20

Computer procedures for finite element analysis

20.1 Introduction

In this chapter we consider some of the steps that are involved in the development of a finite element computer program to carry out analyses for the theory presented in previous chapters. The computer program discussed here may be used to solve any one-, two-, or three-dimensional linear steady-state or transient problem. The program may also be used to solve non-linear problems as will be discussed in Volume 2.

Source listings are not included in the book but may be obtained at no charge from the publisher's internet web site (http://www.bh.com/companions/fem). Any errors reported by readers will be corrected frequently so that up-to-date versions will be available.

The program is an extension of the work presented in the 4th edition.[1,2] The version discussed here is called *FEAPpv* to distinguish the current program from that presented earlier. The program name is an acronym for Finite Element Analysis Program – personal version. It is intended mainly for use in learning finite element programming methodologies and in solving small to moderate size problems on single processor computers. A simple memory management scheme is employed to permit efficient use of main memory with limited need to read and write information to disk.

The current version of *FEAPpv* permits both 'batch' and 'interactive' problem solution. The finite element model of the problem is given as an input file and may be prepared using any text editor capable of writing ASCII file output. A simple graphics capability is also included to display the mesh and results from one- and two-dimensional models in either their undeformed or reference configuration. The available versions for graphics is limited to X-window applications and compilers compatible with the current Compac Fortran 95 compiler for Windows based systems. Experienced programmers should be able to easily adapt the routines to other systems.

Finite element programs can be separated into three basic parts:

1. data input module and preprocessor
2. solution module
3. results module

Figure 20.1 shows a simplified schematic for a typical finite element program system. Each of the modules can in practice be very complex. In the subsequent

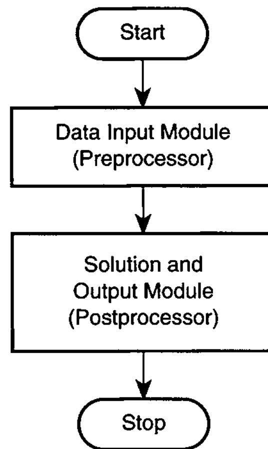


Fig. 20.1 Simplified schematic of finite element program.

sections we shall discuss in some detail the programming aspects for each of the modules. It is assumed that the reader is familiar with the finite element principles presented in this book, linear algebra, and programming in either Fortran or C. Readers who merely intend to use the program may find information in this chapter useful for understanding the solution process; however, for this purpose it is only necessary to read the user instructions available from the web site where the program is downloaded.

This chapter is divided into seven sections. Section 20.2 describes the procedure adopted for data input, necessary to define a finite element problem and basic instructions for data file preparation. The data to be provided consists of nodal quantities (e.g., coordinates, boundary condition data, loading, etc.) and element quantities (e.g., connection data, material properties, etc.).

Section 20.3 describes the memory management routines.

Section 20.4 discusses solution algorithms for various classes of finite element analyses. In order to have a computer program that can solve many types of finite element problems a *command language* strategy is adopted. The command language is associated with a set of compact subprograms, each designed to compute one or at most a few basic steps in a finite element process. Examples in the language are commands to form a global stiffness matrix, as well as commands to solve equations, display results, enter graphics mode, etc. The command language concept permits inclusion of a wide range of solution algorithms useful in solving steady-state and transient problems in either a linear or non-linear mode.

In Section 20.5 we discuss a methodology commonly used to develop element arrays. In particular, numerical integration is used to derive element 'stiffness', 'mass' and 'residual' (load) arrays for problems in linear heat transfer and elasticity. The concept of using basic shape function routines is exploited in these developments (Chapters 8 and 9).

In Section 20.6 we summarize methods for solving the large set of linear algebraic equations resulting from the finite element formulation. The methods may be divided into direct and iterative categories. In a direct solution a variant of Gaussian

elimination is used to factor the problem coefficient matrix (e.g., stiffness matrix) into the product of a lower triangular, diagonal and upper triangular form. A solution (or indeed subsequent resolutions) may then be easily obtained. A direct solution has the advantage that an *a priori* calculation may be made on the number of numerical operations which need to be performed to obtain a solution. On the other hand, a direct solution results in fill-in of the initial, sparse finite element coefficient array – this is especially significant in three-dimensional solutions and results in very large storage and compute times. In the second category iterative strategies are used to systematically reduce a residual equation to zero, and thus yield an acceptable solution to the set of linear algebraic equations. The scheme discussed in this chapter is limited to solution of symmetric equations by a preconditioned conjugate gradient method.

20.2 Data input module

The data input module shown in Fig. 20.1 must obtain sufficient information to permit the definition and solution of each problem by the other modules. In the program discussed in this book the data input module is used to read the necessary geometric, material, and loading data from a file or from information specified by the user using the computer keyboard or mouse. In the program a set of dynamically dimensioned arrays is established which store nodal coordinates, element connection lists, material properties, boundary condition indicators, prescribed nodal forces and displacements, etc. Table 20.1 lists the names of variables which are used in assigning array sizes for mesh data and Table 20.2 indicates some of the main arrays used to store mesh data.

Table 20.1 Control parameters

Variable name	Description	Default
NUMNP	Number of nodal points in mesh	0
NUMEL	Number of elements in mesh	0
NUMMAT	Number of material sets in mesh	0
NDM	Spatial dimension of mesh	none
NDF	Number of degrees of freedom per node (maximum)	none
NEN	Number of nodes per element (maximum)	none
NDD	Number of material property values per set	200

Table 20.2 Variable names used for data storage

Variable name (dimension)	Type	Description
ID(NDF,NUMNP,2)	Integer	(1) Boundary codes; (2) Equation numbers
IE(NIE,NUMMAT)	Integer	Element pointers for degrees of freedom, history pointers, material set type, etc.
IX(NEN1,NUMEL)	Integer	Element connections, set flag, etc.
D(NDD,NUMMAT)	Real	Material property data sets
F(NDF,NUMNP,2)	Real	(1) Nodal forces; (2) and displacements
X(NDM,NUMNP)	Real	Nodal coordinates

The notation used for the arrays often differs from that used in the text. For example, in the text it was found convenient to refer to nodal coordinates as x_i, y_i, z_i, whereas in the program these are called `X(1,i)`, `X(2,i)`, `X(3,i)`, respectively. This change is made so that all arrays used in the program can be dynamically allocated. Thus, if a two-dimensional problem is analysed, space will not be reserved for the `X(3,i)` coordinates. Similarly the nodal displacements in the text were commonly named a_i; in the program these are called `U(1,i)`, `U(2,i)`, etc., where the first subscript refers to the degrees of freedom at a node (from `1` to `NDF`).

20.2.1 Control data and storage allocation

The allocation of the major arrays for storage of mesh and solution variables is performed in a control program as indicated in Fig. 20.2. Since a dynamic memory allocation is used it is not possible to establish absolute values for the maximum number of nodes, elements or material sets. The value for the parameter `NUM_MR` defines the amount of memory available to solve a given problem and is assigned to the main program module; however, if this is not sufficient an error message is given and the program stops execution.

To facilitate the allocation of all the arrays data defining the size of the problem is input by the control program as shown schematically in Fig. 20.2. The required data is shown in Table 20.1; however, the number of nodes, elements and material sets may be omitted and `FEAPpv.f` will use the subsequent input data to determine the actual size required. Using the size data the remaining mesh storage requirements are determined and allocated by the control program.

20.2.2 Element and coordinate data

After a user has determined the mesh layout for a problem solution the data must be transmitted to the analysis program. As an example consider the specification of the nodal coordinate and element connection data for the simple two-dimensional (`NDM` = 2) rectangular region shown in Fig. 20.3, where a mesh of nine four-node rectangular elements (`NUMEL` = 9 and `NEN` =4) and 16 nodes (`NUMNP` = 16) has been indicated. To describe the nodal and element data, values must be assigned to each `X(i,j)` for $i = 1,2$ and $j = 1$ to 16 and to each `IX(k,n)` for $k = 1$ to 4 and $n = 1$ to 9. In the definition of the coordinate array `X`, the subscript i indicates the coordinate direction and the subscript j the node number. Thus, the value of `X(1,3)` is the x coordinate for node 3 and the value of `X(2,3)` is the y coordinate for node 3. Similarly for the element connection array `IX` the subscript k is the local node number of the element and n is the element number. The value of any `IX(k,n)` (for k less than or equal to `NEN`) is the number of a global node. Values of k larger than `NEN` are used to store other data. The convention for the first local node number is somewhat arbitrary. The local node number 1 for element 3 in Fig. 20.3 could be associated with global node 3, 4, 7, or 8. Once the first local node is established the others must follow according to the convention adopted for each particular element type. For example,

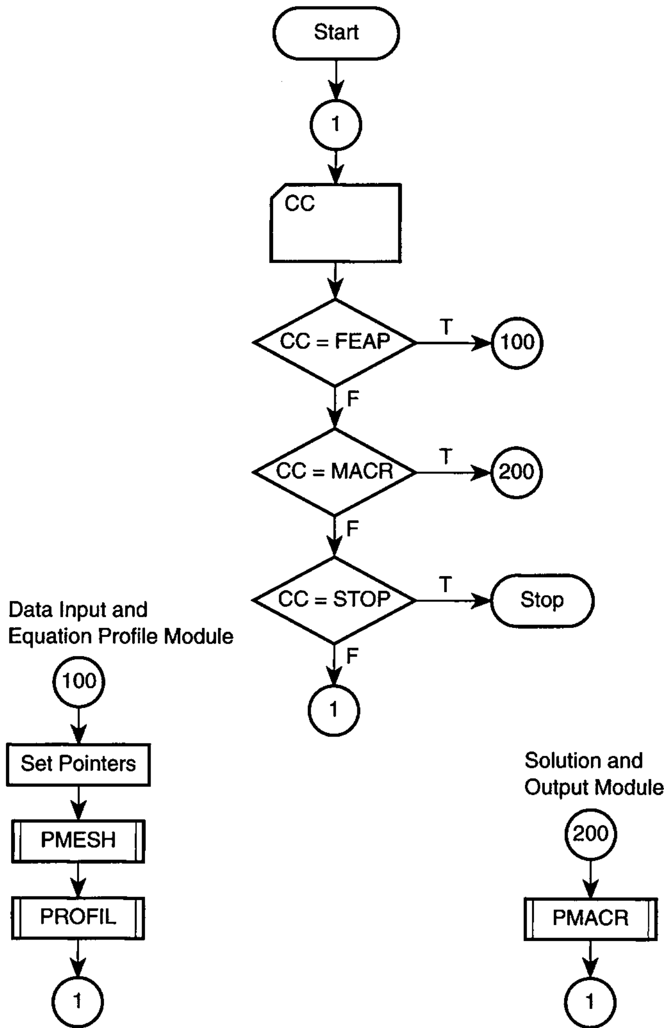


Fig. 20.2 Control program flow chart.

it is conventional to number the connections by a *right-hand rule* and the four-noded quadrilateral element can be numbered according to that shown in Fig. 20.4. If we consider once again element 3 from the mesh in Fig. 20.3 we have four possibilities for specifying the `IX(k,3)` array as shown in Fig. 20.4. The computation of the element arrays from any of the above descriptions must produce the same coefficients for the global arrays and is known as *element invariance* to data input.

Data input modules

In *FEAPpv* two subprograms `PINPUT` and `TINPUT` are available to perform data input operations. For example, all the nodal coordinates may be input using the subprogram

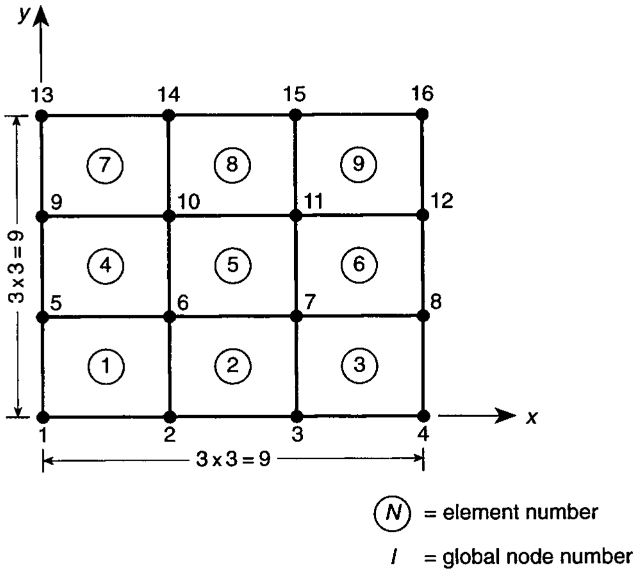
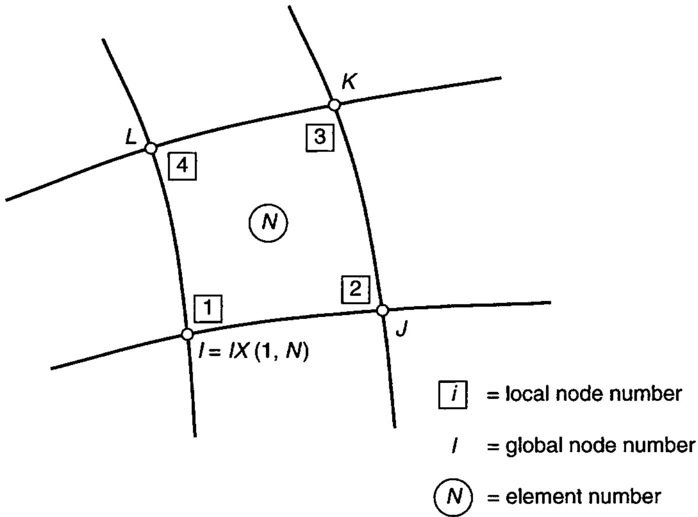


Fig. 20.3 Simple two-dimensional mesh.



Option number	Local node number			
	1	2	3	4
a	3	4	8	7
b	4	8	7	3
c	8	7	3	4
d	7	3	4	8

Fig. 20.4 Typical four-noded element and numbering options.

```
SUBROUTINE XDATA(X,NDM,NUMNP)

IMPLICIT NONE

LOGICAL  ERRCK, PINPUT
INTEGER  NUMNP, NDM , N
REAL*8   X(NDM,NUMNP)

DO N = 1,NUMNP
  ERRCK = PINPUT(X(1,N),NDM}
  IF(ERRCK) THEN
    STOP ' Coordinate error: Node:',N
  ENDIF
END DO ! N

END
```

The above use of the PINPUT routine obtains NDM values from each record and assigns them to the coordinate components of node N. The data input routines obtain their information from the current input file specified by a user. The routines are also used in cases where input is to be provided from the keyboard. These input all data in character mode, and parse the data for embedded function names or parameters (use of functions and parameters is described in the user manual). Users who are extending the capability of the program are encouraged to use the routines to avoid possible errors. The subprogram TINPUT permits character data to precede numerical values use is given as

```
ERRCK = TINPUT(TEXT,M,DATA,N)
```

in which TEXT is a CHARACTER*15 array of size M and DATA is a REAL*8 array of size N.

For cases where integer information is to be input the information must be moved. For example, a simple input routine for the IX data is

```
SUBROUTINE IXDATA(IX,NEN1,NUMEL)

IMPLICIT   NONE

LOGICAL    ERRCK, PINPUT
INTEGER    NUMEL, NEN1 , N, I
INTEGER    IX(NEN1,NUMEL)
REAL*8     RIX(16)

DO N = 1,NUMEL
  ERRCK = PINPUT(RIX,NEN1}
  IF(ERRCK) THEN                 ! Stop on error
    STOP ' Connection error: ELEMENT:',N
  ELSE                           ! Move data to IX
    DO I = 1,NEN1
      IX(I,N) = NINT(RIX(I))
    END DO ! I
  ENDIF
END DO ! N

END
```

While the above form is not optimal it is an expedient method to permit the arbitrary mixing of real and integer data on the same record. In the above two examples the node and element numbers are associated with the record number read. The form used in the routines supplied with *FEAPpv* include the node and element numbers as part of the data record. In this form the inputs need not be sequential nor all data input at one instance.

For a very large problem the preparation of each node and element record for the mesh data would be very tedious; consequently, some methods are provided in *FEAPpv* to *generate* missing data. These include simple interpolation between missing numbers of nodes or elements, use of super-elements to perform generation of *blocks* of nodes and elements, and use of blending function methods. Even with these aids the preparation of the mesh data for nodes and coordinates can be time consuming and users should consider the use of mesh generation programs such as GiD[3] to assist in this task. Generally, however, the data input scheme included in the program is sufficient to solve academic and test examples. Moreover the organization of the mesh input module (subprogram PMESH) is data driven and permits users to interface their own program directly if desired (see below for more information on adding features). The data-driven format of the mesh input routine is controlled by keywords which direct the program to the specific segment of code to be used. In this form each input segment does not interact with any of the others as shown schematically in the flow chart in Fig. 20.5.

20.2.3 Material property specification – multiple element routines

The above discussion considered the data arrays for nodal coordinates and element connections. It is also necessary to specify the material properties associated with each element, loadings, and the restraints to be applied to each node.

Each element has associated property sets, for example in linear isotropic elastic materials Young's modulus E and Poisson's ratio ν describe the material parameters for an isotropic state. In most situations several elements have the same property sets and it is unnecessary to specify properties for each element individually. In the data structure used in *FEAPpv* an element is associated with a material set by a number on the data record for each element. The material properties are then given once for each number. For example, if the region shown in Fig. 20.3 is all the same material, only one material set is required and each element would reference this set. To accommodate the storage of the material set numbers the IX array is increased in size to NEN1 entries and the material set number is stored in the entry IX(NEN1,n) for element n. In *FEAPpv* the material properties are stored in the array D(NDD,NUMMAT), where NUMMAT is the number of different material sets and NDD is the number of allowable properties for each material set (the default for NDD is 200).

Each material set defines the element type to which the properties are to be assigned. In realistic engineering problems several element types may be needed to define the problem to be solved. A simple example involving different element types is shown in

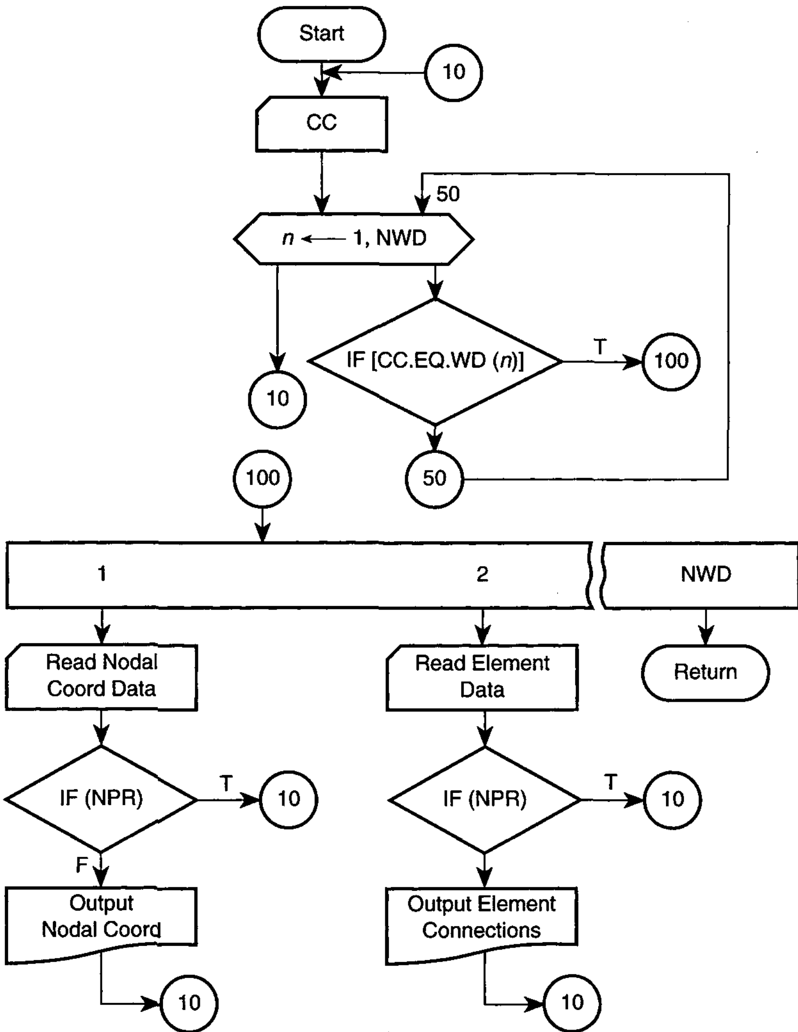


Fig. 20.5 Flow chart for mesh data input.

Fig. 1.4(a) in Chapter 1 where elements 1, 2, 4, and 5 are plane stress elastic elements and element 3 is a truss element. In this case at least two different types of element stiffness formulations must be computed. In *FEAPpv* it is possible to use ten different user provided element formulations in any analysis.† The program has been designed so that all computations associated with each individual element are performed in one element subprogram called ELMTnn, where nn is between 01 and 10 (see Sec. 20.5.3 for a discussion on the organization of ELMTnn). Each element type to be used is specified as part of the material set data. Thus if element type 1, e.g., computations performed by ELMT01, is a plane linear elastic three- or four-noded element and element type 4 is a truss element, the data given for example Fig. 1.4(a) would be:

† In addition, some standard element formulations are provided as described in the user instructions.

(a) *Material properties*

Material set number	Element type	Material property data
1	4	E_1, A_1
2	1	E_2, ν_2

(b) *Element connections*

Element	Material set	Connection
1	2	1 3 4
2	2	1 4 2
3	1	2 5
4	2	3 6 7 4
5	2	4 7 8 5

where E is Young's modulus, ν is Poisson's ratio and A is area. Thus, elements 1, 2, 4, and 5 have material property set 2 which is associated with element type 1 and element 3 has a material property set 1 which is associated with element type 4. It will be seen later that the above scheme leads to a simple organization of an element routine which can input material property sets and perform all the necessary computations for the finite element arrays.

More sophisticated schemes could be adopted; however, for the educational and research type of program described here this added complexity is not warranted.

20.2.4 Boundary conditions - equation numbers

The process of specifying the boundary conditions at nodes and the procedure for imposing specified nodal displacements is closely associated with the method adopted to store the global solution matrix, e.g., the stiffness matrix. In *FEAPpv* the direct solution procedure included uses a variable band (profile) storage for the global solution matrix. Accordingly, only those coefficients within the non-zero profiles are stored.

While the nodal displacements associated with boundary restraints may be imposed using the 'penalty' method described in Chapter 1, a more efficient direct solution results if the rows and columns for these equations are deleted. As an example consider the stiffness matrix corresponding to the problem shown in Fig. 1.1; storing all terms within the upper profile leads to the result shown in Fig. 20.6(a) and requires 54 words, whereas if the equations corresponding to the restrained nodes 1 and 6 are deleted the profile shown in Fig. 20.6(b) results and requires only 32 words. In addition to a reduction in storage requirements, the computer time to solve the equations is also reduced.

To facilitate a compact storage operation in forming the global arrays, a boundary condition array is used for each node. The array is named `ID` and is dimensioned as shown in Table 20.2. During input of data, degrees of freedom with known value or where no unknown exists have a non-zero value assigned to `ID(i,j,1)`. All active

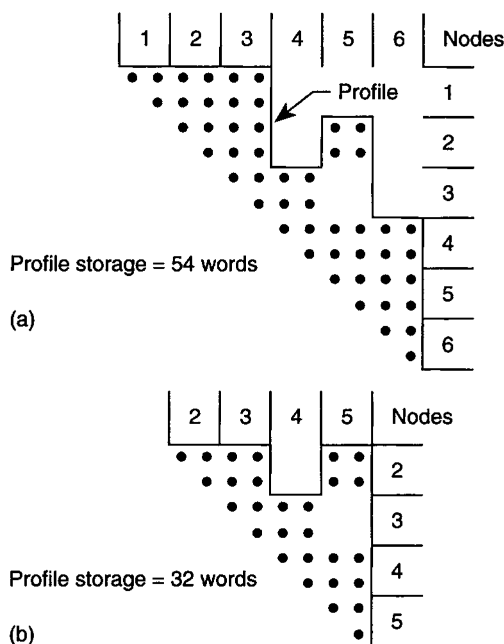


Fig. 20.6 Stiffness matrix: (a) total stiffness storage; (b) storage after deletion of boundary conditions.

degrees of freedom have a zero value in the `ID` array. After the input phase the values in `ID(i,j,2)` are assigned values of the active equation numbers. Restrained DOFs have zero (or negative) values.

Table 20.3 shows the `ID` values for the example shown in Fig. 1.1(a), where it is evident that nodes 1 and 6 are fully restrained.

The numbers for the equations associated with unknowns are constructed from Table 20.3 by replacing each non-zero value with a zero and each zero value by the appropriate equation number. In *FEAPpv* this is performed by subprogram `PROFIL` starting with the degrees of freedom associated with node 1 followed by node 2, etc. The result for the example leads to values shown in Table 20.4, and this information is stored in `ID(i,j,2)`. This information is used to assemble all the global arrays.

Table 20.3 Boundary restraint code values after data input of problem in Fig. 1.1

	Degree of freedom	
Node	1	2
1	1	1
2	0	0
3	0	0
4	0	0
5	0	0
6	1	1

Table 20.4 Compacted equation numbers for problem in Fig. 1.1

	Degree of freedom	
Node	1	2
1	0	0
2	1	2
3	3	4
4	5	6
5	7	8
6	0	0

The above scheme may be modified in a number of ways for either efficiency or to accommodate more general problems. For problems in which the node numbers are input in an order which creates a very large profile it is advisable to employ a program to renumber the nodes for better efficiency (often called bandwidth minimization schemes). Using the renumbered node order the equation numbers may then be constructed.

The solution of mixed formulations which have matrices with zero diagonals requires special care in solving for the parameters. For example in the $\mathbf{q}$, formulation discussed in Sec. 11.2 it is necessary to eliminate all $\tilde{\mathbf{q}}_i$ parameters associated with each $\tilde{\phi}_i$ parameter when a direct method of solution without pivoting is used (e.g., those discussed in Sec. 20.6.1). This may be achieved by numbering the `ID(i,j,2)` entries so that $\tilde{\mathbf{q}}_i$ have smaller equation numbers than the one for the associated $\tilde{\phi}_i$.

The equation number scheme may be further exploited to handle repeating boundaries (see Chapter 9, Sec. 9.18) where nodes on two boundaries are required to have the same displacement but the value is unknown. This is accomplished by setting the equation numbers to the same value (and discard the unused ones). Similarly, regions may be joined by assigning nodes with the same coordinate values the same equation numbers.

All modifications of the above type must be performed prior to computing the profile of the global matrix.

20.2.5 Loading – nodal forces and displacements

In *FEAPpv* the specified nodal forces and displacements associated with each degree of freedom are stored in the array `F(NDF,NUMNP,2)`. The specified force values for degree of freedom i at node j are retained in `F(i,j,1)` and specified values for the corresponding specified displacements in `F(i,j,2)`. The actual value to be used during each phase of an analysis depends on the current value stored in `ID(i,j,1)`. Thus if the value of the `ID(i,j,1)` is zero a force value is taken from `F(i,j,1)` whereas if the value is non-zero a displacement value is taken from `F(i,j,2)`. For the example of Fig. 1.1, an 0.01 settlement of the node 1 can be input by setting `F(1,2,2) = -0.01`, where it is assumed that the second degree of

freedom is a displacement in the vertical direction. Similarly, a horizontal force at node 4 can be specified by setting `F(1,4,1) = 5`, (i.e., X_4 in the figure).

In many problems the loading may be distributed and in these cases the loading must first be converted to nodal forces. In *FEAPpv* there are some provisions included to perform the computation automatically. Users may develop additional schemes for their own problems and add a new input command in the subprogram PMESH. Other options could also be added to compute necessary nodal quantities.

The necessary steps to add a feature in PMESH are:

1. Increase the dimensioned size of the array WD which is a character array to store the command names.
2. Set the value of LIST in the DATA statement to the new number of entries in WD.
3. Add a new statement label entries to the GO TO statement.
4. For each statement label entry add the program statements for the new feature.

The specific instructions to prepare data for *FEAPpv* are contained in the user manual available at the publisher's web site.

20.2.6 Mesh data checking

Once all the data for the geometric, material and loading conditions are supplied *FEAPpv* is ready to initiate execution of the solution module; however prior to this step it is usually preferable to perform some checks on the input data (and any generated values).

After the mesh is input the program will pass to solution mode. During solution additional arrays may be required which can also exceed the available space in the blank common. The most intensive storage requirement is for the global coefficient matrix for the set of linear algebraic equations defining the nodal solution parameters. In direct solution mode a variable band, profile solution scheme is used for simplicity. The solver has the capability of solving both symmetric and unsymmetric coefficient arrays and this is generally adequate for one- and two-dimensional problems of moderate size. However, for three-dimensional applications the storage demands for the coefficient matrix can exceed the capabilities of even the largest computers available at the time of writing this volume. Thus, an alternative iterative scheme is included in *FEAPpv* using a simple preconditioned conjugate gradient solver.

20.3 Memory management for array storage

A single array is partitioned to store all the main data arrays, as well as other arrays needed during the solution and output phases. This is accomplished using a data management system which can define, resize or destroy an integer or real array. Depending on the computer system used real arrays may be defined in the main program module FEAPpv.F in either single precision or double precision form. Using the data management system each array indicated in Table 20.2 is dynamically dimensioned to the size and precision required for each problem. The result is a set of pointers defining

the location in a single array located in blank common. Blank common is defined as

```
REAL*8    HR
INTEGER         MR
COMMON    HR(1),MR(NUM_MR)
```

and pointers are assigned into the array NP stored in the named common POINTERS given by

```
INTEGER              NP
COMMON /POINTERS/ NP(NUM_NP)
```

The size of each array is defined by parameters NUM_MR and NUM_NP. While not strictly defined by programming standards the above size for HR is not limited to 1. By working outside the array bound real arrays may be defined up to size NUM_MR/2 for the double precision indicated. Using this artifice of pointers subroutines may be called as

```
CALL SUBX(MR(NP(5)), HR(NP(33)), ... )
```

where the first argument is integer and the second real. The subroutine would then read

```
SUBROUTINE SUBX(I1, R1, .... )
```

and real names associated with each array as determined by a programmer. At this stage the missing ingredient is assignment of values to each specific pointer. In *FEAPpv* this is accomplished by the subprogram PALLOC. This logical function subprogram associates a number with a name for each variable to be defined, changed or deleted. Each programmer must use a listing of this routine to understand which variable is being defined and whether the variable is to be real or integer. A specification of an array action is accomplished using the assignment statement

```
SETVAL = PALLOC{ NUM , NAME , LENGTH , PRECISION )
```

For example the statement

```
SETVAL = PALLOC{ 43 , 'X' , NDM*NUMNP , 2 )
```

defines the real array for the nodal coordinates to have a size as indicated in Table 20.2. Similarly, the statement

```
SETVAL = PALLOC{ 33 , 'IX' , NEN1*NUMEL , 1 )
```

defines an integer array for the element connection array. Repeating the use of the allocation statement with a different size (either larger or smaller) will redefine the size of the array. Similarly, use of the statement with a zero (0) size deletes the array from the allocation table. Accordingly, use of

```
SETVAL = PALLOC{ 33 , 'IX' , 0 , 1 )
```

would destroy the storage (and values) for the connection data. Thus, using the memory management scheme above it is possible to redefine a mesh in an adaptive solution scheme to add or delete specific element data. Alternatively, data may be used in a temporary manner by allocating and then deleting after use.

20.4 Solution module – the command programming language

At the completion of data input and any checks on the mesh we are prepared to initiate a problem solution. It is at this stage that the particular type of solution mode must be available to the user. In many existing programs only a small number of solution modes are generally included. For example, the program may only be able to solve linear steady-state problems, or in addition it may be able to solve linear transient problems for a single method. In a research mode or indeed in practical engineering problems fixed algorithm programs are often too restrictive and continual modification of the program is necessary to solve specific problems that arise – often at the expense of features needed by another user. For this reason it is desirable to have a program that has modules for various algorithm capabilities and, if necessary, can be modified without affecting other users' capabilities. The program form that we discuss here is basic and the reader can undoubtedly find many ways to improve and extend the capabilities to be able to solve other classes of problems.

The command language concept described in this section has been used by the authors for more than 20 years and, to date, has not inhibited our research activities by becoming outdated. Applications are routinely conducted on personal computers and workstations using an identical program except for graphical display modules.

20.4.1 Linear steady-state problems

A basic aspect of the variable algorithm program *FEAPpv* is a command instruction language which is associated with specific program solution modules for specific algorithms as needed. A user needs only to understand the association between specific commands and the operations carried out by the associated solution modules.

In a steady-state problem we are required to solve the problem given, for example, by

$$\mathbf{r}^{(k)} = \mathbf{f} - \mathbf{K}\mathbf{a}^{(k)} \tag{20.1}$$

where k is an index related to the solution iteration number. We call $\mathbf{r}^{(k)}$ the *residual* of the problem for iteration k and note that a solution results when it is zero. In a data-driven solution mode using the command language of *FEAPpv* the formulation of Eq. (20.1) is given by the command `FORM`, which is a mnemonic for *form residual.* In addition an incremental form of the solution of Eq. (20.1) is adopted in *FEAPpv*. Accordingly we let

$$\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \Delta\mathbf{a}^{(k)} \tag{20.2}$$

and solve the problem

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \mathbf{K}\Delta\mathbf{a}^{(k)} = \mathbf{0} \tag{20.3}$$

Since the problem given by Eq. (20.1) is linear this iterative form *must* converge in one iteration. That is, if we solve the problem for $k = 0$ for any specified $\mathbf{a}^{(0)}$, the residual for $k = 1$ will be zero (to machine precision). The only exceptions to this will be: (*a*) an improperly formulated or implemented finite element formulation for the stiffness and/or the residual; (*b*) an incorrect setting of the necessary boundary conditions to avoid singularity of the resulting stiffness matrix; or (*c*) the problem is so ill-posed that round-off in computer arithmetic leads to significant error in the resulting solution.

In *FEAPpv* the command language statement to form a symmetric stiffness matrix is `TANG`, which is a mnemonic for *tangent stiffness*. An unsymmetric stiffness matrix can be formed by specifying the command `UTAN`. By now the reader should have observed that commands for *FEAPpv* are given by four-character mnemonics. In general, users can use up to 14 characters to issue any command, however, only the first four are interpreted by the program. Thus, if a user desires, the command to form the tangent may be given as `TANGENT`. Finally, to solve the systems of equations given by Eq. (20.3) the command `SOLV` is used. Thus to solve a steady-state problem the three commands issued are:

```
TANGent
FORM
SOLVe
```

The first two commands can be reversed without affecting the algorithm.

The basic structure for all command language statements is:

```
COMMAND OPTION VALUE_1 VALUE_2 VALUE_3
```

Since the above three statements occur so often in any finite element solution strategy a shorthand command option is provided in *FEAPpv* as

```
TANGent,,1
```

where a comma is used to separate the fields and leave a blank option parameter. Any positive non-zero number may be used for the `VALUE_1` parameter.

A user can check that the solution is correct by including another `FORM` command after the `SOLV` statement.

After a solution has been performed for the steady-state problem it is necessary to issue additional commands in order to obtain the solution results. For example, the commands

```
DISPlacement ALL
STREss ALL
```

will output all the nodal displacements and stresses in an *output file* specified at the initiation of running *FEAPpv*. Table 20.5 lists some of the commands available in the program. A complete list is available in the user manual.

The variable algorithm program described by a command language program can often be extended as necessary without need to reprogram the modules. Additional options are described in the user manual.

Table 20.5 Partial list of solutions commands

Command	Option	Value_1	Value_2	Value_3	Description
CHECk					Perform check of mesh (ISW = 2)[1]
DISP	ALL	N1	N2	N3	Output displacement for nodes N1 to N2 at increments of N3 ALL outputs all
DT		V1			Set time increment to V1
FORM					Form equation residual (ISW = 6)
LOOP		N			Loop N times all instructions to a matching NEXT command
MESH					Input changes to mesh
NEXT					End of LOOP instruction
PLOT	OPTION				Enter graphical mode or perform command OPTION
REAC	ALL	N1	N2	N3	Output reactions at nodes N1 to N2 at increments of N3 ALL outputs all (ISW = 6)
SOLV					Solve for new solution increment (after FORM)
STRE	ALL	N1	N2	N3	Output element variables N1 to N2 at increments of N3 ALL outputs all (ISW = 4)
TANGent		N1			Form symmetric tangent Solve if N1 positive (ISW = 3)
TIME					Advance time by DT value
TOL		V1			Set solution tolerance to V1
UTAN		N1			Form unsymmetric tangent (ISW = 3)

20.4.2 Transient solution methods

The integration of second-order differential equations of motion for time-dependent structural systems can be treated using the command language program. The first-order differential equations resulting from the heat equation may also be similarly integrated. For the transient second-order case the residual equation is modified to

$$\mathbf{r}^{(k)} = \mathbf{f} - \mathbf{K}\mathbf{a}^{(k)} - \mathbf{C}\dot{\mathbf{a}}^{(k)} - \mathbf{M}\ddot{\mathbf{a}}^{(k)} \tag{20.4}$$

where $\mathbf{C}$ and $\mathbf{M}$ are damping and mass matrices, respectively, and $\dot{\mathbf{a}}$ and $\ddot{\mathbf{a}}$ are velocity and acceleration, respectively. To solve this problem it is necessary to:

1. specify the time integration method to be used (see Chapter 18);
2. specify the time increment for the integration;
3. specify the number of time steps to perform;
4. form the residual $\mathbf{r}^{(k)}$;
5. form the tangent matrix for the specific time integration method;
6. solve the equation for each time step;
7. report answers as needed.

As an example we consider the Newmark method (GN22) as described in Chapter 18, Sec. 18.33. Using Eq. (18.12) we can define the updates at iteration k as

$$\mathbf{a}_{n+1}^{(k)} = \bar{\mathbf{a}}_{n+1} + \tfrac{1}{2}\beta_2 \Delta t^2 \ddot{\mathbf{a}}_{n+1}^{(k)} \tag{20.5}$$

$$\dot{\mathbf{a}}_{n+1}^{(k)} = \dot{\bar{\mathbf{a}}}_{n+1} + \beta_1 \Delta t \ddot{\mathbf{a}}_{n+1}^{(k)} \tag{20.6}$$

where $\bar{\mathbf{a}}_{n+1}$ and $\dot{\bar{\mathbf{a}}}_{n+1}$ are expressed in terms of solution variables at time n. These equations may also be written in an incremental form as

$$\mathbf{a}_{n+1}^{(k+1)} = \mathbf{a}_{n+1}^{(k)} + \tfrac{1}{2}\beta_2 \Delta t^2 \Delta\ddot{\mathbf{a}}_{n+1}^{(k)} \tag{20.7}$$

$$\dot{\mathbf{a}}_{n+1}^{(k+1)} = \dot{\mathbf{a}}_{n+1}^{(k)} + \beta_1 \Delta t \Delta\ddot{\mathbf{a}}_{n+1}^{(k)} \tag{20.8}$$

Comparing Eq. (20.7) with Eq. (20.3) we obtain

$$\Delta\mathbf{a}_{n+1}^{(k)} = \tfrac{1}{2}\beta_2 \Delta t^2 \Delta\ddot{\mathbf{a}}_{n+1}^{(k)} \tag{20.9}$$

Similarly

$$\Delta\dot{\mathbf{a}}_{n+1}^{(k)} = \beta_1 \Delta t \Delta\ddot{\mathbf{a}}_{n+1}^{(k)} \tag{20.10}$$

Thus, selecting the incremental nodal displacements as the primary unknown, the residual equation for $k+1$ may be written as

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \mathbf{K}^* \Delta\mathbf{a}_{n+1}^{(k)} \tag{20.11}$$

where

$$\mathbf{K}^* = c_1 \mathbf{K} + c_2 \mathbf{C} + c_3 \mathbf{M} \tag{20.12}$$

with

$$c_1 = 1 \qquad c_2 = \frac{2\beta_1}{\beta_2 \Delta t} \qquad c_3 = \frac{2}{\beta_2 \Delta t^2} \tag{20.13}$$

obtained from the relations between the incremental displacement, velocity and acceleration vectors. As we have noted in Chapter 18 the changing of the primary unknown from displacement to acceleration or velocity or, indeed, changing the integration algorithm from Newmark to any other method only changes the residual equation by the parameters c_i which define the tangent matrix $\mathbf{K}^*$. The other changes from different integration algorithms appear in the number of vectors required for the algorithm and the way they are initialized and updated within each time increment.

In program *FEAPpv* the parameters c_i are passed to each element routine as `CTAN(i)` together with the values of the localized nodal displacement, velocity and acceleration vectors. This permits an element module to be programmed in a general manner without knowing which integration method will be used during the solution specified in the command language instructions. In Sec. 20.5 we will discuss the steps needed to program the residual terms, as well as the stiffness and mass terms needed to form the global tangent matrix.

Here we note also that the steady-state algorithm discussed in the previous section merely requires that the velocity and acceleration vectors and the parameters c_2 and c_3 be set to zero before calling an element module. Similarly, for a first-order system the acceleration vector and parameter c_3 are set to zero prior to entering the element module.

The command language instructions to solve a linear transient problem over 50 time steps in which all results are reported at each time is given as

```
TRANS,NEWMark      ! Selects Newmark Method
DT,,0.024          ! Sets time increment to 0.024
TANG               ! Form tangent matrix
LOOP,time,50       ! Loop 50 times to NEXT
  FORM             ! Form residual
  SOLVe            ! Solve equations
  DISP,ALL         ! Output nodal displacements
  STRE,ALL         ! Output element variables
NEXT,time          ! End of LOOP
```

The issuing of the instructions `TRANsient` causes the parameters c_i to be set for the Newmark method. The default for the transient option is the steady-state solution algorithm with $c_1 = 1$ and $c_2 = c_3 = 0$.

20.4.3 Non-linear solutions: Newton's methods

The command language programming instructions may also be used to solve non-linear problems. For example, the steady-state set of non-linear algebraic equations given by the residual equation

$$\mathbf{r}^{(k)} = \mathbf{f} - \mathbf{P}(\mathbf{a}^{(k)}) \tag{20.14}$$

in which $\mathbf{P}$ is a non-linear function of $\mathbf{a}$ is considered. A solution may be obtained by writing a linear approximation for the residual at $k+1$ as

$$\mathbf{r}^{(k+1)} \approx \mathbf{r}^{(k)} - \mathbf{K}_T^{(k)} \Delta\mathbf{a}^{(k)} = \mathbf{0} \tag{20.15}$$

in which $\mathbf{K}_T$ is some non-singular coefficient matrix used to obtain the increments $\Delta\mathbf{a}_{(k)}$. Now the update for $\mathbf{a}_{(k+1)}$ using Eq. (20.2) will not in general make $\mathbf{r}^{(k+1)}$ zero in one iteration.

A common method to generate the coefficient matrix is Newton's method where

$$\mathbf{K}_T^{(k)} = \frac{\partial \mathbf{P}}{\partial \mathbf{a}}\Big|_{\mathbf{a}=\mathbf{a}^{(k)}} \tag{20.16}$$

When properly implemented the norm of the residual should converge at a quadratic asymptotic rate. Thus if $||\mathbf{r}||$ is the norm of the residual then for an approximation close to the solution the ratios for two successive iterations should be

$$\frac{||\mathbf{r}^{(k)}||}{||\mathbf{r}^{(0)}||} = C_1 10^{-q}; \qquad \frac{||\mathbf{r}^{(k+1)}||}{||\mathbf{r}^{(0)}||} = C_2 10^{-2q} \tag{20.17}$$

In general, this is the best one can obtain with the type of algorithm given by Eq. (20.15).

In *FEAPpv* a norm of the solution is computed for each iteration and a check of the current norm versus the initial value is performed as indicated in Eq. (20.17). Once the value of the ratio of the norm is below a specified tolerance, convergence is assumed. The solution tolerance is set using the command language instruction TOL as indicated in Table 20.5 (the default value for the norm is 10^{-12}). The instructions to perform a solution using the algorithm indicated in Eq. (20.15) is given by

```
LOOP,iteration,10     ! Perform a maximum of 10 iterations
  TANG,,1             ! Compute tangent, residual and solve
NEXT,iteration        ! End for LOOP instruction
```

Once the ratio of the norms is reached, *FEAPpv* will exit the iteration loop and execute the instruction following the NEXT statement. If the element module used has a tangent matrix computed using Eq. (20.16) the asymptotic behaviour of Newton's method should be attained. Failure to achieve a quadratic rate of convergence during the last few iterations indicates an incorrect implementation in the element module, a data input error, or extreme sensitivity in the formulation such that round-off prevents the asymptotic rate being reached. One can never achieve convergence beyond that where the round-off limit is reached.

An alternative to the above program is the modified solution method in which the tangent is used from an earlier state. For example, the command language instruction set

```
TANG                  ! Compute tangent
LOOP,iteration,10     ! Perform a maximum of 10 iterations
  FORM                ! Compute residual
  SOLVe               ! Solve equations
NEXT,iteration        ! End for LOOP instruction
```

executes a modified Newton's algorithm and, for general non-linear systems, results in less than a quadratic asymptotic rate of convergence (generally linear or less, so that if iteration k gives a ratio of order 10^{-p}, iteration $k+1$ gives about $10^{-(p+1)}$).

The execution of each TANG, UTAN, FORM, etc. instruction uses the current problem type and time increment to define the parameters c_i along with the current solution values for $\mathbf{a}^{(k)}$, $\dot{\mathbf{a}}^{(k)}$ and $\ddot{\mathbf{a}}^{(k)}$ to calculate a tangent, residual, etc., respectively.

Many additional solution algorithms may be established using the commands available in the program. Some of these are discussed in the user manual where topics ranging from time-dependent loading to general transient, non-linear solution strategies included in *FEAPpv* are described. Authors may be found in Volume 2.

20.4.4 Programming command language statements

The command language module for *FEAPpv* is contained in a set of subprograms whose names begin with PMAC. The routine PMACR calls the other routines and establishes the limits on the number of commands available to the program. Included

```
      SUBROUTINE UMACR1(LCT,CTL,PRT)
      IMPLICIT   NONE

C     Inputs:
C       LCT    - Command character parameters
C       CTL(3) - Command numerical parameters
C       PRT    - Flag, output if true

C     Outputs:
C       N.B. Users are responsible for command actions.

      IMPLICIT  NONE

      LOGICAL   PCOMP,PRT
      CHARACTER LCT*15
      REAL*8    CTL(3)

      CHARACTER      UCT*4
      COMMON /UMAC1/ UCT

C     Set command word to user selected name

      IF(PCOMP(UCT,'MAC1',4)) THEN
        UCT = 'xxxx'
        RETURN
      ELSE
C       Implement user solution step
      ENDIF

      END
```

Fig. 20.7 Structure of a user command subprogram.

in the current command list is an option to access a set of user subprograms named UMACRn where n ranges from 1 to 5. Each user subprogram has a structure as shown in Fig. 20.7. A user is required to select a four character name for xxxx which does not already exist in the command list in PMACR and to program the desired solution step.

It should be noted that all arrays identified in the subprogram PALLOC can be accessed directly using the data management system described in Sec. 20.3. In addition data may be assigned to space in memory using the TEMPn array names that are also available in PALLOC. Thus it is not necessary to pass the names of arrays through the argument list of the subprograms UMACRn. Quite general routines can be created using these routines; however, if a more involved command is deemed necessary by a user the routines PMACRn may be modified to add additional instructions. This is not an option which should be considered without a thorough study of the new solution option needed, as well as, options already available in the commands included.

If it is decided to modify the PMACRn routines it is necessary to:

1. Increase the size of the WD array in subprogram PMACR by the number of commands to be added.

2. Add the new command name to the list in the data statement for WD in subprogram PMACR noting which of the routines PMACRn will have the solution module added (the continue labels indicate the value of n).
3. Increase the value of the variable NWDn in the data statement by the number of commands added for each n.
4. Add the solution module to the subprograms PMACRn. This requires either a modification of a GO TO or an IF-THEN-ELSE program form in addition to adding the statements.

Again users are reminded that extreme care must be exercised when adding commands in this way. Despite the fact that each command involves a specific solution step or steps there are some interactions between instructions that exist. If these are changed in any way the program may not function properly after new commands are added. This is particularly true for setting the parameters NWDn since if these are not correct transfer to incorrect locations in the list can occur.

20.5 Computation of finite element solution modules

20.5.1 Localization of element data

When we want to compute an element array, e.g., an element stiffness matrix, **S**, or an element load or residual vector, **P**, we only need those quantities associated with the one element in question. The nodal and material quantities that are required can be determined from the node and material set numbers stored in the IX array for each element. In the program *FEAPpv* the necessary values are moved from each global array to a set of local arrays before the appropriate element routine, ELMTnn, is called. The process will be called *localization*. The quantities that are localized are:

1. nodal coordinates which are stored in the local array XL(NDM,NEN);
2. nodal displacements, displacement increments, velocity and acceleration which are stored in the array UL(NDF,NEN,5);
3. nodal T-variables which are stored in the array TL(NEN);
4. equation numbers for assembly which are stored in the destination array LD(NEN).

The LD array described in Step 4 above is used to map the element arrays to the global arrays. Accordingly, for the following element array:

$$[LD(1) \quad LD(2) \quad LD(3) \quad \cdots] \begin{bmatrix} S(1,1) & S(1,2) & S(1,3) & \cdots \\ S(2,1) & S(2,2) & \cdots & \cdots \\ \vdots & \vdots & & \end{bmatrix} \begin{bmatrix} P(1) \\ P(2) \\ \vdots \end{bmatrix}$$

the term S(i,j) would be assembled into the global coefficient array (e.g., stiffness matrix) in the position corresponding to row LD(i) and column LD(j). Similarly, P(i) would be assembled into the position corresponding to the LD(i) value. That is, the LD array contains the equation numbers of the global arrays. The LD(i) assignment of the degrees of freedom for each node is made using the data stored in the ID(j,k,2) array as shown in Table 20.2.

The localization process is the same for every type of finite element and is performed in the subprogram PFORM, which organizes all computations associated with elements using the connections given in the IX array. The maximum number of nodes actually connected to an element is determined and assigned to the parameter NEL, which may be less than the maximum NEN, and is determined by finding the largest non-zero entry in the IX array for each element number. Intermediate zero values are interpreted as no node connected. In this way *FEAPpv* permits the mixing of elements with different numbers of connected nodes, e.g., three-noded triangles can be mixed with four-noded quadrilaterals. Also different types of elements can be mixed such as two-noded shell elements with four-noded quadrilaterals.

Since the current value of the nodal displacements and their increments, as well as the nodal velocities and accelerations for transient problems, is localized for all element computations, the program can be used to solve non-linear problems. This is, in fact, the only additional information required over that needed to solve linear problems and will be discussed further in Volume 2.

20.5.2 Element array computations

The efficient computation of element arrays (in both programmer and computer time) is a crucial aspect of any finite element development. The development of sub-programs to evaluate element stiffness and load arrays (or for non-linear problems tangent stiffness and residual arrays) can be efficiently accomplished by a combination of appropriate numerical methods. In order to illustrate a typical development a statement of the essential steps is first given and then some details shown for the two-dimensional linear elastic problem.

A flow chart describing two alternative methods for computing a stiffness matrix is shown in Fig. 20.8. Key steps in the computation are:

1. use of appropriate numerical integration procedures;
2. use of shape function subprograms (which are the same for all problems with the same required continuity);
3. efficient organization of numerical steps.

Gauss–Legendre quadrature formulae are usually utilized to compute element arrays since they provide the highest accuracy for a given number of integration points (see Chapter 9). In some instances it is desirable to use other formulae. For example, if a quadrature formula which samples only at nodes is used, the evaluation of an inertial term leads to a diagonal mass matrix which is more efficient in explicit dynamics calculations.

Shape function subprograms allow a programmer to develop elements for many problems quickly and reliably. A shape function subprogram should evaluate both the shape functions and their derivatives with respect to the global coordinate frame. As an example consider the two-dimensional C_0 problem where we need only first derivatives of each shape function N_i. For the four-noded isoparametric quadrilateral we have

$$N_i = \tfrac{1}{4}(1 + \xi_i \xi)(1 + \eta_i \eta) \tag{20.18}$$

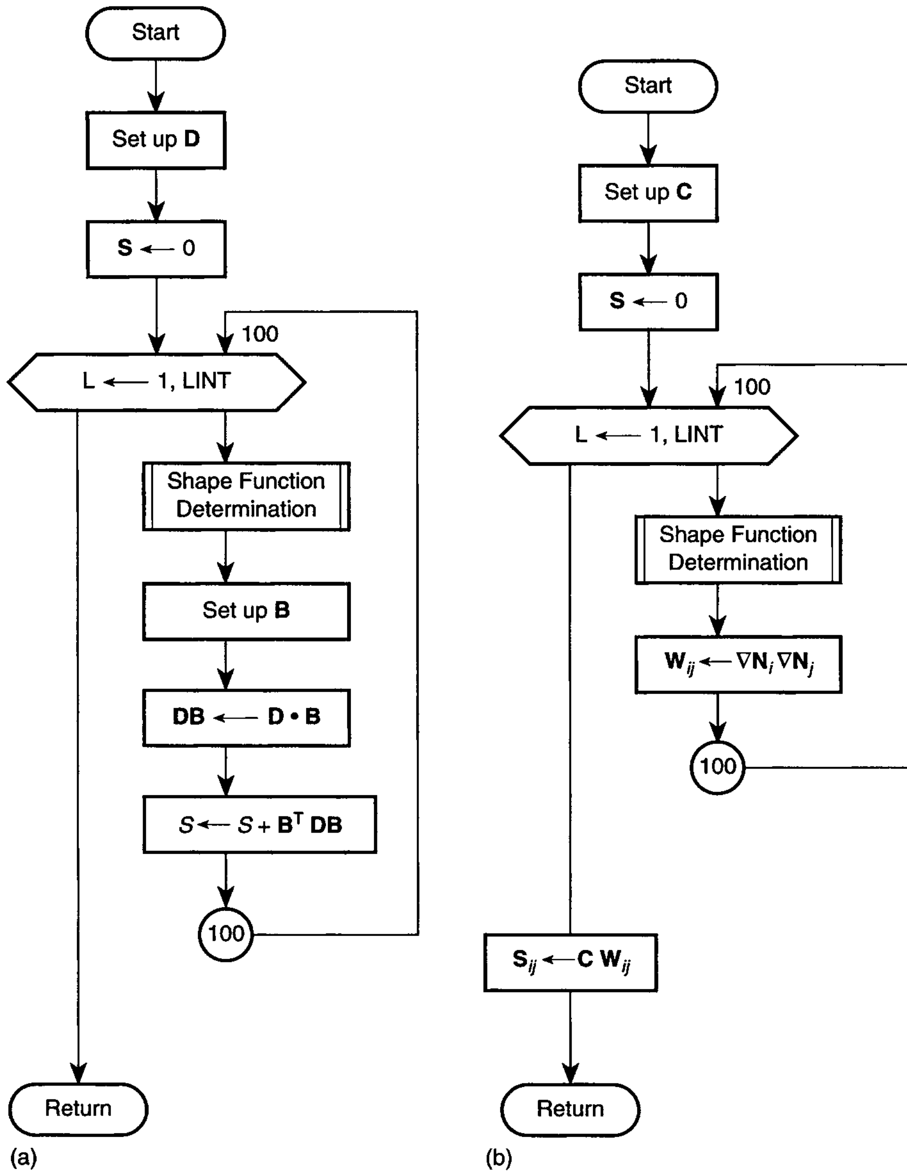


Fig. 20.8 Element stiffness matrix computation: (a) general form; (b) form for constant material properties.

where ξ, η are natural coordinates on the bi-unit square parent element and ξ_i, η_i their values at the four nodes.

Using the isoparametric concept we have

$$x = N_i x_i$$
$$y = N_i y_i \tag{20.19}$$

with derivatives given by

$$\begin{Bmatrix} N_{i,\xi} \\ N_{i,\eta} \end{Bmatrix} = \begin{bmatrix} x_{,\xi} & y_{,\xi} \\ x_{,\eta} & y_{,\eta} \end{bmatrix} \begin{Bmatrix} N_{i,x} \\ N_{i,y} \end{Bmatrix} \tag{20.20}$$

$$\begin{Bmatrix} N_{i,x} \\ N_{i,y} \end{Bmatrix} = \frac{1}{J} \begin{bmatrix} y_{,\eta} & -y_{,\xi} \\ -x_{,\eta} & x_{,\xi} \end{bmatrix} \begin{Bmatrix} N_{i,\xi} \\ N_{i,\eta} \end{Bmatrix} \tag{20.21}$$

where J is the jacobian determinant and $(\ )_{,x}$ denotes the partial derivative $\partial(\ )/\partial x$, etc. The above relations define the steps for the shape function subprogram given in Fig. 20.9 where it is assumed that the nodal coordinates have been transferred to the local coordinate array XL.

This shape function routine can be used for all two-dimensional C_0 problems which use the four-noded element (e.g., two-dimensional plane and axisymmetric elasticity, heat conduction, flow in porous media, fluid flow, etc.). Shape function subprograms can also be used for the generation of mesh data.[4] It is a simple task to extend the shape function routine to higher order elements (e.g., see the listing for subprogram SHAP2 in *FEAPpv* which includes options for up to nine-node quadrilaterals). Using such routines permits the use of elements which have individual edges with either linear or quadratic interpolation.

The generation of the matrix products occurring in the stiffness matrix of elasticity problems deserves special attention since zeros often exist in the **B** and **D** matrices. Several methods can be used to reduce the number of operations performed. The first is to form explicitly the matrix products. While this involves extra hand computations it is in fact elementary if performed on a nodal basis. For example, consider the two-dimensional axisymmetric linear elastic problem where

$$\mathbf{B}_i = \begin{bmatrix} N_{i,r} & 0 \\ 0 & N_{i,z} \\ cN_i/r & 0 \\ N_{i,z} & N_{i,r} \end{bmatrix} \tag{20.22}$$

A two-dimensional plane problem may be considered by replacing r, z by x, y and setting the constant c to zero. For axisymmetry the constant c is unity. For an isotropic linear elastic material the moduli are given by

$$\mathbf{D} = \begin{bmatrix} D_{11} & D_{12} & D_{12} & 0 \\ D_{12} & D_{11} & D_{12} & 0 \\ D_{12} & D_{12} & D_{11} & 0 \\ 0 & 0 & 0 & D_{33} \end{bmatrix} \tag{20.23}$$

where D_{33} is the shear modulus given by $(D_{11} - D_{12})/2$. Thus for a typical nodal pair i and j a contribution to the element stiffness $\mathbf{K}_{ij}$ may be computed using

$$\mathbf{Q}_j = \mathbf{D}\mathbf{B}_j \tag{20.24}$$

and

$$\mathbf{K}_{ij} = \mathbf{B}_i^{\mathrm{T}}\mathbf{Q}_j \tag{20.25}$$

```
      SUBROUTINE SHAPE(SS,XL, J,SHP)

C     Shape function routine for 4-node quadrilateral

      IMPLICIT NONE

      INTEGER II   ,JJ    ,KK
      REAL*8  SS(2),XL(2,4),J,SHP(3,4),SI(4),TI(4),XS(2,2),TEMP
      DATA    SI / -0.5D0,  0.5D0, 0.5D0, -0.5D0/
      DATA    TI / -0.5D0, -0.5D0, 0.5D0,  0.5D0/

C     Compute shape functions and natural coordinate derivatives

      DO II = 1,4
        SHP(1,II) = SI(II)*(0.5D0 + TI(II)*SS(2))
        SHP(2,II) = TI(II)*(0.5D0 + SI(II)*SS(1))
        SHP(3,II) = (0.5D0 + SI(II)*SS(1))*(0.5D0 + TI(II)*SS(2))
      END DO ! II

C     Compute Jacobian and Jacobian determinant

      DO II = 1,2
        DO JJ = 1,2
          XS(II,JJ) = 0.0D0
          DO KK = 1,4
            XS(II,JJ) = XS(II,JJ) + XL(II,KK)*SHP(JJ,KK)
          END DO ! KK
        END DO ! JJ
      END DO ! II
      J = XS(1,1)*XS(2,2) - XS(1,2)*XS(2,1)

C     Transform to X,Y derivatives

      DO II = 1,4
        TEMP = ( XS(2,2)*SHP(1,II) - XS(2,1)*SHP(2,II))/J
        SHP(2,II) = (-XS(1,2)*SHP(1,II) + XS(1,1)*SHP(2,II))/J
        SHP(1,II) = TEMP
      END DO ! II

      END
```

Fig. 20.9 Shape function subprogram for four-noded element.

Thus, using Eqs (20.22) and (20.23) and setting

$$n_j = \frac{c}{r} N_j \tag{20.26}$$

we obtain

$$\mathbf{Q}_j = \begin{bmatrix} (D_{11}N_{j,r} + D_{12}n_j) & D_{12}N_{j,z} \\ (D_{12}N_{j,r} + D_{12}n_j) & D_{22}N_{j,z} \\ (D_{12}N_{j,r} + D_{11}n_j) & D_{12}N_{j,z} \\ D_{33}N_{j,z} & D_{33}N_{j,r} \end{bmatrix} \tag{20.27}$$

and finally the stiffness as

$$\mathbf{K}_{ij} = \begin{bmatrix} (N_{i,r}Q_{11} + n_i Q_{31} + N_{i,z}Q_{41}) & (N_{i,r}Q_{12} + n_i Q_{32} + N_{i,z}Q_{42}) \\ (N_{i,z}Q_{21} + N_{i,r}Q_{41}) & (N_{i,z}Q_{22} + N_{i,r}Q_{42}) \end{bmatrix} \tag{20.28}$$

Accordingly, for each nodal pair it is required to perform 21 multiplications to form each $\mathbf{K}_{ij}$, whereas formal multiplication of $B_i^{\mathrm{T}} D B_j$ including all zero operations would require 48 multiplications. When the element stiffness matrix is symmetric it is only necessary to form the upper or lower triangular parts of **K** (the other half is formed from the symmetry condition). A typical routine for the stiffness computation is given in Figs 20.10 and 20.11 where it is assumed that the quadrature points are available as `SG(1,L)` equal to ξ_L, `SG(2,L)` equal to η_L, and `SG(3,L)` equal to the quadrature weight.

The increments by `NDF` are to keep the stiffness array stored in nodal order with `NDF`×`NDF` submatrix blocks. This is required by *FEAPpv* to maintain proper compatibility with the routine used to assemble the global arrays.

```
      SUBROUTINE ELSTIF(D, XL, AXI, NDF,NDM,NST, S)
      IMPLICIT   NONE

      LOGICAL    AXI
      INTEGER    II,I1, JJ,J1, L, LINT, NDF,NDM,NST
      REAL*8     DV, D11,D12,D33, J, R
      REAL*8     D(*), XL(NDM,4), S(NST,NST)
      REAL*8     SG(3,4), SHP(3,4), Q(4,2), N(4)

      CALL INT2D(2,LINT, SG) ! Set up 2x2 quadrature points

c     Do numerical integration

      DO L = 1,LINT
        CALL SHAPE(SG(1,L),XL, J,SHP)
        DV = J*SG(3,L)          ! SG(3,L) is quadrature weight
        D11 = D(1)*DV           ! D(1) is D_11 modulus
        D12 = D(2)*DV           ! D(2) is D_12 modulus
        D33 = D(3)*DV           ! D(3) is shear modulus

c       Compute n_i = c*N_i/r

        R = 0.0D0               ! R is radius
        DO II = 1,4
          R = R + SHP(3,II)*XL(1,II)
        END DO ! II
        DO II = 1,4
          IF(AXI) THEN
            N(II) = SHP(3,II)/R
          ELSE
            N(II) = 0.0D0
          ENDIF
        END DO ! II
```

Fig. 20.10 Element stiffness calculation. Part 1.

```
c    Compute Q_j = D * B_j

     J1 = 1
     DO JJ = 1,4
       Q(1,1) = D11*SHP(1,JJ) + D12*N(JJ)
       Q(2,1) = D12*SHP(1,JJ) + D12*N(JJ)
       Q(3,1) = D12*SHP(1,JJ) + D11*N(JJ)
       Q(4,1) = D33*SHP(2,JJ)
       Q(1,2) = D12*SHP(2,JJ)
       Q(2,2) = D11*SHP(2,JJ)
       Q(3,2) = D12*SHP(2,JJ)
       Q(4,2) = D33*SHP(1,JJ)

c      Compute stiffness term: k_ij

       I1 = 1
       DO II = 1,JJ
        S(I1  ,J1  ) = S(I1  ,J1  ) + SHP(1,II)*Q(1,1)+N(II)*Q(3,1)
    &                               + SHP(2,II)*Q(4,1)
        S(I1  ,J1+1) = S(I1  ,J1+1) + SHP(1,II)*Q(1,2)+N(II)*Q(3,2)
    &                               + SHP(2,II)*Q(4,2)
        S(I1+1,J1  ) = S(I1+1,J1  ) + SHP(2,II)*Q(2,1)
    &                               + SHP(1,II)*Q(4,1)
        S(I1+1,J1+1) = S(I1+1,J1+1) + SHP(2,II)*Q(2,2)
    &                               + SHP(1,II)*Q(4,2)
        I1 = I1 + NDF
       END DO ! II
       J1 = J1 + NDF
      END DO ! JJ
    END DO ! L

c   Compute lower part by symmetry

    DO II = 1,NST
      DO JJ = 1,II
        S(II,JJ) = S(JJ,II)
      END DO ! JJ
    END DO ! II

    END
```

Fig. 20.11 Element stiffness calculation. Part 2.

An extension to anisotropic problems can be made by replacing the isotropic **D** matrix by the appropriate anisotropic one and then recomputing the $\mathbf{Q}_j$ matrix.

The computation of element stiffness matrices for two-dimensional plane and three-dimensional problems which have constant material properties within an element can be made more efficient than that given above. This is obtained by

noting from Appendix B that the internal energy may be written in indicial form as

$$W(\mathbf{u}) = \tfrac{1}{2}\tilde{u}^i_a D_{abcd} \int_{V_e} N_{i,b} N_{j,d} \, \mathrm{d}V \, u^j_c \tag{20.29}$$

where a, b, c, d are indices from the elasticity equations and range over the space dimension of the problem and i, j are nodal indices which range from 1 to NEL in each element. The element stiffness for the nodal pair i, j may be written as

$$\mathbf{K}^{ij}_{ac} = W^{ij}_{bd} D_{abcd} \tag{20.30}$$

where

$$W^{ij}_{bd} = \int_{V_e} N_{i,b} N_{j,d} \, \mathrm{d}V \tag{20.31}$$

For isotropic materials

$$D_{abcd} = \lambda \delta_{ab} \delta_{cd} + \mu(\delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}) \tag{20.32}$$

where λ and μ are the Lamé elastic constants which are related to the usual elastic constants E and μ as

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}; \qquad \mu = \frac{E}{2(1+\nu)}$$

Thus, the stiffness matrix for an isotropic material is given as

$$K^{ij}_{ac} = \lambda W^{ij}_{ac} + \mu(W^{ij}_{ca} + \delta_{ac} W^{ij}_{bb}) \tag{20.33}$$

Using this approach the steps to compute the element stiffness matrix for plane elasticity are given in Fig. 20.8(b). This procedure for computing stiffness matrices was noted in reference 5 and for plane problems results in about 25% fewer numerical operations than the procedure shown in Fig. 20.8(a). In three dimensions the savings are even greater.

The computation of other element arrays can also be performed using a shape function routine. For example, the computation of the element consistent and diagonal mass matrices by the row sum method (see Appendix I) for transient or eigenvalue computations can be easily constructed. The consistent mass matrix for two- and three-dimensional problems is obtained from

$$\mathbf{M}_{ij} = \mathbf{I} \int_{V_e} \rho N_i N_j \, \mathrm{d}V \tag{20.34}$$

whereas the diagonal mass is computed from

$$\mathbf{M}_{jj} = \mathbf{I} \int_{V_e} \rho N_j \, \mathrm{d}V \tag{20.35}$$

In the above $\mathbf{I}$ is an identity matrix of size NDM and ρ is the mass density. A set of statements to compute the mass matrix for these cases is shown in Fig. 20.12 where the element consistent mass is stored in the square matrix **S** and the diagonal mass matrix is stored in the rectangular array **P**.

The shape function routine may also be used to compute strains, stresses and internal forces in an element. The strains at each point in an element may be

```
C    S(NST,NST) : Consistent mass array
C    P(NDM,NEL) : Diagonal mass array

C    Numerical integration loop

     DO L = 1,LINT
       CALL SHAPE(SG(1,L), XL, J, SHP)
       DMASS = RHO*J*SG(3,L)
       J1 = 1
       DO JJ = 1,NEL
         JMASS   = DMASS*SHP(3,JJ)
         P(1,JJ) = P(1,JJ) + JMASS
         I1 = 1
         DO II = 1,NEL
           S(I1,J1) = S(I1,J1) + SHP((3,II)*JMASS
           I1       = I1 + NDF
         END DO ! II
       J1 = J1 + NDF
       END DO ! JJ
     END DO ! L

C    Copy using identity matrix

     J1 = 0
     DO JJ = 1,NEL
       DO KK = 2,NDM
         P(KK,JJ) = P(1,JJ)
       END DO ! KK
       I1 = 0
       DO II = 1,NEL
         DO KK = 2,NDM
           S(I1+KK,J1+KK) = S(I1+1,J1+1)
         END DO ! KK
         I1 = I1 + NDF
       END DO ! II
       J1 = J1 + NDF
     END DO ! JJ
```

Fig. 20.12 Diagonal (lumped) and consistent mass matrix for an isoparametric element.

computed from

$$\boldsymbol{\varepsilon} = \mathbf{B}_i(\boldsymbol{\xi})_i\tilde{\mathbf{u}}_i \tag{20.36}$$

where $\boldsymbol{\xi}$ is the set of local natural coordinates and $\tilde{\mathbf{u}}_i$ are the nodal displacements at node i. A subprogram to compute the strains for the two-dimensional case given by Eq. (20.22) is shown in Fig. 20.13. Stresses are now computed as usual from

$$\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon} \tag{20.37}$$

or any other relationship expressed in terms of the strains. The above form is more general and efficient than saving the values in the $\mathbf{Q}_i$ matrices during stiffness

```
      SUBROUTINE STRAIN(XL, UL, SHP, NDM,NDF,NEN,NEL, EPS,R, AXI)

      IMPLICIT NONE

      LOGICAL  AXI
      INTEGER  NDM,NDF,NEN,NEL, II
      REAL*8   XL(NDM,*),UL(NDF,NEN,*),SHP(3,*), EPS(4),R

C     Initialize strains and radius

      DO II = 1,4
        EPS(II) = 0.0D0
      END DO ! II
      R = 0.0D0

C     Sum strains from shape functions and nodal values

      DO II = 1,NEL
        EPS(1) = EPS(1) + SHP(1,II)*UL(1,II,1)
        EPS(2) = EPS(2) + SHP(2,II)*UL(2,II,1)
        EPS(3) = EPS(3) + SHP(3,II)*UL(1,II,1)
        EPS(4) = EPS(4) + SHP(1,II)*UL(2,II,1) + SHP(2,II)*UL(1,II,1)
        R      = R      + SHP(3,II)*XL(1,II)
      END DO ! II

C     Modify hoop strain if axisymmetric; zero for plane problem

      IF(AXI) THEN
        EPS(3) = EPS(3)/R
      ELSE
        EPS(3) = 0.0D0
      ENDIF

      END
```

Fig. 20.13 Strain calculation for isoparametric element.

evaluation and then computing the stresses from

$$\boldsymbol{\sigma} = \mathbf{D}\mathbf{B}_i\tilde{\mathbf{u}}_i = \mathbf{Q}_i\tilde{\mathbf{u}}_i \tag{20.38}$$

This would require significant additional storage or saving and retrieving the $\mathbf{Q}_i$ from backing store as given in reference 6. Moreover, it is often desirable to compute the stresses at points other than those used to compute the stiffness matrix as indicated in Chapter 14 for recovery processes. In non-linear problems the computation of strains and stresses must also be performed directly. Thus, for all the above reasons it is desirable to compute strains as necessary using the technique given in Fig. 20.13.

In *FEAPpv* the stresses must also be determined to compute element residuals. One of the main terms in the element residual is the internal stress term and here again shape function routines are useful. The internal force term for problems in elasticity (and, as will be shown in the Volume 2, also for finite deformation inelastic

```
C     Quadrature loop

      DO L = 1,LINT

C       Compute shape functions

        CALL SHAPE(SG(1,L), XL, J, SHP)
        DV = J*SG(3,L)

C       Compute strains

        CALL STRAIN(XL, UL, SHP, NDM,NDF,NEN,NEL, EPS,R, AXI)
        DO II = 1,NEL
          IF(AXI) THEN
            N(II) = SHP(3,II)/R
          ELSE
            N(II) = 0.0D0
          ENDIF
        END DO ! II

C       Compute stresses

        CALL STRESS(EPS, SIG)

C       Compute internal forces

        DO II = 1,NEL
          P(1,II) = P(1,II) - (SHP(1,II)*SIG(1) + SHP(2,II)*SIG(4)
    &                        + N(II)*SIG(3))*DV
          P(2,II) = P(2,II) - (SHP(2,II)*SIG(2) + SHP(1,II)*SIG(4))*DV
        END DO ! II
      END DO ! L
```

Fig. 20.14 Internal force computation.

problems) is given by

$$\mathbf{P}_i = -\int_{V_e} \mathbf{B}_i^{\mathrm{T}} \boldsymbol{\sigma}\, \mathrm{d}V \tag{20.39}$$

The programming steps to compute are given in Fig. 20.14.

The generality of an isoparametric C_0 shape function routine can be exploited to program element routines for other problems. For example, Fig. 20.15 gives the necessary program instructions to compute the 'stiffness' matrix for problems of the quasi-harmonic equation discussed in Chapters 3 and 7.

20.5.3 Organization of element routines

The previous discussion has focused on procedures for determining element arrays. The reader will note that the element square matrices for stiffness and mass were

```
C     Quadrature loop

      DO L = 1,LINT

C       Compute shape functions

        CALL SHAPE(SG(1,L), XL, J, SHP)
        DV = J*SG(3,L)
        KK = D(1)*DV   ! Conductivity times volume

C       For each JJ-node compute the D*B

        DO JJ = 1,NEL
          DO KK = 1,NDM
            Q(KK) = D1*SHP(KK,JJ)
          END DO ! KK

C         For each II-node compute the coefficient matrix

          DO II = 1,JJ
            DO KK = 1,NDM
              S(II,JJ) = S(II,JJ) + SHP(KK,II)*Q(KK)
            END DO ! KK
          END DO ! II
        END DO ! JJ

      END DO ! L
```

Fig. 20.15 Coefficient matrix for quasi-harmonic operator.

both stored in the square array **S** while element vectors were stored in the rectangular array **P**. This was intentional since all aspects of computing element arrays for the program are to be consolidated into a single subprogram called the *element routine*. An element routine is called by the element library subprogram ELMLIB. As given here, the element library provides space for ten element subprograms at any one time, where as noted previously these are named ELMTnn with nn ranging from 01 to 10. This can easily be increased by modifying the subprogram ELMLIB. The subprogram ELMLIB is, in turn, called from the subprogram PFORM which is the routine to loop through all elements and perform the localization step to set up local coordinates XL, displacements, etc., UL and equation numbers for global assembly LD. The subprogram PFORM also uses subprogram DASBLE to assemble element arrays into global arrays and uses subprogram MODIFY to perform appropriate modifications for prescribed non-zero displacements. When an element routine is accessed the value of a parameter ISW is given a value between 1 and 10. The parameter specifies what action is to be performed in the element routine. Each element routine must provide appropriate transfers for each value of ISW. A mock element routine for *FEAPpv* is shown in Fig. 20.16.

```
      SUBROUTINE ELMTnn(D,UL,XL,IX,TL, S,P, NDF,NDM,NST, ISW)

      IMPLICIT   NONE

      INTEGER    NDF,NDM,NST, ISW, IX(NEN1,*)
      REAL*8     D(*),UL(NDF,NEN,*),XL(NDM,*),TL(*), S(NST,*),P(NDF,*)

C     Input and output material set data
      IF(ISW.EQ.1) THEN
        Use D(*) to store input parameters
C     Check element for errors
      ELSEIF(ISW.EQ.2) THEN
        Check element for negative jacobians, etc.
C     Form element coefficient matrix and residual vector
      ELSEIF(ISW.EQ.3 .OR. ISW.EQ.6) THEN
        The S(NST,NST) array stores coefficient matrix
        The P(NDF,NEL) array stores residual vector
C     Output element results (e.g., stress, strain, etc.)
      ELSEIF(ISW.EQ.4) THEN

C     Compute element mass arrays
      ELSEIF(ISW.EQ.5) THEN
        The S(NST,NST) array stores consistent mass
        The P(NDF,NEL) array stores lumped mass
C     Compute element error estimates
      ELSEIF(ISW.EQ.7) THEN

C     Project element results to nodes
      ELSEIF(ISW.EQ.8) THEN

C     Project element error estimator
      ELSEIF(ISW.EQ.9) THEN

C     Augmented lagragian update
      ELSEIF(ISW.EQ.10) THEN

      ENDIF

      END
```

Fig. 20.16 Mock element routine functions.

20.6 Solution of simultaneous linear algebraic equations

A finite element problem leads to a large set of simultaneous linear algebraic equations whose solution provides the nodal and element parameters in the formulation. For example, in the analysis of linear steady-state problems the direct assembly of the element coefficient matrices and load vectors leads to a set of linear algebraic equations. In this section methods to solve the simultaneous algebraic equations are summarized. We consider both *direct* methods where an *a priori* calculation of

the number of numerical operations can be made, and *indirect or iterative* methods where no such estimate can be made.

20.6.1 Direct solution

Consider first the general problem of direct solution of a set of algebraic equations given by

$$\mathbf{K}\mathbf{a} = \mathbf{b} \tag{20.40}$$

where $\mathbf{K}$ is a square coefficient matrix, $\mathbf{a}$ is a vector of unknown parameters and $\mathbf{b}$ is a vector of known values. The reader can associate these with the quantities described previously: namely, the stiffness matrix, the nodal unknowns, and the specified forces or residuals.

In the discussion to follow it is assumed that the coefficient matrix has properties such that row and/or column interchanges are unnecessary to achieve an accurate solution. This is true in cases where $\mathbf{K}$ is symmetric positive (or negative) definite.† Pivoting may or may not be required with unsymmetric, or indefinite, conditions which can occur when the finite element formulation is based on some weighted residual methods. In these cases some checks or modifications may be necessary to ensure that the equations can be solved accurately.[7–9]

For the moment consider that the coefficient matrix can be written as the product of a lower triangular matrix with unit diagonals and an upper triangular matrix. Accordingly,

$$\mathbf{K} = \mathbf{L}\mathbf{U} \tag{20.41}$$

where

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ L_{21} & 1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ L_{n1} & L_{n2} & \cdots & 1 \end{bmatrix} \tag{20.42}$$

and

$$\mathbf{U} = \begin{bmatrix} U_{11} & U_{12} & \cdots & U_{1n} \\ 0 & U_{22} & \cdots & U_{2n} \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & U_{nn} \end{bmatrix} \tag{20.43}$$

† For mixed methods which lead to forms of the type given in Eq. (11.14) the solution is given in terms of a positive definite part for $\tilde{\mathbf{q}}$ followed by a negative definite part for $\tilde{\boldsymbol{\phi}}$. Thus, interchanges are not needed providing the ordering of the equation is defined as described in Sec. 20.2.4.

This form is called a *triangular decomposition* of **K**. The solution to the equations can now be obtained by solving the pair of equations

$$\mathbf{Ly} = \mathbf{b} \tag{20.44}$$

and

$$\mathbf{Ua} = \mathbf{y} \tag{20.45}$$

where $\mathbf{y}$ is introduced to facilitate the separation, e.g., see references 7–11 for additional details.

The reader can easily observe that the solution to these equations is trivial. In terms of the individual equations the solution is given by

$$\begin{aligned} y_1 &= b_1 \\ y_i &= b_i - \sum_{j=1}^{i-1} L_{ij} y_j \qquad i = 2, 3, \ldots, n \end{aligned} \tag{20.46}$$

and

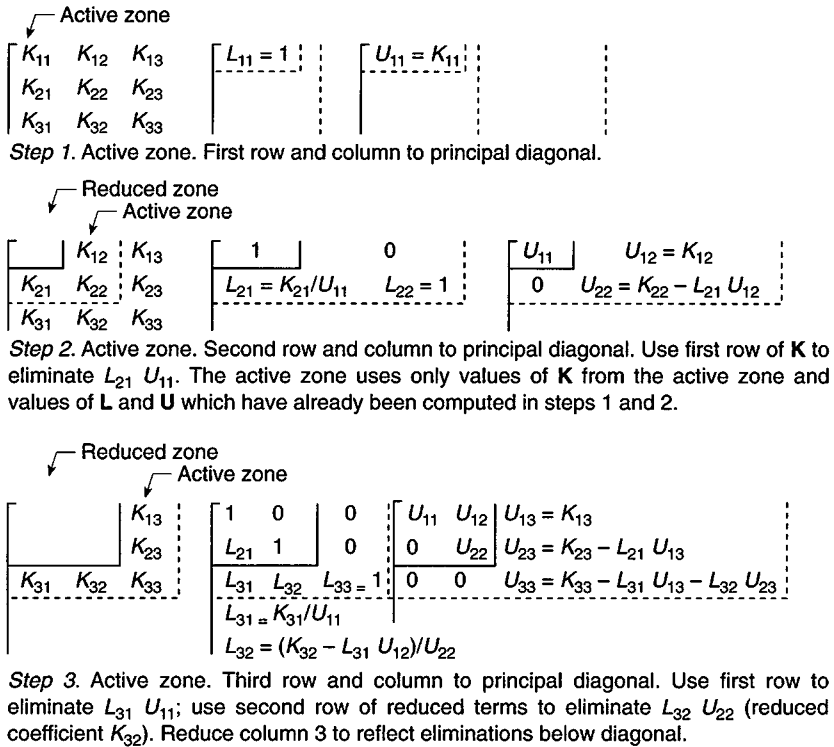
$$\begin{aligned} a_n &= \frac{y_n}{U_{nn}} \\ a_i &= \frac{1}{U_{ii}} \left(y_i - \sum_{j=i+1}^{n} U_{ij} a_j \right) \qquad i = n-2, n-3, \cdots, 1 \end{aligned} \tag{20.47}$$

Equation (20.46) is commonly called *forward elimination* while Eq. (20.47) is called *back substitution.*

The problem remains to construct the triangular decomposition of the coefficient matrix. This step is accomplished using variations on Gaussian elimination. In practice, the operations necessary for the triangular decomposition are performed directly in the coefficient array; however, to make the steps clear the basic steps are shown in Fig. 20.17 using separate arrays. The decomposition is performed in the same way as that used in the subprogram `DATRI` contained in the *FEAPpv* program; thus, the reader can easily grasp the details of the subprograms included once the steps in Fig. 20.17 are mastered. Additional details on this step may be found in references 9–11.

In `DATRI` the Crout form of Gaussian elimination is used to successively reduce the original coefficient array to upper triangular form. The lower portion of the array is used to store $\mathbf{L} - \mathbf{I}$ as shown in Fig. 20.17. With this form, the unit diagonals for $\mathbf{L}$ are not stored.

Based on the organization of Fig. 20.17 it is convenient to consider the coefficient array to be divided into three parts: part one being the region that is fully reduced; part two the region which is currently being reduced (called the active zone); and part three the region which contains the original unreduced coefficients. These regions are shown in Fig. 20.18 where the jth column above the diagonal and the jth row to the left of the diagonal constitute the active zone. The algorithm for the triangular decomposition of an $n \times n$ square matrix can be deduced from Fig. 20.17 and



Step 1. Active zone. First row and column to principal diagonal.

Step 2. Active zone. Second row and column to principal diagonal. Use first row of **K** to eliminate L_{21} U_{11}. The active zone uses only values of **K** from the active zone and values of **L** and **U** which have already been computed in steps 1 and 2.

Step 3. Active zone. Third row and column to principal diagonal. Use first row to eliminate L_{31} U_{11}; use second row of reduced terms to eliminate L_{32} U_{22} (reduced coefficient K_{32}). Reduce column 3 to reflect eliminations below diagonal.

Fig. 20.17 Triangular decomposition of **K**.

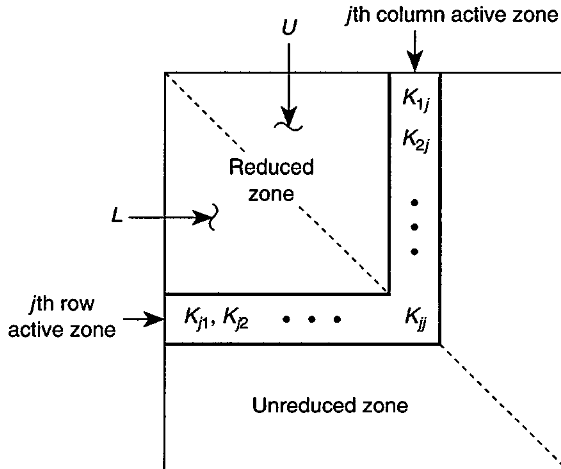


Fig. 20.18 Reduced, active and unreduced parts.

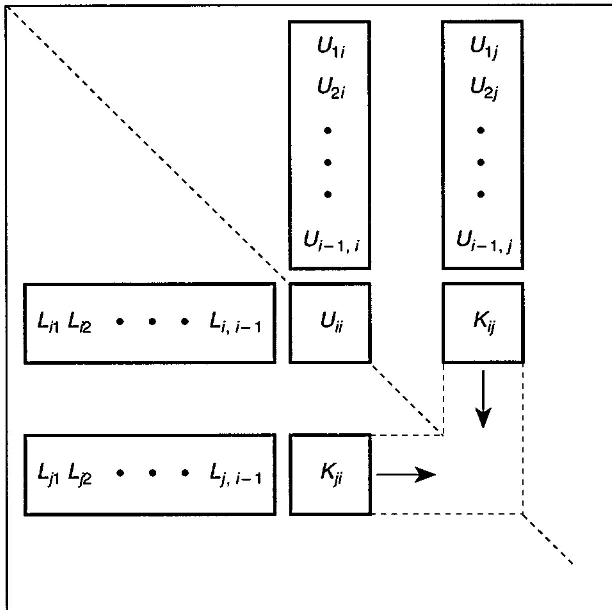


Fig. 20.19 Terms used to construct U_{ij} and L_{ji}.

Fig. 20.19 as follows:

$$U_{11} = K_{11}; \qquad L_{11} = 1 \tag{20.48}$$

For each active zone j from 2 to n,

$$L_{j1} = \frac{K_{j1}}{U_{11}}; \qquad U_{1j} = K_{1j} \tag{20.49}$$

$$\begin{aligned} L_{ji} &= \frac{1}{U_{ii}}\left(K_{ji} - \sum_{m=1}^{i-1} L_{jm}U_{mi}\right) \\ U_{ij} &= K_{ij} - \sum_{m=1}^{i-1} L_{im}U_{mj} \qquad i = 2, 3, \ldots, j-1 \end{aligned} \tag{20.50}$$

and finally

$$\begin{aligned} L_{jj} &= 1 \\ U_{jj} &= K_{jj} - \sum_{m=1}^{j-1} L_{jm}U_{mj} \end{aligned} \tag{20.51}$$

The ordering of the reduction process and the terms used are shown in Fig. 20.19. The results from Fig. 20.17 and Eqs (20.48)–(20.51) can be verified by the reader using the matrix given in the example shown in Table 20.6.

Once the triangular decomposition of the coefficient matrix is computed, several solutions for different right-hand sides **b** can be computed using Eqs (20.46) and (20.47). This process is often called a *resolution* since it is not necessary to recompute

Table 20.6 Example: triangular decomposition of 3 × 3 matrix

$$\mathbf{K} = \begin{bmatrix} 4 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 4 \end{bmatrix} \quad \mathbf{L} = \begin{bmatrix} 1 & & \\ & & \\ & & \end{bmatrix} \quad \mathbf{U} = \begin{bmatrix} 4 & & \\ & & \\ & & \end{bmatrix}$$

Step 1. $L_{11} = 1$, $U_{11} = 4$

$$\begin{bmatrix} & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 4 \end{bmatrix} \quad \begin{bmatrix} 1 & & \\ 0.5 & 1 & \\ & & \end{bmatrix} \quad \begin{bmatrix} 4 & 2 & \\ & 3 & \\ & & \end{bmatrix}$$

Step 2. $L_{21} = \frac{2}{4} = 0.5$, $U_{12} = 2$, $U_{22} = 1$, $U_{22} = 4 - 0.5 \times 2 = 3$

$$\begin{bmatrix} & & 1 \\ & & 2 \\ 1 & 2 & 4 \end{bmatrix} \quad \begin{bmatrix} 1 & & \\ 0.5 & 1 & \\ 0.25 & 0.5 & 1 \end{bmatrix} \quad \begin{bmatrix} 4 & 2 & 1 \\ & 3 & 1.5 \\ & & 3 \end{bmatrix}$$

Step 3. $L_{31} = \frac{1}{4} = 0.25$, $U_{13} = 1$, $L_{32} = \dfrac{2 - 0.25 \times 2}{3} = \dfrac{1.5}{3} = 0.5$

$U_{23} = 2 - 0.5 \times 1 = 1.5$, $L_{33} = 1$, $U_{33} = 4 - 0.25 \times 1 - 0.5 \times 1.5 = 3$

$$\begin{bmatrix} 1 & & \\ 0.5 & 1 & \\ 0.25 & 0.5 & 1 \end{bmatrix} \begin{bmatrix} 4 & 2 & 1 \\ & 3 & 1.5 \\ & & 3 \end{bmatrix} = \begin{bmatrix} 4 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 4 \end{bmatrix}$$

Step 4. Check

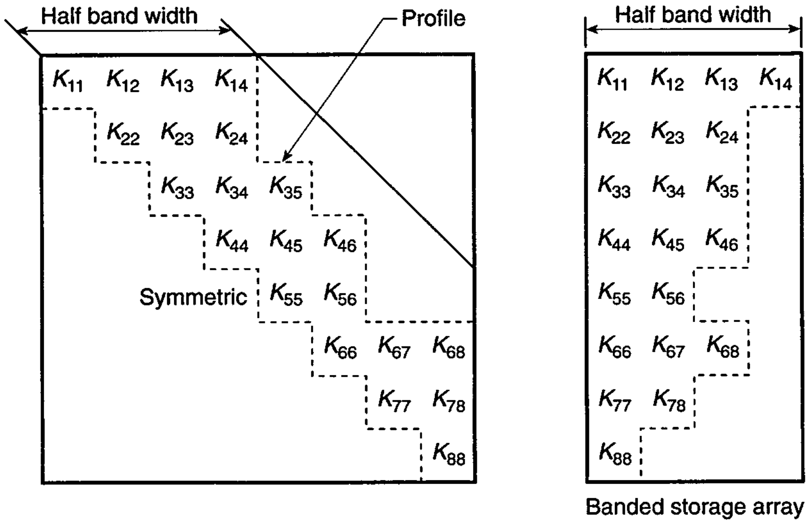
the **L** and **U** arrays. For large size coefficient matrices the triangular decomposition step is very costly while a resolution is relatively cheap; consequently, a resolution capability is necessary in any finite element solution system using a direct method.

The above discussion considered the general case of equation solving (without row or column interchanges). In coefficient matrices resulting from a finite element formulation some special properties are usually present. Often the coefficient matrix is symmetric ($K_{ij} = K_{ji}$) and it is easy to verify in this case that

$$U_{ij} = L_{ji} U_{ii} \tag{20.52}$$

For this problem class it is not necessary to store the entire coefficient matrix. It is sufficient to store only the coefficients above (or below) the principal diagonal and the diagonal coefficients. Equation (20.52) may be used to construct the missing part. This reduces by almost half the required storage for the coefficient array as well as the computational effort to compute the triangular decomposition.

The required storage can be further reduced by storing only those rows and columns which lie within the region of non-zero entries of the coefficient array. Problems formulated by the finite element method and the Galerkin process normally have a symmetric profile which further simplifies the storage form. Storing the upper and lower parts in separate arrays and the diagonal entries of **U** in a third array is used in DATRI. Figure 20.20 shows a typical *profile* matrix and the storage order adopted



I	AD_i
1	K_{11}
2	K_{22}
3	K_{33}
4	K_{44}
5	K_{55}
6	K_{66}
7	K_{77}
8	K_{88}

Diagonals

I	AU_i	AL_i
1	K_{12}	K_{21}
2	K_{13}	K_{31}
3	K_{23}	K_{32}
4	K_{14}	K_{41}
5	K_{24}	K_{42}
6	K_{34}	K_{43}
7	K_{35}	K_{53}
8	K_{45}	K_{54}
9	K_{46}	K_{64}
10	K_{56}	K_{65}
11	K_{67}	K_{76}
12	K_{18}	K_{81}
	•	•
	•	•
	•	•
18	K_{78}	K_{87}

Storage of arrays

J	JD_i
1	0
2	1
3	3
4	6
5	8
6	10
7	11
8	18

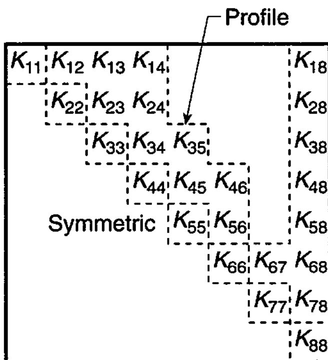


Fig. 20.20 Profile storage for coefficient matrix.

for the upper array `AU`, the lower array `AL` and the diagonal array `AD`. An integer array `JD` is used to locate the start and end of entries in each column. With this scheme it is necessary to store and compute only within the non-zero profile of the equations. This form of storage does not severely penalize the presence of a few large columns/rows and is also an easy form to program a resolution process (e.g., see subprogram `DASOL` in *FEAPpv* and reference 10).

The routines included in *FEAPpv* are restricted to problems for which the coefficient matrix can fit within the space allocated in the main storage array. In two-dimensional formulations, problems with several thousand degrees of freedom can be solved on today's personal computers. In three-dimensional cases however problems are restricted to a few thousand equations. To solve larger size problems there are several options. The first is to retain only part of the coefficient matrix in the main array with the rest saved on backing store (e.g., hard disk). This can be quite easily achieved but the size of problem is not greatly increased due to the very large solve times required and the rapid growth in the size of the profile-stored coefficient matrix in three-dimensional problems.

A second option is to use sparse solution schemes. These lead to significant program complexity over the procedure discussed above but can lead to significant savings in storage demands and compute time – especially for problems in three dimensions. Nevertheless, capacity in terms of storage and compute time is again rapidly encountered and alternatives are needed.

20.6.2 Iterative solution

One of the main problems in direct solutions is that terms within the coefficient matrix which are zero from a finite element formulation become non-zero during the triangular decomposition step. While sparse methods are better at limiting this fill than profile methods they still lead to a very large increase in the number of non-zero terms in the factored coefficient matrix. To be more specific consider the case of a three-dimensional linear elastic problem solved using eight-node isoparametric hexahedron elements. In a regular mesh each interior node is associated with 26 other nodes, thus, the equation of such a node has 81 non-zero coefficients – three for each of the 27 associated nodes. On the other hand, for a rectangular block of elements with n nodes on each of the sides the typical column height is approximately proportional to n^2 and the number of equations to n^3. In Table 20.7 we show the size and approximate number of non-zero terms in $\mathbf{K}$ from a finite formulation for linear elasticity (i.e., with three degrees of freedom per node). The table also indicates the size growth with column height and storage requirements for a direct solution based on a profile solution method.

From the table it can be observed that the demands for a direct solution are growing very rapidly (storage is approximately proportional to n^5) while at the same time the demands for storing the non-zero terms in the stiffness matrix grows proportional to the number of equations (i.e., proportional to n^3 for the block).

Iterative solution methods use the terms in the stiffness matrix directly and thus for large problems have the potential to be very efficient for large three-dimensional problems. On the other hand, iterative methods require the resolution of a set of

Table 20.7

Side nodes	Number of equations	Non-zeros in K		Profile storage data		
		Words ($\times 10^{-6}$)	Mbytes	Col. Ht.	Words ($\times 10^{-6}$)	Mbytes
5	375	0.02	0.12	90	0.03	0.27
10	3000	0.12	0.96	330	0.99	7.92
20	24000	0.96	7.68	1260	30.24	241.82
40	192000	7.68	61.44	4920	944.64	7557.12
80	1536000	61.44	491.52	18440	28323.84	226584.72

equations until the residual of the linear equations, given by

$$\mathbf{r}^{(i)} = \mathbf{b} - \mathbf{K}\mathbf{a}^{(i)} \tag{20.53}$$

becomes less than a specified tolerance.

In order to be effective the number of iterations i to achieve a solution must be quite small – generally no larger than a few hundred. Otherwise, excessive solution costs will result. At the time of writing this book the subject of iterative solution for general finite element problems remains a topic of intense research. There are some impressive results available for the case where **K** is symmetric positive (or negative) definite; however, those for other classes (e.g., unsymmetric or indefinite forms) are generally not efficient enough for reliable use in the solution of general problems.

For the symmetric positive definite case methods based on a preconditioned conjugate gradient method have been particularly effective.[12–14] The convergence of the method depends on the condition number of the matrix **K** – the larger the condition number, the slower the convergence (see reference 9 for more discussion). The condition number for a finite element problem with a symmetric positive definite stiffness matrix **K** is defined as

$$\kappa = \frac{\lambda_n}{\lambda_1} \tag{20.54}$$

where λ_1 and λ_n are the smallest and largest eigenvalue from the solution of the eigenproblem (viz. Chapter 17)

$$\mathbf{K\Phi} = \mathbf{\Phi\Lambda} \tag{20.55}$$

in which $\mathbf{\Lambda}$ is a diagonal matrix containing the individual eigenvalues λ_i and the columns of $\mathbf{\Phi}$ are the eigenvectors $_i$ associated with each of the eigenvalues.

Usually, the condition number for an elasticity problem modelled by the finite element method is too large to achieve rapid convergence and a *preconditioned conjugate* gradient (PCG) is used.[12] A symmetric form of preconditioned system is written as

$$\mathbf{K}_p\mathbf{z} = \mathbf{PKP}^{\mathrm{T}}\mathbf{z} = \mathbf{Pb} \tag{20.56}$$

where

$$\mathbf{P}^{\mathrm{T}}\mathbf{z} = \mathbf{a} \tag{20.57}$$

Now the convergence of the PCG algorithm depends on the condition number of $\mathbf{K}_p$. The problem remains to construct a preconditioner which adequately reduces

the condition number. In *FEAPpv* the diagonal of **K** is used, however, more efficient schemes incorporating also multigrid methods are discussed in references 13 and 14.

20.7 Extension and modification of computer program FEAPpv

The previous sections briefly discussed the basis for the program *FEAPpv* which is available from the publishers web site at no cost. The capabilities of the program are quite significant – mainly due to the flexibility of the command language solution strategy. However, the program can be improved in many ways. Improvements to increase the size of problems which can be solved have already been mentioned. Other improvements include additional command language statements to handle special needs of each user, preprocessors to assist in preparation of input data and postprocessors to permit a wider range of graphical output options. In the latter two instances the program GiD[3] provides features which can greatly assist users in the preparation of mesh data and the display of results†.

In order to facilitate the addition of new input features and/or new command language statements the program *FEAPpv* includes a number of options for users to add subprograms without the need to modify the PMESH or the PMACRn routines.

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† Options to acquire GiD are also provided at the publishers web sit.

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