# Defmod[1]: Finite element code for modeling crustal deformation

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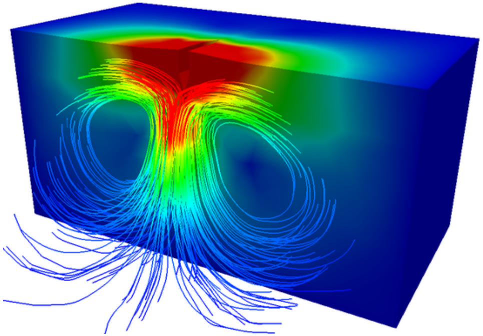

[1]https://bitbucket.org/stali/defmod

## Features

- Can simulate elastodynamic & quasistatic processes (in 2D or 3D) such as:
  - Coseismic (fault) slip or volcanic rifting
  - Postseismic or postrifting deformation due to afterslip, poroelastic rebound and/or viscoelastic relaxation
  - Postglacial rebound and hydrological (un)loading
  - Injection/extraction of fluids from subsurface reservoirs etc.
- Written entirely in Fortran 95
- Uses PETSc's parallel sparse data structures & implicit solver(s)
- Runs on shared and distributed memory machines using MPI
- Scales well on large clusters with hundreds or even thousands of processor cores
- Free to download, use, modify and share (GPL v3)

## Features

Supports:

- Stabilized linear tri, quad, tet & hex elements
- Elastic, viscoelastic, poroelastic and poroviscoelastic rheologies
- Time dependent force/flow and/or traction/flux BC's
- Time dependent linear constraint equations
- Absorbing boundaries for dynamic problems
- Winkler foundation(s)

Note(s):

- Fault slip/opening and displacement/velocity/pressure BC's can be specified using linear constraint equations
- Isostasy can be simulated using Winkler foundation(s)

## Physics

Cauchy's equation of motion:

$$\int_\Omega (\sigma_{ij,j} + f_i - \rho \ddot{u}_i) d\Omega = 0$$

Semi discrete form using the finite element method:

$$M\ddot{u} + C\dot{u} + Ku = f$$

$$C = \alpha M + \beta K$$

– M is the mass matrix
– K is the stiffness matrix
– C is the damping matrix
– $\alpha$ and $\beta$ are Rayleigh damping coefficients

## Constraint Equations

Implemented using Lagrange Multipliers (LM's)

$$M\ddot{u} + C\dot{u} + Ku + G^T\lambda = f$$

$$Gu = l$$

- $G$ is the constraint matrix
- $\lambda$ is the force required to enforce the constraint
- $l$ is the value of the constraint (e.g., prescribed slip or displacements)

## Explicit Solver for Dynamic problems

For problems without constraints we perform explicit time integration using a central differencing scheme for $\ddot{u}$ and a backward differencing scheme for $\dot{u}$

$$\begin{aligned} u^{t+\Delta t} =& M^{-1}\left[\Delta t^2(f - Ku^t) - \Delta t C(u^t - u^{t-\Delta t})\right] + \\ & 2u^t - u^{t-\Delta t} \end{aligned}$$

- $M$ is assumed to be lumped (i.e., diagonal)
- Time step is restricted by

  $$\Delta t_{critical} \sim L/c;\ c = \sqrt{E/\rho}$$

  where L is the (smallest) element edge length

For problems with constraints we use the "Forward Increment Lagrange Multiplier Method" of Carpenter et al. [1991]

## Implicit Solver for Quasistatic problems

- With linear constraints (LM's)

$$\begin{vmatrix} K & G^T \\ G & 0 \end{vmatrix} \begin{vmatrix} u \\ \lambda \end{vmatrix} = \begin{vmatrix} f \\ l \end{vmatrix}$$

  System is indefinite and solved using ASM preconditioned GMRES

- Without constraints

$$\begin{vmatrix} K \end{vmatrix} \begin{vmatrix} u \end{vmatrix} = \begin{vmatrix} f \end{vmatrix}$$

  System is symmetric positive definite and CG can be used instead (`-ksp_type cg`)

Note: PETSc can be configured with many sparse solvers and preconditioners that can be engaged at runtime using simple command line options

## Implicit Solver for Quasistatic problems

- For problems involving viscoelasticity we use the time-stepping algorithm proposed by Melosh and Raefsky [1980]
- For poroelastic problems we also have to account for the continuity equation which results in the coupled system [Zienkiewicz and Shiomi, 1984]:

$$K_e u - Hp = f$$

$$H^T \dot{u} + S\dot{p} + K_c p = q$$

where $K_e$ and $K_c$ are solid and fluid stiffness matrices, $H$ is the coupling matrix, $S$ is the compressibility matrix, $p$ the pressure vector and $q$ the in/out flow

The equations are solved using an incremental loading scheme [Smith and Griffiths, 2004]

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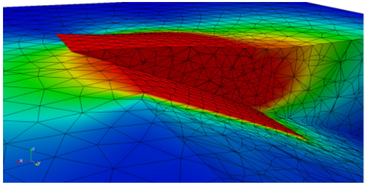
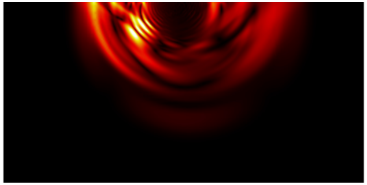
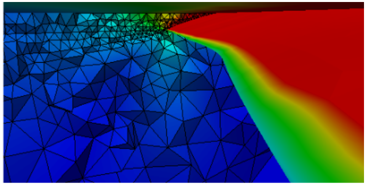
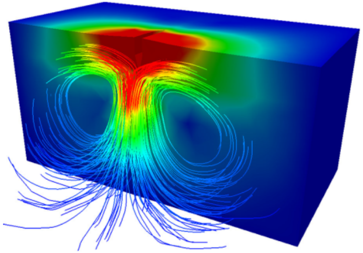
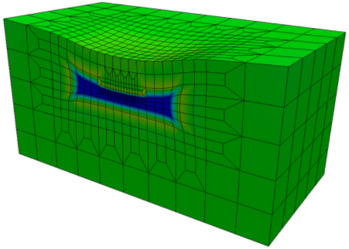
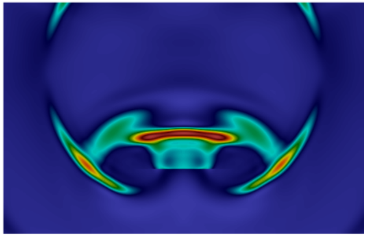
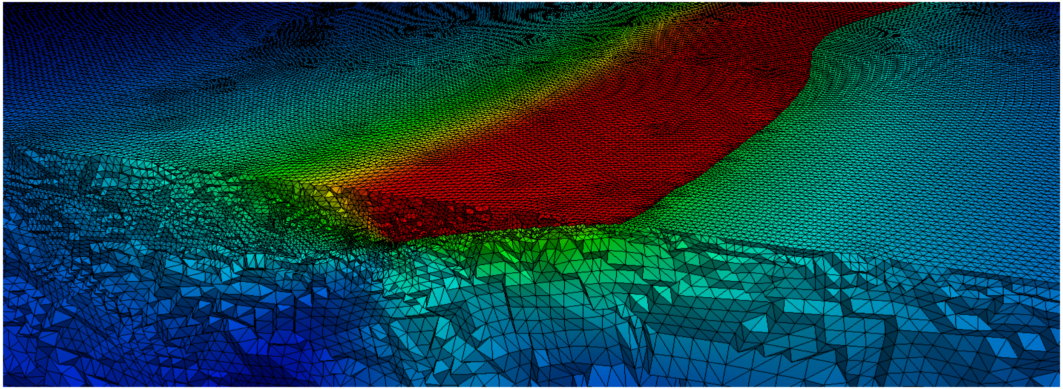
## Applications

Many ...

## Applications

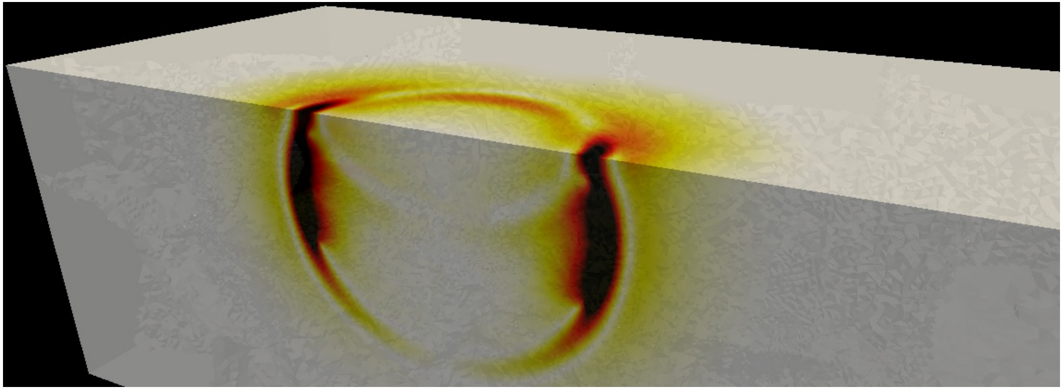
Including problems with non-trivial fault geometries



Model with $\sim 8$ million tet elements, with slip on the entire subduction interface, implicitly solved, from start to finish, in $\sim 120$ secs on 256 Xeon E5-2660 cores

## Applications

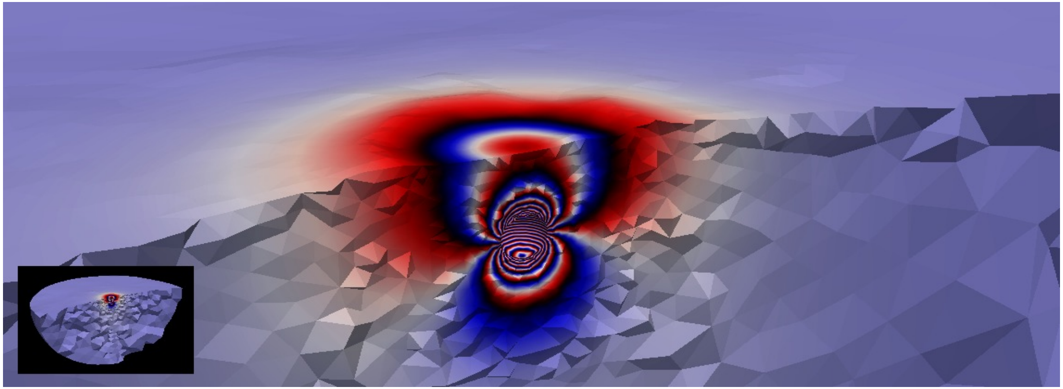
Complex loading histories



Model with $\sim 6$ million tet elements, with a slipping strike slip fault, explicitly solved (includes 2000 time steps), from start to finish, in $\sim 47.5$ secs on 128 cores

## Applications

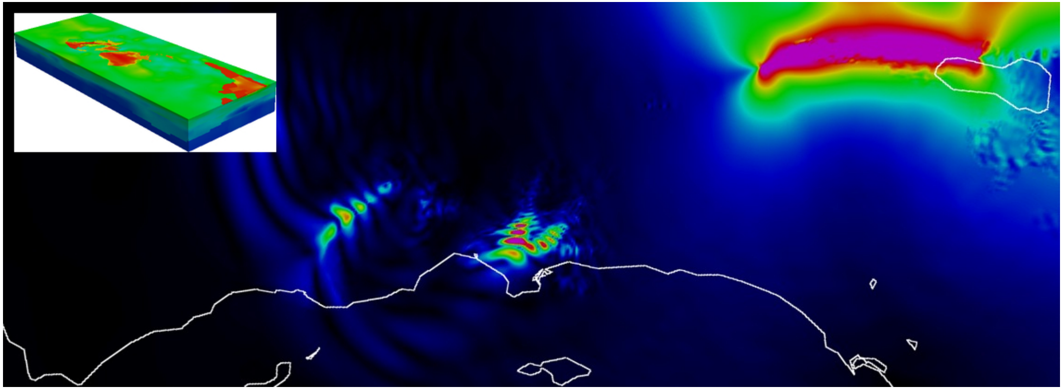
Realistic topography



Model (mesh built by T. Masterlark) containing a spherical magma chamber, with traction loading on the chamber wall, implicitly solved, from start to finish, in $\sim 1.5$ secs on 4 cores

## Applications

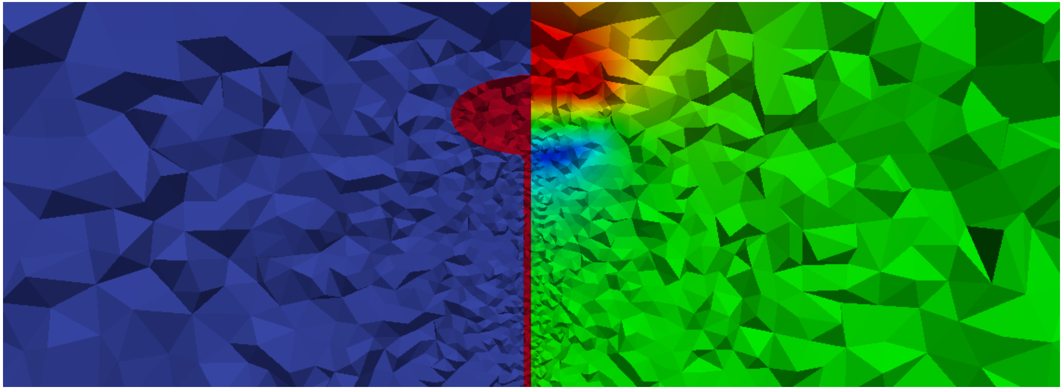
Heterogeneous (3D) material properties



A full 200 sec simulation of long-period ($\sim 0.075$ Hz) ground motion in Southern California, using SCEC's CVM-S4, due to slip on the Southern San Andreas Fault takes $\sim 100$ secs on 256 cores

## Applications

Fully coupled multiphysics



Model containing a porous, permeable magma chamber; Mass flux at the base of the conduit results in $\Delta P$ (left) which then causes uplift (right)

## I/O

Input

- A single ASCII file is used for ease of use and easy manipulation of mesh/BCs for runs driven by shell scripts
- Currently all processor cores access the same ASCII input file[2] to read on-core (i.e., local) mesh data

Output

- Each processor core writes its own ASCII output (VTK) for on-core elements/nodes that can be directly visualized using ParaView
- Output frequency can be specified in the input file (e.g., write output after every 50 time steps)

[2]Can take a few minutes for runs involving more than 1K processor cores; E.g., 3 mins to partition, read and map a $\sim$16 million (hex) element mesh on 1K cores of Lonestar (TACC) cluster

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1 Element data
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0 Nodal Data
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000  Material data
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0 Applied (nodal) force data
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0 Start and end time(s) for applied force
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1 Total simulation time
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1 Time step
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1 Output frequency
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1 Write total displacements
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit quad 5
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000
3.0E10 0.25 3000
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit-v quad 5 Enable viscoelasticity
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0
10.0 0.00 1 1
10.0 10.0 1 1
0.00 10.0 0 0
20.0 0.00 1 1
20.0 10.0 1 1
3.0E10 0.25 3000 1.0E18 1.0
3.0E10 0.25 3000 1.0E18 1.0
5 -10.0E10 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit-p quad 5 Enable poroelasticity
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0 1
10.0 0.00 1 1 1
10.0 10.0 1 1 1
0.00 10.0 0 0 1
20.0 0.00 1 1 1
20.0 10.0 1 1 1
3.0E10 0.25 3000 1.0E18 1.0 1E-6 1.0 0.05 2.2E9
3.0E10 0.25 3000 1.0E18 1.0 1E-6 1.0 0.05 2.2E9
5 -10.0E10 0.0 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0 0.0
```

## Input file example

```
$ cat examples/two_quads_qs.inp
implicit-pv quad 5 Enable poroviscoelasticity
2 6 2 0 2 0 0
0.0 0.1 1 1
1 2 3 4 1
2 5 6 3 2
0.00 0.00 0 0 1
10.0 0.00 1 1 1
10.0 10.0 1 1 1
0.00 10.0 0 0 1
20.0 0.00 1 1 1
20.0 10.0 1 1 1
3.0E10 0.25 3000 1.0E18 1.0 1E-6 1.0 0.05 2.2E9
3.0E10 0.25 3000 1.0E18 1.0 1E-6 1.0 0.05 2.2E9
5 -10.0E10 0.0 0.0 0.0 0.0
6 -10.0E10 0.0 0.0 0.0 0.0
```

## Build and Execution

```
$ ssh lonestar.tacc.utexas.edu
$ module load petsc
$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all

$ mpirun -np 2 ./defmod -f examples/two_quads_qs.inp
Reading input file ...
Partitioning mesh ...
Forming [K] ...
Forming RHS ...
Setting up solver ...
Solving ...
Recovering stress ...
Cleaning up ...
Finished
```

## Build and Execution

```
$ ssh lonestar.tacc.utexas.edu
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$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all
```

```
$ mpirun -np 2 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
Reading input file ...
Partitioning mesh ...
Forming [K] ...
Forming RHS ...
Setting up solver ...
Solving ...
0 KSP Residual norm 6.484684701823e+00
1 KSP Residual norm 2.983375739070e-15
Recovering stress ...
Cleaning up ...
Finished
```

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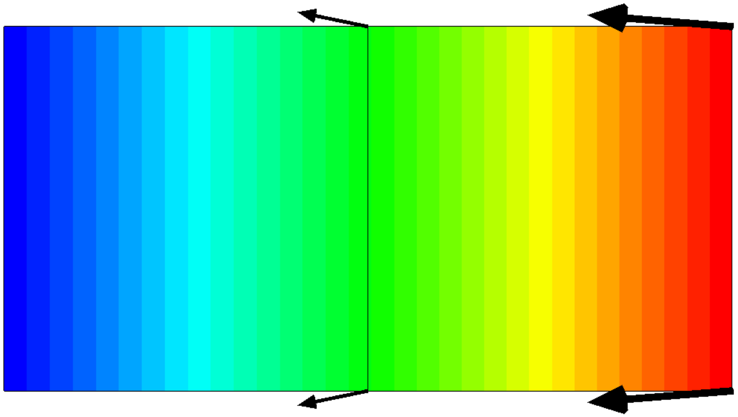
```
$ mpirun -np 2 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
Reading input file ...
Partitioning mesh ...
Forming [K] ...
Forming RHS ...
Setting up solver ...
Solving ...
0 KSP Residual norm 6.484684701823e+00
1 KSP Residual norm 2.983375739070e-15
Recovering stress ...
Cleaning up ...
Finished
```

By default output is written in VTK format and can be easily visualized using ParaView, VisIt etc.

## Result



## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0 Constraint Eqn's
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3 Equation 1 {Ux5+Ux8-2Ux13=0.0}
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0 Start and end time(s)
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3 Equation 2 {Uy5+Uy8-2Uy13=0.0}
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1 Equation 9 {Ux9=1.0}
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1 Equation 10 {Uy9=1.0}
 0.0 1.0 9
 1.0 0.0 1.0
```

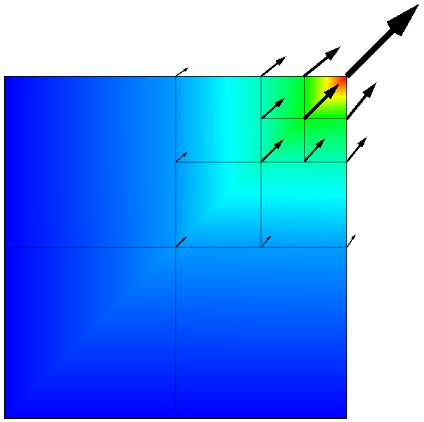
## Input file with constraints

```
$ cat examples/quadtree_qs.inp

implicit quad 12
10 19 1 10 0 0 0
1.0 0.25 1 1
1 2 5 4 1
...
0.0 0.0 0 0
...
7.5E10 0.25 3000.0
3
 1.0 0.0 5
 1.0 0.0 8
-2.0 0.0 13
 0.0 0.0 0.0
⇝
```

```
⇝
3
 0.0  1.0 5
 0.0  1.0 8
 0.0 -2.0 13
 0.0  0.0 0.0
...
1
 1.0 0.0 9
 1.0 0.0 1.0
1
 0.0 1.0 9
 1.0 0.0 1.0
```

Note: Any constraint that is specified remains active throughout the simulation; A zero value is assumed (for *u* or *p*) unless specified otherwise

## Result



Note: Displacements at hanging nodes are average of their corresponding edge nodes

## More examples ...

- Displacement BC in 3D

  $Uy_9=10.0$

  ```
  1
   0.0 1.0 0.0 9
  10.0 0.0 0.0
  ```

- Pressure head BC in 3D (for poroelastic problem)

  $P_9=1.0E3$

  ```
  1
   0.0 0.0 0.0 1.0 9
  1.0E3 0.0 0.0
  ```

- Fault slip between two coincident nodes (in x-direction)

  $Ux_{13}$-$Ux_{81}=10.0$

  ```
  2
   1.0 0.0 0.0 13
  -1.0 0.0 0.0 81
  10.0 0.0 0.0
  ```

## More examples ...

- Displacement BC in 3D
  $Uy_9 = 10.0$
  ```
  1
   0.0 1.0 0.0 9
  10.0 0.0 0.0
  ```

- Pressure head BC in 3D (for poroelastic problem)
  $P_9 = 1.0E3$
  ```
  1
   0.0 0.0 0.0 1.0 9
  1.0E3 0.0 0.0
  ```

- Fault slip between two coincident nodes (in x-direction)
  $Ux_{13} - Ux_{81} = 10.0$
  ```
  2
   1.0 0.0 0.0 13
  -1.0 0.0 0.0 81
  10.0 0.0 0.0
  ```

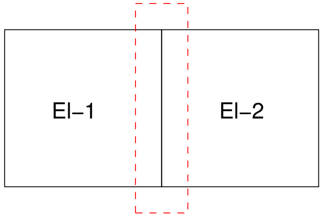
## More examples ...

- Displacement BC in 3D
  $Uy_9=10.0$
  ```
  1
   0.0 1.0 0.0 9
  10.0 0.0 0.0
  ```

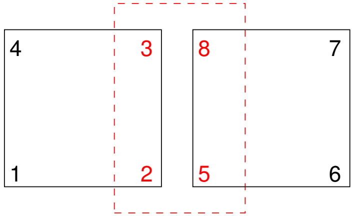
- Pressure head BC in 3D (for poroelastic problem)
  $P_9=1.0E3$
  ```
  1
   0.0 0.0 0.0 1.0 9
  1.0E3 0.0 0.0
  ```

- Fault slip between two coincident nodes (in x-direction)
  $Ux_{13}-Ux_{81}=10.0$
  ```
  2
   1.0 0.0 0.0 13
  -1.0 0.0 0.0 81
  10.0 0.0 0.0
  ```

## Fault slip



Element view



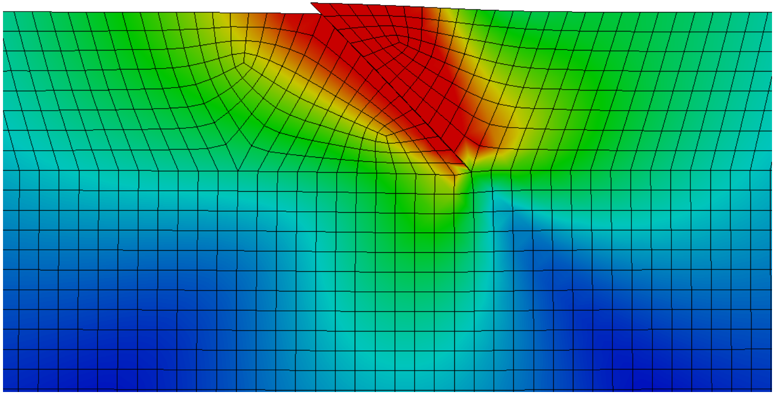
Nodal view (exploded)

To enforce slip we need to specify the relative displacement/opening between coincident nodes {3 & 8} and {2 & 5}

For example the relative displacement (Y coordinate) between nodes {3 & 8} can be written as $\mathtt{Uy}_3 - \mathtt{Uy}_8 = 1.0$ and is specified (between 0.1 – 0.5 seconds) as:

```
 2
  0  1  3
  0 -1  8
 1.0 0.1 0.5
```

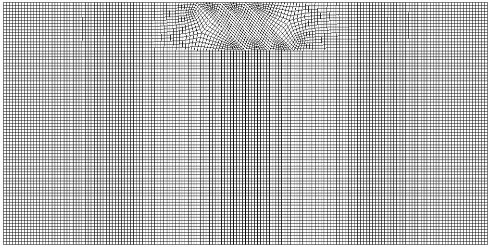
## Fault slip



## Example

```
$ cat examples/2d_fault_dyn.inp
```

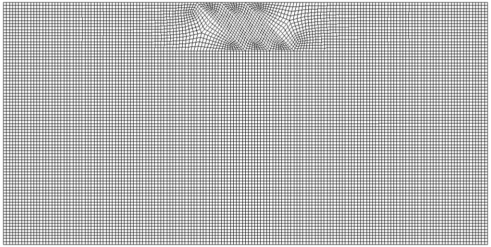
```
explicit quad 12
18796 19036 2 48 0 0 200
75 0.025 40 0
0.0 0.01
...
2
 0 -1 1832
 0  1 1619
 0.1 0.2 2.7
...
2
 1 0 1832
-1 0 1619
 0.1 0.2 2.7
...
```



## Example

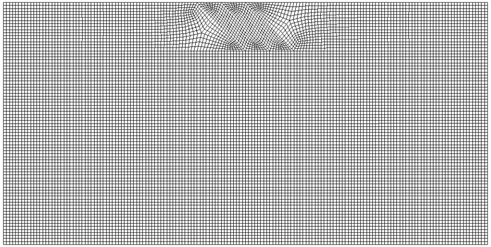
```
$ cat examples/2d_fault_dyn.inp
```

```
explicit quad 12
18796 19036 2 48 0 0 200 ABC's
75 0.025 40 0
0.0 0.01
...
2
 0 -1 1832
 0  1 1619
 0.1 0.2 2.7
...
2
 1 0 1832
-1 0 1619
 0.1 0.2 2.7
...
```



## Example

```
$ cat examples/2d_fault_dyn.inp

explicit quad 12
18796 19036 2 48 0 0 200
75 0.025 40 0
0.0 0.01 Damping coefficients
...
2
 0 -1 1832
 0  1 1619
 0.1 0.2 2.7
...
2
 1 0 1832
-1 0 1619
 0.1 0.2 2.7
...
```



## Example (Dynamic)

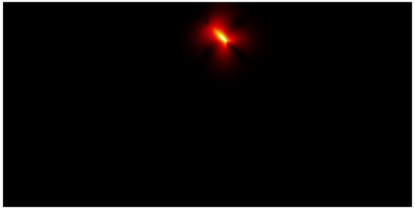
T=0.0 sec

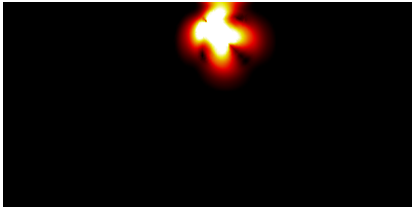
Displacement

Velocity (100x)

## Example (Dynamic)

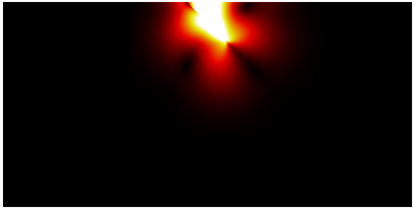
T=2.5 sec


Displacement

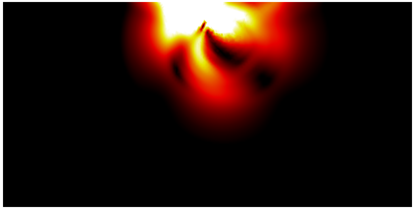

Velocity (100x)

## Example (Dynamic)

T=5.0 sec



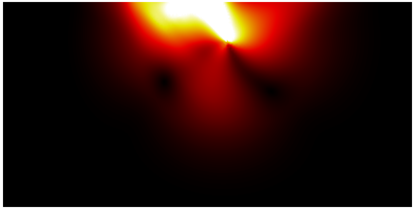
Displacement

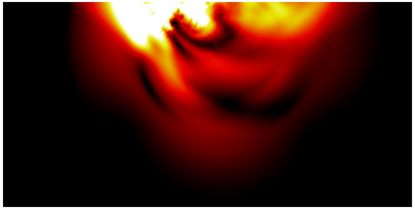


Velocity (100x)

## Example (Dynamic)

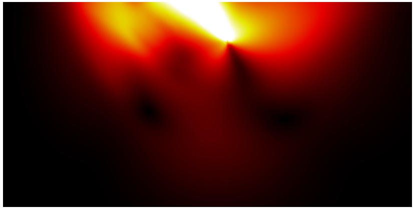
T=7.5 sec

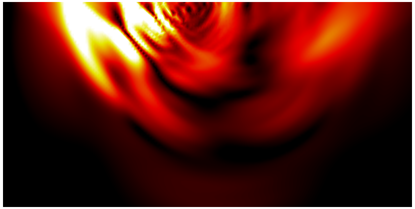

Displacement


Velocity (100x)

## Example (Dynamic)

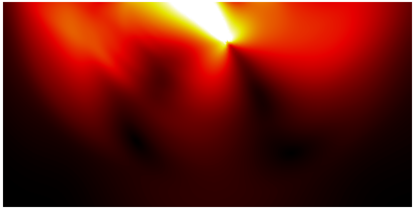
T=10.0 sec


Displacement

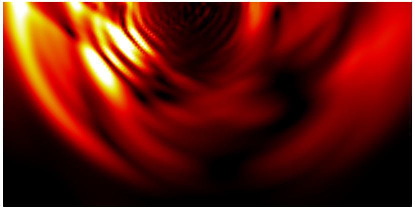

Velocity (100x)

## Example (Dynamic)

T=12.5 sec



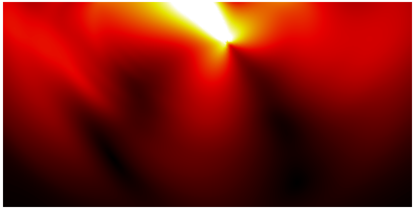
Displacement

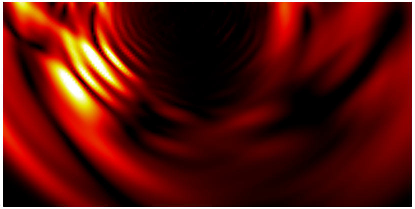


Velocity (100x)

## Example (Dynamic)

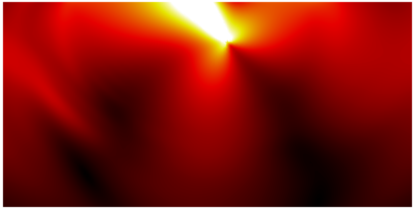
T=15.0 sec

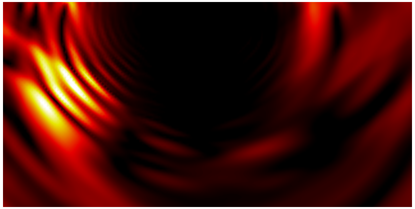

Displacement


Velocity (100x)

## Example (Dynamic)

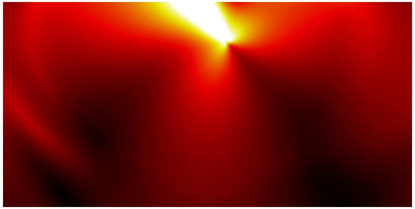
T=17.5 sec

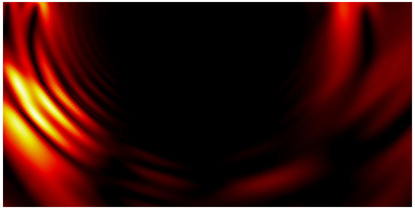

Displacement


Velocity (100x)

## Example (Dynamic)

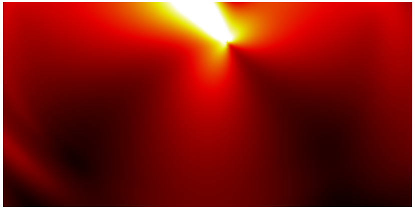
T=20.0 sec

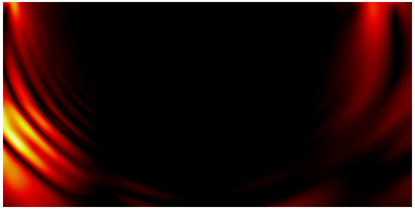

Displacement


Velocity (100x)

## Example (Dynamic)

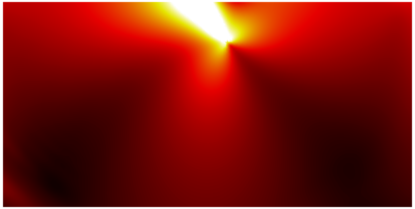
T=22.5 sec

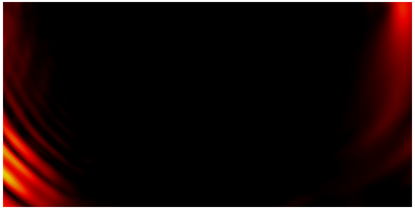

Displacement


Velocity (100x)

## Example (Dynamic)

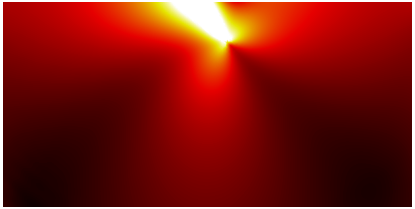
T=25.0 sec


Displacement


Velocity (100x)

## Example (Dynamic)

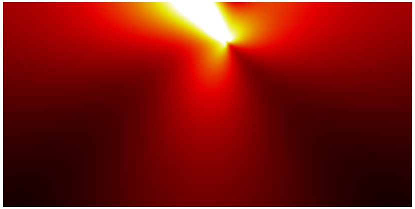
T=27.5 sec


Displacement

Velocity (100x)

## Example (Dynamic)

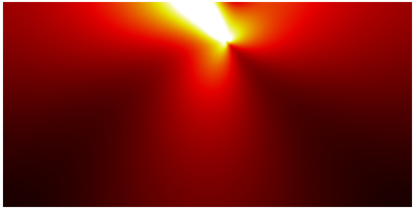
T=30.0 sec


Displacement

Velocity (100x)

## Example (Dynamic)

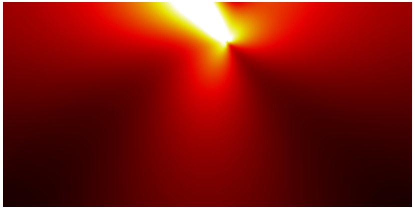
T=32.5 sec

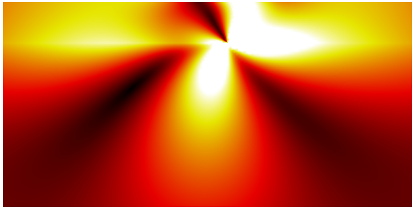

Displacement

Velocity (100x)

## Example (Quasistatic)

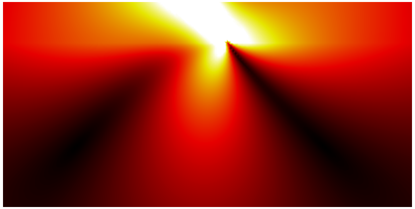
T=0.0 years

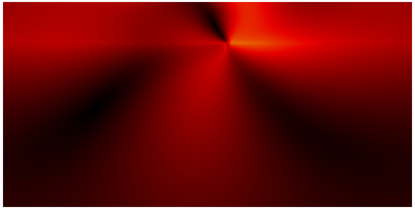

Displacement


Velocity (20x)

## Example (Quasistatic)

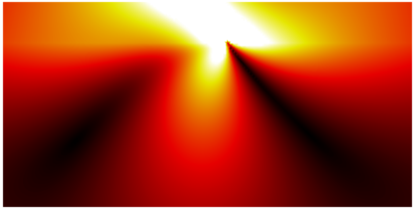
T=5.0 years

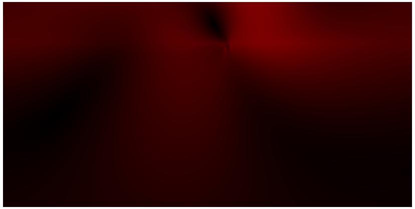

Displacement


Velocity (20x)

## Example (Quasistatic)

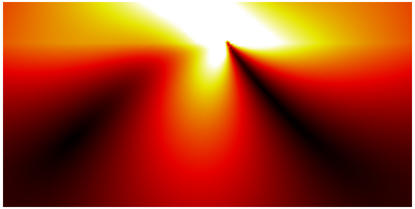
T=10.0 years


Displacement


Velocity (20x)

## Example (Quasistatic)

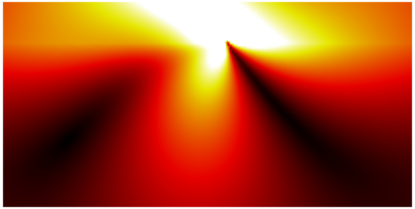
T=15.0 years


Displacement

Velocity (20x)

## Example (Quasistatic)

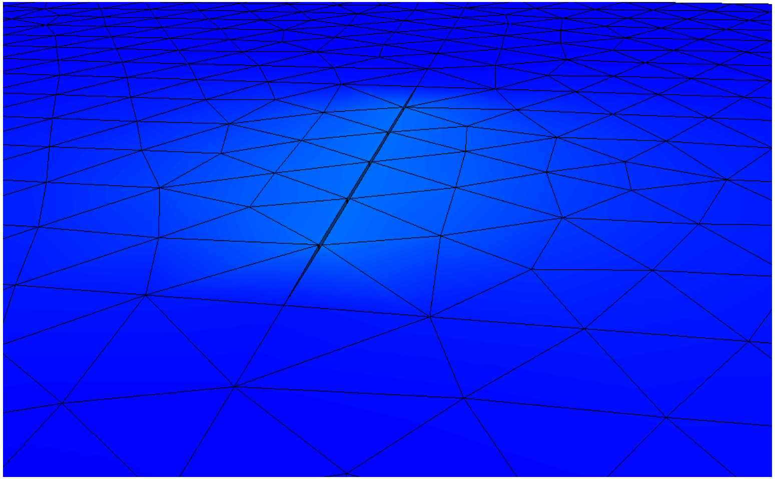
T=20.0 years


Displacement

Velocity (20x)

## Example (3D Quasistatic)

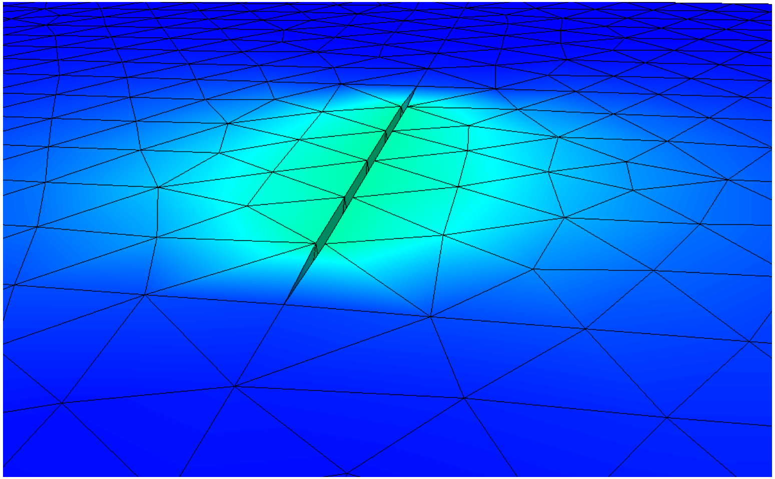
T=0.0 years (Rifting starts)



Displacement

## Example (3D Quasistatic)

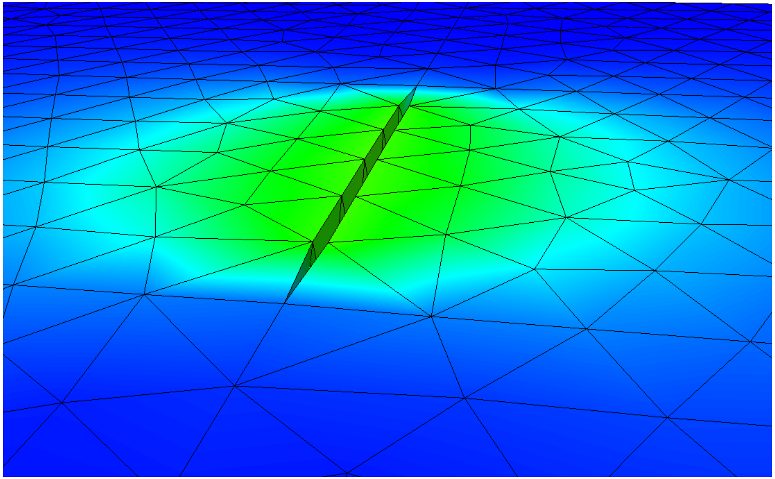
T=1.0 years (Rifting ...)



Displacement

## Example (3D Quasistatic)

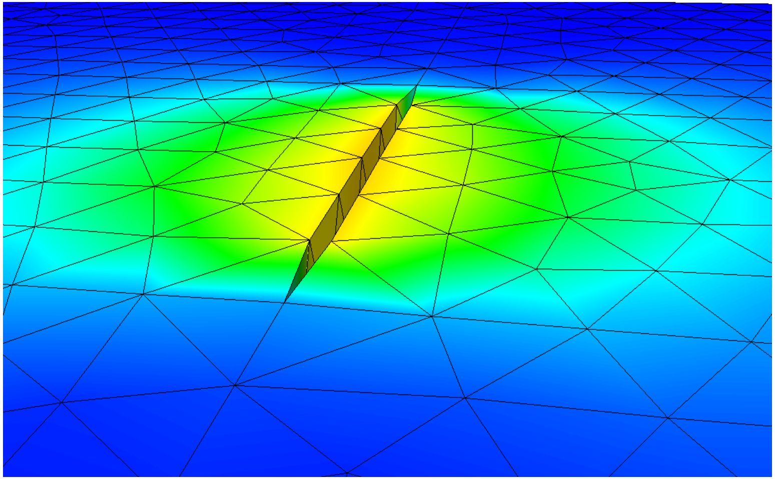
T=2.0 years (Rifting ...)



Displacement

## Example (3D Quasistatic)

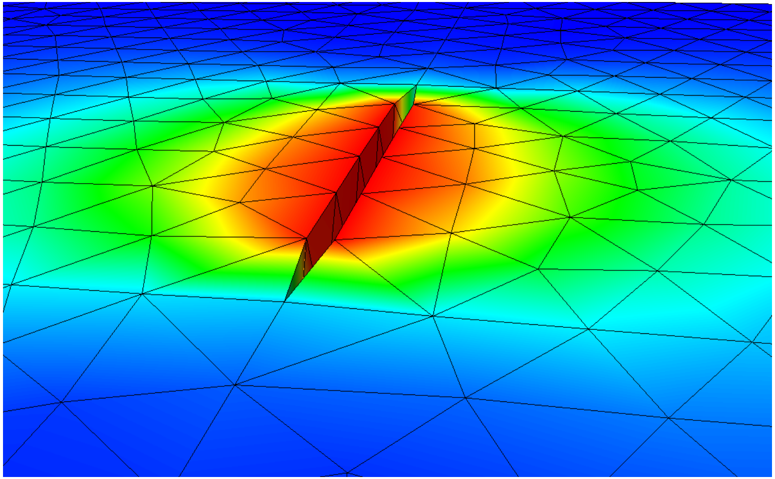
T=3.0 years (Rifting ...)



Displacement

## Example (3D Quasistatic)

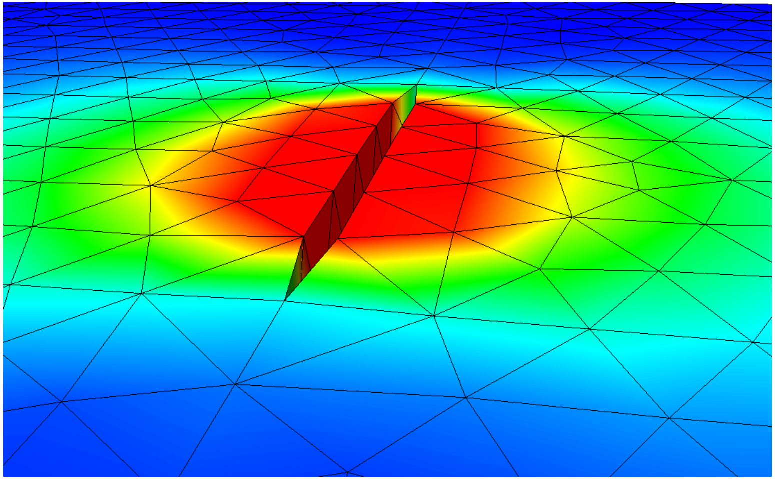
T=4.0 years (Rifting ...)



Displacement

## Example (3D Quasistatic)

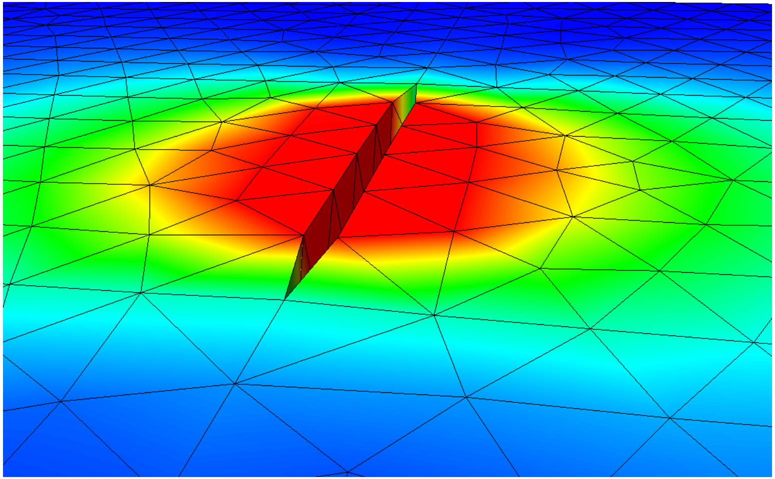
T=5.0 years (Rifting ends)



Displacement

## Example (3D Quasistatic)

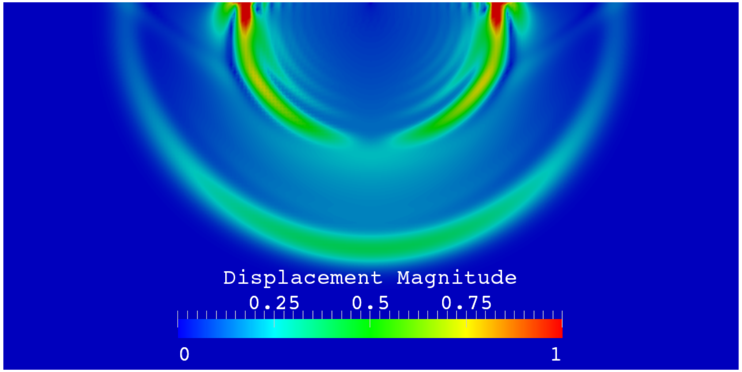
T=10.0 years (Postrifting viscous relaxation)



Displacement

## Example (2D Dynamic with ABCs)

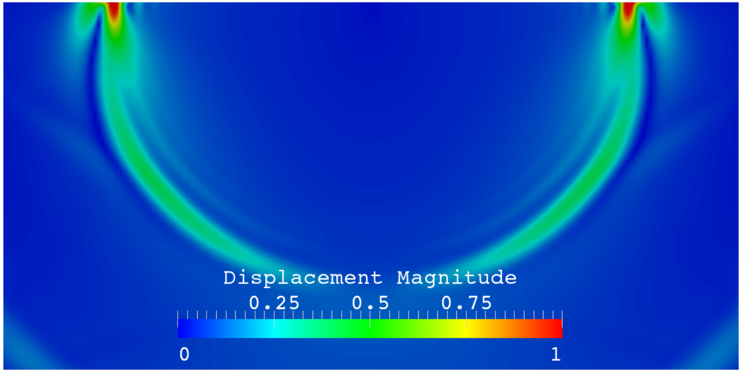
Time step 250



Note: Full computational domain is shown

## Example (2D Dynamic with ABCs)

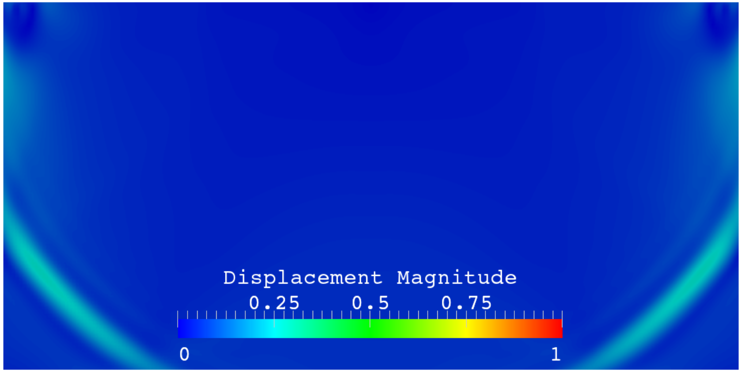
Time step 500



Note: Full computational domain is shown

## Example (2D Dynamic with ABCs)

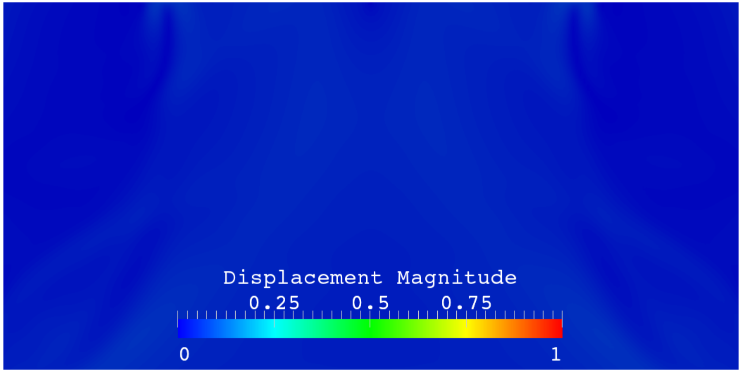
Time step 750



Note: Full computational domain is shown

## Example (2D Dynamic with ABCs)

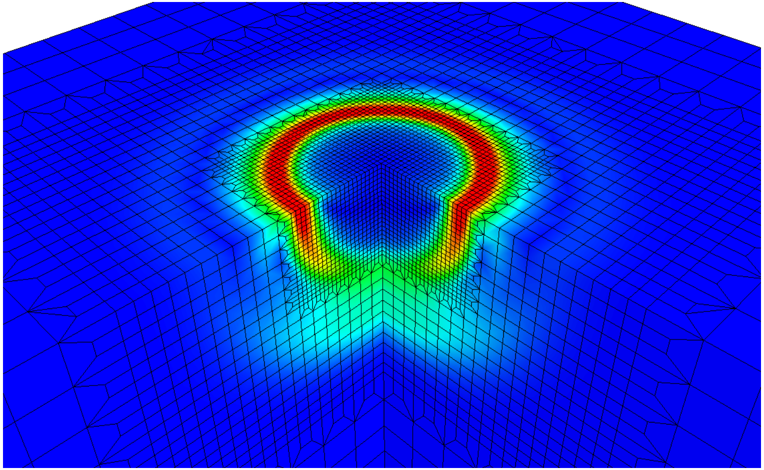
Time step 1000



Note: Full computational domain is shown

## Example (3D Dynamic)

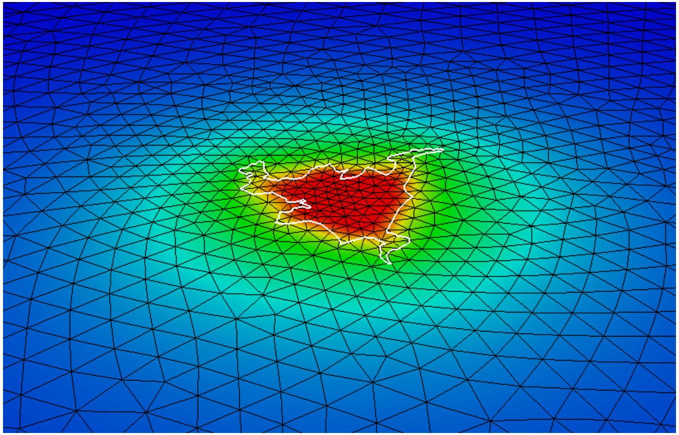
T=3.0 secs



Velocity

## Example (3D with Traction BCs)

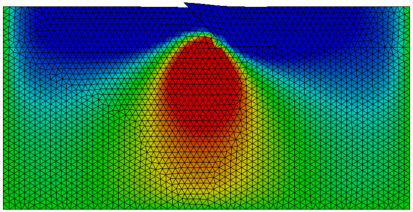
Deformation due to lake[3] loading



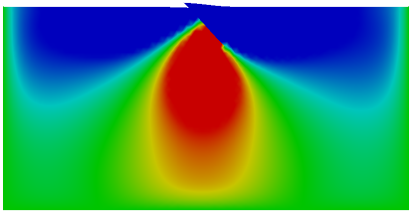
[3]Shoreline is shown in white

## Example (2D Poroelasticity)

Pore pressure change following an earthquake at time step 0



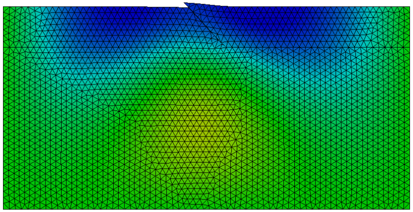
(i) with a permeable fault zone



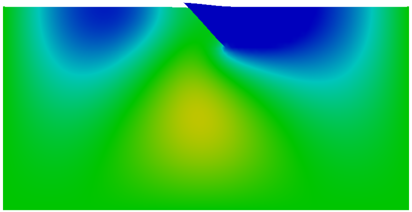
(ii) with an impermeable fault zone

## Example (2D Poroelasticity)

Pore pressure change following an earthquake at time step 5



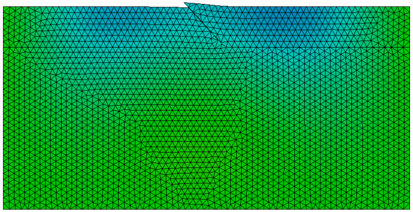
(i) with a permeable fault zone



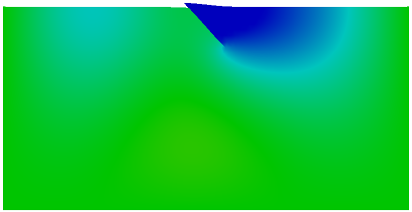
(ii) with an impermeable fault zone

## Example (2D Poroelasticity)

Pore pressure change following an earthquake at time step 10



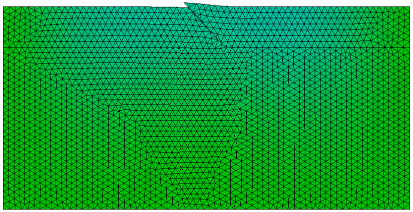
(i) with a permeable fault zone



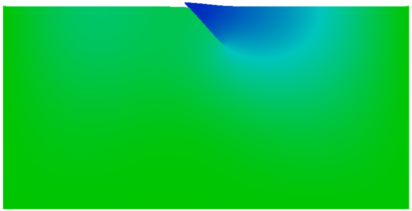
(ii) with an impermeable fault zone

## Example (2D Poroelasticity)

Pore pressure change following an earthquake at time step 15



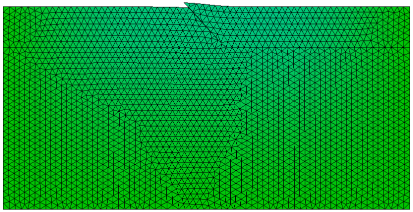
(i) with a permeable fault zone

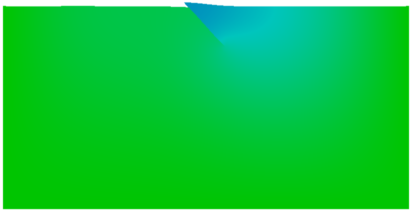


(ii) with an impermeable fault zone

## Example (2D Poroelasticity)

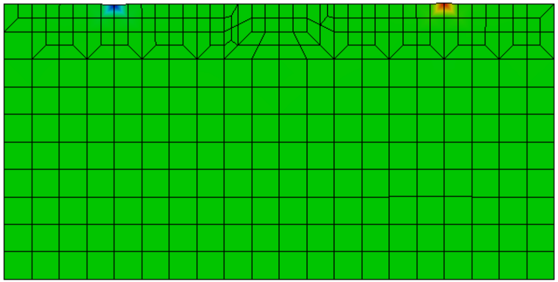
Pore pressure change following an earthquake at time step 20


(i) with a permeable fault zone


(ii) with an impermeable fault zone

## Example (2D Poroelasticity)

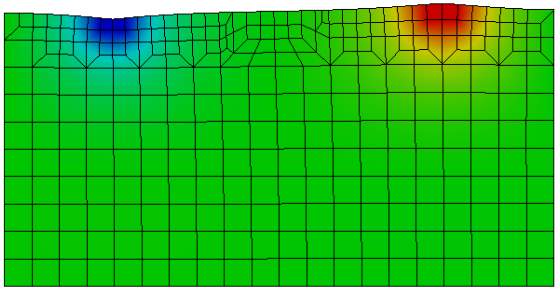
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

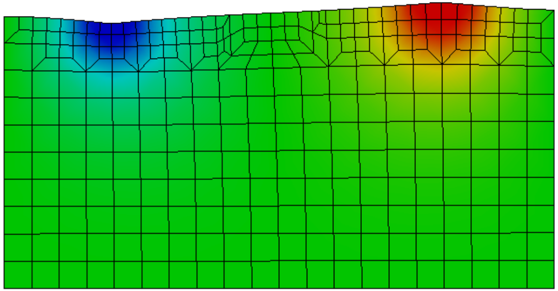
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

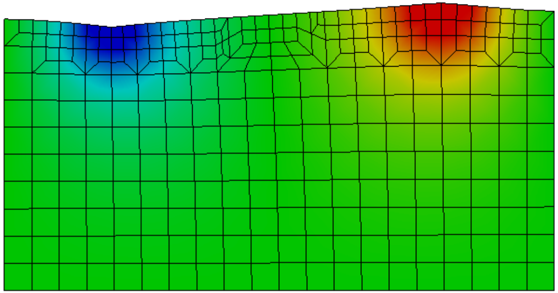
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

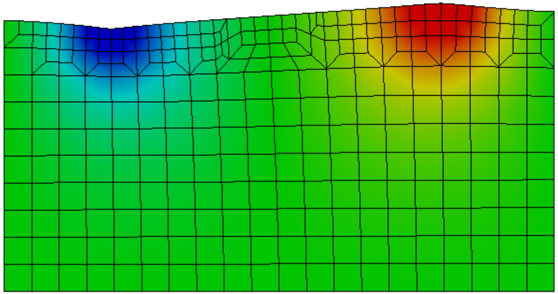
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

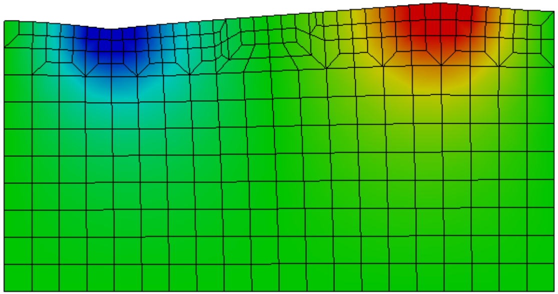
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

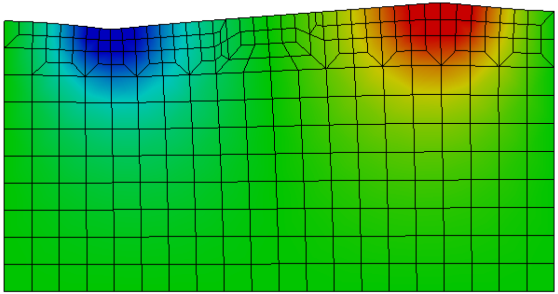
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

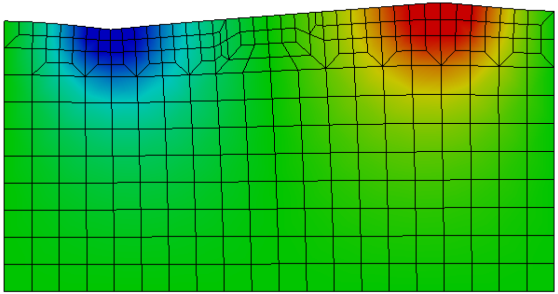
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

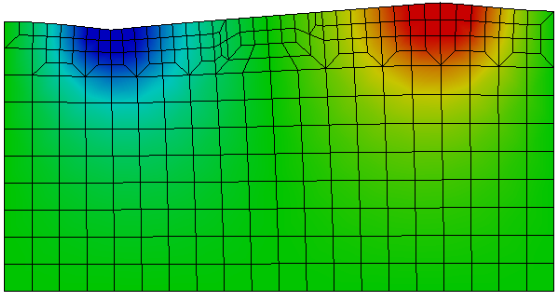
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production on

## Example (2D Poroelasticity)

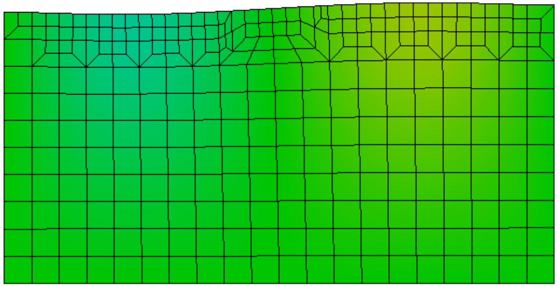
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production off

## Example (2D Poroelasticity)

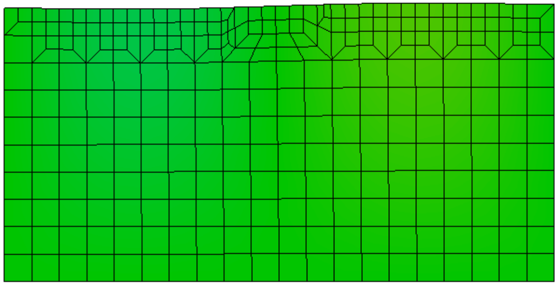
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production off

## Example (2D Poroelasticity)

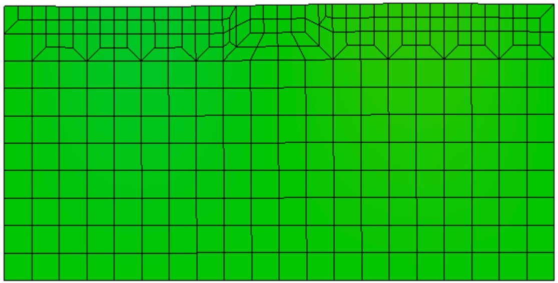
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production off

## Example (2D Poroelasticity)

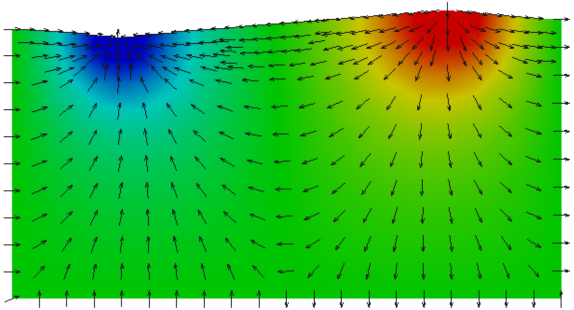
Pore pressure change due to injection (top right) and withdrawl (top left) of fluid in a saturated reservoir



Production off

## Example (2D Poroelasticity)

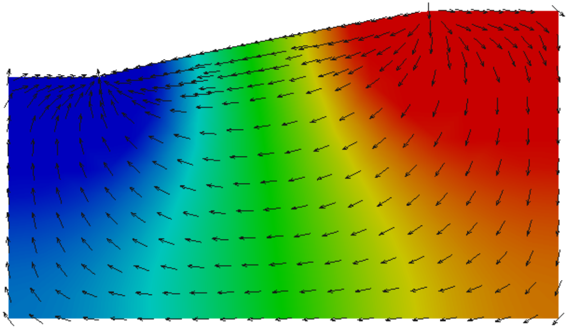
Fluid velocity vectors (unscaled) during steady production



With flow BC

## Example (2D Poroelasticity)

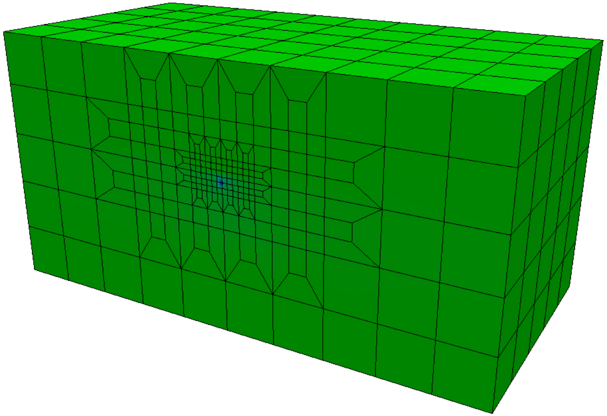
Fluid velocity vectors (unscaled) during steady production



With no-flow BC

## Example (3D Poroelasticity)

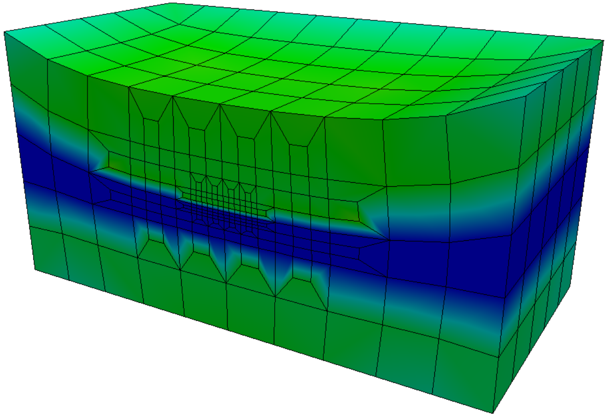
Pore pressure change due to withdrawl of fluid from a confined reservoir; Permeability ratio b/w reservoir and surrounding rock = 1.0E6



Note: In 3D, both (stabilized) linear tet or hex elements can be used

## Example (3D Poroelasticity)

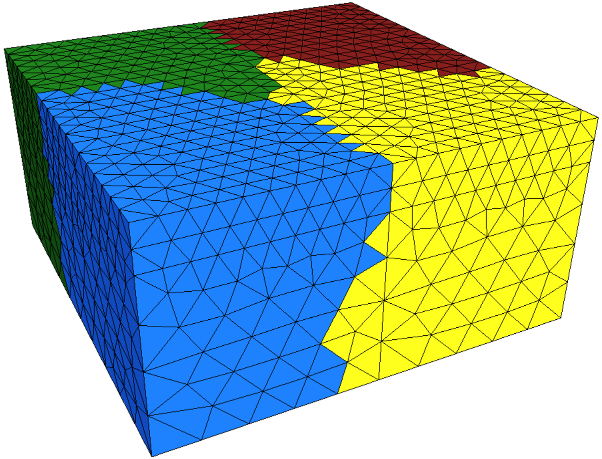
Pore pressure change due to withdrawl of fluid from a confined reservoir; Permeability ratio b/w reservoir and surrounding rock = 1.0E6



Note: In 3D, both (stabilized) linear tet or hex elements can be used

## Parallelism

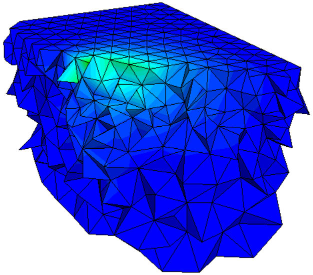
Each processor core owns only a part of the mesh, part of the stiffness matrix, part of the load/solution vector and writes its own VTK output



A mesh partitioned (using METIS) to run on 4 processor cores

## Parallelism

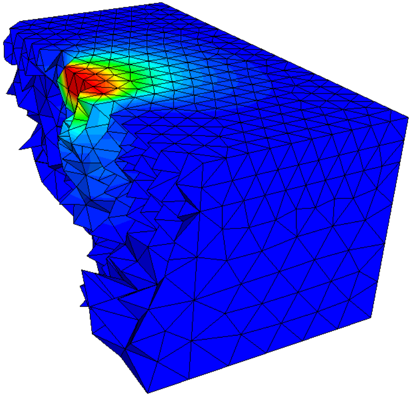
Each processor core owns only a part of the mesh, part of the stiffness matrix, part of the load/solution vector and writes its own VTK output



Visualization of subdomain(s) 1

## Parallelism

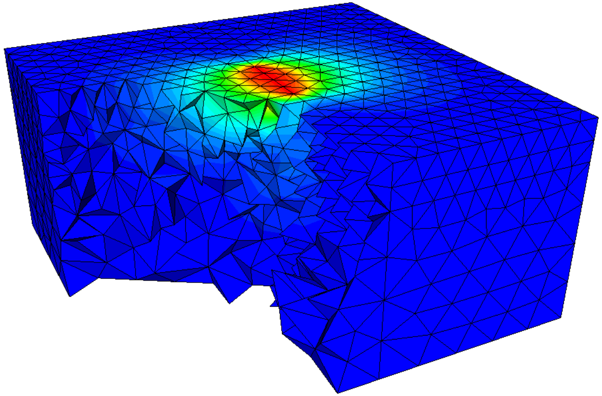
Each processor core owns only a part of the mesh, part of the stiffness matrix, part of the load/solution vector and writes its own VTK output



Visualization of subdomain(s) 1, 2

## Parallelism

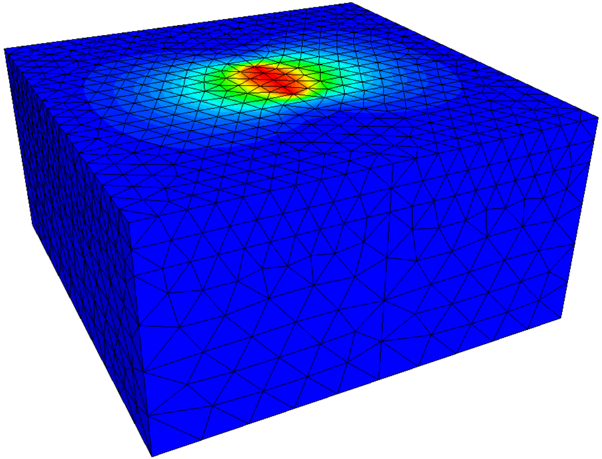
Each processor core owns only a part of the mesh, part of the stiffness matrix, part of the load/solution vector and writes its own VTK output



Visualization of subdomain(s) 1, 2, 3

## Parallelism

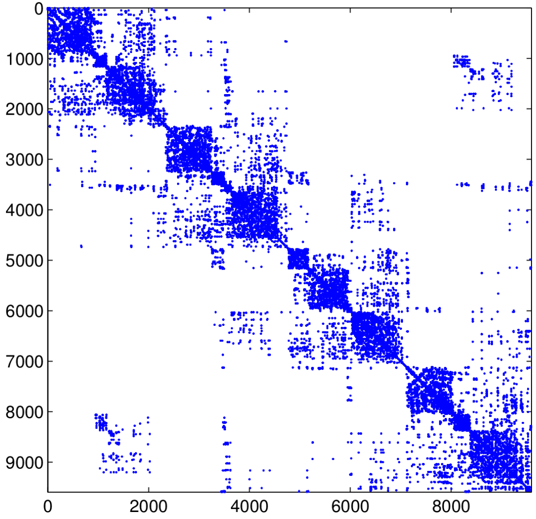
Each processor core owns only a part of the mesh, part of the stiffness matrix, part of the load/solution vector and writes its own VTK output



Visualization of subdomain(s) 1, 2, 3 and 4

## Parallelism

The resulting stiffness matrix, distributed (row wise) across 4 processor cores



## Limitations

- Due to the use of a serial mesh partitioner (METIS), the largest problem Defmod can solve on most current generation clusters (having $16-128$ GB of RAM on node 0) is limited to 125-1000 million unknowns
- Beyond 4000 cores, the 'I' part in 'I/O' is likely to become a bottleneck as all cores will have to access the same input file to read part of the mesh they own (skipping rest) during the initialization phase

## Solver performance

On the Trestles cluster (SDSC) for a problem with $\sim$ 25 million unknowns ...

| CPU Cores Used # | DOF per core | Explicit Dynamic Solver Efficiency | Implicit Quasistatic Solver Efficiency[4] |
|---|---|---|---|
| 128 | 195.2K | 1.00 | 1.00 |
| 256 | 97.6K | 0.97 | 0.92 |
| 512 | 48.4K | 0.93 | 0.89 |
| 1024 | 24.4K | 0.80 | 0.87 |

- On most current generation clusters, parallel efficiency of $\sim$ 90% or more can be achieved as long as DOF/core is $> 37.5K$
- Ideally DOF/core should be b/w 37.5-250K for explicit dynamic problems and b/w 37.5-125K for implicit quasistatic problems (assuming 1GB RAM/core, unbalanced mesh and default solver settings)

[4] Maximum iterations were fixed

## Examples

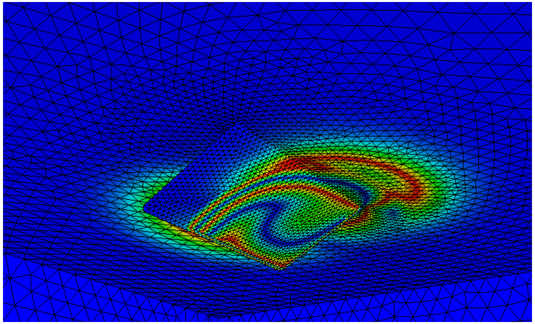
- Sample files are provided in the `examples` directory
- For more details look at the following files[5] in order:

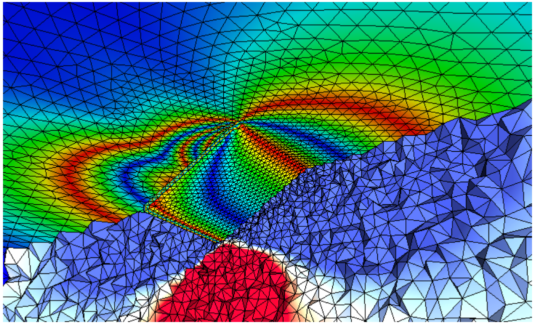
  1. `two_quads_qs.inp`
  2. `quadtree_qs.inp`
  3. `cube_qs.inp`
  4. `2d_point_load_dyn.inp`
  5. `2d_fault_dyn.inp`
  6. `2d_per_fault_poro_qs.inp`
  7. `3d_rift_visco_qs.inp`
  8. `3d_reservoir_poro_qs.inp`

[5] Some of the files are commented

## Showcase application(s)

Investigating source processes; Estimating slip distribution and/or poroviscoelastic properties of rock using (high rate) GPS + InSAR


Elastodynamic deformation due to a slipping thrust fault


Quasistatic deformation due to afterslip and poroviscoelastic relaxation

## TODO

In order of priority

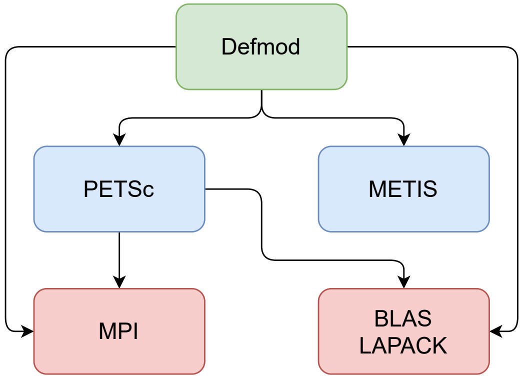
1. Code optimization (soon)
   - Use adaptive time-stepping for quasistatic problem(s)
   - Use AMG as default preconditioner for quasistatic problem(s)
   - Reduce (local) memory footprint by using exact preallocation
2. Solution of the adjoint problem (planned)

## Source files

| Name | Description |
|---|---|
| `petsc*.h` | Header file(s) |
| `m_utils.F90` | Simple utilities (area of triangle/quadrilateral etc.) |
| `m_elems.F90` | Element definitions, shape functions, their derivatives etc. |
| `m_local.F90` | Element level routines to compute stiffness/mass matrix, stress tensor etc. |
| `m_global.F90` | Routines that need access to on-rank arrays (nodal coordinates, element connectivity etc.) |
| `main.F90` | Main code (partitioner/mapper, solver(s) etc.) |

More on installation ...

## Dependencies



## Laptop/PC running Debian

```
$ sudo apt-get install gcc gfortran make python cmake git
$ curl -O https://ftp.mcs.anl.gov/pub/petsc/release-snapshots/petsc-lite-3.16.tar.gz
$ tar -xzf petsc-lite-3.16.tar.gz
$ cd petsc-3.16.*
$ export PETSC_DIR=$PWD PETSC_ARCH=arch-linux2-c-opt
$./configure --with-cc=gcc --with-fc=gfortran --download-mpich
              --download-fblaslapack --download-metis --with-debugging=0
$ make all
$ export PATH=$PATH:$PETSC_DIR/$PETSC_ARCH/bin
$ cd ..
$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all
$ mpiexec -n 2 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
```

Note: Above instructions can be used on any computer that runs Debian (or Ubuntu); See `http://www.debian.org/ports/` for supported architectures

## Laptop/PC running Debian

```
$ sudo apt-get install libmpich-dev liblapack-dev libmetis-dev make python git
$ curl -O https://ftp.mcs.anl.gov/pub/petsc/release-snapshots/petsc-lite-3.16.tar.gz
$ tar -xzf petsc-lite-3.16.tar.gz
$ cd petsc-3.16.*
$ export PETSC_DIR=$PWD PETSC_ARCH=arch-linux2-c-opt
$./configure --with-metis --with-debugging=0

$ make all

$ cd ..
$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all
$ mpiexec -n 2 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
```

Note: Above instructions can be used on any computer that runs Debian (or Ubuntu); See `http://www.debian.org/ports/` for supported architectures

## Laptop/PC running Debian

```
$ sudo apt-get install libpetsc-real-dev libmetis-dev make git
```

```
$ export PETSC_DIR=/usr/lib/petsc
```

```
$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all FPPFLAGS=-DPETSC_HAVE_METIS LDLIBS=-lmetis
$ mpiexec -n 2 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
```

Note: Above instructions can be used on any computer that runs Debian (or Ubuntu); See `http://www.debian.org/ports/` for supported architectures

## Linux clusters

On typical Linux clusters, MPI and BLAS/LAPACK are almost always preinstalled and all we have to do is:

```
$ curl -O https://ftp.mcs.anl.gov/pub/petsc/release-snapshots/petsc-lite-3.16.tar.gz
$ tar -xzf petsc-lite-3.16.tar.gz
$ cd petsc-3.16.*
$ export PETSC_DIR=$PWD
$ ./configure --with-mpi-dir=/path/to/mpi --download-metis --with-debugging=0
$ make all
```

NOTE: `/path/to/mpi` above is simply the MPI installation directory, which can be be found using:

```
$ which mpif90 | rev | cut -c12- | rev
```

```
$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all
$ mpiexec -n 2 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
```

## Linux clusters

On many Linux clusters, such as those available via XSEDE or at large supercomputing centers, PETSc is usually preinstalled. E.g., on the Lonestar cluster at TACC (UTexas) all we have to do is:

```
$ ssh lonestar.tacc.utexas.edu
$ module load petsc

$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all
$ ibrun[6] -n 2 -o 0 ./defmod -f examples/two_quads_qs.inp -ksp_monitor
```

[6] via Scheduler

## Linux clusters

Similarly, on the Comet cluster at SDSC all we have to do is:

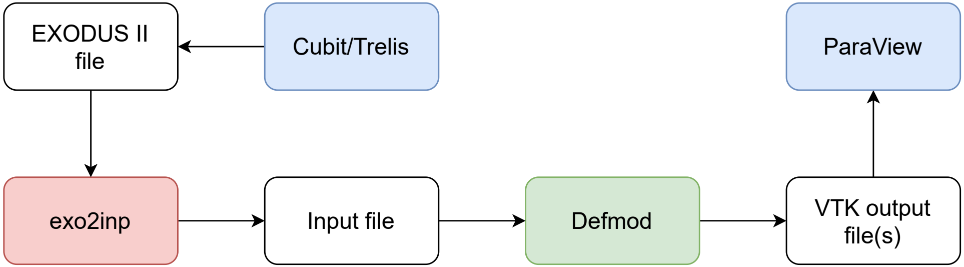
```
$ ssh comet.sdsc.edu
$ module load petsc

$ git clone https://bitbucket.org/stali/defmod
$ cd defmod
$ make all PETSC_DIR=$PETSCHOME
$ ibrun[7] ./defmod -f examples/two_quads_qs.inp -ksp_monitor
```

[7] via Scheduler

## Other Linux distributions and operating systems

- Those using non-Debian based distributions should see the `INSTALL` file included with the source
- Any standard conforming C/Fortran 95 compiler will work. The ones that have been tested and are known to work include:
  - AOCC (free)
  - Clang/Flang (free)
  - Cray
  - GCC (free)
  - Intel
  - Open64 (free)
  - PGI (free)
  - Oracle/Sun Studio (free)
- Apple macOS and MS Windows users can install all required dependencies using Homebrew and Cygwin/WSL, respectively

## Suggested workflow



Note: The `exo2inp` utility is available at `https://bitbucket.org/stali/defmod-utils/`

## Derivative work

Dr. Chunfang Meng at MIT has developed a sophisticated hybrid solver which can simulate dynamic rupture due to quasistatic loading in poroviscoelastic media, and is useful for studying processes such as induced or triggered seismicity. See https://doi.org/10.1016/j.cageo.2016.11.014 for details.

He has combined the hybrid solver with OpenSWPC, a parallel, higher-order finite difference code developed by Takuto Maeda at ERI (University of Tokyo). For more information about this mixed (FE-FD) approach, see https://doi.org/10.1016/j.cageo.2018.01.015.

Dr. Meng has also extended the code to incorporate fault zone inhomogeneities (damage) as well as the ability to model slip/rupture on truly intersecting faults. For details, see https://doi.org/10.1785/0220190083 and https://doi.org/10.1785/0220190234, respectively.

Defmod has also been incorporated into Esh3D for solving Eshelby's inclusion problem in full and half space. See https://doi.org/10.1029/2018EA000442 for details.

## Acknowledgements

- PETSc team for providing a first class Fortran API and support
- Greg Lyzenga/Jay Parker (JPL) for providing the 3D viscoelastic strain rate matrices
- Chris Kyriakopoulos (UC Riverside) for his help in validating Defmod with ABAQUS
- XSEDE award for testing and benchmarking code on x86 Linux clusters

For more information visit `https://bitbucket.org/stali/defmod`

A short preprint describing Defmod is available at `http://arxiv.org/abs/1402.0429`

Some useful utilities/scripts are available at `https://bitbucket.org/stali/defmod-utils`