PyLith v3.0 Tutorial

Quasi-static Simulations with No Fault

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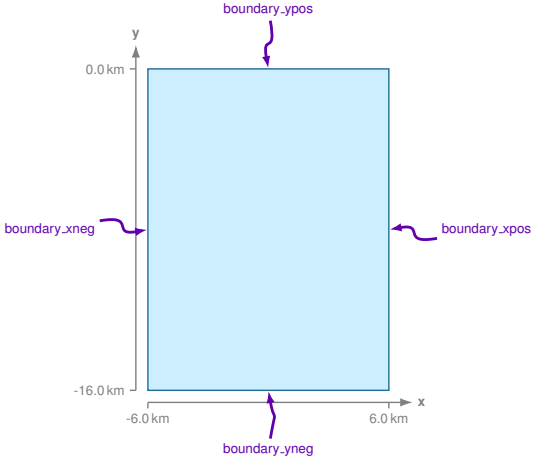
Axial and Shear Deformation of a 2D Box: `examples/box-2d`



Solve the static and quasistatic boundary elasticity equation in a 2D box with uniform material properties.

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Steps in example

Step 1 **Axial extension with Dirichlet (displacement) boundary conditions**

Step 2 **Shear deformation with Dirichlet (displacement) boundary conditions**

Step 3 **Shear deformation with Dirichlet (displacement) and Neumann (traction) boundary conditions**

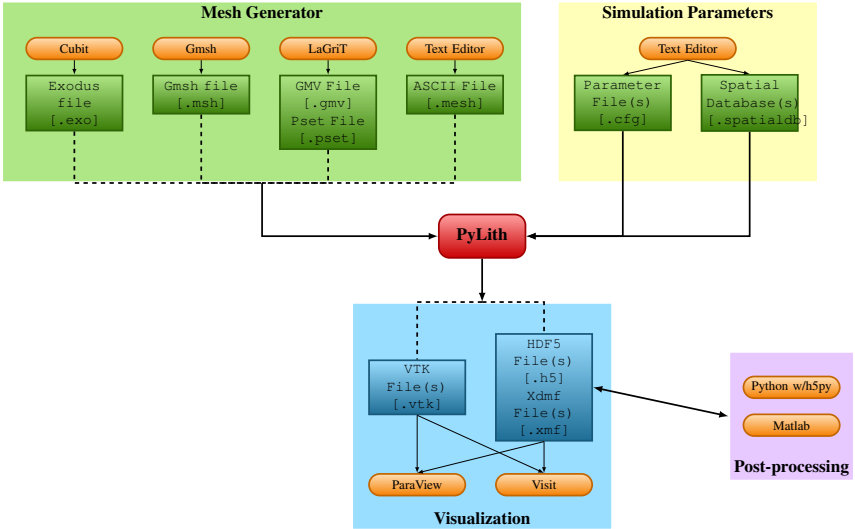
Step 4 Same as Step 2 but with initial conditions equal to the analytical solution

Step 5 Shear deformation with time-dependent Dirichlet (displacement) and Neumann (traction) boundary conditions

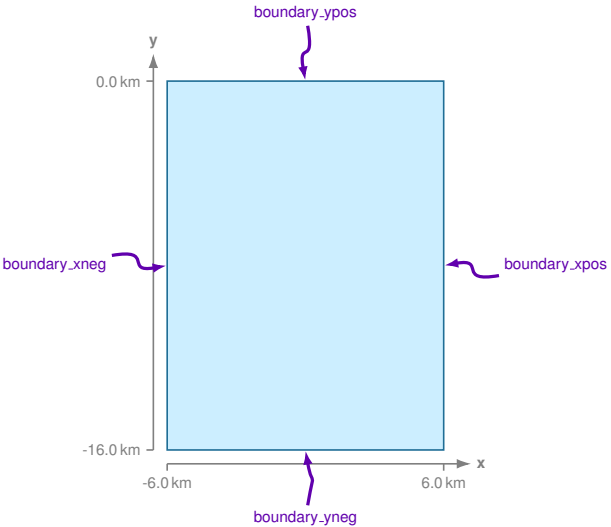
Concepts covered

- Ingredients for a PyLith simulation
- PyLith `MeshIOAscii` mesh format
- PyLith `.cfg` paremeter files
- `ZeroDB`, `UniformDB`, and `SimpleDB` spatial databases
- Dirichlet (displacement) boundary conditions
- Neumann (traction) boundary conditions
- Running a simulation
- Visualization of simulation results using Paraview

Overview of a PyLith simulation

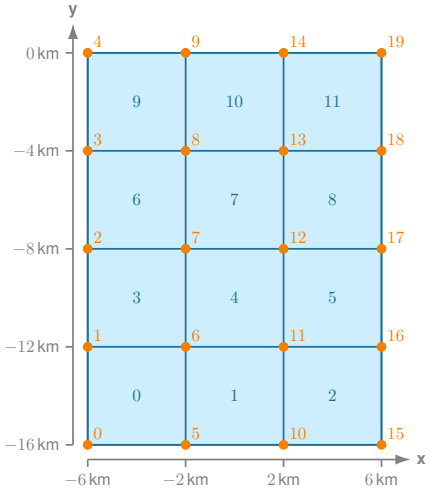


Geometry


boundary_ypos
y
0.0 km
boundary_xneg
boundary_xpos
-16.0 km
x
-6.0 km
6.0 km
boundary_yneg

Creating the finite-element mesh

For this very simple example, we create the mesh by hand



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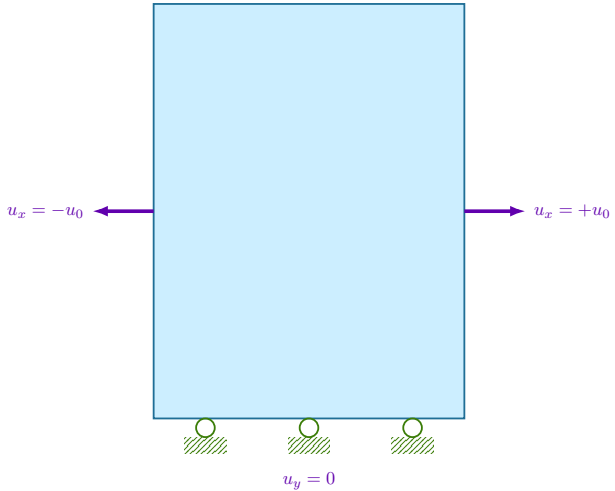
Files used in simulations

Files are in directory `examples/box-2d`

README.md	Brief description of the various examples
*.cfg	PyLith parameter files
*.mesh	Finite-element mesh file generated manually using a text editor
*.spatialdb	Spatial database files
viz	Directory containing ParaView Python scripts and other files for visualizing results
output	Directory containing simulation output; created automatically when running the simulations

Step 1: Overview

Axial extension in the x direction



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Step 1: Physics

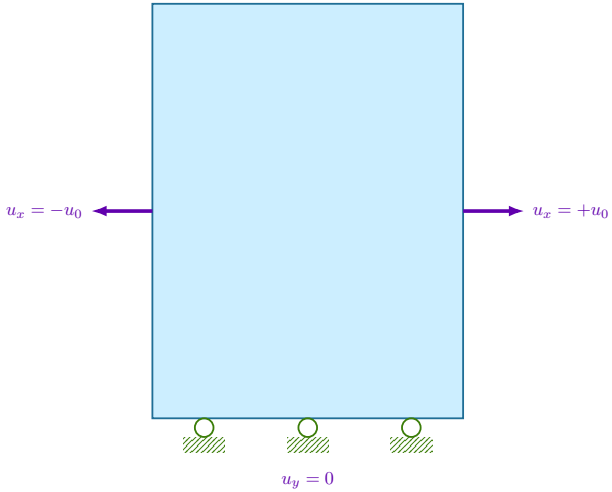
$$\vec{s} = \begin{pmatrix} \vec{u} \end{pmatrix}^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = -u_0$ on boundary_xneg

$u_x = +u_0$ on boundary_xpos

$u_y = 0$ on boundary_yneg



PyLith

Step 1: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = -u_0$ on boundary_xneg

$u_x = +u_0$ on boundary_xpos

$u_y = 0$ on boundary_yneg

Step 1: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = -u_0$ on boundary_xneg

$u_x = +u_0$ on boundary_xpos

$u_y = 0$ on boundary_yneg

```
# These are the defaults; not included in pylithapp.cfg.
[pylithapp.problem]
solution = pylith.problems.SolnDisp

[pylithapp.problem.solution.subfields]
displacement.basis_order = 1
```

Step 1: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = -u_0$ on boundary_xneg

$u_x = +u_0$ on boundary_xpos

$u_y = 0$ on boundary_yneg

```
# These are the defaults; not included in pylithapp.cfg.
[pylithapp.problem]
materials = [elastic]
materials.elastic = pylith.materials.Elasticity

[pylithapp.problem.materials.elastic]
elastic.bulk_rheology = pylith.materials.IsotropicLinearElastic
```

Step 1: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = -u_0$ on boundary_xneg

$u_x = +u_0$ on boundary_xpos

$u_y = 0$ on boundary_yneg

```
[pylithapp.problem]
bc = [bc_xneg, bc_xpos, bc_yneg]
bc.bc_xneg = pylith.bc.DirichletTimeDependent
bc.bc_xpos = pylith.bc.DirichletTimeDependent
bc.bc_yneg = pylith.bc.DirichletTimeDependent

[pylithapp.problem.bc.bc_xpos]
constrained_dof = [0]
label = boundary_xpos
...
```

Step 1: Input files

quad.mesh Finite-element mesh as a text file

pylithapp.cfg PyLith parameter file common to all steps

step01_axialdisp.cfg PyLith parameter file

Step 1: Run the simulation

```
pylith step01_axialdisp.cfg

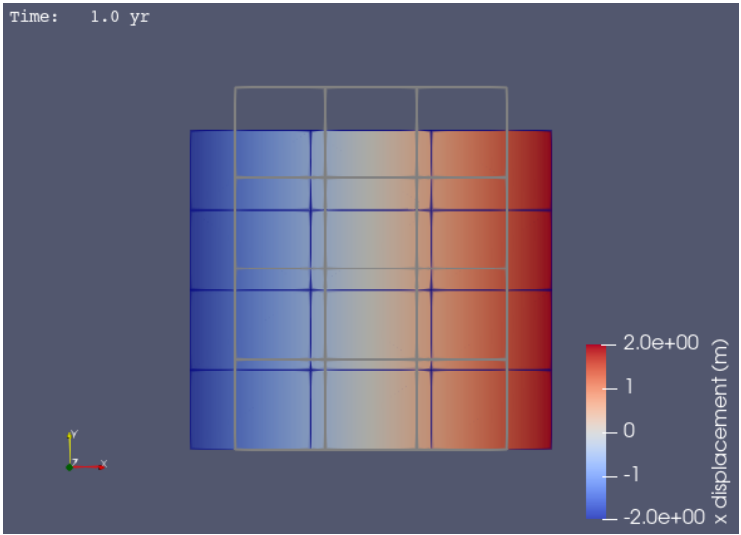
# Output
 >> /software/unix/py39-venv/pylith-debug/lib/python3.9/site-packages/pylith/meshio/MeshIOObj.py:44:read
 -- meshioascii(info)
 -- Reading finite-element mesh
 >> /src/cig/pylith/libsrc/pylith/meshio/MeshIO.cc:94:void pylith::meshio::MeshIO::read(topology::Mesh *)
 -- meshioascii(info)
 -- Component 'reader': Domain bounding box:
    (-6000, 6000)
    (-16000, -0)

# -- many lines omitted --

 -- Solving problem.
0 TS dt 0.01 time 0.
    0 SNES Function norm 1.245882095312e-02
    Linear solve converged due to CONVERGED_ATOL iterations 1
    1 SNES Function norm 6.738354969624e-18
  Nonlinear solve converged due to CONVERGED_FNORM_ABS iterations 1
1 TS dt 0.01 time 0.01
 >> /software/unix/py39-venv/pylith-debug/lib/python3.9/site-packages/pylith/problems/Problem.py:201:finalize
 -- timedependent(info)
 -- Finalizing problem.
```

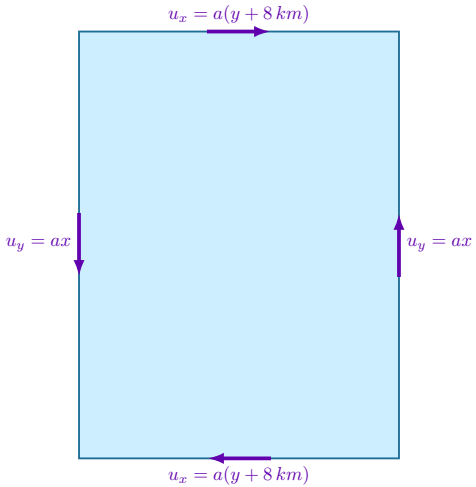
Step 1: Visualize results

Run the `viz/plot_dispwarp.py` Python script from within ParaView



Step 2: Overview

Simple shear deformation using Dirichlet (displacement) boundary conditions



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Step 2: Physics

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

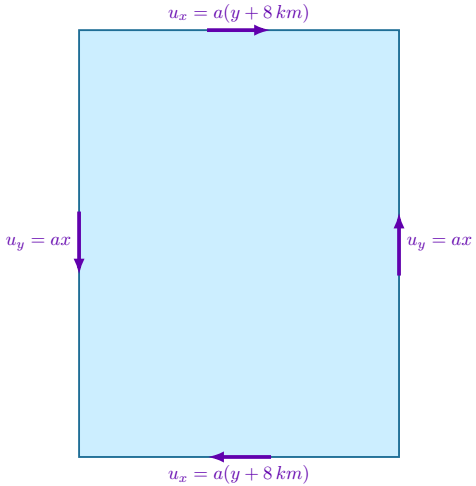
$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = ax$ on boundary_xneg

$u_x = ax$ on boundary_xpos

$u_y = a(y + 8\text{km})$ on boundary_yneg

$u_y = a(y + 8\text{km})$ on boundary_ypos



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Step 2: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = ax$ on boundary_xneg

$u_x = ax$ on boundary_xpos

$u_y = a(y + 8\mathrm{km})$ on boundary_yneg

$u_y = a(y + 8\mathrm{km})$ on boundary_ypos

Step 2: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = ax$ on boundary_xneg

$u_x = ax$ on boundary_xpos

$u_y = a(y + 8\text{km})$ on boundary_yneg

$u_y = a(y + 8\text{km})$ on boundary_ypos

```
# These are the defaults; not included in pylithapp.cfg.
[pylithapp.problem]
solution = pylith.problems.SolnDisp

[pylithapp.problem.solution.subfields]
displacement.basis_order = 1
```

Step 2: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = ax$ on boundary_xneg

$u_x = ax$ on boundary_xpos

$u_y = a(y + 8\text{km})$ on boundary_yneg

$u_y = a(y + 8\text{km})$ on boundary_ypos

```
# These are the defaults; not included in pylithapp.cfg.
[pylithapp.problem]
materials = [elastic]
materials.elastic = pylith.materials.Elasticity

[pylithapp.problem.materials.elastic]
elastic.bulk_rheology = pylith.materials.IsotropicLinearElastic
```

Step 2: Physics to simulation parameters

$$\vec{s} = \begin{pmatrix} \vec{u} \end{pmatrix}^T$$

$$\nabla \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$u_x = ax$ on boundary_xneg

$u_x = ax$ on boundary_xpos

$u_y = a(y + 8\text{km})$ on boundary_yneg

$u_y = a(y + 8\text{km})$ on boundary_ypos

```
[pylithapp.problem]
bc = [bc_xneg, bc_yneg, bc_xpos, bc_ypos]
bc.bc_xneg = pylith.bc.DirichletTimeDependent
bc.bc_yneg = pylith.bc.DirichletTimeDependent
bc.bc_xpos = pylith.bc.DirichletTimeDependent
bc.bc_ypos = pylith.bc.DirichletTimeDependent

[pylithapp.problem.bc.bc_xpos]
constrained_dof = [1]
label = boundary_xpos
...
```

Step 2: Input files

quad.mesh Finite-element mesh as a text file

pylithapp.cfg PyLith parameter file common to all steps

step02_sheardisp.cfg PyLith parameter file

sheardisp_bc_xneg.spatialdb Displacement field on boundary_xneg

sheardisp_bc_xpos.spatialdb Displacement field on boundary_xpos

sheardisp_bc_yneg.spatialdb Displacement field on boundary_yneg

sheardisp_bc_ypos.spatialdb Displacement field on boundary_ypos

Step 2: Run the simulation

```
pylith step02_sheardisp.cfg

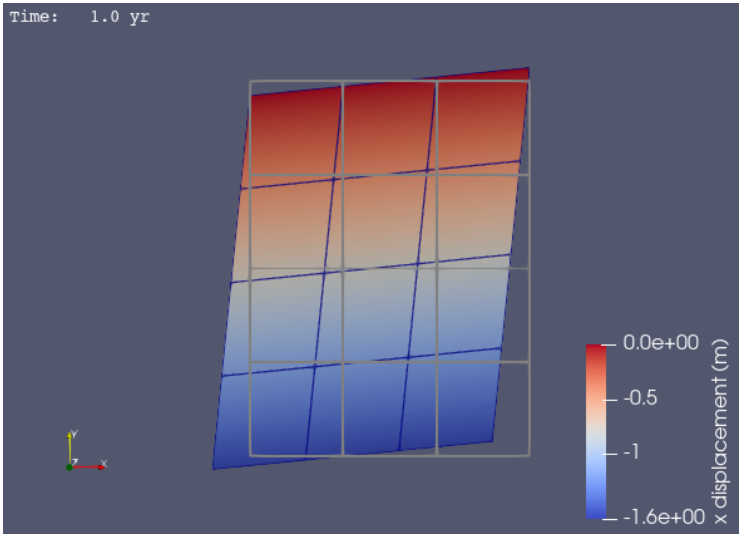
# Output
 >> /software/unix/py39-venv/pylith-debug/lib/python3.9/site-packages/pylith/meshio/MeshIOObj.py:44:read
 -- meshioascii(info)
 -- Reading finite-element mesh
 >> /src/cig/pylith/libsrc/pylith/meshio/MeshIO.cc:94:void pylith::meshio::MeshIO::read(topology::Mesh *)
 -- meshioascii(info)
 -- Component 'reader': Domain bounding box:
    (-6000, 6000)
    (-16000, -0)

# -- many lines omitted --

 -- Solving problem.
0 TS dt 0.01 time 0.
    0 SNES Function norm 2.239977678460e-03
    Linear solve converged due to CONVERGED_ATOL iterations 1
    1 SNES Function norm 1.964321818484e-18
  Nonlinear solve converged due to CONVERGED_FNORM_ABS iterations 1
1 TS dt 0.01 time 0.01
 >> /software/unix/py39-venv/pylith-debug/lib/python3.9/site-packages/pylith/problems/Problem.py:201:finalize
 -- timedependent(info)
 -- Finalizing problem.
```

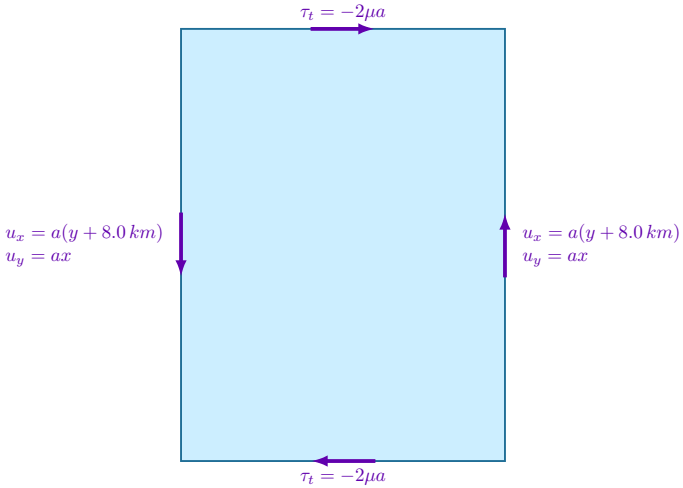
Step 2: Visualize results

Run the `viz/plot_dispwarp.py` Python script from within ParaView



Step 3: Overview

Simple shear deformation using Dirichlet (displacement) and Neuammn (traction) boundary conditions



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Step 3: Physics

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

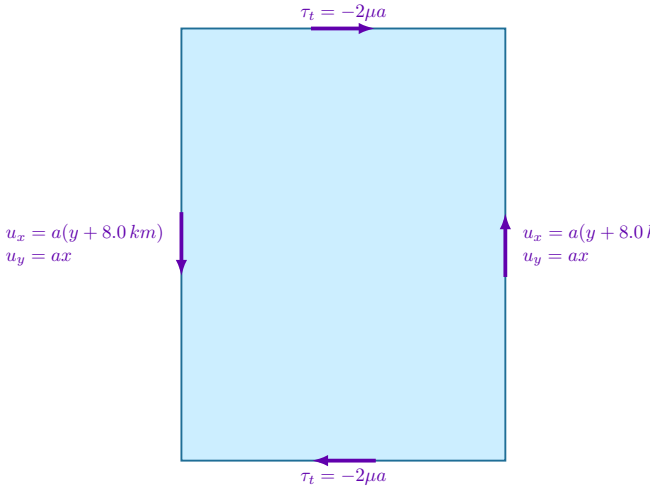
$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$$\left.\begin{aligned} u_x &= a(y + 8\text{km}) \\ u_y &= ax \end{aligned}\right\} \text{ on boundary\_xneg}$$

$$\left.\begin{aligned} u_x &= a(y + 8\text{km}) \\ u_y &= ax \end{aligned}\right\} \text{ on boundary\_xpos}$$

$\tau_t = -2\mu a$ on boundary_yneg

$\tau_t = -2\mu a$ on boundary_ypos



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Step 3: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$$\left.\begin{array}{c} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xneg}$$

$$\left.\begin{array}{c} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xpos}$$

$\tau_t = -2\mu a$ on boundary_yneg

$\tau_t = -2\mu a$ on boundary_ypos

Step 3: Physics to simulation parameters

$$\vec{s} = \left(\ \vec{u} \ \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

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$$\left.\begin{array}{c} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xpos}$$

$\tau_t = -2\mu a$ on boundary_yneg

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```
# These are the defaults; not included in pylithapp.cfg.
[pylithapp.problem]
solution = pylith.problems.SolnDisp

[pylithapp.problem.solution.subfields]
displacement.basis_order = 1
```

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$$\left.\begin{array}{c} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xneg}$$

$$\left.\begin{array}{c} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xpos}$$

$$\tau_t = -2\mu a \text{ on boundary\_yneg}$$

$$\tau_t = -2\mu a \text{ on boundary\_ypos}$$

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materials = [elastic]
materials.elastic = pylith.materials.Elasticity

[pylithapp.problem.materials.elastic]
elastic.bulk_rheology = pylith.materials.IsotropicLinearElastic
```

Step 3: Physics to simulation parameters

$$\vec{s} = \left(\vec{u} \right)^T$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\vec{u}) = \vec{0}$$

$$\left.\begin{array}{l} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xneg}$$

$$\left.\begin{array}{l} u_x = a(y + 8\text{km}) \\ u_y = ax \end{array}\right\} \text{ on boundary\_xpos}$$

$\tau_t = -2\mu a$ on boundary_yneg

$\tau_t = -2\mu a$ on boundary_ypos

```
[pylithapp.problem]
bc = [bc_xneg, bc_yneg, bc_xpos, bc_ypos]
bc.bc_xneg = pylith.bc.DirichletTimeDependent
bc.bc_xpos = pylith.bc.DirichletTimeDependent
bc.bc_yneg = pylith.bc.NeumannTimeDependent
bc.bc_ypos = pylith.bc.NeumannTimeDependent

[pylithapp.problem.bc.bc_xpos]
constrained_dof = [0, 1]
label = boundary_xpos
...
```

Step 3: Input files

quad.mesh Finite-element mesh as a text file

pylithapp.cfg PyLith parameter file common to all steps

step03_sheardisptract.cfg PyLith parameter file

sheardisp_bc_xneg.spatialdb Displacement field on boundary_xneg

sheardisp_bc_xpos.spatialdb Displacement field on boundary_xpos

Step 3: Run the simulation

```
pylith step03_sheardisptract.cfg

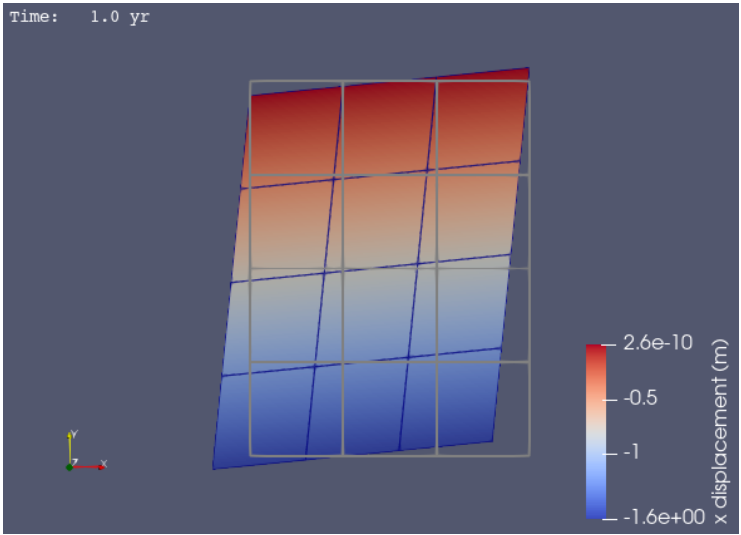
# Output
 >> /software/unix/py39-venv/pylith-debug/lib/python3.9/site-packages/pylith/meshio/MeshIOObj.py:44:read
 -- meshioascii(info)
 -- Reading finite-element mesh
 >> /src/cig/pylith/libsrc/pylith/meshio/MeshIO.cc:94:void pylith::meshio::MeshIO::read(topology::Mesh *)
 -- meshioascii(info)
 -- Component 'reader': Domain bounding box:
    (-6000, 6000)
    (-16000, -0)

# -- many lines omitted --

 -- Solving problem.
0 TS dt 0.01 time 0.
    0 SNES Function norm 6.059797141590e-03
    Linear solve converged due to CONVERGED_ATOL iterations 1
    1 SNES Function norm 2.140441363908e-18
  Nonlinear solve converged due to CONVERGED_FNORM_ABS iterations 1
1 TS dt 0.01 time 0.01
 >> /software/unix/py39-venv/pylith-debug/lib/python3.9/site-packages/pylith/problems/Problem.py:201:finalize
 -- timedependent(info)
 -- Finalizing problem.
```

Step 3: Visualize results

Run the `viz/plot_dispwarp.py` Python script from within ParaView



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