end type BOX_Type
  type, private :: Node_Type
    type (Info_Type) :: Info
    type (BOX_Type), dimension(:), pointer :: BOX_Array
  end type Node_Type
  type, private :: Path_Type
    type (BOX_Type), pointer :: BP
  end type Path_Type
```

Root_BAP *(BOX array pointer) and* **Path** *(array of* **BOX** *type) are allocated when* **Max_Level** *increases. A zero value for* **Max_Level** *signals that* **Root_BAP** *has not been initialized.*

```
  type (BOX_Type), dimension(:), pointer, private :: Root_BAP, Trav_BAP
  type (Path_Type), dimension(:), allocatable, private :: Path
  integer, private, save :: Max_Level = 0
contains
  subroutine Look_Up( Item )
    type (Info_Type), intent(in) :: Item
    integer :: Level
! start subroutine Look_Up
    Trav_BAP => Root_BAP                          ! Copy Root_BAP to Trav_BAP
    do Level = Max_Level, 1, -1
      do
        if (associated( Trav_BAP(Level) % Next_NP )) then
          if (Item % Key == Trav_BAP(Level) % Next_NP % Info % Key) then
            call Modify_Target( Trav_BAP(Level) % Next_NP )
            return
          else if ( Item % Key &
             > Trav_BAP(Level) % Next_NP % Info % Key) then
            Trav_BAP => Trav_BAP(Level) % Next_NP % BOX_Array
            cycle                               ! Keep looking at the same level
          end if
        end if
        exit                     ! This level found null or "<"; go to next level
      end do
      Path(Level) % BP => Trav_BAP(Level)                         ! Copy pointer
    end do
    call Insert_Target( )                        ! All levels found null or "<"
    return
  contains

    subroutine Insert_Target( )
      type (Node_Type), pointer :: New_NP
      integer :: Level, L
    ! start subroutine Insert_Target
```

Generate the level for the new node that will be inserted. Allocate the node and allocate its **BOX** *array with pointer for each level. Copy data into the new node.*

```
      call Get_Level( L )
      allocate( New_NP )
      allocate( New_NP % BOX_Array(L) )
      New_NP % Info = Item
      New_NP % Info % Data(3) = L
```

Use **`Path`** *to link the new node into the skip list at each level. If the level of the new node exceeds* **`Max_Level`***, a new* **`Root_BAP`** *will be generated and the higher levels will be linked to it.*

```
      do Level = 1, min( L, Max_Level )
        New_NP % BOX_Array(Level) = Path(Level) % BP
        Path(Level) % BP % Next_NP => New_NP
      end do
      if (L > Max_Level) call New_Root( New_NP, L )
      return
    end subroutine Insert_Target

    subroutine Get_Level( L )
      :
    end subroutine Get_Level

    subroutine Modify_Target( Arg_NP )
      :
    end subroutine Modify_Target

    subroutine New_Root( New_NP, L )
      :
    end subroutine New_Root

  end subroutine Look_Up

  subroutine Print_List( )
! start subroutine Print_List
    Trav_BAP => Root_BAP
    do while (associated( Trav_BAP(1) % Next_NP ))
      print *, Trav_BAP(1) % Next_NP % Info
      Trav_BAP => Trav_BAP(1) % Next_NP % BOX_Array      ! Advance to next node
    end do
    return
  end subroutine Print_List

end module D25_M
```

7.5 COMPARISON OF ALGORITHMS

A sequence of 1,024 character strings, with 27 duplicates and 997 different strings, was generated randomly (see the electronically distributed file **`dxf.txt`**). These were then inserted into an array, a linked list, a simple binary search tree, an AVL tree, B trees of order 2, 4, and 32, and a skip list. Comparisons and other relevant operations were counted during the tests.

An array (with binary search) required 9,765 comparisons and 245,314 moves.

A linked list required 261,245 comparisons.

A simple binary search tree required 12,363 comparisons and reached level 20. Considerably worse performance might be expected with nonrandom input data.

An AVL tree required 9,858 comparisons and 668 rotations; the maximum level was 11.

A B tree of order 2 (level 30) required 38,285 comparisons and 5,066 moves; order 4 (level 7) required 14,613 comparisons and 2,807 moves; order 32 (level 3) required 11,165 comparisons and 12,327 moves.

A skip list required 14,825 comparisons; the final maximum level was 9. (This test employed the “good” random number generator in the electronic version of the skip list module. One intrinsic **`random_number`** subroutine required more than 19,000 comparisons.)

Conclusions:

For maintaining an expanding list in internal storage, the two best choices, among the alternatives described in this book, are an AVL tree and a skip list. The AVL tree requires fewer comparisons, but rotations are rather expensive. The skip list is more complicated, but would probably be more efficient over all.

POSSIBLE ANSWER to Exercise 5, Section 1.2 (page 35):

```
! Binary search in ordered array (with recursion).
  pure function Search (Array, Key) result (Location)
    real, intent(in), dimension(:) :: Array
    real, intent(in) :: Key
    integer :: Location(2)
! start function Search
    Location = Recursive_Binary_Search( 0, size(Array) + 1 )
    return
  contains
    pure recursive function Recursive_Binary_Search( L_1, L_2 ) &
        result( L_R )
      integer, intent(in) :: L_1, L_2
      integer, dimension(2) :: L_R
      integer :: Middle
  ! start function Recursive_Binary_Search
      if (L_2 - L_1 <= 1) then
        L_R = (/ L_1, L_2 /)                       ! Array constructor
      else
        Middle = (L_1 + L_2) / 2
        if (Key > Array(Middle)) then
          L_R = Recursive_Binary_Search( Middle, L_2 )
        else if (Key < Array(Middle)) then
          L_R = Recursive_Binary_Search( L_1, Middle )
        else
          L_R = Middle                        ! Whole array assignment
        end if
      end if
      return
    end function Recursive_Binary_Search
  end function Search
```

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