RocFrac User's Guide

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Chapter 1

RocFrac Command Statements

The purpose of RocFrac is to simulate complex dynamic fracture problems using an explicit Cohesive Volumetric Finite Element (CVFE) scheme. RocFrac can handle large deformations, moving interfaces, and non-linear material response.

1.1 Compiling

The source files and makefile for the analysis code resides in the directory Rocfrac/Source in the RocStar tree. The source files and makefile for the preprocessor *rfracprep* reside in the directory Rocfrac/utilities/RocfracPrep. The preprocessor *rfracprep* is automatically build within the Rocstar suite.

1.2 Sequence Needed to Run a Problem

This section describes the sequence of execution needed to run RocFrac. In general there are 4 steps involved: create the finite element mesh, partition the mesh and add cohesive elements (if required), solution and post-processing.

1.2.1 Create Finite Element Mesh/Steps needed with Patran

The first step is to create the finite element mesh. As of this writing there is only one practical way to create the volumetric finite element mesh and that is to use the commercial package Patran. Please refer to the Patran documentation on how to use Patran for creating meshes. If Patran is used at NCSA then the user is limit to creating meshes no greater then roughly 1 million elements before needing to submit the Patran job as batch. Once the mesh and boundary conditions have been created the file needs to be exported to a Patran Neutral File. The file should have the same prefix as that found in the control deck file under the option ***PREFIX**. The ending suffix of the neutral file must end in '*.pat*' or '*.out*'. Thus, the name convention is ***PREFIX.***out or ***PREFIX***.pat. This file should be placed in the *Modin* directory in located in the *Rocfrac* directory of the Rocstar suite.

1.2.1.1 Geometry Creation

There are no special considerations to be address. The geometry can be created just as one would proceed to do for a finite element calculation.

1.2.1.2 Mesh Creation

There are no special considerations that need to be taken when creating a finite element mesh, just engineering judgment. Note, however, that the only elements currently supported by Rocfrac are: 4 and 10 node tetrahedral elements for an Arbitrary Euler Lagrange (***ALE**) calculation and 8 node hexahedral, 4 and 10 node tetrahedral for non-ALE calculations. Currently the use of mixed meshes in modeling the geometry is not permitted.

For very large meshes it is useful to split the mesh into sections if possible. An example is a 4 segment rocket with no case. Each segment can be meshed independently and written to a Patran neutral file. The mesh files are then placed in *Rocfrac/Modin* with the the file name ***PREFIX***.#.out where # is the number of the segment starting from 1. Note: each mesh's numbering of elements and nodes must start from 1.

1.2.1.3 Monitoring nodes and elements

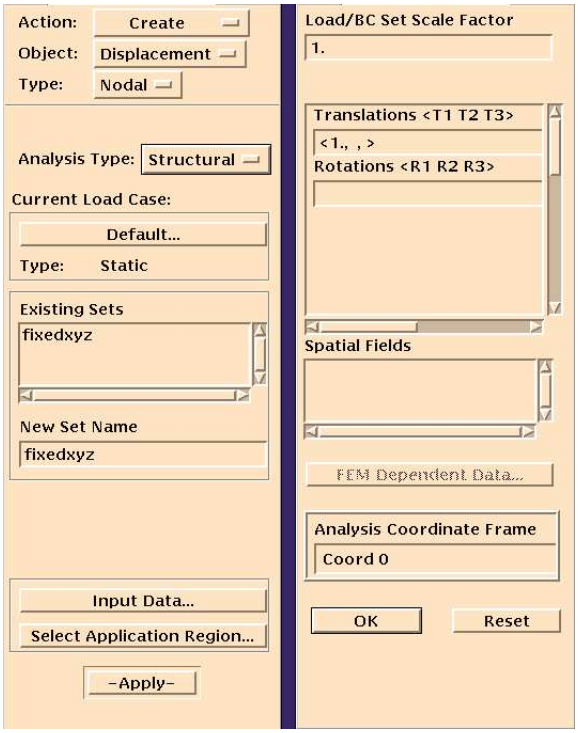
To specify nodes or elements to monitor during the simulation use the Create -> Temperature Boundary Conditions dialog. Actual values give as boundary condition is ignored, BC is only used to mark monitored nodes and elements.

1.2.1.4 Boundary Condition Flags

The boundary conditions set in Patran are not the actual boundary conditions for the model, but instead represent flags that denote the actual boundary conditions.

Setting the Displacement Boundary Condition Flags

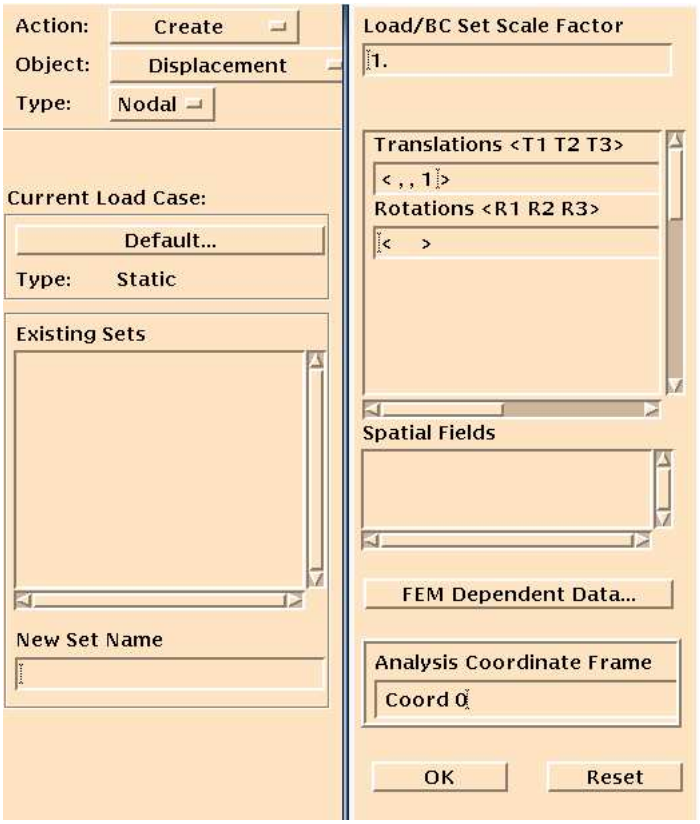
The way to set the boundary condition for the displacement boundary conditions is to assign the U_x fixed displacement the appropriate flag as that found in the control deck option ***BOUNDARY** (See Section 2.1.19). For example, if the top of a specimen is to be fixed in all three directions then the U_x fixed displacement should be given a value of 1.0 in Patran, which will correspond to the boundary condition specified in card 1 under the ***BOUNDARY** option.



Patran dialog box to set displacement boundary conditions

Setting the Mesh Motion Boundary Condition Flags

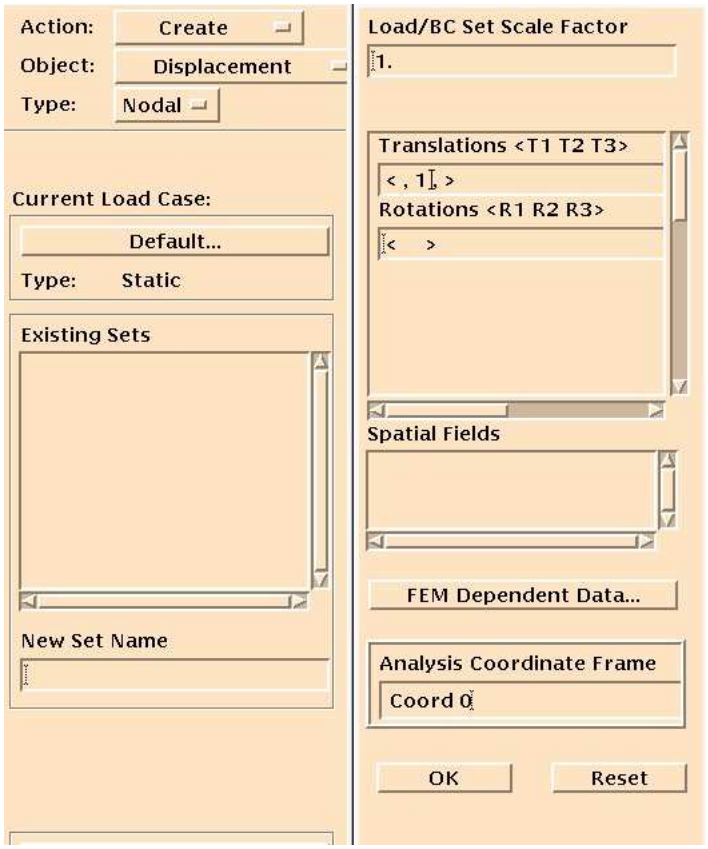
The way to set the boundary condition for the mesh motion boundary conditions is to use the 'create displacement dialog box' and assign the U_z displacement the appropriate flag as that found in the control deck option ***BOUNDARYMM** (See Section 2.1.20). For example, if the top of a specimen is to have fixed velocities in all three directions then the U_z displacement should be given a value of 1.0 in Patran, which will correspond to the boundary condition specified as card 1 under the ***BOUNDARYMM** option.



Setting the Mesh Motion Boundary Condition Flags

Setting the Thermal Boundary Conditions

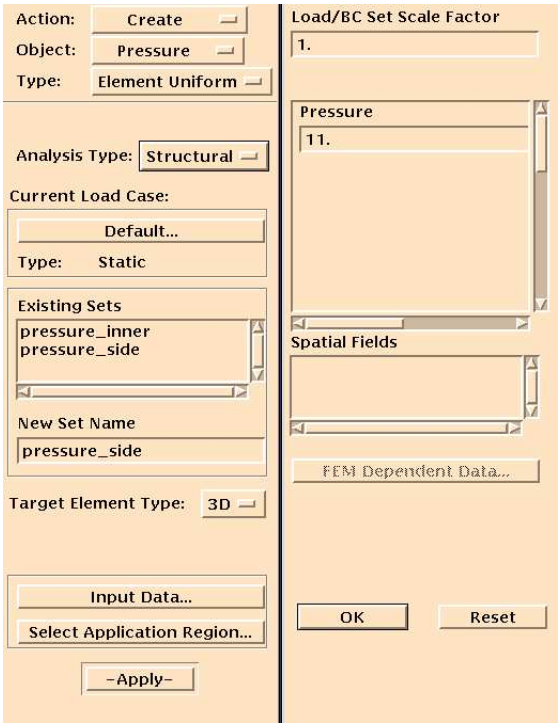
The way to set the boundary condition for the thermal boundary conditions is to use the 'create displacement dialog box' and assign the U_y displacement the appropriate flag as that found in the control deck option ***BOUNDARYHT** (See Section 2.1.20). For example, if the top of a specimen is to have fixed temperature then the U_y displacement should be given a value of 1.0 in Patran, which will correspond to the boundary condition specified as card 1 under the ***BOUNDARYHT** option.



Setting the Thermal Boundary Condition Flags

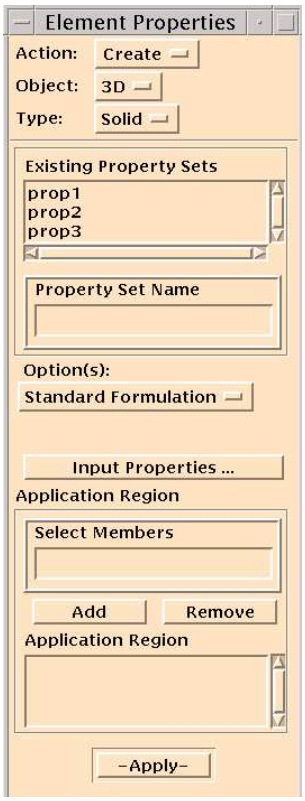
1.2.2 Controlling what surface is in contact with the the fluids domain

To specify which surfaces are in contact with the fluids domain we use Patran's '*apply pressure*' dialog box. On the surfaces that are in contact with the fluids domain use a pressure value equal to 1 for non-inert surfaces or 2 for inert surfaces . To specify a surface that is not in contact with the fluids domain we use a pressure value of 0. To specify a surface that is between two solids domain use the value of 4 on one surface and 5 on the opposite surface.



1.2.3 Setting element flags

To specify the element flags using Patran for the volumetric flags we use the 'properties' option. Assign an element property to each volume where you want a different property. Note that you should not use the material property window.



1.2.4 Run rfracprep

The Patran Neutral Files should be placed in the *Rocfrac/ModIn* directory. The program *rfracprep* creates the cohesive elements (if needed) and partitions the mesh using the program METIS. It currently only supports the inclusion of cohesive elements everywhere in the domain and only between tetrahedral elements. To run type: *rfracprep* in the same directory as the Rocfrac-Control.txt file. Execution is self-explanatory and two command line options are available; *-np* # tells *rfracprep* how many processors to partition the mesh and *-un* # (where # is the units conversion factor) is used to convert the units of the geometry. *rfracprep* will then create each processor's input file in the directory *Rocfrac/Rocin/* and each volumetric mesh file will be called *<prefix>.####.hdf* where #### corresponds to the processor's id. It will also create the 2D (SurfMesh.####.hdf) interface meshes needed to be registered with RocCom via RocFrac. The final file that needs to be created by your favorite editor (emacs/vi..) is the input control deck file RocfracControl.txt, see Section 2.1.

1.2.5 Run RocFrac

The program RocFrac is part of the RocStar code, so it must be run within the RocStar framework. In order to run it in Stand-Alone mode (i.e. no other RocStar modules are needed), the option 'SolidAlone Rocflo Rocfrac Rocburn' can be specified, thus allowing for a Rocfrac alone analysis problem. In order to run a stand alone problem, the pressure and burning rate needs to be applied within RocFrac since these quantities are not supplied from the fluid or burning modules. During the analysis the results output files are written to the *Rocfrac/Rocout/* directory. These HDF files consist of: surface meshes results (isolid_*.hdf), volume meshes (solid_*hdf), and restart quantities (solid_bnd*.hdf). Note, as of this writing, for the restart, it must be restarted on the same number of processors for each run.

1.2.6 Run the Post-processor

The isolid_*.hdf and solid_*.hdf files are used in *Rocketeer* to view the results. The solid_bnd*.hdf files are not to be used in *Rocketeer*, there're only used for restarting.

1.3 File Management

- *RocfracControl.txt* - control deck input file. See Section 2.1 for a description of the control deck parameters. This file should be placed in the Rocfrac/ directory in the GenX tree.
- Modin/<prefix>.pat - Patran Neutral File.
- Rocin/<prefix>.####.inp - each processor's input file.
- *.res* - output file, summarizes the input data from the control deck.
- Rocout/*.hdf - Rocketeer input and restart.

Chapter 2

Executive Control Section

This section describes the keywords and specifications for the input control deck file. The control deck file contains keyword statements that correspond to the analysis. The format definitions are as follows: A - character, F - real, I - integer. Keyword cards must begin with a * in column 1. These keywords and keyword specifics are based on Abaqus's. For a more in-depth description the reader should consult the abaqus keyword manual.

2.1 Executive System Parameters

2.1.1 *PREFIX: Define the prefix extension for IO files.

This option allows the user to specify what the prefix extensions are for the input files and the output files. The prefix should be no more then 20 characters in length. NOTE: ALWAYS NEEDED

Option	Format	Entry
First card:		
1	A	prefix name

2.1.2 *NRUN: Define the timing parameters** (Obsolete)

This option is used to specify the parameters needed to obtain a stable solution. NOTE: ALWAYS NEEDED

Option	Format	Entry
First card:		
2	I	divide the courant condition time step by

Note: typical values are 1.0-4.0 depending on whether ALE was specified.

2.1.3 *DYNAMIC:

This option is used to specify the parameters needed to obtain a stable solution. NOTE: ALWAYS NEEDED

‡**Optional Parameters:**

SCALE FACTOR

Factor to multiply the Courant limit, typical values are .8 - .9 without ALE and .5-.8 with ALE

First card: No cards

2.1.4 *ALE: Enable ALE

This option is used to run an ALE simulation (the default is off if not specified).

Option	Format	Entry

First card:

2	I	mesh motion stability parameter

Note: typical values are between .1-.3

2.1.5 *IOPARAM: Output options

This option is used to specify the output interval to write results to a file that will later be post-processed. If the option is not given then the default is to never output the results to a file.

Option	Format	Entry

First card:

1	I	time step interval for output

2.1.6 *IOFORMAT: Format of input files

This option is used to specify the format of the input file. If the value equals 1 then the input files are ASCII and if the value equals 0 then the input files are binary.

2.1.7 *POVIO: Output POV-RAY format

This option is used to specify that the outer boundary of the mesh should be written to a file for further analysis with the pov-ray ray tracing program. The output files need first to be run through the post pov-ray program. If the option is not given then the default is not to write any pov-ray files.

Option	Format	Entry

First card:

1	F	value to magnify the displacement
2	I	time step to start the output
3	I	interval for output

2.1.8 *HYPERELASTIC: hyperelastic material model

Specifies a hyperelastic volumetric elements material model.

‡**Optional Parameters:**

NEOHOOKINC
Specifies the Incompressible neo-Hookean model

ARRUDA-BOYCE
Specifies the ARRUDA-BOYCE material model, good for filled rubbers

Option	Format	Entry
First card:		
1	I	total number of materials
Following cards:		
1	F	Young's Modulus
2	F	Poisson's Ratio
3	F	Density
4	F	Thermal Expansion Coefficient

2.1.9 *MICROMECHANICAL: micromechanical material model

Specifies a micromechanical volumetric elements material model.

‡**Optional Parameters:**

MODEL=HUANG
Specifies the micromechanical model developed by Prof. Huang

MODEL=MATOUS ** (under development)
Specifies the micromechanical model developed by Karl Matous

Option	Format	Entry
First card:		
1	F	Matrix Young's Modulus
2	F	Matrix Poisson's Ratio
2	F	Matrix volume fraction
3	F	Composite Density
1	I	total number of particles
Following cards:		
1	F	Particle Young's Modulus
2	F	Particle Poisson's Ratio
3	F	Particle volume fraction
4	F	Particle size

2.1.10 *ELASTIC: elastic material model

Specifies a elastic volumetric elements material model.

‡**Optional Parameters:**

NLGEOM
Specifies finite rotations

Option	Format	Entry
First card:		
1	I	total number of materials
Following cards:		
1	F	Young's Modulus
2	F	Poisson's Ratio
3	F	Density
4	F	Thermal Expansion Coefficient

2.1.11 *MATVOL: Volumetric element material properties** (Obsolete)

Specifies the volumetric elements material properties. NOTE: ALWAYS NEEDED

Option	Format	Entry
First card:		
1	I	total number of materials
Following cards:		
1	F	Young's Modulus
2	F	Poisson's Ratio
3	F	Density
4	F	Thermal Expansion Coefficient
5	F	Material type analysis

For card 5, the current options are:

0 - non-linear arruda-boyce

1 - large deformation, linear material

2 - small deformation, linear material

-1 - Neo-Hookean Incompressible

11 - Neo-Hookean Incompressible, Node based formulation

13 - large deformation, linear material, Node based formulation

2.1.12 *MATCOH: Cohesive element properties

Specifies the cohesive elements properties.

Option	Format	Entry
First card:		
1	I	total number of properties
Following cards:		
1	F	Critical normal opening displacement
2	F	Critical tangential opening displacement
3	F	Critical tensial stress
4	F	Critical shearing stress
5	F	Initial Stress threshold

2.1.13 *PLOAD: Static Pressure Load

Defines the pressure value for a static pressure load on a triangular surface elements. Need a .press file to give a list of the surface triangles where the pressure is applied.

Option	Format	Entry
First card:		
1	I	Pressure

2.1.14 *PLOAD1: Dynamic Pressure Load

Specifies that the load changes with each time step, the pressure values are read in from an input file for each time step. The file name should be no longer then 20 characters.

Option	Format	Entry
First card:		
1	A	file name containing the nodal pressure values

2.1.15 *DUMMYTRACT: Assigns a traction when Rocfrac Stand alone is used

The magnitude of the traction force applied, the region that the traction gets applied to is specified in the RocFracUpdateInbuff subroutine.

‡**Optional Parameters:**

INTERFACE = SF
Apply pressure on surfaces marked Fluid/Solid interface
INTERFACE = S
Apply pressure on surfaces marked Solid interface
INTERFACE = ALL
Apply pressure on all surfaces

Option	Format	Entry

Option	Format	Entry
First card:		
1	F	Traction magnitude value

2.1.16 *DUMMYFLUX: Assigns a heat flux when Rocfrac Stand alone is used

The magnitude of the heat flux applied, the region that the traction gets applied to is specified in the RocFracUpdateInbuff subroutine.

Option	Format	Entry
First card:		
1	F	Traction magnitude value

2.1.17 *DUMMYBURN: Assigns a burn rate when Rocfrac Stand alone is used

The magnitude of the burn rate applied, the region that the traction gets applied to is specified in the RocFracUpdateInbuff subroutine.

Option	Format	Entry
First card:		
1	F	Traction magnitude value

2.1.18 *END: Denotes end of control deck input

Place at the end of the control deck input key variables. No options. NOTE: ALWAYS NEEDED

2.1.19 *BOUNDARY: Displacement Boundary Conditions

Specifies the meaning of the boundary condition flags set in the meshing program. A *zero* indicates that the boundary condition is an imposed velocity and a *one* is for an imposed force. Only the last three parameters should be changed to the specific value for each card. Note ***BOUNDARY** is not used by the analysis code but only by the preprocessor, hence ***BOUNDARY** should always be placed before the ***END** option.

Option	**Format**	**Entry**
First to number of boundary flags:		
10 0 0	3E	value x, value y, value z
20 0 0	3E	value x, value y, value z

2.1.20 *BOUNDARYMM: Mesh Motion Boundary Conditions

Specifies the meaning of the mesh motion boundary condition flags set in the meshing program. A *zero* indicates that the boundary condition is an imposed velocity and a *one* is for an imposed force.

Option	**Format**	**Entry**
First to number of boundary flags:		
10 0 0	3E	value x, value y, value z
20 0 0	3E	value x, value y, value z

2.1.21 *BOUNDARYHT: Thermal Boundary Conditions

Specifies the meaning of the thermal boundary condition flags set in the meshing program. A *zero* indicates that the boundary condition is an imposed temperature and a *one* is for an imposed heat flux.

Option	**Format**	**Entry**
First to number of boundary flags:		
10 0 0	3E	value x, value y, value z
20 0 0	3E	value x, value y, value z

2.1.22 *INITIAL CONDITION: assigns the initial conditions

The magnitude of the initial conditions of the simulation.

‡**Optional Parameters:**

TYPE = TEMPERATURE
Initial reference temperature.

Option	**Format**	**Entry**

Option	**Format**	**Entry**
First card:		
1	F	Initial Temperature

2.1.23 *ELEMENT: Element Type

Specifies the volumetric element type.

‡**Optional Parameters:**

V3D4

4 node tetrahedral

V3D4NCC

4 node tetrahedral, node based element, lumped using circumcenter

V3D4N

4 node tetrahedral, node based element, lumped using centroid

V3D10R

10 node tetrahedral, reduced integration

V3D10

10 node tetrahedral

V3D8ME

8 node hexahedral mixed enhanced

2.1.24 *DAMPING

Specifies artifical damping.

2.1.25 *HEAT TRANSFER

Specifies material properties for heat transfer analysis

Option	Format	Entry
First card:		
1	I	total number of materials
Following cards:		
1	F	Thermal conductivity, κ
2	F	Specific heat at constant pressure, C_p

2.1.26 *PROBE

Monitors variables at a point in space given in Cartesian coordinates. Note: the node closest to the specified coordinates will be flag to be monitored. Probe data is written to the Rocout directory.

Option	Format	Entry
1	I	total number of probes

Following cards:

1	3E	Coor. x, Coor. y, Coor. z

Chapter 3

Three-dimensional solid element library

This section defines the three-dimensional solid (continuum) elements available in RocFrac.

3.1 Volumetric Stress/Displacement Elements:

- **V3D4** 4-node linear tetrahedron
- **V3D10** 10-node quadratic tetrahedron
- **V3D8** 8-node hexahedral

Warning: Element type **C3D4** is a constant stress tetrahedron. This element only provides accurate results in general cases with very fine meshing.

Active degrees of freedom:
1, 2, 3 (u_x,u_y, u_z)

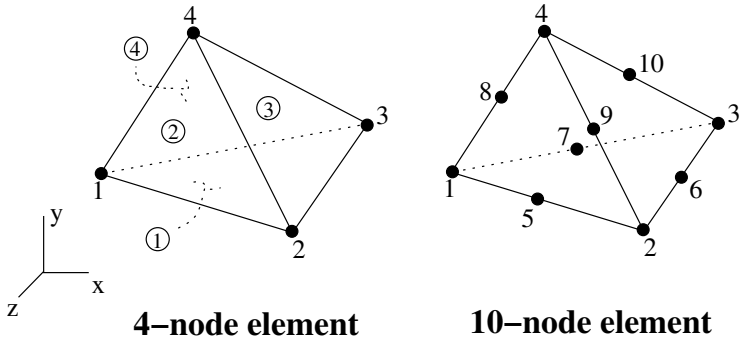


Figure 3.1: Node ordering and face numbering for tetrahedral elements

3.2 Cohesive Stress/Displacement Elements:

- **C3D6** 6-node linear triangular prism with 3-point gauss integration.
- **C3D12** 12-node quadratic triangular prism (NOT YET IMPLEMENTED)

Active degrees of freedom:
1, 2, 3 (Δu_x,Δu_y, Δu_z)

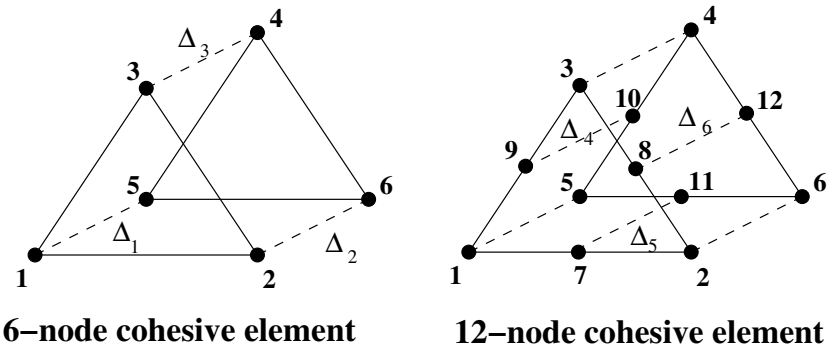


Figure 3.2: Node ordering for cohesive elements

Chapter 4

RocFrac Input File (old format)

The Input Files (i.e. the <prefix>/<prefix>.N#.inp files, where N# is the processors id) are used to communicate the analysis model into Rocfrac standalone version. Each processor has its own input file. File format was replace in Gen3 with HDF formatted files.

4.1 Data Format

The input files format is as follows:

Packet 01: Version Number

Data Card 1

VERS VERS = Version Number of Analysis Code

Packet 02: Node Data

Data Card 1

N1, Aux, Aux, Aux, Aux N1 = Number of Nodes Aux = Auxilllary flags (not applicable)

Data Card 2 (Repeated N1 times)

ID X Y NDFLAG1 X = X Cartesian Coordinate of Node Y = Y Cartesian Coordinate of Node Z = Z Cartesian Coordinate of Node NFLAG1 = Generic Flag of Node (not applicable)

Packet 03: Structural Boundary Conditions

Data Card 1

NumBC, AuxFlag

NumBC = Number of Boundary Condition Flags
AuxFlag = Auxillary Flag (not applicable)

Data Card 2 (Repeated NumBC times)

NodeID BCFLAG1 BCFLAG2

NodeID = Node Identification
BCFLAG1 = Boundary Condition Flag 1
BCFLAG2 = Boundary Condition Flag 2 (not applicable)

Packet 04: Mesh Motion Boundary Conditions

Data Card 1

NumBC, AuxFlag

NumBC = Number of Boundary Condition Flags
AuxFlag = Auxillary Flag (not applicable)

Data Card 2

NodeID BCFLAG1 BCFLAG2

NodeID = Node Identification
BCFLAG1 = Boundary Condition Flag 1
BCFLAG2 = Boundary Condition Flag 2 (not applicable)

Packet 05: Element Data

Data Card 1

```
NumElemProp
  ElemPropId
    NumElemType
      ElemType, NumEl, NumElBndry
        MatId, ElemConn, AUX

          NumElemProp = Total Number of Element Properties
          ElemPropId = Element Property Id
          NumElemType = Number of Element Types
          ElemType:
            1D - Bar0002, Bar0003, Bar0004
            2D - tri0003, tri0004, tri0006,tri0007, tri0009, tri0013
             2D - quad004, quad005, quad008,quad009, quad014,
quad015
            3D - tet0004, tet0010, tet0016
              3D - wedge06, wedge07, wedge15, wedge16,
wedge20,wedge21, wedge24, wedge52
                    3D - hex0008, hex0009=26,
hex0020,hex0021,hex0026,hex0027,hex0032,hex0064
          NumEl = Total Number of 'ElemType' Elements
          NumElBndry = Total Number of Partition Border 'ElemType'
Elements
          MatId = Element Material Id
          ElemConn = Element corner nodes followed by additional
nodes
          AUX = Auxillary Input (not applicable)
```

Data Card 2

```
IMAT, LND, AUX, AUX

          IMAT = Material ID
          LND = Element corner nodes followed by additional nodes
          NumElTot = Number of Elements Total
          AUX = Auxillary Input (not applicable)
          AUX = Auxillary Input (not applicable)
```

Packet 06: Parallel Communication

Data Card 1

```
NumNeigh

          NumNeigh = Number of Neighboring Processors
```

Data Card 2 (Repeated NumNeigh times)

```
NeighID,NumNodeShare

          NeighID = Neighbor's ID
          NumNodeShare = Number of Shared Nodes with NeighID
```

Data Card 3 (Repeated NumNodeShare times)

NodeShareID NodeShareID = ID of shared node

Packet Type 99:

Data Card 1

99 Signals End of Input File

Chapter 5

Example Problems

5.1 Layered Two Material Cantilever Beam

This example is of a cantilever beam composed of two materials. The top half of the beam is composed of a rubber and the bottom half steel, shown in Figure 5.1. The rubber has a Young's Modulus of 0.991 GPa, Poisson's ratio of .46, Density of 956.0 kg/m^3 and is to be modeled using the NeoHookean Incompressible material model. The steel has a Young's Modulus of 210 GPa, Poisson's ratio of .27, density = 7870.9 kg/m^3 and is to be modeled using small displacements and linear material response. The traction load is 100.0 and the points are all fixed at the wall.

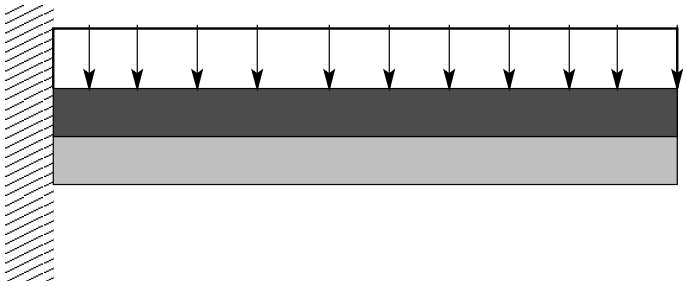


Figure 5.1: Geometry and loading condition

The input files for a four processor run can be found in cvs at /CSAR/brtnfld/GenXData/Beam2Mat.