

# Rocfrac Development Guide

by Scot Breitenfeld<sup>1</sup>

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<sup>1</sup>This file is currently maintained by SCOT BREITENFELD, brtnfld@uiuc.edu. Please send comments or error corrections to that address.

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# Chapter 1

## Theory and Concepts

For an introduction to the fundamental theories and concepts behind the Cohesive Volumetric Finite Element (CVFE) scheme the reader is encouraged to review Jeff Baylor's 1995 UIUC Thesis "A numerical Simulation of impact-induced damage of composite materials".

### 1.1 Code Structure

This section describes the basic algorithm and structure of the code.

The code uses for the direct integration the explicit central-difference method which approximates the nodal displacements, accelerations and velocities as

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t \dot{\mathbf{u}}_n + \frac{1}{2} \Delta t^2 \ddot{\mathbf{u}}_n, \quad (1.1)$$

$$\dot{\mathbf{u}}_{n+1} = \dot{\mathbf{u}}_n + \frac{\Delta t}{2} (\ddot{\mathbf{u}}_n + \ddot{\mathbf{u}}_{n+1}), \quad (1.2)$$

$$\ddot{\mathbf{u}}_{n+1} = -\mathbf{M}^{-1} (\mathbf{R}_{in_{n+1}} - \mathbf{R}_{co_{n+1}} + \mathbf{R}_{ex}). \quad (1.3)$$

Where,  $\Delta t$  is the time step,  $\mathbf{M}$  is the lumped mass matrix, and  $\mathbf{R}_{in}$ ,  $\mathbf{R}_{co}$ ,  $\mathbf{R}_{ex}$  are the global internal force, cohesive force and external force vectors, respectively. In the numerical implementation the sum within the brackets of equation 1.3 is replaced with one vector called  $\mathbf{R}_{net}$ , yet the argument name used in the subroutines that calculate the respective force vectors still retains the original force variable naming.

The numerical algorithm is as follows:

- Data input.
- Set initial conditions (  $\mathbf{u}(0)$ ,  $\dot{\mathbf{u}}(0)$ ,  $\ddot{\mathbf{u}}(0)$  ).
- Solution time increment loop:
  - Update the nodal displacements.

$$u_{n+1} = u_n + \Delta t \dot{u}_n + \frac{1}{2} \Delta t^2 \ddot{u}_n$$

- Update mesh position.
- Calculate the mesh normals at the nodes.
- Update mass matrix due to change in undeformed configuration.
- Calculate  $R\_bar$ .
- Calculate mesh velocity vector.
- Compute the internal force vector  $R_{co}$ .
- Calculate the mesh acceleration.
- Compute the internal force vector  $R_{in}$ .
- Update the nodal velocity and accelerations.

$$\ddot{u}_{n+1} = M^{-1} R_{net_{n+1}},$$

$$\dot{u}_{n+1} = \dot{u}_n + \frac{\Delta t}{2} (\ddot{u}_n + \ddot{u}_{n+1}).$$

- Apply displacement boundary conditions.

## 1.2 Call Graph

This section describes the call graph of the subroutines. The main driver code is called `rocfrac.f`. The call graph is pictured in Figure 1.1. Not that the calls to the MPI libraries are not included.

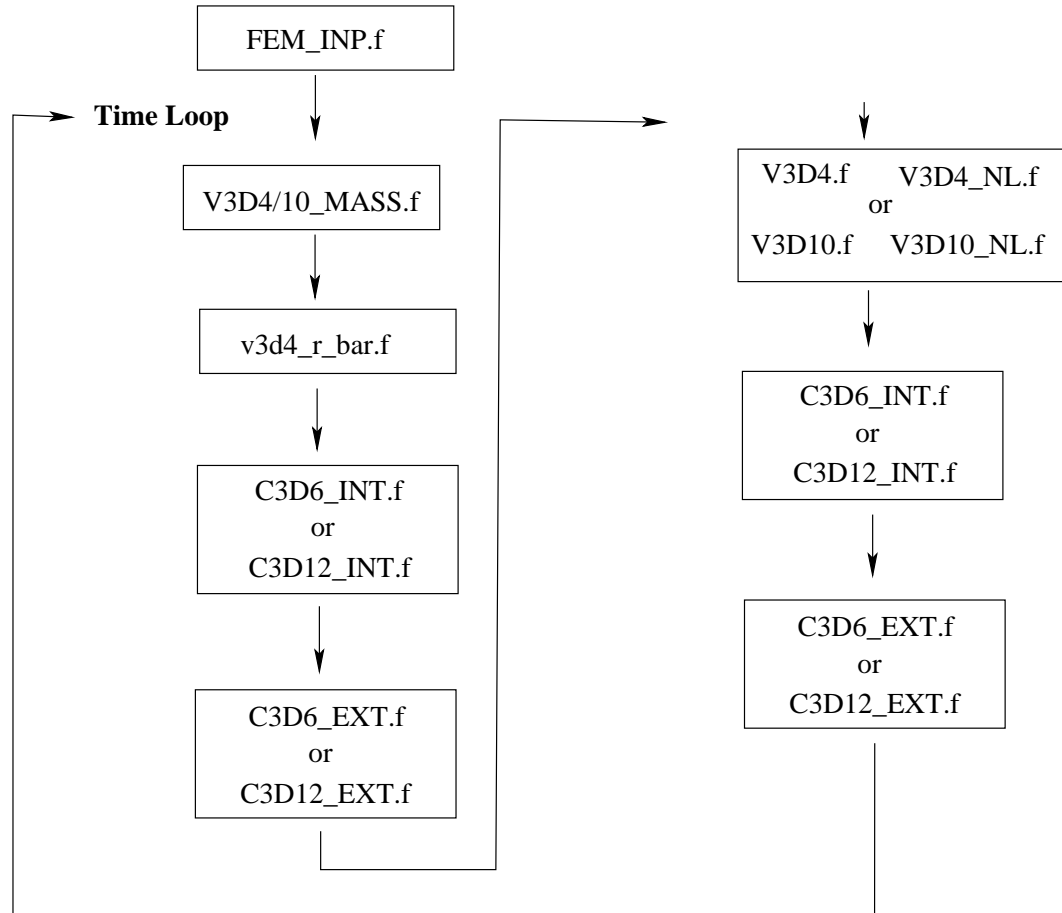


Figure 1.1: Call Tree for rocfrac

## Chapter 2

# Subroutines and Functions

This section contains a detail listing of the subroutines and functions and their purpose, notes, inputs and output.

### 2.1 Rocfrac/Rocfrac/Source/angle\_rad\_3d.f90

NAME

`angle_rad_3d`

FUNCTION

returns the angle in radians between two rays in 3D.

NOTES

The routine always computes the SMALLER of the two angles between two rays. Thus, if the rays make an (exterior) angle of 1.5 radians, the (interior) angle of 0.5 radians will be reported.

Formula:

$$X \cdot Y = \text{Norm}(X) * \text{Norm}(Y) * \text{Cos} ( \text{Angle}(X,Y) )$$

## 2.2. ROCFRAC/ROCFRAC/SOURCE/CAUCHYSTRESSPRINC.F90

### INPUTS

real X1, Y1, Z1, X2, Y2, Z2, X3, Y3, Z3, are three points  
which define the rays. The rays are:  
( X1-X2, Y1-Y2, Z1-Z2 ) and ( X3-X2, Y3-Y2, Z3-Z2 ).

### OUTPUT

real ANGLE\_RAD\_3D, the angle between the two rays, in radians.  
This value will always be between 0 and PI. If either ray has  
zero length, then the angle is returned as zero.

## **2.2 Rocfrac/Rocfrac/Source/CauchyStressPrinc.f90**

### NAME

CauchyStressPrinc

### FUNCTION

Determines the Cauchy stress tensor for materials defined in  
principal directions

### INPUTS

ndime --> number of dimensions  
xmu --> mu coefficient  
xlamb --> lambda coefficient  
detf --> determinant of F, i.e. J



### 2.3. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90

---

stret --> vector containing the stretches

btens --> matrix containing the the principal directions

#### OUTPUT

sigma --> Cauchy stress tensor

sprin --> principal stresses

## **2.3 Rocfrac/Rocfrac/Source/arruda\_boyce.f90**

#### NAME

ARRUDA\_BOYCE

#### FUNCTION

Arruda-Boyce constitutive model, returns

2nd Piola-Kirchhoff Stresses

#### INPUTS

F11,F12,F13,F21,F22,F23,F31,F32,F33 -- componets

of the deformation gradient [F]

mu, kappa -- material parameters

ielem -- element id number

#### OUTPUT

S11,S22,S33,S12,S23,S13 -- componets of

the 2nd Piola-Kirchhoff Stresses

2.4.

ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/SOLVE\_X

USES

rs, Solve\_x

## **2.4 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/Solve\_x**

NAME

Solve\_x

FUNCTION

Solve for the x

INPUTS

xmu -- mu

i -- element id

stretch -- principle stretch

OUTPUT

x -- x

## **2.5 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/rs**

NAME

rs

FUNCTION

## 2.5. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/RS

calls the recommended SEQUENCE of  
subroutines from the eigensystem SUBROUTINE package (eispack)  
to find the eigenvalues and eigenvectors (IF desired)  
of a REAL symmetric matrix.

### INPUTS

nm must be set to the row DIMENSION of the two-dimensional  
array parameters as declared in the calling PROGRAM  
DIMENSION statement.  
n is the order of the matrix a.  
a CONTAINS the REAL symmetric matrix.  
matz is an INTEGER variable set equal to zero IF  
ONLY eigenvalues are desired. otherwise it is set to  
any non-zero INTEGER for both eigenvalues and eigenvectors.

### OUTPUT

w CONTAINS the eigenvalues in ascending order.  
z CONTAINS the eigenvectors IF matz is not zero.  
ierr is an INTEGER output variable set equal to an error  
completion code described in the documentation for tqlrat  
and tql2. the normal completion code is zero.  
fv1 and fv2 are temporary storage arrays.

### NOTES

## 2.6. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/PYTHAG

questions and comments should be directed to burton s. garbow,  
mathematics and computer science div, argonne national laboratory  
this version dated august 1983.

## **2.6 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/pythag**

NAME

pythag

FUNCTION

finds  $\text{SQRT}(a^{**2}+b^{**2})$  without overflow or destructive underflow

## **2.7 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/tql1**

NAME

tql1

FUNCTION

finds the eigenvalues of a symmetric  
tridiagonal matrix by the ql method.

INPUTS

n is the order of the matrix.

d CONTAINS the diagonal elements of the input matrix.

## 2.7. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/TQL1

e CONTAINS the subdiagonal elements of the input matrix  
in its last n-1 positions. e(1) is arbitrary.

### OUTPUT

d CONTAINS the eigenvalues in ascending order. IF an  
error EXIT is made, the eigenvalues are correct and  
ordered for indices 1,2,...ierr-1, but may not be  
the smallest eigenvalues.

e has been destroyed.

ierr is set to

zero            for normal RETURN,  
j               IF the j-th eigenvalue has not been  
determined after 30 iterations.

### USES

pythag for  $\text{SQRT}(a*a + b*b)$  .

### NOTES

this SUBROUTINE is a translation of the algol PROCEDURE tq11,  
num. math. 11, 293-306(1968) by bowdler, martin, reinsch, and  
wilkinson.

handbook for auto. comp., vol.ii-linear algebra, 227-240(1971).

questions and comments should be directed to burton s. garbow,

## 2.8. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/TQL2

mathematics and computer science div, argonne national laboratory  
this version dated august 1983.

## **2.8 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/tql2**

### NAME

tql2

### FUNCTION

Finds the eigenvalues and eigenvectors  
of a symmetric tridiagonal matrix by the ql method.  
the eigenvectors of a full symmetric matrix can also  
be found IF tred2 has been used to reduce this  
full matrix to tridiagonal form.

### NOTES

this SUBROUTINE is a translation of the algol PROCEDURE tql2,  
num. math. 11, 293-306(1968) by bowdler, martin, reinsch, and  
wilkinson.  
handbook for auto. comp., vol.ii-linear algebra, 227-240(1971).  
questions and comments should be directed to burton s. garbow,  
mathematics and computer science div, argonne national laboratory  
this version dated august 1983.

### INPUTS

## 2.8. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/TQL2

nm must be set to the row DIMENSION of two-dimensional array parameters as declared in the calling PROGRAM DIMENSION statement.

n is the order of the matrix.

d CONTAINS the diagonal elements of the input matrix.

e CONTAINS the subdiagonal elements of the input matrix in its last n-1 positions. e(1) is arbitrary.

z CONTAINS the transformation matrix produced in the reduction by tred2, IF performed. IF the eigenvectors of the tridiagonal matrix are desired, z must contain the identity matrix.

### OUTPUT

d CONTAINS the eigenvalues in ascending order. IF an error EXIT is made, the eigenvalues are correct but unordered for indices 1,2,...,ierr-1.

e has been destroyed.

z CONTAINS orthonormal eigenvectors of the symmetric tridiagonal (or full) matrix. IF an error EXIT is made, z CONTAINS the eigenvectors associated WITH the stored eigenvalues.

ierr is set to

zero            for normal RETURN,

## 2.9. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/TRED1

j                    IF the j-th eigenvalue has not been  
determined after 30 iterations.

### USES

pythag for  $\text{SQRT}(a*a + b*b)$  .

## **2.9 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/tred1**

### NAME

tred1

### FUNCTION

Reduces a REAL symmetric matrix  
to a symmetric tridiagonal matrix using  
orthogonal similarity transformations.

### INPUTS

nm must be set to the row DIMENSION of two-dimensional  
array parameters as declared in the calling PROGRAM  
DIMENSION statement.  
n is the order of the matrix.  
a CONTAINS the REAL symmetric input matrix. ONLY the  
lower triangle of the matrix need be supplied.

### OUTPUT



## 2.10. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/TRED2

a CONTAINS information about the orthogonal transformations used in the reduction in its strict lower triangle. the full upper triangle of a is unaltered.  
d CONTAINS the diagonal elements of the tridiagonal matrix.  
e CONTAINS the subdiagonal elements of the tridiagonal matrix in its last n-1 positions. e(1) is set to zero.  
e2 CONTAINS the squares of the corresponding elements of e.  
e2 may coincide WITH e IF the squares are not needed.

### NOTES

this SUBROUTINE is a translation of the algol PROCEDURE tred1, num. math. 11, 181-195(1968) by martin, reinsch, and wilkinson. handbook for auto. comp., vol.ii-linear algebra, 212-226(1971). questions and comments should be directed to burton s. garbow, mathematics and computer science div, argonne national laboratory this version dated august 1983.

## **2.10 Rocfrac/Rocfrac/Source/arruda\_boyce.f90/tred2**

### NAME

tred2

### FUNCTION

reduces a REAL symmetric matrix to a

## 2.10. ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.F90/TRED2

symmetric tridiagonal matrix using and accumulating  
orthogonal similarity transformations.

### INPUTS

nm must be set to the row DIMENSION of two-dimensional  
array parameters as declared in the calling PROGRAM  
DIMENSION statement.

n is the order of the matrix.

a CONTAINS the REAL symmetric input matrix. ONLY the  
lower triangle of the matrix need be supplied.

### OUTPUT

d CONTAINS the diagonal elements of the tridiagonal matrix.

e CONTAINS the subdiagonal elements of the tridiagonal  
matrix in its last n-1 positions. e(1) is set to zero.

z CONTAINS the orthogonal transformation matrix  
produced in the reduction.

a and z may coincide. IF distinct, a is unaltered.

### NOTES

this SUBROUTINE is a translation of the algol PROCEDURE tred2,  
num. math. 11, 181-195(1968) by martin, reinsch, and wilkinson.  
handbook for auto. comp., vol.ii-linear algebra, 212-226(1971).  
questions and comments should be directed to burton s. garbow,

### 2.11. ROCFRAC/ROCFRAC/SOURCE/CAL\_SHDX.F90

mathematics and computer science div, argonne national laboratory  
this version dated august 1983.

## **2.11 Rocfrac/Rocfrac/Source/cal\_shdx.f90**

### NAME

cal\_shdx

### FUNCTION

computes shape fn. values and parametric derivatives at Gauss pts.

### INPUTS

meshpos -- mesh coordinates  
ndim -- dimension of problem  
nnode -- number of nodes  
nintk -- number of integration points  
surf\_eleme -- connectivity of surf\_elem  
iface -- face number of tetrahedral

### OUTPUT

shdx -- shape fn. derivatives

## **2.12 Rocfrac/Rocfrac/Source/shcalc\_3d10.f90**

### NAME

shcalc\_3d10

### 2.13. ROCFRAC/ROCFRAC/SOURCE/AINV.F90

---

#### FUNCTION

EVALUALTE SHAPE FUNCTION AND ITS DERIVATIVES FOR 10-NODE TET.

#### AUTHOR

written by Changyu Hwang Nov. 20, 2001

## 2.13 Rocfrac/Rocfrac/Source/ainv.f90

#### NAME

ainv

#### FUNCTION

Computes the det and inverse of a (3x3) matrix

#### USED BY

shcalc, shcalc\_3d10

#### INPUTS

ndim -- size of input array (must be 3)

ajac -- Input array (ndim x ndim)

#### OUTPUT

ajacin -- inverse of ajac

det -- determinate of ajac

## 2.14 Rocfrac/Rocfrac/Source/shcalc.f90

NAME

shcalc

FUNCTION

EVALUALTE SHAPE FUNCTION AND ITS DERIVATIVES FOR 4-NODE TET.

## 2.15 Rocfrac/Rocfrac/Source/v3d4\_r\_bar.f90

NAME

v3d4\_r\_bar

FUNCTION

—

Caluculates R for the ALE forumulation for  
the 4-node tetrahedral

INPUTS

d\_bar -- Displacement from mesh motion and  
surface regression  
numnp -- Number of Nodes  
NumElv -- Number of volumetric elements  
lmctet -- Element connectivity  
meshcoor -- mesh coordinates

## 2.16. ROCFRAC/ROCFRAC/SOURCE/VOL\_ELEM\_MAT.F90

---

nstart -- starting element number

nend -- ending element number

### OUTPUT

—

Rbar -- R additional internal force from ALE

## 2.16 Rocfrac/Rocfrac/Source/vol\_elem\_mat.f90

### NAME

VOL\_ELEM\_MAT

### FUNCTION

Forms the material compliance matrix, [C] for an isotropic material

-1

Note:  $[E] = [C]$  and  $\{\epsilon\} = [C]\{\sigma\}$

### INPUTS

e -- Young's modulus

xnu -- Poisson's ratio

numat\_vol -- number of volumetric elements

Integration -- = 1 pseudo-Reduced integration (split Cijkl)

= 0 Cijkl

### OUTPUT

ci -- elastic stiffness constants  
cj -- split stiffness constants

## 2.17 Rocfrac/Rocfrac/Source/v3d4n\_nl.f90

NAME

v3d4n\_nl

FUNCTION

Computes the internal force vector for a 4-node tetrahedral  
NODE BASED ELEMENT for finite deformations.

INPUTS

NumNP -- Number of nodes  
NumEL -- Number of elements  
coord -- number of coordinates  
disp -- Nodal Displacement  
nodes -- Nodal connectivity  
NumElNeigh -- Number of elements in contact with node  
ElConn -- Element connectivity  
alpha -- volume ratio  
Ahat -- undeformed volume of node  
NumMatVol -- number of materials

## 2.18. ROCFRAC/ROCFRAC/SOURCE/VOL\_ELEM\_MAT.F90

xmu -- material parameter

xlamba -- material parameter

### OUTPUT

Rnet -- internal force vector

## **2.18 Rocfrac/Rocfrac/Source/vol\_elem\_mat.f90**

### NAME

VOL\_ELEM\_MAT

### FUNCTION

Caluculates the volume and surface area for tetraderal  
elements

## **2.19 Rocfrac/Rocfrac/Source/principal\_stress.f90**

### NAME

principal\_stress

### FUNCTION

Computes Principal Values of Symmetric Second Rank Tensor

### INPUTS

S = Symmetric Second-Rank Tensor Stored as a Vector



## 2.20. ROCFRAC/ROCFRAC/SOURCE/MAX\_DT\_SOLID.F90

---

P = Principal Values

.. The Components of S Must be Stored in the Following Orders

2-D Problems, S11,S12,S22

3-D Problems, S11,S12,S13,S22,S23,S33

OUTPUTS

SVonMises -- VonMises Stress

## 2.20 Rocfrac/Rocfrac/Source/max\_dt\_solid.f90

NAME

max\_dt\_solid

FUNCTION

Determines the maximum time step

INPUTS

glb -- global array

OUTPUT

dt\_courant -- maximum time step

## 2.21 Rocfrac/Rocfrac/Source/jacobi.f90

NAME

jacobi

FUNCTION

## 2.22. ROCFRAC/ROCFRAC/SOURCE/FEMINP.F90

---

Evaluates the stretches and principal directions given the b matrix using the Jacobi iteration. Adapted from numerical recipes

### INPUTS

btens --> left Cauchy-Green tensor

### OUTPUT

stret --> vector containing the stretches

princ --> matrix containing the three principal column vectors

## 2.22 Rocfrac/Rocfrac/Source/feminp.f90

### NAME

feminp

### FUNCTION

READ INPUT INFORMATION (i.e. Analysis Deck File)

### INPUTS

glb -- global array

myid -- processor id (starting at 0)

## 2.23 Rocfrac/Rocfrac/Source/feminp/PREFIX\_SUB

### NAME

PREFIX\_SUB

## 2.24. ROCFRAC/ROCFRAC/SOURCE/FEMINP/ALE\_SUB

---

### FUNCTION

Reads prefix keyword (i.e. Analysis Deck File)

### INPUTS

glb -- global array

## 2.24 Rocfrac/Rocfrac/Source/feminp/ALE\_SUB

### NAME

ALE\_SUB

### FUNCTION

ALE keyword turns on ALE routines

### INPUTS

glb -- global array

## 2.25 Rocfrac/Rocfrac/Source/feminp/ALE\_SUB

### NAME

ALE\_SUB

### FUNCTION

Courant limit multiplier

### INPUTS

glb -- global array

keywd -- keywd for control deck

2.26.

ROCFRAC/ROCFRAC/SOURCE/FEMINP/MATMODEL\_HYPERELASTIC

## **2.26 Rocfrac/Rocfrac/Source/feminp/MATMODEL\_HYPERELA**

NAME

MATMODEL\_HYPERELASTIC

FUNCTION

reads material model type, and the  
hyperelastic material parameters

INPUTS

glb -- global array  
keywd -- keywd for control deck

OUTPUT

tmp\_E -- Young's Modulus  
tmp\_xnu -- Possion's ratio  
tmp\_rho -- Density  
tmp\_alpha -- thermal coefficient of expansion  
tmp\_iSolnType -- material type model

## **2.27 Rocfrac/Rocfrac/Source/feminp/MATMODEL\_ELASTIC**

NAME

MATMODEL\_ELASTIC

## 2.28. ROCFRAC/ROCFRAC/SOURCE/FEMINP/BOUNDARY\_SUB

### FUNCTION

reads material model type, and the  
elastic material parameters

### INPUTS

glb -- global array  
keywd -- keywd for control deck

### OUTPUT

tmp\_E -- Young's Modulus  
tmp\_xnu -- Possion's ratio  
tmp\_rho -- Density  
tmp\_alpha -- thermal coefficient of expansion  
tmp\_iSolnType -- material type model

## **2.28 Rocfrac/Rocfrac/Source/feminp/BOUNDARY\_SUB**

### NAME

BOUNDARY\_SUB

### FUNCTION

This option is used to prescribe boundary conditions  
at nodes.

## 2.29. ROCFRAC/ROCFRAC/SOURCE/FEMINP/BOUNDARY\_SUB

### INPUTS

glb -- global array

## **2.29 Rocfrac/Rocfrac/Source/feminp/BOUNDARY\_SUB**

### NAME

BOUNDARY\_SUB

### FUNCTION

This option is used to prescribe mesh motion boundary conditions at nodes.

### INPUTS

glb -- global array

## **2.30 Rocfrac/Rocfrac/Source/feminp/ELEMENT\_SUB**

### NAME

ELEMENT\_SUB

### FUNCTION

Specifies the element type

### 2.31. ROCFRAC/ROCFRAC/SOURCE/BC\_ENFORCE.F90

---

#### INPUTS

glb -- global array

## 2.31 Rocfrac/Rocfrac/Source/bc\_enforce.f90

#### NAME

bc\_enforce

#### FUNCTION

Enforces the structural boundary conditions

#### INPUTS

numbound -- number of nodes with enforced boundary  
conditions

numnp -- number of nodes

id -- element id

r -- imposed type of boundary condition

slope -- loading amplitude slope

prop -- proportion of amplitude for loading

vb -- imposed velocity

ab -- imposed acceleration

delta -- time increment

Rnet -- sum of forces

xm -- lumped nodal mass matrix

## 2.32.

*ROCFRAC/ROCFRAC/SOURCE/ARRUDA\_BOYCE.CAUCHY.F90*

---

DampEnabled -- flag for damping

CurrTime -- current time

### OUTPUT

v -- nodal velocity with bc

a -- nodal acceleration with bc

d -- nodal displacement with bc

## **2.32 Rocfrac/Rocfrac/Source/arruda\_boyce.cauchy.f90**

### NAME

ARRUDA\_BOYCE\_CAUCHY

### FUNCTION

Arruda-Boyce constitutive model, returns Cauchy Stress

### INPUTS

F11,F12,F13,F21,F22,F23,F31,F32,F33 -- componets

of the deformation gradient [F]

mu, kappa -- material parameters

ielem -- element id number

### OUTPUT

Cchy11, Cchy22, Cchy33,Cchy12,Cchy13,Cchy23 -- componets

of the Cauchy stress tensor



### 2.33. ROCFRAC/ROCFRAC/SOURCE/VOLRATIO.F90

---

USES

rs, Solve\_x

## 2.33 Rocfrac/Rocfrac/Source/VolRatio.f90

NAME

VolRatio

FUNCTION

Calculates the Volume Ratio for the node based elements  
using either the circumcenter of centroid.

INPUTS

n1,n2,n3,n4 -- node number

coor -- nodeal coordinates

numnp -- number of nodes

NdMassLump -- = 1 then circumcenter method  
                  = 0 then centroid method

OUTPUT

AlphaR -- Ratio of the Volume for a node

## 2.34 Rocfrac/Rocfrac/Source/UpdateMassMatrix.f90

NAME

UpdateMassMatrix

## 2.35. ROCFRAC/ROCFRAC/SOURCE/ROCFRACMAIN

---

### FUNCTION

Updates the mass matrix due to change in undeformed configuration. Calls the appropriate mass matrix subroutine and handles the parallel communication.

### INPUTS

glb -- global variables

### USES

GENX\_RocFrac, V3D4\_MASS, V3D4N\_MASS, V3D10\_MASS

## 2.35 Rocfrac/Rocfrac/Source/RocFracMain

### NAME

RocFracMain.f90

### FUNCTION

3D Dynamic Explicit Code with ALE formulation for regressing boundaries Finite Element Analysis Code with additional fracture simulation using cohesive elements.

### USAGE

Finite Element code to solve the 3-Dimensional TRANSIENT structural problem

### USES

### 2.36. ROCFRAC/ROCFRAC/SOURCE/ROCFRACMAIN

---

RocFracSubInterface, UpdateStructuralSoln, feminp, VolRatio, vol\_elem\_mat,  
RocFracInterfaceInitial, RocFracInterfaceBuff, UpdateMassMatrix, V3D4\_volum  
max\_dt\_solid, UpdateRbar,v3d4\_ale,V3D10\_ALE,FluidPressLoad, TractPressLoad,  
UpdateStructural,principal\_stress,bc\_enforce

Global variables stored in modules : GENX\_RocFrac,GENX\_RocFracComm,GENX\_Roc

#### COPYRIGHT

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#### AUTHOR

principal : M.S. Breitenfeld, P.H. Geubelle

- email : brtnfld@uiuc.edu, geubelle@uiuc.edu

contributing : Changyu Huang, Amit Acharya

#### CREATION DATE

2001

## **2.36 Rocfrac/Rocfrac/Source/RocFracMain**

#### NAME

RocFracInterfaceBuff

#### FUNCTION

Passes the variables to the fluid code. It transfers the new mesh

### 2.37. ROCFRAC/ROCFRAC/SOURCE/INTEGRALCHECK.F90

velocity and displacement to the interface mesh arrays that are registered with RocCom

## **2.37 Rocfrac/Rocfrac/Source/IntegralCheck.f90**

NAME

CheckIntegral

FUNCTION

Sums the conservation quantities over all the processors. MPI\_REDUCE

INPUTS

glb -- global array

OUTPUT

IntegralArray -- Conservation term:

1. Volume
2. Mass
3. x-momentum
4. y-momentum
5. z-momentum
6. energy
7. burning area
8. non-burning area

2.38. ROCFRAC/ROCFRAC/SOURCE/GENX\_ROCFRACINTERP.F90

**2.38 Rocfrac/Rocfrac/Source/GENX\_RocFracInterp.f90**

NAME

GENX\_RocFracInterp

FUNCTION

Global module for interface variables

**2.39 Rocfrac/Rocfrac/Source/GENX\_RocFracComm.f90**

NAME

GENX\_RocFracComm

FUNCTION

Global MPI array modules

**2.40 Rocfrac/Rocfrac/Source/GENX\_RocFrac.f90**

NAME

GENX\_RocFrac

FUNCTION

Global variable module

**2.41 Rocfrac/Rocfrac/Source/FluidPressLoad.f90**

NAME

## 2.42. ROCFRAC/ROCFRAC/SOURCE/LOCCHR.F90/LOCCHR

---

FluidPressLoad

### FUNCTION

Transforms the pressure given in the deformed state to the undeformed configuration. This subroutine is for the formulation where all quantities are with respect to the undeformed configuration. Assumes the pressure (tractions) are constant over the surface of the triangle.

1-3 for 4 node tet (i.e. 3 node triangles)

4-6 for 10 node tet (i.e. 6 node triangles, mid-side nodes get traction)

## 2.42 Rocfrac/Rocfrac/Source/locchr.f90/locchr

### NAME

locchr

### FUNCTION

Locates the keyword value after a keyword

### INPUTS

text -- character string

varna -- variable name to search for

lvari -- length of the variable name

kpos0 -- initial position in 'text' so start looking for varna

#### OUTPUT

kpos1 -- Start of keyword value in string

kpos2 -- End of keyword value in string

### **2.43 Rocfrac/Rocfrac/Source/locchr.f90/conchr**

#### NAME

conchr

#### FUNCTION

To determine if a control deck keyword is specified

#### INPUTS

text -- character string

varna -- variable name to search for

lvvari -- length of the variable name

kpos0 -- initial position in 'text' so start looking for varna

#### OUTPUT

key -- 0 = no, 1 = yes

## 2.44 Rocfrac/Rocfrac/Source/locchr.f90/dtext

NAME

dtext

FUNCTION

To determine the string length

INPUTS

text -- character string

OUTPUT

l11 -- length of string

## 2.45 Rocfrac/Rocfrac/Source/locchr.f90/dtext

NAME

dtext

FUNCTION

Converts a character string to an integer

INPUTS

char -- character string



## *2.46. ROCFRAC/ROCFRAC/SOURCE/LOCCHR.F90/RCHAR*

---

### OUTPUT

key -- integer

## **2.46 Rocfrac/Rocfrac/Source/locchr.f90/rchar**

### NAME

rchar

### FUNCTION

Converts a character string to a real

### INPUTS

char -- character string

### OUTPUT

key -- real

## **2.47 Rocfrac/Rocfrac/Source/ALEUpdateMassMatrix.f90**

### NAME

ALEUpdateMassMatrix

### FUNCTION

Updates the nodal coordinates as a result  
of the regressing boundaries. Calculates

## 2.47.

*ROCFRAC/ROCFRAC/SOURCE/ALEUPDTEMASSMATRIX.F90*

---

the new lumped inverse mass matrix from the new  
nodal coordinates, MPI calls handle  
communication between partition boundaries

### USED BY

RocfracMain

### USES

GENX\_RocFrac -- Global variables  
V3D4\_MASS, V3D4N\_MASS, V3D10\_MASS

### INPUTS

glb -- global array

### OUTPUTS

xmass -- Inverse lumped mass matrix