FEAP - - A Finite Element Analysis Program

Version 8.6 Parallel User Manual

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Chapter 1

INTRODUCTION

1.1 General features

This manual describes features for the parallel version of the general purpose *Finite Element Analysis Program* (*FEAP*). It is assumed that the reader of this manual is familiar with the use of the serial version of *FEAP* as described in the basic user manual.[1] It is also assumed that the reader of this manual is familiar with the finite element method as describe in standard reference books on the subject (e.g., *The Finite Element Method*, 7th edition, by O.C. Zienkiewicz, R.L. Taylor, et al. [2, 3, 4]).

The current version of the parallel code modifies the serial version of *FEAP* to interface to the PETSc library system (version 3.13.2) available from Argonne National Laboratories.[5, 6] In addition the METIS[7] and ParMETIS[8] libraries are used to partition each mesh for parallel solution. The present parallel version of *FEAP* may only be used in a UNIX/Linux (including Mac OS X) environment and includes an integrated set of modules to perform:

1. Input of data describing a finite element model;
2. An interface to METIS[7] to perform a graph partitioning of the mesh *nodes*. A stand alone module exists to also use ParMETIS[8] to perform the graph partitioning for very large problems;
3. An interface to PETSc[5, 6, 9] to perform the parallel solution steps;
4. Construction of solution algorithms to address a wide range of applications; and
5. Graphical and numerical output of solution results.

1.2 Problem solution

The solution of a problem using the parallel versions starts from a standard input file for a serial solution. This file must contain all the data necessary to define nodal coordinate, element connection, boundary condition codes, loading conditions, and material property data. That is, if it were possible, this file must be capable of solving the problem using the serial version. However, at this stage of problem solving the only solution commands included in the file are those necessary to partition the problem for the number of processors to be used in the parallel solution steps.

1.3 Graph partitioning

To use the parallel version of *FEAP* it is first necessary to construct a standard input file for the *serial* version of *FEAP*. Preparation of this file is described in the *FEAP* User Manual.[1]

1.3.1 METIS version

After the file is constructed and its validity checked, a *serial execution* of the *parallel FEAP* program built in the `parfeap` directory may be performed. Using the `GRAPh` solution command statement followed by an `OUTDomains` solution command will generate the needed parallel execution input files. To use this option a basic form for the input file is given as:

```
FEAP * * Start record and title
  ...
Control and mesh description data
  ...
END  mesh

<Initial condition data for transient problems>

BATCh
  GRAPh node numd     ! METIS partitions 'numd' nodal domains
  OUTDomains          ! Creates 'numd' partitioned meshes
END batch
  ...
STOP
```

where the `node` on the `GRAPh` command is optional. Options for `OUTDomains` are explained below in Sect. 1.3.3 Using these commands, *METIS*[7] will split a problem into `numd` partitions by partitioning the node graph and output `numd` *input files* for a subsequent parallel solution of the problem.

The initial condition data is only required for transient solutions in which inital data is non-zero. Otherwise this data is omitted. The form of the initial condition data is described in the basic User manual.[1]

For efficiency of assembly, it is necessary to pre-allocate matrix memory requirements. In PETSc, there are two basic matrix formats: *AIJ* and *BAIJ*. By default *FEAP* stores the pre-allocation information in the partitioned input files in the *AIJ* format when using `OUTDomains`. This format is compatible with most of PETSc's solver options. However, if one wishes to use a solver that requires (or benefits) from the *BAIJ* (blocked) format, then one can issue the command

```
OUTDomains,BAIJ
```

The block size can optionally be controlled by:

```
OUTDomains,BAIJ,,<nsbk>
```

The block size `nsbk` can be any (integer) factor of `ndf` and defaults to `ndf` if not specified. Note that in the *BAIJ* format, degrees of freedom with Dirichlet boundary are included in the matrix assembly. Issuing `OUTDomains,AIJ` forces *AIJ* format. In this format it is also possible to include the degrees of freedom with Dirichlet boundary conditions in the matrix assembly (as is required for certain PETSc solvers). This is done by setting the boundary equation flag to unity:

```
OUTDomains,AIJ,1,<nsbk>
```

In this format, one can optionally provide PETSc with a hint to the equation block size `nsbk`. As with *BAIJ*, this value defaults to `ndf` if not specified.

1.3.2 ParMETIS: Parallel graph partitioning

A stand alone parallel graph partitioner also exists.[1] The parallel partitioner, `partition` (located in the `$(FEAPHOME8_4)/parfeap/partition` subdirectory), uses *ParMETIS*[8] to perform the construction of the nodal split. To use this program it is necessary to have a *FEAP* input file that contains *all* the nodal coordinate and *all* the element connection records. That is, there must be a file with the form:

[1] This is only needed for problems so large that they can not be partitioned with METIS.

```
FEAP * * Start record and title
  Control record

COORdinates
  All nodal coordinate records
  ...
ELEMent
  All element connection records
  ...
  remaining mesh statemnts
  ...
END  mesh
```

The flat form for an input file may be created from any *FEAP* input file using the solution command:

```
OUTMesh
```

This creates an input file with the same name and the extender ".`rev`". If a `TIE` mesh manipulation command is used the output mesh will remove unused nodes and renumber the node numbers.

Once the flat input file exists a parallel partitioning is performed by executing the command

```
mpirun -n nump partition numd Ifile
```

where `nump` is the number of processors that `ParMETIS` uses, `numd` is the number of mesh partitions to create and `Ifile` is the name of the flat *FEAP* input file. For an input file originally named `Ifile`, the program creates a graph file with the name `graph.file`. The graph file contains the following information:

1. The processor assignment for each node (numnp)
2. The pointer array for the nodal graph (numnp+1)
3. The adjacency lists for the nodal graph

To create the partitioned mesh input files the flat input file is used again (in the same directory containing the `graph.file`) in a *serial execution* of the parallel *FEAP* together with the solution commands

```
GRAPh FILE
OUTDomains
```

See the next section for a discussion of possible options for `OUTDomains`.

It is usually also possible to also create the `graph.file` in parallel without separately running `partition` from the command line by using the command set

```
OUTMesh
GRAPh PARTition numd
OUTDomains
```

where `numd` is the number of domains to create. For this to work the program `mpirun` must be in your path. Here, the parameter `nump` is equal to `numd`.[2] The use of the command `OUTMesh` is required to ensure that a flat input file is available and after execution it is destroyed.

1.3.3 Structure of parallel meshes

It is assumed that `numd` represents the number of processors to be used in the parallel solution. Each partition is assigned `numpn` nodes. The number can differ slightly among the various partitions but is approximately the total number of nodes in the problem divided by `numd`. In the current release, no weights are assigned to the node or the node graph edges to reflect possible differences in solution or communication effort. Each partitioned input file also contains *ghost nodes* for effecting the evaluation of element residuals. The sum of the nodes in a partition (`numpn`) and its ghost nodes defines the total number of nodes in each partitioned data file (i.e., the total number of nodes, `numnp`, in each mesh partition).

In the parallel solution the global equations are numbered sequentially from 1 to the total number of equations in the problem (`numteq`). The nodes in partition 1 are associated with the first set of equations, the nodes in partition 2 the second set, etc. For each partition, the stiffness and/or the mass matrix is also partitioned and each partition matrix has two parts: (a) a diagonal block for all the nodes in the partition (i.e., `numpn` nodes) and, (b) off diagonal blocks associated with the ghost nodes as shown in Figure 1.1. In solving a set of linear equations

$$\mathbf{K}\, d\mathbf{u} = \mathbf{R}$$

associated with an implicit solution step, the solution vector $d\mathbf{u}$ and the residual $\mathbf{R}$ are also split according to each partition. The residual for each partition contains only

[2] Use of this command set requires the path to the location of the `partition` program to be set in the `pstart.F` file located in the `parfeap` directory.

the terms associated with the equations of the partition. The solution vector, however, has both the terms associated with the partition as well as those associated with the equations of its ghost nodes. In this way, it is only necessary to exchange values for the displacement quantities associated with the respective ghost nodes after each solution iteration. This optimizes the communication costs.

In the next chapter we describe how the input data files for each partition are organized.

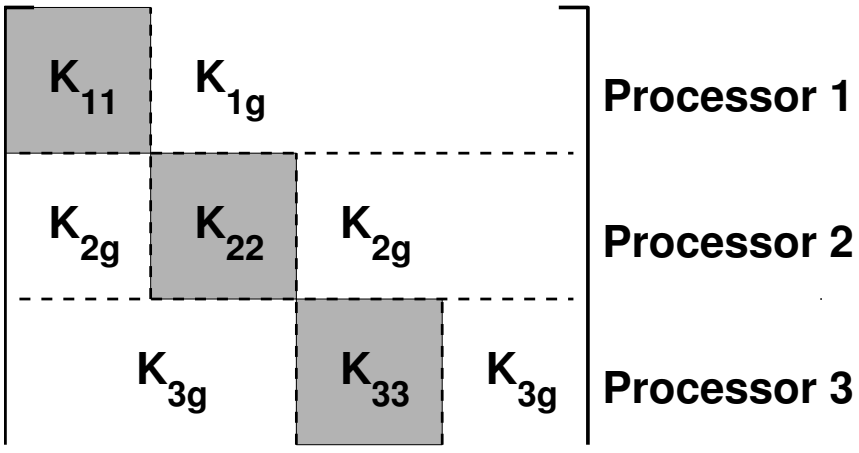

Figure 1.1: Structure of stiffness matrix in partitioned equations.

Chapter 2

Input files for parallel solution

After using the *METIS* or the *ParMETIS* partitioning algorithm on the total problem (for example, that given by say the mesh file `Ifilename`) *FEAP* produces `numd` files for the partitions and these serve as input for the parallel solution. Each new input file is named `Ifilename_0001`, etc. up to the number of partitions specified (i.e., `numd` partitions).

The first part of each file contains a standard *FEAP* input file for the nodes and elements belonging to the partition. This is followed by a set of commands that begin with `DOMAin` and end with `END DOMAin`. *All of the data contained between the* `DOMAin` *and* `END DOMAin` *is produced automatically by FEAP* when using `OUTDomains`.

The file structure for a parallel solution is shown in Figure 2.1 and is provided only to describe how the necessary data is given to each partition. *No changes are allowed to be made to these statements.*

2.1 Basic structure of parallel file

Each part of the data following the `END MESH` statement performs a specific task in the parallel solution. It is important that the data not be altered in any way as this can adversely affect the solution process. Below we describe the role each data set plays during the solution.

2.1.1 DOMAIN - Domain description

The `DOMAIN` data defines the number of nodes belonging to this partition (`numpn`), the number of total nodes in the problem (`numtn`) and the number of total equations in the

```
FEAP * * Start record and title
  ...
Control and mesh description data for a partition
  ...
END MESH

DOMAin
  numpn  numtn  numteq

FORMat <AIJ,BAIJ>

<BCIN BLOCked nsbk>   (Required for BAIJ)

LOCAl to GLOBal node numbers
  ...

GETData POINter    nget_pnt
  ...

GETData VALUes     nget_val
  ...

SENDdata POINter   nsend_pnt
  ...

SENDdata VALUes    nsend_val
  ...

MATRix storage
  ...

<EQUAtion> numbers (If BCIN is not present)
  ...

END DOMAIN

BATCh ! Optional initial conditions
  INITial DISPlacements
END BATCH
  ... List of initial conditions

INCLude solve.filename

STOP
```

Figure 2.1: Input file structure for parallel solution.

problem (`numteq`). Note that the number of nodes in the partition (`numpn`) is always less or equal to the number of nodes given on the control record (`numnp`) due to the presence of the ghost nodes. The sum over all partitions of the number of nodes in each partition (`numpn`) is equal to the total number of nodes in the problem (`numtn`).

2.1.2 FORMat - Format of matrix equations

This data set defines the format assumed for the matrix pre-allocation data as well as the local to global node number data. The valid options are `AIJ` and `BAIJ`; `AIJ` is the default.

2.1.3 BCIN BLOCked - Boundary equations in assembly

This data set is optional. For matrix formats that include the degrees of freedom associated with Dirichlet boundary conditions in the matrix assembly, this command will be present. It takes a single numerical parameter indicating the blocking size which is always an (integer) factor of `ndf`.

2.1.4 LOCal to GLOBal node numbering

Each record in this set defines three values: (1) a local node number in the partition; (2) the global node associated with the local number; and (3) the global equation block number associated with the local node. The first `numpn` records in the set are the nodes associated with the current partition the remaining records with the ghost nodes.

2.1.5 GETData and SENDdata - Ghost node get and send

The current partition retrieves (`GETData`) the solution values for its ghost nodes from other partitions. The data is divided into two parts: (1) A `POINTER` part which defines the number of values to obtain from each partition and (2) The `VALUes` list of *local node* numbers needing values. The pointer data is given as

```
GETData POINter nparts
  np_1
  np_2
   ...
  np_nparts
```

where `np_i` defines the number of values to get from partition-i (note the number should always be a zero for the current partition). The nodal values list is given as

```
GETData VALUes nvalue
  local_node_1
  local_node_2
   ...
  local_node_nvalue
```

The `local_node_i` numbers are grouped so that the first `np_1` are obtained from processor 1, the next `np_2` from processor 2, etc. The `local_node_1` is the number of a local ghost node to be obtained from another processor and may appear only *once* in the list of `GETData VALUes`.

A corresponding pair of lists is given for the data to be sent (`SEND`data) to the other processors. The lists have identical structure to the `GETData` lists and are given by

```
SENDdata POINter nparts
  np_1
  np_2
   ...
  np_nparts
```

and

```
SENDdata VALUes nvalue
  local_node_1
  local_node_2
   ...
  local_node_nvalue
```

where again the `local_node_i` numbers are grouped so that the first `np_1` are sent to processor 1, the next `np_2` to processor 2, etc. It is possible for a local node number to appear more than once in the `SENDdata VALUes` list as it could be a ghost node for more than one other partition. `np_i` should be zero for input file `Ifilename_000i`.

2.1.6 MATRix storage – equation structure

Each equation in the global matrix consists of the number of terms that are associated with the current partition and the number of terms associated with other partitions. This information is provided for each equation (or equation block when in *BAIJ* format)

by the `MATRix storage` data set. Each record in the set is given by the global equation number followed by the number of terms associated with the current partition and then the number of terms associated with other partitions. The use of this data is critical to obtain rapid assembly of the global matrices by PETSc. If it is incorrect the assembly time will be very large compared to the time needed to compute the matrix coefficients or even solve the equations.

When the matrix format is *BAIJ* the data is given for each block equation. Thus, the first `nsbk` equations are associated with block 1, the second with block 2, etc. The total number of equations `numteq` for this form is `numtn` $\times$ `nsbk`. Here, each record of the `MATRix storage` data is given by the global block number, the number of blocks associated with the current partition and the number of blocks associated with other partitions.

When the optional `BCIN` command is present, every node has `ndf` equations independent of any boundary conditions. If a degree-of-freedom (DOF) is of displacement type we assemble a unit value on the diagonal and all off-diagonal entries are zero. That is, the equations for any DOF a that are fixed will be assembled as:

$$1\, du_a = R_a = d\bar{u}$$

where $d\bar{u}$ denotes a specified valued for the solution. In some cases, this can improve the efficiency of the solver and for some solvers it is required, e.g. the Prometheus multi-grid pre-conditioner and GAMG the geometric-algebraic multi-grid pre-conditioner.

2.1.7 EQUAtion number data

This data set is not present when the boundary equations are assembled (`BCIN`). However, when the equations are in *AIJ* format and `BCIN` has not been set, then it is necessary to fully describe the equation numbering associated with each node in the partition. This is provided by the `EQUAtion` number data set. The set consists of `numnp` records which contain the *local* node number followed by the *global* equation number for every degree-of-freedom associated with the node. If a degree-of-freedom is restrained (i.e., of displacement or Dirichlet type) the equation is not active and a zero appears. This form results in fewer unknown values but may not be used with any equation solution requiring all equations to be present (in particular, Prometheus and GAMG).

2.1.8 END DOMAIN record

The parallel domain data is terminated by the `END DOMAIN` record. It is followed by the solution commands.

2.1.9 Initial conditions

Following the domain data the list of any initial conditions applied to a transient problem will appear. The initial conditions must be fully specified in the original input data file.

Initial conditions for displacements will appear as shown in Fig. 2.1. However, if rate type conditions are applied the data will appear as

```
BATCh   ! Initial rate conditions
  TRANsient type c1 c2 c3
  INITial RATE
END BATCH
  .... List of rate conditions
```

where `type` is one of the standard feap transient solution algorithms and `c1,c2,c3` are the values of the transient solution parameters. For example, if the Newmark method is used then `type` will be output as `NEWMark` and `c1,c2` will be the values of the β, γ Newmark parameters. The final parameter `c3` is not used by Newark but appears as unity.

If both initial displacements and intial rates are specified then both `BATCh--END` pairs of data will appear in the domain input file.

Chapter 3

Solution process

Once the parallel input mesh files are created an execution of the parallel version of feap may be performed using, for example, the command line statement

```
mpirun -n $NPROC $FEAPHOME8_6/parfeap/feap -ksp_type cg -pc_type jacobi
```

or the command line statement

```
mpirun -n $NPROC $FEAPHOME8_6/parfeap/feap -ksp_type cg -pc_type gamg
```

(for details on using other solvers as well as optional parameters for these choices see the `makefile` in the `parfeap` subdirectory). The parameters setting the number of processors (`NPROC`) and the execution path (`FEAPHOME8_6`) must be defined before issuing the command. This can be done by setting shell environment variables.

Once parallel *FEAP* starts, the input file should be set to `Ifilename_0001` where `filename` is the name of the solution file to be solved. Each processor reads its input file up to the `END DOMAIN` statement and then starts processing command language statements.

In a parallel solution using *FEAP* the same command language statements must be provided for each partition. This is accomplished by the statement

```
INCLude solve.filename
```

appearing after the `END DOMAin` statement, where `filename` is the name of the input data file with the leading `I` and the trailing partition number removed. Thus for the file named `Iblock_0001` the command is given as `solve.block`. All solution commands are then placed in a file with this name and can include both `BATCh` and `INTEractive` commands. For example a simple solution may be given by the commands

```
BATCh
  PETSc ON
  TOL ITER 1.d-07 1.d-08 1.d+20
  TANGent,,1
END

INTEractive
```

placed in the `solve.filename` file. Note that both batch and interactive modes of solution are optionally included. Interactive commands need only be entered once and are sent to other processors automatically. In the subsequent subsections we describe some of the special commands that control the parallel execution mode of *FEAP*

3.1 Command language statements

Most of the standard command language statements available in the serial version of *FEAP* (see users manual [1]) may be used in the parallel version of feap. New commands are available also that are specifically related to performing a parallel solution.

3.1.1 PETSc Command

The `PETSc` command is used to activate the parallel solution process. The command

```
PETSc <ON,OFF>
```

may be used to turn on and off the parallel execution. It is only required for single processor solutions and is optional when two or more processors are used in the solution process. When required, it should always be the first solution command. It is automatically included in the default `solve.filename` generated by `OUTDomains`.

The command may also be used with the `VIEW` parameter to create outputs for the tangent matrix, solution residual or mass matrix. Thus, use as

```
PETSc VIEW
MASS
PETSc NOVIew
```

will create a file named `mass.m` that contains all the non-zero values of the *total* mass matrix. The parameter `VIEW` turns on output arrays and this remains in effect for all

commands until the command is given with the `NOVIew` parameter. The file is created in a format that may be directly used by MATLAB.[10] *This command should only be used with small problems to verify the correctness of results as large files will result otherwise.*

3.2 Solution of linear equations

The parallel version of *FEAP* can use most all of the SLES (linear solvers) available in PETSc as well as the parallel multigrid solver GAMG. This also includes most of the direct solvers that can optionally be built with PETSc. The actual type of linear solver used is specified on the `mpirun` line and several useful examples are contained in the `makefile` located in the `parfeap` directory (see, Sect. 3 above). Once the solution is initiated the solution of linear equations is performed whenever a `TANG,,1` or `SOLVe` command is given.

The types of solvers and the associated pre-conditioners tested to date are described in Table 3.1. This is only a small sampling of the many options available in PETSc.

Solver	Preconditioner	Matrix format/Notes
CG	Jacobi	AIJ and BAIJ formats
CG	Hypre with Boomerang	AIJ format
CG	ML/Trilinos	AIJ format
CG	GAMG	AIJ with BCIN format
MINRES	Jacobi	AIJ and BAIJ formats
GMRES	Jacobi	AIJ and BAIJ formats
GMRES	Block Jacobi	Often gives indefinite factor.
GMRES	ASM(ILU)	
SuperLU	(direct)	AIJ format (has BLAS conflict on Mac OS X $\geq$ 10.7.5)
MUMPS	(direct)	AIJ format

Table 3.1: Linear solvers and pre-conditioners tested.

The solvers, together with the necessary options for preconditioning are specified on the `mpirun` line. For convenience, it is recommended to place these in the provided `makefile` and to run them with the `make` command. Several options are pre-provided in the distributed makefile.

3.2.1 Tolerance for iterative equation methods

The basic form of iterative solution for linear equations in PETSc is a Krylov subspace scheme. These methods terminate their iterations based on assumed tolerances and can be changed as desired.

Termination tolerances for the solvers are given by either

```
TOL ITER rtol atol dtol
```

or

```
ITER TOL rtol atol dtol
```

where `rtol` is the tolerance for the preconditioned equations, `atol` the tolerance for the original equations and `dtol` a value at which divergence is assumed. The default values are:

$$\text{rtol} = 1.\text{d} - 8 \quad ; \quad \text{atol} = 1.\text{d} - 16 \quad \text{and} \quad \text{dtol} = 1.\text{d} + 16$$

For many problems it is advisable to check that the actual solution is accurate when using iterative methods since termination of the iterative solution is performed based on the `rtol` value. A check should be performed using the command sequence

```
TANG,,1
LOOP,,1
  FORM
  SOLV
NEXT
```

since the `TANG` command has significant set up costs, especially for multi-grid methods. Indeed, for some problems more than one iteration is needed in the loop.

3.2.2 GLIST & GNODE: Output of results with global node numbers

In normal execution each partition creates its own output file (e.g., `Ofilename_0001`, etc.) with printed data given with the *local* node and element numbers of the processor's input data file. In some cases the global node numbers are known and it is desired to identify which processor to which the node is associated. This may be accomplished by including a `GLISt` command in the solution statements along with the list of *global* node numbers to be output. The option is restricted to 3 lists, each with a maximum of 100 nodes. The command sequence is given by:

```
BATCh
  GLISt,,<1,2,3>
END
  list of global node numbers, 8 per record
! blank termination record
```

The list will be converted by each processor into the local node numbers to be output using the command

```
DISP LIST <1,2,3>
```

The command may also be used with `VELOcity, ACCEleration, and STREss`; see the relevant manual pages in the *FEAP* Users Manual.[1]

It is also possible to directly output the *global* node number associated with individual *local* node numbers using the command statement

```
DISP GNODe nstart nend ninc
```

where *nstart* and *nend* are *global* node numbers. This command form also may be used with `VELOcity, ACCEleration, and STREss`.

3.3 Eigenproblem solution for modal problems

The computation of the natural modes and frequencies of free vibration of an undamped linear structural problem requires the solution of the general linear eigenproblem

$$\mathbf{K}\,\mathbf{\Phi} = \mathbf{M}\,\mathbf{\Phi}\,\mathbf{\Lambda}$$

In the above $\mathbf{K}$ and $\mathbf{M}$ are the stiffness and mass matrices, respectively, and $\mathbf{\Phi}$ and $\mathbf{\Lambda}$ are the normal modes and frequencies squared. Normally, the constraint

$$\mathbf{\Phi}^T\mathbf{M}\,\mathbf{\Phi} = \mathbf{I}$$

is used to scale the eigenvectors. In this case one also obtains the relation

$$\mathbf{\Phi}^T\mathbf{K}\,\mathbf{\Phi} = \mathbf{\Lambda}$$

3.3.1 Subspace method solutions

The subspace algorithm contained in *FEAP* has been extended to solve the above problem in a parallel mode. The use of the subspace algorithm requires a linear solution of the equations

$$\mathbf{K}\,\mathbf{x} = \mathbf{y}$$

for each vector in the subspace and for each subspace iteration. The parallel subspace solution is performed using the command set

```
TANGent
MASS <LUMPed,CONSistent>
PSUBspace <print> nmodes <nadded>
```

where `nmodes` is the desired number of modes, `nadded` is the number of extra vectors used to accelerate the convergence (default is maximum of `nmodes` and 8) and `print` produces a print of the subspace projections of $\mathbf{K}$ and $\mathbf{M}$. The accuracy of the computed eigenvalues is the maximum of $1.\mathrm{d}-12$ and the value set by the `TOL` solution command. The method may be used with either a lumped or a consistend mass matrix.

If it is desired to extract 10 eigenvectors with 8 added vectors and 20 iterations are needed to converge to an acceptable error it is necessary to perform 360 solutions of the linear equations. Thus, for large problems the method will be very time consuming.

3.3.2 Arnoldi/Lanczos method solutions

In order to reduce the computational effort for eigenproblems the Arnoldi/Lanczos methods implemented in the ARPACK module available from Rice University[11] has been modified to work with the parallel version of *FEAP*.

Two modes of the ARPACK solution methods are included in the program:

1. Mode 1: Solves the problem reformed as

   $$\mathbf{M}^{-1/2}\,\mathbf{K}\,\mathbf{M}^{-1/2}\,\mathbf{\Psi} = \mathbf{\Psi}\,\mathbf{\Lambda}$$

   where

   $$\mathbf{\Phi} = \mathbf{M}^{-1/2}\,\mathbf{\Psi}$$

   This form is most efficient when the mass matrix is diagonal (lumped) and, thus, in the current release of parallel *FEAP* is implemented only for diagonal (lumped) mass forms. This mode form is specified by the solution command set

```
TANGent
MASS LUMPed
PARPack LUMPed  nmodes <maxiters> <eigtol>
```

where `nmodes` is the number of desired modes. Optionally, `maxiters` is the number of iterations to perform (default is 300) and `eigtol` the solution tolerance on eigenvalues (default is the maximum of $1.d-12$ and the values set by the command `TOL`).

2. Mode 3: Solves the general linear eigenproblem directly and requires solution of the linear problem

$$\mathbf{K}\,\mathbf{x} = \mathbf{y}$$

for each iteration. Fewer iterations are normally required than in the subspace method, however, the method is generally far less efficient than the Mode 1 form described above. This form is given by the set of commands

```
TANGent
MASS <LUMPed,CONSistent>
PARPack <SYMMetric> nmodes <maxiters> <eigtol>
```

Use of the command `MASS` alone also will employ a consistent mass (or the mass produced by the quadrature specified).

3.4 Graphics output

During a solution the graphics commands may be given in a standard manner. However, each processor will open a graphics window and display only the parts that belong to that processor. Scaling is also done processor by processor unless the `PLOT RANGe` command is used to set the range for the plot values.

3.4.1 GPLOt command

An option does exist to collect all the results together and present on a single graphics window. This option also permits postscript outputs to be constructed and saved in files. To collect the results together it is necessary to write the results to disk for each item to be graphically presented. This is accomplished using the `GPLOt` command. This command has the options

```
GPLOt DISPlacement n
GPLOt STREss       n
GPLOt PSTRess      n
```

where `n` denotes the component of a displacement (`DISP`), nodal stress (`STRE`) or principal stress (`PSTRE`). Each use of the command creates a file for each processor with the form

```
Gproblem_domain.xyyyy
```

where `problem_domain` is the name of the problem file for the `domain`; `x` is `d, s` or `p` for a displacement, stress or principal stress, respectively; and `yyyy` is a unique plot number (it will be between 0001 and 9999).

3.4.2 NDATa command

Once the `GPLOt` files have been created they may be plotted using a *serial execution* of the parallel *FEAP* program (i.e., using the original pre-partioning step file `Ifilename`). The command may be given in `INTEractive` mode only as one of the options:

```
Plot > NDATa DISPl   n
Plot > NDATa STREss  n
Plot > NDATa PSTRess n
```

where `n` is the value of `yyyy` used to write the file.

WARNING: Plots by *FEAP* use substantial memory and thus this option may not work for very large problems. One should minimize the number of commands used during input of the problem description (i.e., remove input commands in the mesh that create new memory).

3.4.3 Paraview

An alternate scheme for plotting parallel solutions can be achieved by use of the Paraview[1] system. This is a convenient open source tool that can be used with *FEAP*.

[1] See `http://www.paraview.org`.

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Appendix A

Installation

The installation of the parallel version of *FEAP* is accomplished after first building a serial version (see *FEAP Installation Manual* for instructions to build the serial version).

A.1 Installing PETSc

In order to build the parallel version it is necessary to have an installed version of PETSc[5, 6] that includes Metis, and ParMetis[12]. It is further important to install several of the optional pre-conditioner and solver packages.

In the appropriate "`.bash_xxx`" file it is useful (but not necessary) to insert lines similar to

```
export PETSC_DIR=/Users/rlt/Software/petsc-3.13.2
export PETSC_ARCH=gnu-opt
```

This saves on some typing later on.

The files, manuals, and installation instruction for PETSc may be downloaded from:

```
http://www.mcs.anl.gov/petsc
```

However in short, after downloading and unpacking the source file the PETSc libraries need to be built (and tested). Our typical (non-debugging) installation is performed as follows:

```
export PETSC_DIR=/Users/rlt/Software/petsc-3.13.2
export PETSC_ARCH=gnu-opt
cd $PETSC_DIR
./configure --download-{parmetis,superlu_dist,openmpi, \
   ml,hypre,metis,mumps,scalapack,blacs} --with-debugging=0
```

Once the configuration is completed the PETSc library is compiled using:

```
make PETSC_DIR=/Users/rlt/Software/petsc-3.13.2 PETSC_ARCH=gnu-opt all
```

and tested using

```
make PETSC_DIR=/Users/rlt/Software/petsc-3.13.2 PETSC_ARCH=gnu-opt test
```

This will create a PETSc system that includes Metis, ParMetis, SuperLU, MUMPS, GAMG, ML/Trilinos, Hypre as well as an MPI environment. (ScaLapack and BLACS are needed by MUMPS.) Of these only Metis and ParMetis are required – assuming you already have an MPI environment. Leave off the `--with-debugging=0` flag if you want to build a debugging version. In general it is best to build both a debugging and non-debugging version.

The above instructions assume use of a `bash` shell. For other operating systems or shells see the PETSc documentation at [6]. Not all the listed packages are needed but these tend to be useful for a wide variety of problem classes.

A.2 Installing parallel *FEAP*

Optionally one can include the ARPAck modules in the build. To do so, first build the archive `archivelib.a` in the directory `packages/arpack/archive` using the command `make install`. Then build the archive `parpacklib.a` in the directory `parfeap/packages/arpack` using the command `make install`.

With the PETSc libraries available the parallel executable for *FEAP* is built from the `parfeap` subdirectory using the command

```
make install
```

If the ARPAck libraries have been built one should edit the `makefile` to ensure that they are linked by uncommenting the appropriate lines.

Appendix B

Solution Command Manual Pages

FEAP has a few options that are used only to solve parallel problems. The commands are additions to the *command language* approach in which users write each step using available commands. The following pages summarize the commands currently added to the parallel version of *FEAP*.

```
disp,gnod,<n1,n2,n3>
```

Other options of this command are described in the *FEAP* User Manual. The command `DISP`lacement may be used to print the current values of the solution *generalized displacement* vector associated with the *global node numbers* of the original mesh. The command is given as

```
disp,gnod,n1,n2,n3
```

prints out the current solution vector for global nodes `n1` to `n2` at increments of `n3` (default increment = 1). If `n2` is not specified only the value of node `n1` is output. If both `n1` and `n2` are not specified only the first node solution is reported.

```
glist,,n1
   <values>
```

The command `GLISt` is used to specify lists of *global* node numbers for output of nodal values. It is possible to specify up to three different lists where the list number corresponds to `n1` (default = 1). The list of nodes to be output is input with up to 8 values per record. The input terminates when less than 8 values are specified or a blank record is encountered. No more than 100 items may be placed in any one list.

List outputs are then obtained by specifying the command:

```
name,list,n1
```

where `name` may be `DISP`lacement,`VELO`city,`ACCE`leration, or `STRE`ss and `n1` is the desired list number.

Example:

```
BATCh
  GLISt,,1
END
1,5,8,20

BATCh
  DISP,LIST,1
   ...
END
```

The global list of nodes is processed to determine the processor and the associated local node number. Each processor then outputs its active values (if any) and gives both the local node number in the partition as well as the global node number.

```
gplo disp n
gplo velo n
gplo acce n
gplo stre n
```

Use of plot commands during execution of the parallel version of *FEAP* create the same number of graphic windows as processors used to solve the problem. Each window contains only the part of the problem contained on that processor.

The use of the `GPLOt` command is used to save files containing the results for all nodal dispacements, velocities, accelerations or stresses in the total problem. The only action occuring after the use of this command is the creation of a file containing the current results for the quantity specified. Repeated use of the command creates files with different names.

These results may be processed by a serial run of the problem using the mesh for the total problem. To display the nodal values command `NDATa` is used. See manual page on `NDATa`.

```
grap,,num_d
grap node num_d
grap file
grap part num_d
```

The use of the `GRAPh` command activates the interface to the *METIS* multilevel partioner. The graph partition into `num_d` parts is performed based on a nodal graph. The nodal partition divides the total number of nodes (i.e., `numnp` values) into `num_d` nearly equal parts.

If the `GRAPh` command is given with the option `file` the graph data is input from the file `graph.filename` where `filename` is the same as the input file without the leading `I` character. The data contained in the `graph.filename` is created using the stand alone `partitioner` program which employs the *PARMETIS* multilevel partitioner.

It is also possible to execute *PARMETIS* to perform the partitioning directly during a mesh input. It is necessary to have a mesh which contains all the nodal coordinate and element data in the input file. This is accomplished using the command set

```
OUTMesh
GRAPh PARTition num_d
OUTDomains
```

where `num_d` is the number of domains to create. The command `OUTMesh` creates a file with all the nodal and element data and is destroyed after execution of the `GRAPh` command.

```
iter,,,icgit
iter,bpcg,v1,icgit
iter,ppcg,v1,icgit
iter,tol,v1,v2,v3
```

The `ITERative` command sets the mode of solution to iterative for the linear algebraic equations generated by a `TANGent`. Currently, iterative options exist only for symmetric, positive definite tangent arrays, consequently the use of the `UTANgent` command should be avoided. An iterative solution requires the sparse matrix form of the tangent matrix to fit within the available memory of the computer.

Serial solutions

In the serial version the solution of the equations is governed by the relative residual for the problem (i.e., the ratio of the current residual to the first iteration in the current time step). The tolerance for convergence may be set using the `ITER,TOL,v1,v2` option. The parameter `v1` controls the relative residual error given by

$$(\mathbf{R}^T\mathbf{R})_i^{1/2} \leq v1\,(\mathbf{R}^T\mathbf{R})_0^{1/2}$$

and, for implementations using `PETSc` the parameter `v2` controls the absolute residual error given by

$$(\mathbf{R}^T\mathbf{R})_i^{1/2} \leq v2$$

The default for `v1` is `1.0d-08` and for `v2` is `1.0d-16`. By default the maximum number of iterations allowed is equal to the number of equations to be solved, however, this may be reduced or increased by specifying a positive value of the paramter `icgit`.

The symmetric equations are solved by a preconditioned conjugate gradient method. Without options, the preconditioner is taken as the diagonal of the tangent matrix. Options exist to use the diagonal nodal blocks (i.e., the $ndf \times ndf$ nodal blocks, or reduced size blocks if displacement boundary conditions are imposed) as the preconditioner. This option is used if the command is given as `ITERative,BPCG`. Another option is to use a banded preconditioner where the non-zero profile inside a specified half band is used. This option is used if the command is given as `ITERative,PPCG,v1`, where `v1` is the size of the half band to use for the preconditioner.

The iterative solution options currently available are not very effective for poorly conditioned problems. Poor conditioning occurs when the material model is highly non-

linear (e.g., plasticity); the model has a long thin structure (like a beam); or when structural elements such as frame, plate, or shell elements are employed. For compact three dimensional bodies with linear elastic material behavior the iterative solution is often very effective.

Another option is to solve the equations using a direct method (see, the `DIRE`ct command language manual page).

Parallel solutions

For the parallel version the control of the PETSc preconditioned iterative solvers is controlled by the command

```
ITER TOL itol atol dtol
```

where `itol` is the tolerance for the *preconditioned* equations (default $1.d-08$), `atol` is the tolerance for the original equations (default $1.d-16$) and `dtol` is a divergence protection when the equations do not converge (default $1.d+16$).

```
ndat disp n
ndat velo n
ndat acce n
ndat stre n
```

This command is used in a serial execution of parallel *FEAP* using the mesh for the total problem. It is necessary for files to be created during a parallel execution using the `GPLOt` command (See manual page on `GPLOt`).

The command is given by

```
NDATa DISPlacement num
```

where the parameter `num` is the number corresponding to the order the `DISPlacement` are created. Thus, the command sequence

```
NDATa DISPlacement 2
NDATa STREss       2
```

would display the results for the second files created for the displacements and stresses.

Note this command is Plot level command.

```
outd,<aij>
outd,aij,1,<bsize>
outd,baij,,<bsize>
```

The use of the `OUTDomains` command may only be used after the `GRAPh` command partitions the mesh into `num_d` parts (see `GRAPh` command language page for details).

Using the command `OUTDomains,AIJ` or `OUTDomains,BAIJ` creates `num_d` input files for a subsequent parallel solution in which the matrix format will be created in *AIJ* or *BAIJ* format, respectively; *AIJ* is the default.

The parameter `bsize` defines the block size and *must be an integer divisor of* `ndf`. That is if `ndf = 6` then `bsize` may be 1, 2, 3, or 6. By default each block in the equations has a size `ndf`. The setting of the block size can significantly reduce the amount of storage needed to store the sparse coefficient matrix created by `TANGent` or `UTANgent` when a problem has a mix of element types and the matrix is in *BAIJ* format. For example if a problem has a large number of solid elements with 3 degrees of freedom per node and additional frame or shell elements with 6 degrees of freedom per node, specifying `bsize = 3` can save considerable memory. Further the setting of the block size can improve the rate of convergence of iterative and direct solvers.

The use of the unity flag in `OUTDomains,AIJ,1` forces the inclusion of all, even prescribed, degrees of freedom in the matrix assembly for *AIJ* format. This permits the use of blocking for *AIJ* format matrices – something that is in general not possible if prescribed degrees of freedom are not assembled. This is the default behavior for *BAIJ* format matrices.

```
pets
pets on
pets off
pets view
pets noview
```

The use of the `PETSc` command activates(`on`) or deactivates(`off`) parallel solution options, respectively. To turn on parallel computing the command may be given in the simple form: `PETSc`. When more than one partition is created, i.e., the number of solution processors is 2 or more, the `PETSc` option is on by default. The command must be the first command of the command language program when only 1 processor is used.

The option `PETSc VIEW` will result in the creation of debug files containing important parallel matrices and vectors. The output is in `MATLAB` sparse format. This option should only be used for very small problems to check that a formulation produces correct results (i.e., there is another set of terms to which a comparison is to be made). The option is turned off using the statement `PETSc NOVIew`. The default is `NOVIew`.

```
stre,gnod,<n1,n2,n3>
```

Other options for this command are given in the *FEAP* User Manual. The `STREss` command is used to output nodal stress results at *global node numbers* `n1` to `n2` at increments of `n2` (default = 1).

The command specified as:

```
stre,gnode,n1,n2,n3
```

prints out the stresses for global nodes n1 to n2 at increments of n3 (default increment = 1). If n2 is not specified only the value of node n1 is output. If both n1 and n2 are not specified only the first node solution is reported.

```
tol,,v1
tol,ener,v1
tol,emax,v1
tol,iter,v1,v2,v3
```

The `TOL` command is used to specify the solution tolerance values to be used at various stages in the analysis. Uses include:

1. Convergence of nonlinear problems in terms of the norm of energy in the current iterate (the inner, dot, product of the displacement increment and the solution residual vectors).
2. Convergence of iterative solution of linear equations.
3. Convergence of the subspace eigenpair solution which is measured in terms of the change in subsequent eigenvalues computed.

The basic command, `TOL,,tol`, without any arguments sets the parameter *tol* used in the solution of non-linear problems where the command sequence

```
LOOP,,30
  TANG,,1
NEXT
```

is given. In this case, the loop is terminated either when the number of iterations reaches 30 (or whatever number is given in this position) or when the *energy error* is less than *tol*. The energy error is given by

$$E_i = (d\mathbf{u}^T\mathbf{R})_i \leq tol\,(d\mathbf{u}^T\mathbf{R})_0 = E_0$$

in which $\mathbf{R}$ is the residual of the equatons and $d\mathbf{u}$ is the solution increment. The default value of *tol* for the solution of nonlinear problems is 1.0d-16.

The `TOL` command also permits setting a value for the energy below which convergence is assumed to occur. The command is issued as `TOL,ENER`gy,`v1` where `v1` is the value of the converged energy (i.e., it is equivalent to the tolerance times the maximum energy value). Normally, *FEAP* performs nonlinear iterations until the value of the energy is less than the `TOL`erance value times the value of the energy from the first iteration

as shown above. However, for some transient problems the value of the initial energy is approaching zero (e.g., for highly damped solutions which are converging to some steady state limit). In this case, it is useful to specify the energy for convergence relative to early time steps in the solution. Convergence will be assumed if either the normal convergence criteria or the one relative to the specified maximum energy is satisfied.

The `TOL` command also permits setting the maximum energy value used for convergence. The command is issued as

```
TOL,EMAXimum,v1
```

where `v1` is the value of the maximum energy quantity. Note that the `TIME` command sets the maximum energy to zero, thus, the value of `EMAX`imum must be reset after each time step using, for example, a set of commands:

```
LOOP,time,n
  TIME
  TOL,EMAX,5.e+3
  LOOP,newton,m
    TANG,,1
  NEXT
  etc.
NEXT
```

to force convergence check against a specified maximum energy. The above two forms for setting the convergence are nearly equivalent; however, the `ENER`gy tolerance form can be set once whereas the `EMAX`imum form must be reset after each time command.

The command

```
TOL ITERation itol atol dtol
```

is used to control the solution accuracy when an *iterative* solution process is used to solve the equations

$$\mathbf{K}\, d\mathbf{u} = \mathbf{R}$$

In this case the parameter *itol* sets the relative error for the solution accuracy, i.e., when

$$(\mathbf{R}^T\mathbf{R})_i^{1/2} \le itol\, (\mathbf{R}^T\mathbf{R})_0^{1/2}$$

The parameter *atol* is only used when solutions are performed using the `KSP` schemes in a `PETSc` implementation to control the absolute residual error

$$(\mathbf{R}^T\mathbf{R})_i^{1/2} \le atol$$

The `dtol` parameter is used to terminate the solution when divergence occurs. The default for `itol` is `1.0d-08`, that for `atol` is `1.0d-16` and for `dtol` is `1.0d+16`.

Appendix C

Program structure

C.1 Introduction

This section describes the parallel infrastructure for the general purpose finite element program, *FEAP*.[1] The current version of the parallel code modifies the serial version of *FEAP* to interface to the PETSc library system available from Argonne National Laboratories.[5, 6] In addition the METIS[7] and ParMETIS[8] libraries are used to partition each mesh for parallel solution.

The necessary modifications and additions for the parallel features are contained in the directory `parfeap`. There are four sub-directories contained in `parfeap`:

1. `packages`: Contains the subdirectory `arpack` with the files needed for the (optional) ARPACK eigen solution module (see Section 3.3).

2. `partition`: Contains the program and include file used to construct the nodal graph partition using ParMETIS (see Section 1.3).

3. `unix`: Contains the subprogram files for UNIX based systems.

Appendix D

Parallel Validation

The validation of the parallel portion of FEAP has been performed on a number of different basic problems to verify that the parallel extension of FEAP will solve such problems and that the parallel version performs properly in the sense that it scales with processor number in an acceptable manner. Furthermore, a series of comparison tests have been performed to verify that the parallel version of the program produces the same answers as the serial version. Because of the enormous variety of analyses that one can perform with FEAP, it is not possible to provide parallel tests for all possible combinations of program features. Nonetheless, below one will find some basic validation tests that highlight the performance of the parallel version of the code on a variety of problems.

All validation tests were performed on a cluster of AMD Opteron 250 processors, connected together via a Quadrics QsNet II interconnect. Code performance is often strongly related to the computational sub-systems employed. All tests reported utilized GCC v3.3.4, MPI v1.2.4, PETSc v2.3.2-p3, AMD ACML (BLAS/LAPACK) v3.5.0, ParMetis v3.1, Prometheus v1.8.5, and ARPACK ©2001. The batch scheduler assures that no other jobs are running on the same compute nodes during the runs. All runs have utilized the algebraic multigrid solver Prometheus in blocked form with coordinate information. Run times are as reported from PETSc summary statistics from a single run; Mflops are those associated with PETSc's KSPsolve object; Number of solves is the total number of $Ax = b$ solves during the KSP iterations in the total problem, and Scaling % of ideal is computed as $(\text{Mflops}_{np}/np)/(\text{Mflops}_2/2) \times 100$.

D.1 Timing Tests

D.1.1 Linear Elastic Block

In this test a linear elastic unit block discretized into $70 \times 70 \times 70$ 8-node brick elements is clamped on one face and loaded on the opposite face with a uniform load in all coordinate directions. In blocked form there are 1,073,733 equations in this problem.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	129.20	1241	13	-
4	71.69	2171	13	87
8	35.77	4646	14	94
16	21.30	8347	14	84
32	13.19	14561	14	73

D.1.2 Nonlinear Elastic Block

In this test a nonlinear neohookean unit block discretized into $50 \times 50 \times 50$ 8-node brick elements is clamped on one face and loaded on the opposite face with a uniform load in all coordinate directions. In blocked form there are 397,953 equations in this problem. To solve the problem, to default tolerances, takes 4 Newton iterations within which there are on average 12 KSP iterations.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	166.7	1142	53	-
4	82.66	2356	54	103
8	43.48	4642	53	102
16	27.15	7846	56	86
32	15.58	13988	52	77

D.1.3 Plasticity

In this test one-quarter of a plate with a hole is modeled using 364500 8-node brick elements and pulled in tension beyond yield. The problem involves 10 uniform size load steps which drives the plate well into the plastic range; each load step takes between 3 and 10 Newton iterations. There are 1,183,728 equations. Due to the large number

of overall KSP iterations needed for this problem, it has only been solved using 8, 16, and 32 processors. Scaling is thus computed relative to the 8 processor run.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	-	-	-	-
4	-	-	-	-
8	220.80	4434	2973	-
16	107.70	8425	2908	95
32	59.03	15645	2868	88

D.1.4 Box Beam: Shells

In this test a box beam is modeled using 40000 linear elastic 4-node shell elements (6-dof per node). The beam has a 1 to 1 aspect ratio with each face modeled by 100×100 elements. One end is fully clamped and the other is loaded with equal forces in the three coordinate directions. There are 242,400 equations; the block size is 6×6.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	49.43	510	195	-
4	16.37	1619	190	159
8	12.46	1972	188	97
16	5.03	5246	181	129
32	3.28	8177	184	100

D.1.5 Linear Elastic Block: 10-node Tets

In this test the linear elastic unit block from the first test is re-discretized using 10-node tetrahedral elements. As in the 8-node brick case, there are 1,073,733 equations in this problem. In the table below, we also provide the ratio of times for the "same" problem when solved using 8-node brick elements. This indicates the difficulty in solving problems (iteratively) that emanate from quadratic approximations. Essentially, per dof, tets solve in the ideal case 1.5 times slower.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal	Slow down vs. Brick
2	216.8	1299	30	-	1.7
4	110.4	2615	30	101	1.5
8	56.62	5059	29	97	1.6
16	31.44	9370	30	90	1.5
32	17.07	17659	28	85	1.3

D.1.6 Transient

In this test a short (2 to 1 aspect ratio) neohookean beam is subjected to a step displacement in the axial direction. The modeling employs symmetry boundary conditions on three orthogonal planes. The beam is discretized into uniform size 8-node brick elements $10 \times 10 \times 20$ for a total of 7623 equations. The dynamic vibrations of the material are followed for 40 time steps using Newmark's method. The steep drop off in performance should be noted. This is due to the small problems size. There is too little work for each processor to be effectively utilized here.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	95.37	1079	1385	-
4	58.91	1687	1420	78
8	39.03	2645	1382	61
16	32.15	3138	1376	36
32	33.61	3123	1371	18

D.1.7 Mock turbine

In this test we model a mock turbine fan blade with 12 fins. The system is loaded using an $R\omega^2$ body force term which is computed consistently. Overall there are 1,080,000 8-node brick elements in the mesh and 3,415,320 equations. It should be noted that problem, at roughly 3.5 million equations, provides enough work for the processors that even at 32 processors there is no degradation of performance. The scaling is perfect.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	854.3	806	116	-
4	362.4	1931	112	120
8	172.9	4085	110	127
16	88.99	8232	115	128
32	46.68	16159	112	125

D.1.8 Mock turbine Small

In this test we model again a mock turbine fan blade with 12 fins. The system is loaded using an $R\omega^2$ body force term which is computed consistently. Overall, however, there are only 552960 8-node brick elements in the mesh and 1,771,488 equations.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	347.40	1097	125	-
4	199.50	1878	132	86
8	91.63	4064	122	93
16	47.68	8024	126	91
32	26.32	15400	119	88

D.1.9 Mock turbine Tets

In this test we model again a mock turbine fan blade with 12 fins. The system is loaded using an $R\omega^2$ body force term which is computed consistently. This time however we utilize 10-node tetrahedral elements with a model that has 1,771,488 equations. This computation can be directly compared to the small mock turbine benchmark. The slow down is given in the last column of the table below.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal	Slow Down vs. Brick
2	507.7	1193	126	-	1.5
4	304.2	1934	129	81	1.5
8	131.0	4675	131	98	1.4
16	70.01	8860	134	93	1.5
32	41.83	16238	127	85	1.6

D.1.10 Eigenmodes of Mock Turbine

In this test we look at the computation of the first 5 eigen modes of the small (552960 element) mock turbine model. Again, the mesh is composed of 8-node brick elements and the model has 1,771,488 equations. A lumped mass is utilized and the algorithm tested is the ARPA symmetric option. Due to the large number of inner-outer iterations the timing runs are done only for 8, 16, and 32 processors. Scaling is thus computed relative to the 8 processor run.

Number Processors	Time (sec)	Mflops (KSP Solve)	Number Solves	Scaling % Ideal
2	-	-	-	-
4	-	-	-	-
8	916.9	3757	2744	-
16	507.1	7122	2876	95
32	248.3	14042	2723	93

D.2 Serial to Parallel Verification

Serial to parallel code verification is reported upon below. For all test run, the program is run in serial mode (with a direct solver) and in parallel mode on 4 processors (forcing inter- and intra-node communications). Then various computation output quantities are compared between the parallel and serial runs. In all cases, it is observed that the outputs match to the computed accuracy.

D.2.1 Linear elastic block

In this test a linear elastic unit block discretized into $5 \times 5 \times 5$ 8-node brick elements is clamped on one face and loaded on the opposite face with a uniform load in all coordinate directions. The displacements are compared at global nodes 100 and 200 and the maximum overall principal stress is also determined from both runs. All values are seen to be identical. For the parallel runs, the processor number containing the value is given in parenthesis and the reported node number is the local processor node number.

Serial Displacements						
Node	x-coor	y-coor	z-coor	x-disp	y-disp	z-disp
100	6.00E-01	8.00E-01	4.00E-01	-1.3778E-01	1.1198E+00	1.1241E+00
200	2.00E-01	6.00E-01	1.00E+00	-4.1519E-01	2.3568E-01	2.6592E-01

Serial Max Principal Stress	
Node	Stress
1	4.0881E+02

Parallel Displacements						
(P)Node	x-coor	y-coor	z-coor	x-disp	y-disp	z-disp
(4)49	6.00E-01	8.00E-01	4.00E-01	-1.3778E-01	1.1198E+00	1.1241E+00
(2)38	2.00E-01	6.00E-01	1.00E+00	-4.1519E-01	2.3568E-01	2.6592E-01

Parallel Max Principal Stress	
(P)Node	Stress
(3)1	4.0881E+02

Note: Processor 3's local node 1 corresponds to global node 1.

D.2.2 Box Beam

In this test a linear elastic unit box-beam discretized into $4 \times 20 \times 20$ 4-node shell elements is clamped on one face and loaded on the opposite face with a uniform load in all coordinate directions. The displacements are compared at global nodes 500 and 1000 and the maximum overall principal bending moment is also determined from both runs. All values are seen to be identical. For the parallel runs, the processor number containing the value is given in parenthesis and the reported node number is the local processor node number.

Serial Displacements/Rotations						
Node	x-coor	y-coor	z-coor	x-disp x-rot	y-disp y-rot	z-disp z-rot
500	8.00E-01	1.00E-01	1.00E+00	3.6632E-03 4.4272E-02	-3.2924E-03 -7.3033E-04	2.3266E-03 -2.1595E-02
1000	1.00E+00	3.00E-01	2.00E-01	2.2972E-02 4.8140E-02	1.5303E-03 2.8224E-02	1.6876E-02 -1.3278E-01

Serial Max Principal Bending Moment	
Node	Stress
1	1.7091E+01

Parallel Displacements/Rotations						
(P)Node	x-coor	y-coor	z-coor	x-disp x-rot	y-disp y-rot	z-disp z-rot
(1)29	8.00E-01	1.00E-01	1.00E+00	3.6632E-03 4.4272E-02	-3.2924E-03 -7.3033E-04	2.3266E-03 -2.1595E-02
(2)280	1.00E+00	3.00E-01	2.00E-01	2.2972E-02 4.8140E-02	1.5303E-03 2.8224E-02	1.6876E-02 -1.3278E-01

Parallel Max Principal Bending Moment	
(P)Node	Stress
(4)1	1.7091E+01

Note: Processor 4's local node 1 corresponds to global node 1.

D.2.3 Linear Elastic Block: Tets

In this test a linear elastic unit block discretized into 162 10-node tetrahedral elements is clamped on one face and loaded on the opposite face with a uniform load in all coordinate directions. The displacements are compared at global nodes 55 and 160 and the maximum overall principal stress is also determined from both runs. All values are seen to be identical. For the parallel runs, the processor number containing the value is given in parenthesis and the reported node number is the local processor node number.

Serial Displacements						
Node	x-coor	y-coor	z-coor	x-disp	y-disp	z-disp
55	8.33E-01	0.00E+00	1.67E-01	4.9509E-01	4.3175E-01	4.2867E-01
160	8.33E-01	1.67E-01	5.00E-01	2.1305E-01	4.2030E-01	4.1548E-01

Serial Max Principal Stress	
Node	Stress
8	9.0048E+01

Parallel Displacements						
(P)Node	x-coor	y-coor	z-coor	x-disp	y-disp	z-disp
(3)23	8.33E-01	0.00E+00	1.67E-01	4.9509E-01	4.3175E-01	4.2867E-01
(1)17	8.33E-01	1.67E-01	5.00E-01	2.1305E-01	4.2030E-01	4.1548E-01

Parallel Max Principal Stress	
(P)Node	Stress
(4)6	9.0048E+01

Note: Processor 4's local node 6 corresponds to global node 8.

D.2.4 Mock Turbine: Modal Analysis

In this test we examine a small mock turbine model with 30528 equations, where the discretization is made with 8-node brick elements. We compute using the serial code (subspace method) the first 5 eigenvalues using a lumped mass. With the parallel code, we compute the same eigenvalues using a parallel eigensolve (implicitly restarted Arnoldi). The computed frequencies and from the first 5 modes are compared and seen to be the same within the accuracy of the computation.

Serial Eigenvalues $(\text{rad/sec})^2$				
Mode 1	Mode 2	Mode 3	Mode 4	Mode 5
8.10609997E-02	8.13523152E-02	8.13523152E-02	9.33393875E-02	9.33393875E-02
Parallel Eigenvalues $(\text{rad/sec})^2$				
8.10609790E-02	8.13522933E-02	8.13522972E-02	9.33393392E-02	9.33393864E-02

The comparison of eigenvectors is a bit harder for this problem because of repeated eigenvalues. The first eigenvalue is not repeated and it can easily be seen that the serial and parallel codes have produced the same eigenmode (up to an arbitrary scaling factor). Eigenvalues 2 and 3 are repeated and thus the vectors computed are, permissibly, drawn from a subspace and thus direct comparison is not evident. The same holds for eigenvalues 4 and 5; though, it can be observed that vector 4 from the serial computation does closely resemble vector 5 from the parallel computations – i.e. they appear to be drawn from a similar region of the subspace.

As a test of the claim of differing eigenmodes due to selection of different eigenvectors from a subspace, we also compute the first 5 modes of an asymmetric structure that does not possess repeated eigenvalues. The basic geometry is that of perturbed cube. The first 5 eigenvalues and modes are compared and show proper agreement to within the accuracy of the computations for both the eigenvalues and the eigenmodes.

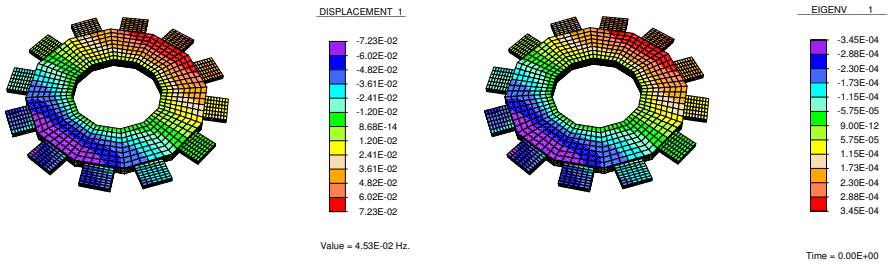

Figure D.1: Comparison of Serial (left) to Parallel (right) mode shape 1 degree of freedom 1.

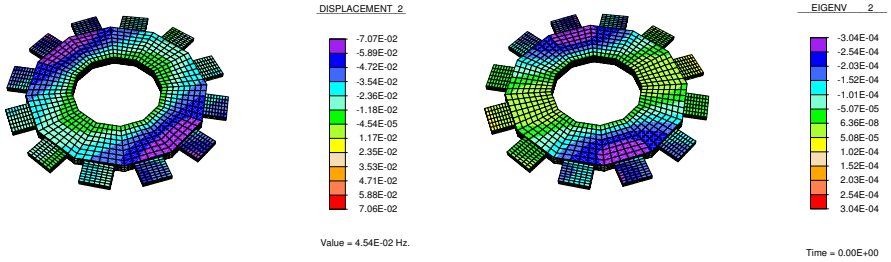

Figure D.2: Comparison of Serial (left) to Parallel (right) mode shape 2 degree of freedom 2.

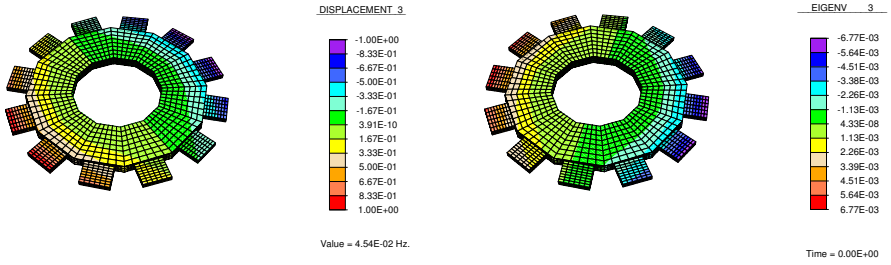

Figure D.3: Comparison of Serial (left) to Parallel (right) mode shape 3 degree of freedom 3.

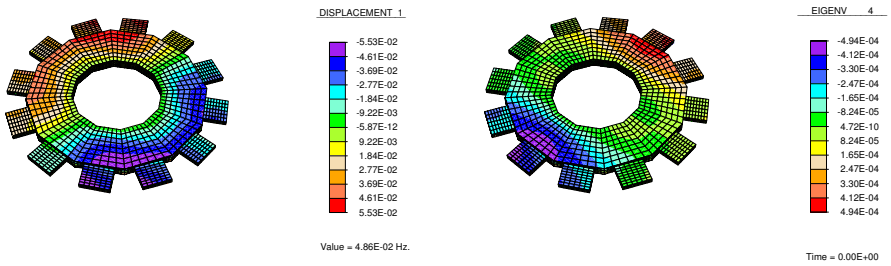

Figure D.4: Comparison of Serial (left) to Parallel (right) mode shape 4 degree of freedom 1.

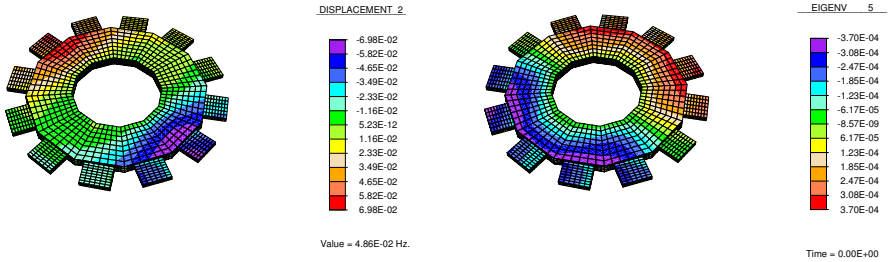

Figure D.5: Comparison of Serial (left) to Parallel (right) mode shape 5 degree of freedom 2.

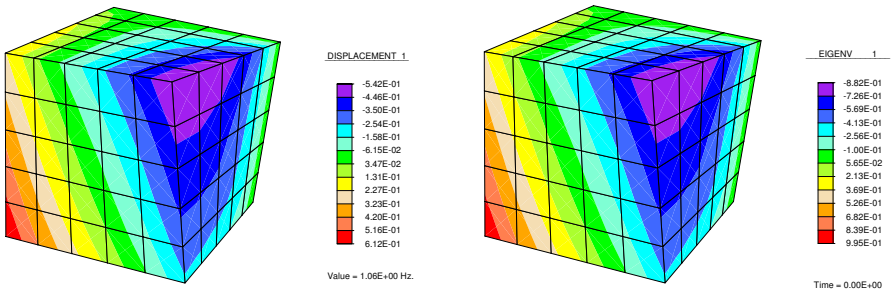

Figure D.6: Comparison of Serial (left) to Parallel (right) mode shape 1 degree of freedom 1.

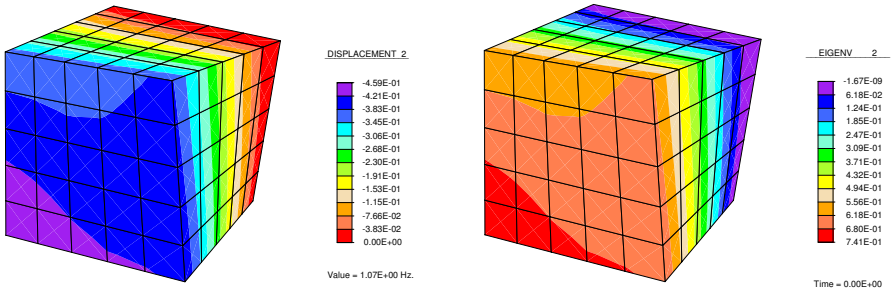

Figure D.7: Comparison of Serial (left) to Parallel (right) mode shape 2 degree of freedom 2.

Serial Eigenvalues $(\text{rad/sec})^2$				
Mode 1	Mode 2	Mode 3	Mode 4	Mode 5
4.46503673E+01	4.52047021E+01	9.08496135E+01	2.32244552E+02	3.04152767E+02
Parallel Eigenvalues $(\text{rad/sec})^2$				
4.46503674E+01	4.52047021E+01	9.08496136E+01	2.32244552E+02	3.04152767E+02

D.2.5 Transient

This test involves a mixed element test with shells, bricks, and beams under a random dynamic load. The basic geometry consists of a cantilever shell with a brick block above it which has an embedded beam protruding from it. The loading is randomly prescribed on the top of the structure and the time histories are followed and compared for the displacements at a particular point, the first stress component in a given element, and the 1st principal stress and von Mises stress at a particular node. The time history is followed for 20 time steps. The time integration is performed using Newmark's method. Agreement is seen to be perfect to the accuracy of the computations.

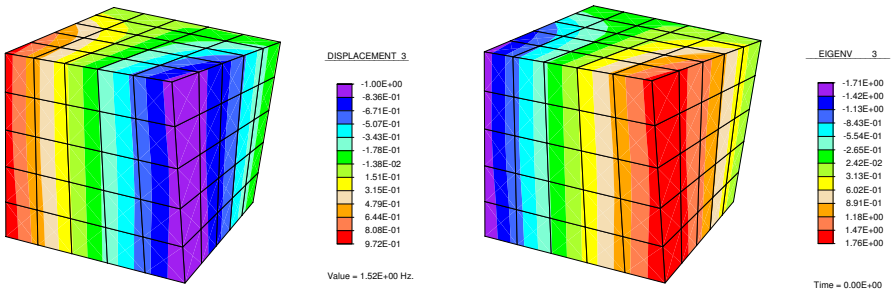

Figure D.8: Comparison of Serial (left) to Parallel (right) mode shape 3 degree of freedom 3.

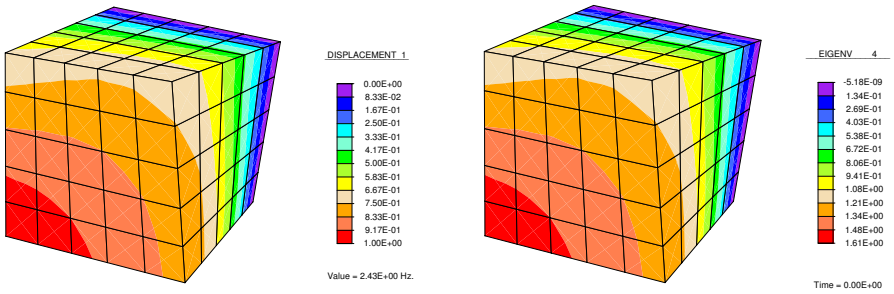

Figure D.9: Comparison of Serial (left) to Parallel (right) mode shape 4 degree of freedom 1.

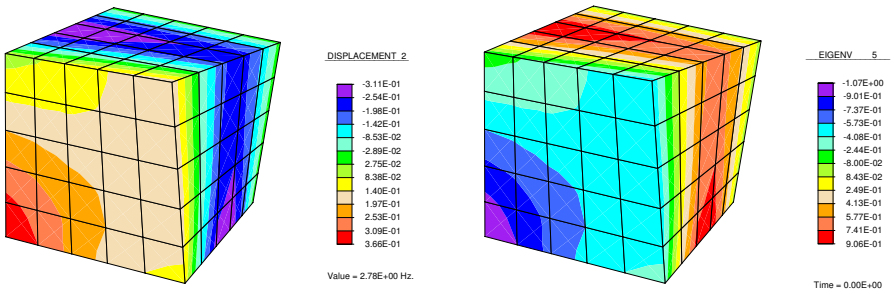

Figure D.10: Comparison of Serial (left) to Parallel (right) mode shape 5 degree of freedom 2.

	z-Displacement at (0.6,1,1)		σ_{xx} in Element 1	
Time	Serial Value	Parallel Value	Serial Value	Parallel Value
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2.5000E-01	2.5181E-04	2.5181E-04	3.9640E-02	3.9640E-02
5.0000E-01	6.0174E-04	6.0174E-04	1.3681E-01	1.3681E-01
7.5000E-01	8.3328E-04	8.3328E-04	1.9837E-01	1.9837E-01
1.0000E+00	1.1250E-03	1.1250E-03	2.2532E-01	2.2532E-01
1.2500E+00	4.2010E-04	4.2010E-04	1.5061E-01	1.5061E-01
1.5000E+00	-7.1610E-04	-7.1610E-04	-1.5312E-01	-1.5312E-01
1.7500E+00	-1.3485E-03	-1.3485E-03	-3.7978E-01	-3.7978E-01
2.0000E+00	-2.2463E-03	-2.2463E-03	-4.2376E-01	-4.2376E-01
2.2500E+00	-1.8943E-03	-1.8943E-03	-4.4457E-01	-4.4457E-01
2.5000E+00	-9.1891E-04	-9.1891E-04	-2.9013E-01	-2.9013E-01
2.7500E+00	-6.8862E-04	-6.8862E-04	-1.4539E-02	-1.4539E-02
3.0000E+00	3.8305E-05	3.8306E-05	1.1134E-03	1.1139E-03
3.2500E+00	7.4499E-05	7.4499E-05	-1.1587E-01	-1.1587E-01
3.5000E+00	-1.4893E-04	-1.4893E-04	1.1732E-01	1.1732E-01
3.7500E+00	1.9767E-04	1.9767E-04	4.3679E-02	4.3678E-02
4.0000E+00	-1.8873E-04	-1.8873E-04	-2.1461E-01	-2.1461E-01
4.2500E+00	5.7747E-04	5.7747E-04	2.6870E-01	2.6871E-01
4.5000E+00	1.3268E-03	1.3268E-03	3.2132E-01	3.2132E-01
4.7500E+00	1.3859E-03	1.3859E-03	1.3378E-01	1.3378E-01
5.0000E+00	2.5241E-03	2.5241E-03	6.6854E-01	6.6854E-01

Stresses at Global Node 1				
Time	Serial Values		Parallel Values	
Step	I_1 Principal	von Mises	I_1 Principal	von Mises
1	7.5561E-02	9.5922E-02	7.5561E-02	9.5922E-02
2	2.4364E-01	3.0328E-01	2.4364E-01	3.0328E-01
3	3.4447E-01	4.2623E-01	3.4447E-01	4.2623E-01
4	4.0833E-01	5.1265E-01	4.0833E-01	5.1265E-01
5	2.5260E-01	3.1018E-01	2.5260E-01	3.1018E-01
6	1.5934E-01	3.6208E-01	1.5934E-01	3.6208E-01
7	3.5077E-01	7.7659E-01	3.5077E-01	7.7659E-01
8	4.3971E-01	9.8767E-01	4.3971E-01	9.8767E-01
9	4.4131E-01	9.8761E-01	4.4131E-01	9.8761E-01
10	2.5587E-01	5.6437E-01	2.5587E-01	5.6437E-01
11	1.2681E-01	2.3667E-01	1.2681E-01	2.3667E-01
12	2.3099E-02	3.6287E-02	2.3099E-02	3.6286E-02
13	9.8640E-02	2.2004E-01	9.8640E-02	2.2004E-01
14	2.0000E-01	2.4597E-01	2.0000E-01	2.4597E-01
15	1.1798E-01	1.6039E-01	1.1798E-01	1.6039E-01
16	1.8668E-01	4.2255E-01	1.8668E-01	4.2255E-01
17	4.3432E-01	5.2267E-01	4.3432E-01	5.2267E-01
18	5.8732E-01	7.3503E-01	5.8732E-01	7.3503E-01
19	2.7197E-01	3.7066E-01	2.7197E-01	3.7066E-01
20	1.1706E+00	1.4434E+00	1.1706E+00	1.4434E+00

D.2.6 Nonlinear elastic block: Static analysis

In this test a unit neo-hookean block is clamped on one side and subjected to surface load on the opposite side. The displacements at two random nodes are compared as well as the max equivalent shear stress (von Mises) over the entire mesh. All values are seen to be the same between the serial and parallel computation.

Serial Displacements						
Node	x-coor	y-coor	z-coor	x-disp	y-disp	z-disp
50	0.00E+00	0.00E+00	1.67E-01	0.0000E+00	0.0000E+00	0.0000E+00
100	1.67E-01	0.00E+00	3.33E-01	5.6861E-04	1.0501E-04	1.5672E-04

Serial Maximum Equivalent Shear
0.881

Parallel Displacements						
(P)Node	x-coor	y-coor	z-coor	x-disp	y-disp	z-disp
(2) 27	0.00E+00	0.00E+00	1.67E-01	5.8777E-17	4.9956E-18	-6.3059E-17
(2) 54	1.67E-01	0.00E+00	3.33E-01	5.6861E-04	1.0501E-04	1.5672E-04

Note: Processor 2's nodes 27 and 54 correspond to global nodes 50 and 100.

Parallel Maximum Equivalent Shear
0.881

D.2.7 Nonlinear elastic block: Dynamic analysis

In this test a non-linear neo-hookean block is subjected to a step displacement at one end while the other is end is clamped. The time history of the displacement at the center of the block is followed. The time integration is performed using Newmark's method. Agreement is seen to be perfect to the accuracy of the computation.

x-Displacement		
Time	Serial Run (Node 172)	Parallel Run (Node 25, Processor 3)
0.0000E+00	0.0000E+00	0.0000E+00
1.0000E-02	-6.6173E-07	-6.6173E-07
2.0000E-02	1.1588E-05	1.1588E-05
3.0000E-02	-4.8502E-05	-4.8502E-05
4.0000E-02	-4.8177E-05	-4.8177E-05
5.0000E-02	2.6189E-04	2.6189E-04
6.0000E-02	7.8251E-04	7.8251E-04
7.0000E-02	1.0785E-03	1.0785E-03
8.0000E-02	9.7015E-04	9.7015E-04
9.0000E-02	7.7567E-04	7.7567E-04
1.0000E-01	8.2252E-04	8.2252E-04

Note: Local node 25 of processor 3 corresponds to global node 172.

D.2.8 Plastic plate

In this test a small version of the quarter plastic plate from the timing runs is used with 4500 8-node brick elements. The problem involves 10 uniform size load steps which

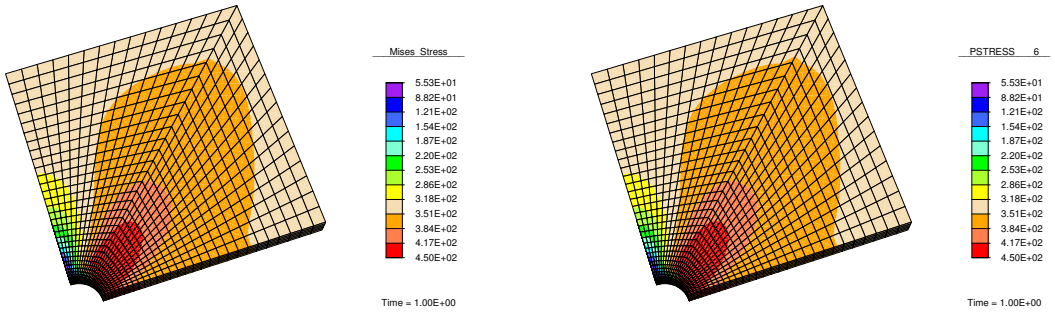

Figure D.11: von Mises stresses at the end of the loading. (left) serial, (right) parallel

drives the plate well into the plastic range. The displacement history is followed for a point on the loaded edge of the plate. As seen in the tables the parallel and serial runs match. Also shown are the contours of the von Mises stresses at the end of the run with the plastic zone emanating from the plate hole; these also match perfectly within the accuracy of the computation.

y-Displacement		
Load Step	Serial Run (Node 5700)	Parallel Run (Node 1376, Part. 4)
0.0000E+00	0.0000E+00	0.0000E+00
1.0000E-01	1.5260E-02	1.5260E-02
2.0000E-01	3.0520E-02	3.0520E-02
3.0000E-01	4.5780E-02	4.5780E-02
4.0000E-01	6.1039E-02	6.1039E-02
5.0000E-01	7.6308E-02	7.6308E-02
6.0000E-01	9.1639E-02	9.1639E-02
7.0000E-01	1.0707E-01	1.0707E-01
8.0000E-01	1.2264E-01	1.2264E-01
9.0000E-01	1.3848E-01	1.3848E-01
1.0000E+00	1.5519E-01	1.5519E-01

Note: Local node 1376 on processor 4 corresponds to global node 5700.

D.2.9 Transient plastic

This test involves a mixed element test with shells, bricks, and beams under a random dynamic load with load sufficient to cause extensive plastic yielding in the system. The basic geometry consists of a cantilever shell with a brick block above it which has a an embedded beam protruding from it. The loading is randomly prescribed on the top of

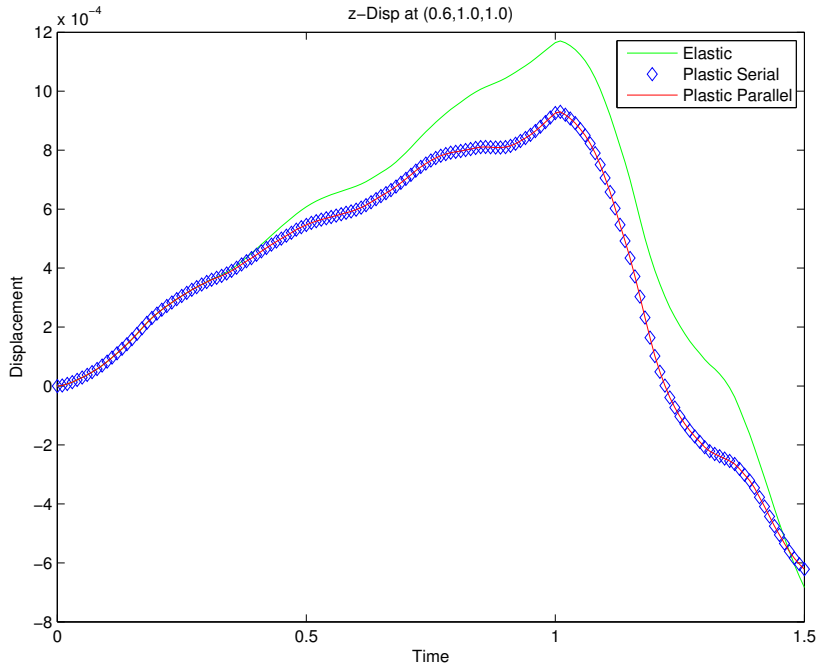

Figure D.12: Z-displacement for the node located at (0.6, 1.0, 1.0).

the structure and the time histories are followed and compared for the displacements at a particular point, the first stress component in a given element, and the 1st principal stress and von Mises stress at a particular node. The time history is followed for 150 time steps. The time integration is performed using Newmark's method. As a benchmark the elastic response (from the serial computation) is also shown in each figure. The agreement between the parallel and serial runs is seen to be perfect.

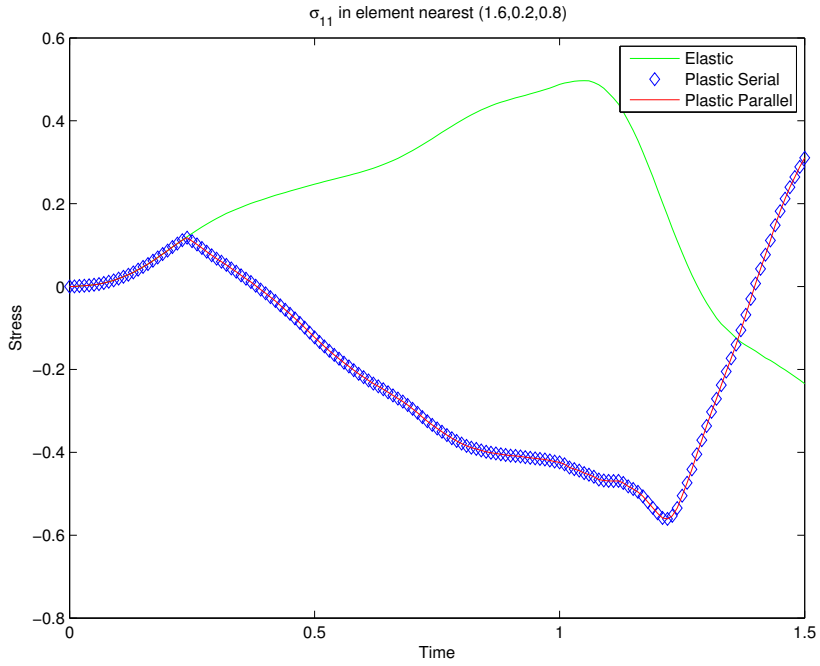

Figure D.13: 11-component of the stress in the element nearest (1.6, 0.2, 0.8).

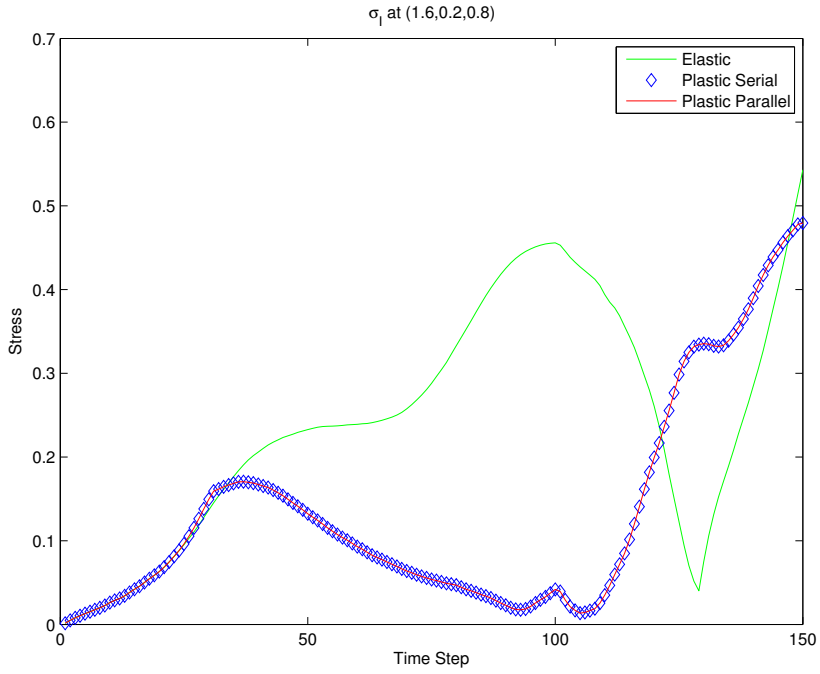

Figure D.14: 1st principal stress at the node located at (1.6, 0.2, 0.8).

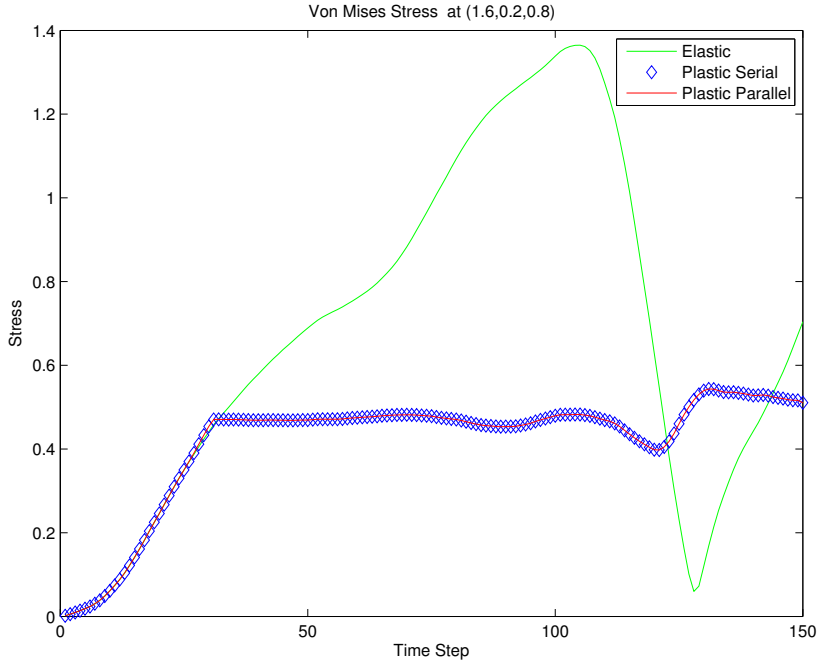

Figure D.15: von Mises stress at the node located at (1.6, 0.2, 0.8).

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