GEL01_axi_swell_A.Flowers_Comments

July 14, 2025

1 Axisymmetric cylinder swelling

- Swelling of a gel cylinder
- This is an axisymmetric simulation

2 Degrees of freedom

- Displacement: u
- pressure: p
- chemical potential: mu
- concentration: c

3 Units

- Length: mm
- Mass: kg
- Time: s
- Mass density: kg/mm^3
- Force: milliN
- Stress: kPa
- Energy: microJ
- Temperature: K
- Amount of substance: mol
- Species concentration: mol/mm^3
- Chemical potential: milliJ/mol
- Molar volume: mm^3/mol
- Species diffusivity: mm^2/s
- Gas constant: microJ/(mol K)

3.0.1 Software:

- Dolfinx v0.8.0

In the collection "Example Codes for Coupled Theories in Solid Mechanics,"

By Eric M. Stewart, Shawn A. Chester, and Lallit Anand.

https://solidmechanicscoupledtheories.github.io/

4 Import modules

[ ]:
```
# Import FEnicSx/dolfinx
import dolfinx

# For numerical arrays
import numpy as np

# For MPI-based parallelization
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()

# PETSc solvers
from petsc4py import PETSc

# specific functions from dolfinx modules
from dolfinx import fem, mesh, io, plot, log
from dolfinx.fem import (Constant, dirichletbc, Function, functionspace,␣
 ↪Expression )
from dolfinx.fem.petsc import NonlinearProblem
from dolfinx.nls.petsc import NewtonSolver
from dolfinx.io import VTXWriter, XDMFFile

# specific functions from ufl modules
import ufl
from ufl import (TestFunctions, TrialFunction, Identity, grad, det, div, dev,␣
 ↪inv, tr, sqrt, conditional ,\
                 gt, dx, inner, derivative, dot, ln, split, exp, eq, cos, sin,␣
 ↪acos, ge, le, outer, tanh,\
                 cosh, atan, atan2)

# basix finite elements (necessary for dolfinx v0.8.0)
import basix
from basix.ufl import element, mixed_element

# Matplotlib for plotting
import matplotlib.pyplot as plt
plt.close('all')

# For timing the code
from datetime import datetime

# Set level of detail for log messages (integer)
# Guide:
# CRITICAL  = 50, // errors that may lead to data corruption
# ERROR     = 40, // things that HAVE gone wrong
```

```
# WARNING   = 30, // things that MAY go wrong later
# INFO      = 20, // information of general interest (includes solver info)
# PROGRESS  = 16, // what's happening (broadly)
# TRACE     = 13, // what's happening (in detail)
# DBG       = 10  // sundry
#
log.set_log_level(log.LogLevel.WARNING)
```

5 Define geometry

[ ]:
```
# Create mesh
R0 = 2.5  # radius of bar
H0 = 2.5  # height of bar
domain = mesh.create_rectangle(MPI.COMM_WORLD, [[0.0,0.0], [R0,H0]],\
                         [8,8], mesh.CellType.triangle, diagonal=mesh.
 ↪DiagonalType.crossed)

x = ufl.SpatialCoordinate(domain)
```

Identify boundaries of the domain

[ ]:
```
# Identify the boundaries of the  rectangle mesh
#
def xBot(x):
    return np.isclose(x[0], 0)
def xTop(x):
    return np.isclose(x[0], R0)
def yBot(x):
    return np.isclose(x[1], 0)
def yTop(x):
    return np.isclose(x[1], H0)

# Mark the sub-domains
boundaries = [(1, xBot),(2,xTop),(3,yBot),(4,yTop)]

# Identify the bottom left corner
def Ground(x):
        return np.isclose(x[0], 0) and np.isclose(x[1], 0)


# Build collections of facets on each subdomain and mark them appropriately.
facet_indices, facet_markers = [], [] # initalize empty collections of indices␣
 ↪and markers.
fdim = domain.topology.dim - 1 # geometric dimension of the facet (mesh␣
 ↪dimension - 1)
for (marker, locator) in boundaries:
```

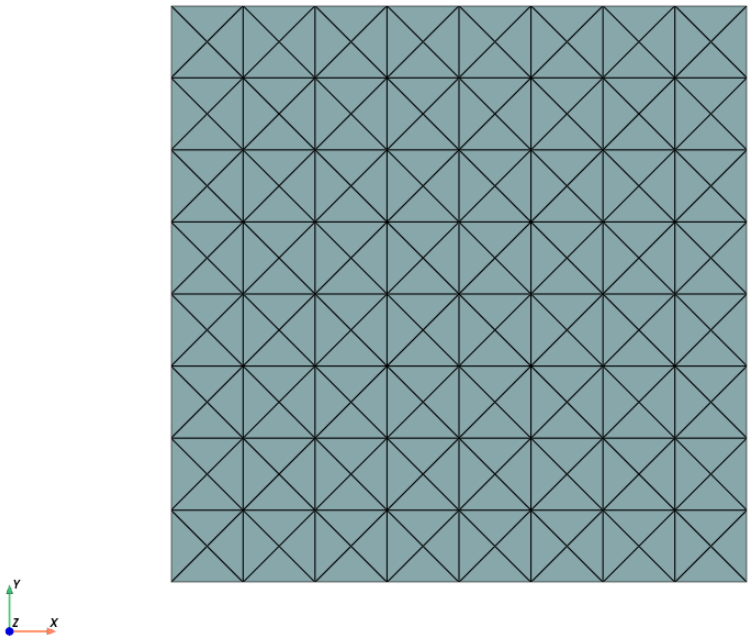
```
    facets = mesh.locate_entities(domain, fdim, locator) # an array of all the␣
 ↪facets in a
                                                         # given subdomain␣
 ↪("locator")
    facet_indices.append(facets)                         # add these facets to␣
 ↪the collection.
    facet_markers.append(np.full_like(facets, marker))   # mark them with the␣
 ↪appropriate index.

# Format the facet indices and markers as required for use in dolfinx.
facet_indices = np.hstack(facet_indices).astype(np.int32)
facet_markers = np.hstack(facet_markers).astype(np.int32)
sorted_facets = np.argsort(facet_indices)
#
# Add these marked facets as "mesh tags" for later use in BCs.
facet_tags = mesh.meshtags(domain, fdim, facet_indices[sorted_facets],␣
 ↪facet_markers[sorted_facets])
```

Visualize reference configuration

[ ]:
```
import pyvista
pyvista.set_jupyter_backend('html')
from dolfinx.plot import vtk_mesh
pyvista.start_xvfb()

# initialize a plotter
plotter = pyvista.Plotter()

# Add the mesh.
topology, cell_types, geometry = plot.vtk_mesh(domain, domain.topology.dim)
grid = pyvista.UnstructuredGrid(topology, cell_types, geometry)
plotter.add_mesh(grid, show_edges=True)

plotter.view_xy()

#labels = dict(xlabel='X', ylabel='Y',zlabel='Z')
labels = dict(xlabel='X', ylabel='Y')
plotter.add_axes(**labels)

plotter.screenshot("results/bar_mesh.png")

from IPython.display import Image
Image(filename='results/bar_mesh.png')

# # Use the following  commands for a  zoom-able  view
# if not pyvista.OFF_SCREEN:
#     plotter.show()
```

```
# else:
#     plotter.screenshot("axi_cylinder_mesh.png")
```

[ ]:



5.1 Define boundary and volume integration measure

[ ]:
```
# Define the boundary integration measure "ds" using the facet tags,
# also specify the number of surface quadrature points.
ds = ufl.Measure('ds', domain=domain, subdomain_data=facet_tags,␣
 ↪metadata={'quadrature_degree':2})

# Define the volume integration measure "dx"
# also specify the number of volume quadrature points.
dx = ufl.Measure('dx', domain=domain, metadata={'quadrature_degree': 2})

# Create facet to cell connectivity required to determine boundary facets.
domain.topology.create_connectivity(domain.topology.dim, domain.topology.dim)
domain.topology.create_connectivity(domain.topology.dim, domain.topology.dim-1)
domain.topology.create_connectivity(domain.topology.dim-1, domain.topology.dim)

# #  Define facet normal
```

```
n2D = ufl.FacetNormal(domain)
n = ufl.as_vector([n2D[0], n2D[1], 0.0]) # define n as a 3D vector for later use
```

6 Material parameters

[ ]:
```
# Set the locking stretch to a large number to model a Neo-Hookean material
#
Gshear_0= Constant(domain,PETSc.ScalarType(1000.0))          # Shear modulus, kPa
lambdaL = Constant(domain,PETSc.ScalarType(100))             # Locking stretch,␣
 ↪Neo-Hookean material
Kbulk   = Constant(domain,PETSc.ScalarType(1000*Gshear_0))  # Bulk modulus, kPa
Omega   = Constant(domain,PETSc.ScalarType(1.00e5))          # Molar volume of␣
 ↪fluid
D       = Constant(domain,PETSc.ScalarType(5.00e-3))         # Diffusivity
chi     = Constant(domain,PETSc.ScalarType(0.1))             # Flory-Huggins␣
 ↪mixing parameter
theta0  = Constant(domain,PETSc.ScalarType(298) )            # Reference␣
 ↪temperature
R_gas   = Constant(domain,PETSc.ScalarType(8.3145e6))        # Gas constant
RT      = Constant(domain,PETSc.ScalarType(8.3145e6*theta0))
#
phi0    = Constant(domain,PETSc.ScalarType(0.999))                # Initial␣
 ↪polymer volume fraction
mu0     = Constant(domain,PETSc.ScalarType(ln(1.0-phi0) + phi0 )) # Initial␣
 ↪chemical potential
c0      = Constant(domain,PETSc.ScalarType((1/phi0) - 1))         # Initial␣
 ↪concentration
```

7 Simulation time-control related parameters

[ ]:
```
t    = 0.0        # initialization of time
Ttot = 3600*6     # total simulation time
ttd  = 300        # Decay time constant
dt   = 100        # Fixed step size

# Boundary condition expression for increasing  the chemical potential
#
def muRamp(t):
    return mu0*exp(-t/ttd)
```

8 Function spaces

```
[ ]: # Define function space, both vectorial and scalar
     #
     U2 = element("Lagrange", domain.basix_cell(), 2, shape=(2,)) # For displacement
     P1 = element("Lagrange", domain.basix_cell(), 1) # For pressure, chemical␣
      ↪potential and  species concentration
     #
     TH = mixed_element([U2, P1, P1, P1])  # Taylor-Hood style mixed element
     ME = functionspace(domain, TH)        # Total space for all DOFs

     # Define actual functions with the required DOFs
     w = Function(ME)
     u, p, mu, c = split(w)  # displacement u, pressure p, chemical potential mu,␣
      ↪and concentration c

     # A copy of functions to store values in the previous step for time-stepping
     w_old = Function(ME)
     u_old,  p_old, mu_old, c_old = split(w_old)

     # Define test functions
     u_test, p_test,  mu_test, c_test = TestFunctions(ME)

     # Define trial functions needed for automatic differentiation
     dw = TrialFunction(ME)
```

9 Initial conditions

- The initial conditions for $\mathbf{u}$ and p are zero everywhere.
- These are imposed automatically, since we have not specified any non-zero initial conditions.
- We do, however, need to impose the uniform initial conditions for $\mu = \mu_0$ and $\hat{c} = \hat{c}_0$ which correspond to $\phi_0 = 0.999$. This is done below.

```
[ ]: # Assign initial  normalized chemical potential  mu0 to the domain
     w.sub(2).interpolate(lambda x: np.full((x.shape[1],),  mu0))
     w_old.sub(2).interpolate(lambda x: np.full((x.shape[1],), mu0))

     # Assign initial  value of normalized concentration  c0 to the domain
     w.sub(3).interpolate(lambda x: np.full((x.shape[1],),  c0))
     w_old.sub(3).interpolate(lambda x: np.full((x.shape[1],), c0))
```

10 Subroutines for kinematics and constitutive equations

[ ]:
```
# Special gradient operators for axisymmetric functions
#
#---------------------------------------------------
# Gradient of vector field u
#---------------------------------------------------
def axi_grad_vector(u):

    grad_u = grad(u)

    axi_grad_33_exp = conditional(eq(x[0], 0), 0.0, u[0]/x[0])

    axi_grad_u = ufl.as_tensor([[grad_u[0,0], grad_u[0,1], 0],
                  [grad_u[1,0], grad_u[1,1], 0],
                  [0, 0, axi_grad_33_exp]])

    return axi_grad_u

#---------------------------------------------------
# Gradient of scalar field y
# (just need an extra zero for dimensions to work out)
#---------------------------------------------------
def axi_grad_scalar(y):

    grad_y = grad(y)

    axi_grad_y = ufl.as_vector([grad_y[0], grad_y[1], 0.])

    return axi_grad_y
#---------------------------------------------------
# Axisymmetric deformation gradient
#---------------------------------------------------
def F_axi_calc(u):

    dim = len(u)                # dimension of problem (2)

    Id = Identity(dim)          # 2D Identity tensor

    F = Id + grad(u)            # 2D Deformation gradient

    F33_exp =  1.0 + u[0]/x[0]  # axisymmetric F33, R/R0

    F33 = conditional(eq(x[0], 0.0), 1.0, F33_exp) # avoid divide by zero at r=0

    F_axi =  ufl.as_tensor([[F[0,0], F[0,1], 0],
                  [F[1,0], F[1,1], 0],
```

```
                  [0, 0, F33]]) # Full axisymmetric F

    return F_axi

#-----------------------------------------------------
# Effective stretch lambdaBar
#-----------------------------------------------------
def lambdaBar_calc(u):
    F = F_axi_calc(u)
    C = F.T*F
    I1 = tr(C)
    lambdaBar = sqrt(I1/3.0)
    return lambdaBar

#-----------------------------------------------------
# Calculate zeta
#-----------------------------------------------------
def zeta_calc(u):
    lambdaBar = lambdaBar_calc(u)
    # Use Pade approximation of Langevin inverse
    z    = lambdaBar/lambdaL
    z    = conditional(gt(z,0.95), 0.95, z) # Keep simulation from blowing up
    beta = z*(3.0 - z**2.0)/(1.0 - z**2.0)
    zeta = (lambdaL/(3*lambdaBar))*beta
    return zeta

#-----------------------------------------------------
# Calculate zeta0
#-----------------------------------------------------
def zeta0_calc():
    # Use Pade approximation of Langevin inverse (A. Cohen, 1991)
    z    = 1/lambdaL
    z    = conditional(gt(z,0.95), 0.95, z) # Keep from blowing up
    beta0 = z*(3.0 - z**2.0)/(1.0 - z**2.0)
    zeta0 = (lambdaL/3)*beta0
    return zeta0

#-----------------------------------------------------
# Subroutine for calculating the elastic jacobian Je
#-----------------------------------------------------
def Je_calc(u,c):
    F = F_axi_calc(u)
    detF = det(F)
    #
    detFs = 1.0 + c          # = Js
    Je    = (detF/detFs)     # = Je
    return   Je
```

```
#-------------------------------------------
# Subroutine for calculating the Piola  stress
#-------------------------------------------
def Piola_calc(u,p):
    F     = F_axi_calc(u)
    zeta  = zeta_calc(u)
    zeta0 = zeta0_calc()
    Piola = (zeta*F - zeta0*inv(F.T) ) - J*p*inv(F.T)/Gshear_0
    return Piola

#-------------------------------------------------------------
# Subroutine for calculating the normalized species flux
#-------------------------------------------------------------
def Flux_calc(u, mu, c):
    F = F_axi_calc(u)
    #
    Cinv = inv(F.T*F)
    #
    Mob = (D*c)/(Omega*RT)*Cinv
    #
    Jmat = - RT* Mob * axi_grad_scalar(mu)
    return Jmat
```

[ ]:
```
##A.FLowers Comments

# Special gradient operators for axisymmetric functions
#-----------------------------------------------------
# Gradient of vector field u
#-----------------------------------------------------
def axi_grad_vector(u):
##Used in axissymmetric FE modeling to compute modified gradient of a vector␣
 ↪field
    grad_u = grad(u)
##u= scalar function; grad(u)= vector gradient. given in Jacobian matrix
    axi_grad_33_exp = conditional(eq(x[0], 0), 0.0, u[0]/x[0])
##Used to compute the hoop strain; Cyndrical coordinates
##Scalar expression represents (3,3) component of axisymmetric deformation␣
 ↪gradient / strain tensor
##Avoids division by zero at the axis point of r=0

    axi_grad_u = ufl.as_tensor([[grad_u[0,0], grad_u[0,1], 0],
##gradient tensor from 2D axisymmetric displacement field
##Gradient of radial displacement (r)
                    [grad_u[1,0], grad_u[1,1], 0],
##Gradient of axial displacement (z)
                    [0, 0, axi_grad_33_exp]])
```

```
##Hoop strain in circumferential direction; this is from the symmetry (theta)
    return axi_grad_u
##Gives 3x3 tensor representing full displacement gradient in axisymmetric␣
 ↪coordinates

#-----------------------------------------------------
# Gradient of scalar field y
# (just need an extra zero for dimensions to work out)
#-----------------------------------------------------
def axi_grad_scalar(y):
##Defining function for scalar FEniCS
    grad_y = grad(y)
##Standard gradient computed from scalar field y; this is 2D vector in (r,z)␣
 ↪plane
    axi_grad_y = ufl.as_vector([grad_y[0], grad_y[1], 0.])
##Pads 2D gradient with zero in theta-direction; 3D vector in cylindircal␣
 ↪coordinates (r,z,theta)
    return axi_grad_y
##Gives 3D gradient vector

#-----------------------------------------------------
# Axisymmetric deformation gradient
#-----------------------------------------------------
def F_axi_calc(u):

    dim = len(u)                # dimension of problem (2)
##u= 2D displacement field
    Id = Identity(dim)          # 2D Identity tensor
##Creates 2x2 identity tensor
    F = Id + grad(u)            # 2D Deformation gradient
##Defines 2D deformation gradient
    F33_exp =  1.0 + u[0]/x[0]  # axisymmetric F33, R/R0
##Computes circumferential stretch. Term reflects hoop (theta) stretch due to␣
 ↪radial displacement
    F33 = conditional(eq(x[0], 0.0), 1.0, F33_exp) # avoid divide by zero at r=0
##Avoids division by zero
    F_axi =  ufl.as_tensor([[F[0,0], F[0,1], 0],
                  [F[1,0], F[1,1], 0],
                  [0, 0, F33]]) # Full axisymmetric F
##Builds 3x3 deformation gradient in cylindrical coordinates
    return F_axi
##Gives tensor for use in strain energy and stress

#-----------------------------------------------------
# Effective stretch lambdaBar
#-----------------------------------------------------
def lambdaBar_calc(u):
```

```
    F = F_axi_calc(u)
##Computes 3x3 deformation gradient tensor F for axisymmetric
    C = F.T*F
##Computers right Cauchy-Green deformation tensor; measuring stretch relative␣
 ↪to reference configuration, used in finite strain elasticity
    I1 = tr(C)
##First invariant of C; represents sum of squared prinipal stretches
    lambdaBar = sqrt(I1/3.0)
##Computes isochoric (Volume-preserving) average stretch
##Invariant under rotation and insensitive to volumetric changes when in␣
 ↪isocheric energy term
    return lambdaBar
##Gives scalar effective stretch value

#-----------------------------------------------------
# Calculate zeta
#-----------------------------------------------------
def zeta_calc(u):
    lambdaBar = lambdaBar_calc(u) # Use Pade approximation of Langevin inverse
##Computes isochoric effective stretch
    z    = lambdaBar/lambdaL
##Limit stretch of polymer chains; closer value is to 1, closer it is to max.␣
 ↪extension, with the material becoming more stiff
    z    = conditional(gt(z,0.95), 0.95, z) # Keep simulation from blowing up
##Numerical safegaurd to prevent blow-up
    beta = z*(3.0 - z**2.0)/(1.0 - z**2.0)
##Pade approx. of inverse Langevin; used to relate average chain stretch to␣
 ↪applied force in non-Gaussian polymer models
    zeta = (lambdaL/(3*lambdaBar))*beta
##Scales material response entering stress calculation in Gent or Arruda-Boyce␣
 ↪models; rescales beta
    return zeta
##Gives scalar, varying deformation and reflects finite extensibility of␣
 ↪polymer chains

#-----------------------------------------------------
# Calculate zeta0
#-----------------------------------------------------
def zeta0_calc(): # Use Pade approximation of Langevin inverse (A. Cohen, 1991)
    z    = 1/lambdaL
##Limit stretch of polymer chain
    z    = conditional(gt(z,0.95), 0.95, z) # Keep from blowing up
##Numerical safegaurd; ensuring numerical stability
    beta0 = z*(3.0 - z**2.0)/(1.0 - z**2.0)
##Pade approx. of inverse Langevin; representing stretch energy per chain
    zeta0 = (lambdaL/3)*beta0
```

```
##Initial modulus scaling factor from chain; finite extensibility correction␣
 ↪factor
    return zeta0
##Gives constant value; used to enforce zero-stress reference

#-----------------------------------------------------
# Subroutine for calculating the elastic jacobian Je
#-----------------------------------------------------
def Je_calc(u,c):
    F = F_axi_calc(u)
##Computes axisymmetric deformation gradient F of displacement field
    detF = det(F)
##Computes total volume ratio; how much element has expanded / compressed␣
 ↪compared to reference volume
    detFs = 1.0 + c          # = Js
##Define swelling volume ratio
##c= swlling-related variable; 1+c= volume expansion due to chemical absorption
    Je    = (detF/detFs)     # = Je
##Computes elastic volume change; mechanical deformation after accounting for␣
 ↪volume change from swelling
    return   Je
##Gives mechanical output of deformation
##Used for elastic energy density functions, stress calculations, and␣
 ↪thermodynamic coupling with chemical potentials

#-----------------------------------------------
# Subroutine for calculating the Piola  stress
#-----------------------------------------------
def Piola_calc(u,p):
    F     = F_axi_calc(u)
##Computes deformation gradient F in axisymmetric coordinates from displacement␣
 ↪field
    zeta  = zeta_calc(u)
##Computes scalar energy quantity (either osmotic pressure of chemical␣
 ↪potential energy)
    zeta0 = zeta0_calc()
##Reference value, in undeformed or initial state
    Piola = (zeta*F - zeta0*inv(F.T) ) - J*p*inv(F.T)/Gshear_0
##Enforce incompressibility (volumetric constraints) common in gel mechanics or␣
 ↪incompressible elasticity
    return Piola
##Gives full, first Piola-Kirchhoff stress tensor P

#-------------------------------------------------------------
# Subroutine for calculating the normalized species flux
#-------------------------------------------------------------
```

```
def Flux_calc(u, mu, c):
    F = F_axi_calc(u)
##Computes deformation gradient tensor F in axisymmetric coordinates; measuring␣
 ↪stretch and shear
    Cinv = inv(F.T*F)
##Computes inverse of right Cauchy-Green deformation tensor
##Geometric nonlinearity due to large deformation; helps transform diffusivity /
 ↪ mobility from reference configuration to the current
    Mob = (D*c)/(Omega*RT)*Cinv
##Defines effective mobility tensor M; modifies diffusion based on deformation
    Jmat = - RT* Mob * axi_grad_scalar(mu)
##Computes flux via Fick's Law (chemical potential, not concentration)
##Species flux in material coordinates driven by chemical potential gradients␣
 ↪modulated by deformation, concentration, and thermal energy
    return Jmat
##Gives reference configuration material flux vector
```

11 Evaluate kinematics and constitutive relations

[ ]:
```
# Kinematics
F = F_axi_calc(u)
J = det(F)  # Total volumetric jacobian
#
lambdaBar = lambdaBar_calc(u)
#
# Elastic volumetric Jacobian
Je     = Je_calc(u,c)
Je_old = Je_calc(u_old,c_old)

#  Normalized Piola stress
Piola = Piola_calc(u, p)

#  Normalized species  flux
Jmat = Flux_calc(u, mu, c)
```

[ ]:
```
##A.Flowers Comments

# Kinematics
F = F_axi_calc(u)
##Computes deformation gradient tensor F from displacement field in␣
 ↪axisymmetric coordinates; captures stretch and shear from displacement
J = det(F)  # Total volumetric jacobian
##Total Jacobian determinant measuring volume change due to deformation; ratio␣
 ↪of current to referene volume
##J couples with pressure in incompressibility and appears in transport models␣
 ↪(such as osmosis) as coupling between defomration and chemical concetration
```

```
lambdaBar = lambdaBar_calc(u)
# Elastic volumetric Jacobian
Je     = Je_calc(u,c)
##Elastic Jacobian at present time; mechanical volume change, excluding swelling
Je_old = Je_calc(u_old,c_old)
##Elastic Jacobian at previous time; shows evolution

#  Normalized Piola stress
Piola = Piola_calc(u, p)
##Computes total stress in material using displacement and pressure field; then␣
 ↪used in momentum balace, determining response under deformation and swelling

#  Normalized species  flux
Jmat = Flux_calc(u, mu, c)
##Computes species flux vector; considers deformation, chemical potential, and␣
 ↪concentration. Pertinent to chemical transport in deforming materials␣
 ↪(swelling gels) where mechanics and diffusion are coupled
##Flux of mobile species (solvent and ions); how fast they are moving through␣
 ↪material, driven by chemical potential gradients and modified by mechanical␣
 ↪deformation
##C evolves through mass conservation (diffusion)
```

12 Weak forms

[ ]:
```
# Residuals:
# Res_0: Balance of forces (test fxn: u)
# Res_1: Pressure variable (test fxn: p)
# Res_2: Balance of mass   (test fxn: mu)
# Res_3: Auxiliary variable (test fxn: c)

# Time step field, constant within body
dk = Constant(domain, PETSc.ScalarType(dt))

# The weak form for the equilibrium equation
Res_0 = inner(Piola, axi_grad_vector(u_test) )*x[0]*dx

# The weak form for the pressure
Res_1 = dot((p*Je/Kbulk + ln(Je)) , p_test)*x[0]*dx

# The weak form for the mass balance of solvent
Res_2 = dot((c - c_old)/dk, mu_test)*x[0]*dx \
        -  Omega*dot(Jmat , axi_grad_scalar(mu_test) )*x[0]*dx

# The weak form for the concentration
fac = 1/(1+c)
```

```
fac1 =  mu - ( ln(1.0-fac)+ fac + chi*fac*fac)
fac2 = - (Omega*Je/RT)*p
fac3 = - (1./2.) * (Omega/(Kbulk*RT)) * ((p*Je)**2.0)
fac4 = fac1 + fac2 + fac3
#
Res_3 = dot(fac4, c_test)*dx

# Total weak form
Res = Res_0 + Res_1 + Res_2 + Res_3

# Automatic differentiation tangent:
a = derivative(Res, w, dw)
```

[ ]:
```
##A.Flowers Comments

# Residuals:
# Res_0: Balance of forces (test fxn: u)
# Res_1: Pressure variable (test fxn: p)
# Res_2: Balance of mass   (test fxn: mu)
# Res_3: Auxiliary variable (test fxn: c)

# Time step field, constant within body
dk = Constant(domain, PETSc.ScalarType(dt))
##Defines constant scalar due to FEniCS (time step size)

# The weak form for the equilibrium equation
Res_0 = inner(Piola, axi_grad_vector(u_test) )*x[0]*dx
##Computes double contraction (Frobenius) between stress tensor and gradient;␣
 ↪internal virtual work density at a material point
##Main driving force of displacement solution under swelling and pressure

# The weak form for the pressure
Res_1 = dot((p*Je/Kbulk + ln(Je)) , p_test)*x[0]*dx
##Adds term to pressure residual enforcing compressibility / volume constraint␣
 ↪via pressure, elastic volume change, and bulk modulus
##p=pressure field (unknown) acting as Lagrange multiplier; apperas when␣
 ↪pressure is solved as a field, and is not given (balancing swelling and␣
 ↪elasticity)

# The weak form for the mass balance of solvent
Res_2 = dot((c - c_old)/dk, mu_test)*x[0]*dx \
##Weak form of transient accumulation of mobile species
        -  Omega*dot(Jmat , axi_grad_scalar(mu_test) )*x[0]*dx
##Weak form of divergence of flux; drives species redistribution due to␣
 ↪chemical gradients and deformation
```

```
##Overall enforces chemical species conservation; change in concentration =␣
 ↪inflow/outflow due to chemical potential gradients accounting for␣
 ↪deformation of medium and axisymmetric geometry

# The weak form for the concentration
fac = 1/(1+c)
##Computes volume fraction of polymer
fac1 =  mu - ( ln(1.0-fac)+ fac + chi*fac*fac)
##Encodes Flory-Huggins chemical potential
fac2 = - (Omega*Je/RT)*p
##Accounts for mechanical pressure contribution due to chemical potential
fac3 = - (1./2.) * (Omega/(Kbulk*RT)) * ((p*Je)**2.0)
##Compressibility correction due to bulk deformation from free energy stored
fac4 = fac1 + fac2 + fac3
##Residual contributions; difference between computed chemical potential and␣
 ↪its theoretical value based on thermodynamics, mechanics, and compressibility

Res_3 = dot(fac4, c_test)*dx
##Residual term in variational form for solving chemical␣
 ↪potential-concentration coupling in swelling gel model
##Thermodynamic consistency condition; ensures chemical potential used in flux␣
 ↪equation is thermodynamically correct, given concentration and mechanical␣
 ↪state
##Nonlinear coupled system, with momentum balance, mass transport, and␣
 ↪thermodynamic closure

# Total weak form
Res = Res_0 + Res_1 + Res_2 + Res_3
##Total residual of FE; combining mechanics, thermodynamics, and mass transport␣
 ↪in a swelling gel model
##Formula enabling coupled multiphysics behavior; characteristics in swelling␣
 ↪gels, ionic polymers, hydrogel actuators

# Automatic differentiation tangent:
a = derivative(Res, w, dw)
##Solves nonlinear variational problem in FEniCS, computing Jacobian matrix
```

13 Set-up output files

[ ]:
```
# Set up projection problem for fixing visualization issues
# of fields in  the axisymmetric simulation
#
def setup_projection(u, V):

    trial = ufl.TrialFunction(V)
    test  = ufl.TestFunction(V)
```

```
    a = ufl.inner(trial, test)*x[0]*dx
    L = ufl.inner(u, test)*x[0]*dx

    projection_problem = dolfinx.fem.petsc.LinearProblem(a, L, [], \
        petsc_options={"ksp_type": "cg", "ksp_rtol": 1e-16, "ksp_atol": 1e-16,␣
 ↪"ksp_max_it": 1000})

    return projection_problem
```

[ ]:
```
# results file name
results_name = "gel_axi_swell"

# Function space for projection of results
U1 = element("DG", domain.basix_cell(), 1, shape=(2,))  # For 2d vector
P0 = element("DG", domain.basix_cell(), 1)              # For  scalar
T1 = element("DG", domain.basix_cell(), 1, shape=(3,3)) # For stress tensor

V1 = fem.functionspace(domain, P0) # Scalar function space
V2 = fem.functionspace(domain, U1) # Vector function space
V3 = fem.functionspace(domain, T1) # Tensor function space

# basic fields to write to output file
u_vis = Function(V2)
u_vis.name = "disp"

p_vis = Function(V1)
p_vis.name = "p"

mu_vis = Function(V1)
mu_vis.name = "mu"

c_vis = Function(V1)
c_vis.name = "c"


# calculated fields to write to output file
phi = 1/(1+c)
phi_vis = Function(V1)
phi_vis.name = "phi"
phi_expr = Expression(phi,V1.element.interpolation_points())

# Project the volumetric Jacobian J for visualization
#
J_projection = setup_projection(J, V1)
J_vis = J_projection.solve()
J_vis.name = "J"
```

```
# Project the effective stretch lambdabar for visualization
#
lambdaBar_projection = setup_projection(lambdaBar, V1)
lambdaBar_vis = lambdaBar_projection.solve()
lambdaBar_vis.name = "lambdaBar"

# Project the Piola stress tensor for visualization
#
Piola_projection = setup_projection(Piola, V3)
Piola_temp = Piola_projection.solve()

T   = Piola_temp*F.T/J
T0   = T - (1/3)*tr(T)*Identity(3)
Mises = sqrt((3/2)*inner(T0, T0))
Mises_projection = setup_projection(Mises, V1)
Mises_vis = Mises_projection.solve()
Mises_vis.name = "Mises"

P11 = Function(V1)
P11.name = "P11"
P11_expr = Expression(Piola_temp[0,0],V1.element.interpolation_points())
P22 = Function(V1)
P22.name = "P22"
P22_expr = Expression(Piola_temp[1,1],V1.element.interpolation_points())
P33 = Function(V1)
P33.name = "P33"
P33_expr = Expression(Piola_temp[2,2],V1.element.interpolation_points())

# set up the output VTX files.
file_results = VTXWriter(
    MPI.COMM_WORLD,
    "results/" + results_name + ".bp",
    [  # put the functions here you wish to write to output
        u_vis, p_vis, mu_vis, c_vis, phi_vis, J_vis, P11, P22, P33,
        lambdaBar_vis,Mises_vis,
    ],
    engine="BP4",
)

def writeResults(t):

       # Re-project some fields. This is necessary here to remove visual␣
 ↪artifacts which arise
       # due to the axisymmetric formulation as r -> 0
       #
       Piola_temp     = Piola_projection.solve()
```

```
        Mises_vis      = Mises_projection.solve()
        J_vis          = J_projection.solve()
        lambdaBar_vis  = lambdaBar_projection.solve()

        # Output field interpolation
        u_vis.interpolate(w.sub(0))
        p_vis.interpolate(w.sub(1))
        mu_vis.interpolate(w.sub(2))
        c_vis.interpolate(w.sub(3))
        phi_vis.interpolate(phi_expr)
        P11.interpolate(P11_expr)
        P22.interpolate(P22_expr)
        P33.interpolate(P33_expr)

        # Write output fields
        file_results.write(t)
```

14 Infrastructure for pulling out time history data (displacement, force, etc.)

[ ]:
```
# This is actually not neede here for this simulation


# # Identify point for reporting displacement and temperature at a given point
# pointForDisp = np.array([R0,H0,0.0])

# bb_tree = dolfinx.geometry.bb_tree(domain,domain.topology.dim)
# cell_candidates = dolfinx.geometry.compute_collisions_points(bb_tree,␣
 ↪pointForDisp)
# colliding_cells = dolfinx.geometry.compute_colliding_cells(domain,␣
 ↪cell_candidates, pointForDisp).array

# # boundaries = [(1, xBot),(2,xTop),(3,yBot),(4,yTop)]
# # Compute the reaction force using the Piola stress field
# RxnForce = fem.form(2*np.pi*P22*x[0]*ds(4))
```

15 Analysis Step

[ ]:
```
# Give the step a descriptive name
step = "Swell"
```

15.1 Boundary conditions

[ ]:
```
# Constant for applied displacement
mu_cons = Constant(domain,PETSc.ScalarType(muRamp(0)))

# Recall the sub-domains names and numbers
# boundaries = [(1, xBot),(2,xTop),(3,yBot),(4,yTop)]

# Find the specific DOFs which will be constrained
xBot_u1_dofs = fem.locate_dofs_topological(ME.sub(0).sub(0), facet_tags.dim,␣
 ↪facet_tags.find(1))
yBot_u2_dofs = fem.locate_dofs_topological(ME.sub(0).sub(1), facet_tags.dim,␣
 ↪facet_tags.find(3))
#
xTop_mu_dofs = fem.locate_dofs_topological(ME.sub(2), facet_tags.dim,␣
 ↪facet_tags.find(2))
yTop_mu_dofs = fem.locate_dofs_topological(ME.sub(2), facet_tags.dim,␣
 ↪facet_tags.find(4))

# Build Dirichlet BCs
bcs_1 = dirichletbc(0.0, xBot_u1_dofs, ME.sub(0).sub(0)) # u1 fix - xBot
bcs_2 = dirichletbc(0.0, yBot_u2_dofs, ME.sub(0).sub(1)) # u2 fix - yBot
#
bcs_3 = dirichletbc(mu_cons, xTop_mu_dofs, ME.sub(2))    # mu_cons - xTop
bcs_4 = dirichletbc(mu_cons, yTop_mu_dofs, ME.sub(2))    # mu_cons - yTop

bcs = [bcs_1, bcs_2, bcs_3, bcs_4]
```

[ ]:
```
##A.Flowers Comments

# Constant for applied displacement
mu_cons = Constant(domain,PETSc.ScalarType(muRamp(0)))
##Defines chemically driven control parameters; simulates ramping up the␣
 ↪chemical potential at the boundary during swelling (constant field)

# Recall the sub-domains names and numbers
# boundaries = [(1, xBot),(2,xTop),(3,yBot),(4,yTop)]

# Find the specific DOFs which will be constrained
xBot_u1_dofs = fem.locate_dofs_topological(ME.sub(0).sub(0), facet_tags.dim,␣
 ↪facet_tags.find(1))
yBot_u2_dofs = fem.locate_dofs_topological(ME.sub(0).sub(1), facet_tags.dim,␣
 ↪facet_tags.find(3))
##Dirichlet boundary conditions; radial displacement and axial displacement

xTop_mu_dofs = fem.locate_dofs_topological(ME.sub(2), facet_tags.dim,␣
 ↪facet_tags.find(2))
```

```
yTop_mu_dofs = fem.locate_dofs_topological(ME.sub(2), facet_tags.dim,␣
 ↪facet_tags.find(4))
##Retrieves DOFs in chemical potential field

# Build Dirichlet BCs
bcs_1 = dirichletbc(0.0, xBot_u1_dofs, ME.sub(0).sub(0)) # u1 fix - xBot
bcs_2 = dirichletbc(0.0, yBot_u2_dofs, ME.sub(0).sub(1)) # u2 fix - yBot
##Define Dirichlet boundary conditions for vector displacement field on 2D␣
 ↪axisymmetric mesh
##Bottom edge fixed (x) radially
##Bottom edge fixed (y) axially

bcs_3 = dirichletbc(mu_cons, xTop_mu_dofs, ME.sub(2))    # mu_cons - xTop
bcs_4 = dirichletbc(mu_cons, yTop_mu_dofs, ME.sub(2))    # mu_cons - yTop
##Given value of chemical potential , modeling contact with external␣
 ↪environment (i.e. fluid in swelling gel)
##Top right edge set chemical potential (externally)
##Top center edge set for axisymmetric top

bcs = [bcs_1, bcs_2, bcs_3, bcs_4]
##Implements boundary conditions to solver
##Prevent horizontal slip (radial), fix vertical movement (axial), set␣
 ↪envrionment potential (chemical potential), ensure top boundary exposure␣
 ↪(chemical potential)
```

15.2 Define the nonlinear variational problem

[ ]:
```
# Set up nonlinear problem
problem = NonlinearProblem(Res, w, bcs, a)

# the global newton solver and params
solver = NewtonSolver(MPI.COMM_WORLD, problem)
solver.convergence_criterion = "incremental"
solver.rtol = 1e-8
solver.atol = 1e-8
solver.max_it = 50
solver.report = True

#  The Krylov solver parameters.
ksp = solver.krylov_solver
opts = PETSc.Options()
option_prefix = ksp.getOptionsPrefix()
opts[f"{option_prefix}ksp_type"] = "preonly"
opts[f"{option_prefix}pc_type"] = "lu" # do not use 'gamg' pre-conditioner
opts[f"{option_prefix}pc_factor_mat_solver_type"] = "mumps"
opts[f"{option_prefix}ksp_max_it"] = 30
ksp.setFromOptions()
```

16 Initialize arrays for storing output history

[ ]:
```
# # Arrays for storing output history
# totSteps = 100000
# timeHist0 = np.zeros(shape=[totSteps])
# timeHist1 = np.zeros(shape=[totSteps])
# timeHist2 = np.zeros(shape=[totSteps])
# timeHist3 = np.zeros(shape=[totSteps])
# #
# timeHist3[0] = mu0 # Initialize the chemical potential

# Initialize a counter for reporting data
ii=0

# Write initial state to file
writeResults(t=0.0)
```

16.1 Start calculation loop

[ ]:
```
# Print  message for simulation start
print("-------------------------------------")
print("Simulation Start")
print("-------------------------------------")
# Store start time
startTime = datetime.now()

# Time-stepping solution procedure loop
while (round(t + dt, 9) <= Ttot):

    # increment time
    t += dt
    # increment counter
    ii += 1

    # update time variables in time-dependent BCs
    mu_cons.value = float(muRamp(t))

    # Solve the problem
    try:
        (iter, converged) = solver.solve(w)
    except: # Break the loop if solver fails
        print("Ended Early")
        break

    # Collect results from MPI ghost processes
    w.x.scatter_forward()
```

```
    # Write output to file
    writeResults(t)

    # Update DOFs for next step
    w_old.x.array[:] = w.x.array

    # Print progress of calculation
    if ii%1 == 0:
        now = datetime.now()
        current_time = now.strftime("%H:%M:%S")
        print("Step: {} | Increment: {}, Iterations: {}".\
              format(step, ii, iter))
        print("      Simulation Time: {} s  of  {} s".\
              format(round(t,4), Ttot))
        print()

# close the output file.
file_results.close()

# End analysis
print("-----------------------------------------")
print("End computation")
# Report elapsed real time for the analysis
endTime = datetime.now()
elapseTime = endTime - startTime
print("-----------------------------------------")
print("Elapsed real time:  {}".format(elapseTime))
print("-----------------------------------------")
```

```
-----------------------------------
Simulation Start
-----------------------------------
Step: Swell | Increment: 1, Iterations: 6
      Simulation Time: 100.0 s  of  21600 s

Step: Swell | Increment: 2, Iterations: 6
      Simulation Time: 200.0 s  of  21600 s

Step: Swell | Increment: 3, Iterations: 6
      Simulation Time: 300.0 s  of  21600 s

Step: Swell | Increment: 4, Iterations: 6
      Simulation Time: 400.0 s  of  21600 s

Step: Swell | Increment: 5, Iterations: 5
      Simulation Time: 500.0 s  of  21600 s

Step: Swell | Increment: 6, Iterations: 5
```

```
      Simulation Time: 600.0 s  of  21600 s

Step: Swell | Increment: 7, Iterations: 5
      Simulation Time: 700.0 s  of  21600 s

Step: Swell | Increment: 8, Iterations: 5
      Simulation Time: 800.0 s  of  21600 s

Step: Swell | Increment: 9, Iterations: 5
      Simulation Time: 900.0 s  of  21600 s

Step: Swell | Increment: 10, Iterations: 5
      Simulation Time: 1000.0 s  of  21600 s

Step: Swell | Increment: 11, Iterations: 5
      Simulation Time: 1100.0 s  of  21600 s

Step: Swell | Increment: 12, Iterations: 5
      Simulation Time: 1200.0 s  of  21600 s

Step: Swell | Increment: 13, Iterations: 5
      Simulation Time: 1300.0 s  of  21600 s

Step: Swell | Increment: 14, Iterations: 5
      Simulation Time: 1400.0 s  of  21600 s

Step: Swell | Increment: 15, Iterations: 5
      Simulation Time: 1500.0 s  of  21600 s

Step: Swell | Increment: 16, Iterations: 5
      Simulation Time: 1600.0 s  of  21600 s

Step: Swell | Increment: 17, Iterations: 5
      Simulation Time: 1700.0 s  of  21600 s

Step: Swell | Increment: 18, Iterations: 5
      Simulation Time: 1800.0 s  of  21600 s

Step: Swell | Increment: 19, Iterations: 4
      Simulation Time: 1900.0 s  of  21600 s

Step: Swell | Increment: 20, Iterations: 4
      Simulation Time: 2000.0 s  of  21600 s

Step: Swell | Increment: 21, Iterations: 4
      Simulation Time: 2100.0 s  of  21600 s

Step: Swell | Increment: 22, Iterations: 4
```

```
      Simulation Time: 2200.0 s  of  21600 s

Step: Swell | Increment: 23, Iterations: 4
      Simulation Time: 2300.0 s  of  21600 s

Step: Swell | Increment: 24, Iterations: 4
      Simulation Time: 2400.0 s  of  21600 s

Step: Swell | Increment: 25, Iterations: 4
      Simulation Time: 2500.0 s  of  21600 s

Step: Swell | Increment: 26, Iterations: 4
      Simulation Time: 2600.0 s  of  21600 s

Step: Swell | Increment: 27, Iterations: 4
      Simulation Time: 2700.0 s  of  21600 s

Step: Swell | Increment: 28, Iterations: 4
      Simulation Time: 2800.0 s  of  21600 s

Step: Swell | Increment: 29, Iterations: 4
      Simulation Time: 2900.0 s  of  21600 s

Step: Swell | Increment: 30, Iterations: 4
      Simulation Time: 3000.0 s  of  21600 s

Step: Swell | Increment: 31, Iterations: 4
      Simulation Time: 3100.0 s  of  21600 s

Step: Swell | Increment: 32, Iterations: 4
      Simulation Time: 3200.0 s  of  21600 s

Step: Swell | Increment: 33, Iterations: 4
      Simulation Time: 3300.0 s  of  21600 s

Step: Swell | Increment: 34, Iterations: 4
      Simulation Time: 3400.0 s  of  21600 s

Step: Swell | Increment: 35, Iterations: 4
      Simulation Time: 3500.0 s  of  21600 s

Step: Swell | Increment: 36, Iterations: 4
      Simulation Time: 3600.0 s  of  21600 s

Step: Swell | Increment: 37, Iterations: 4
      Simulation Time: 3700.0 s  of  21600 s

Step: Swell | Increment: 38, Iterations: 4
```

```
      Simulation Time: 3800.0 s  of  21600 s

Step: Swell | Increment: 39, Iterations: 4
      Simulation Time: 3900.0 s  of  21600 s

Step: Swell | Increment: 40, Iterations: 4
      Simulation Time: 4000.0 s  of  21600 s

Step: Swell | Increment: 41, Iterations: 4
      Simulation Time: 4100.0 s  of  21600 s

Step: Swell | Increment: 42, Iterations: 4
      Simulation Time: 4200.0 s  of  21600 s

Step: Swell | Increment: 43, Iterations: 4
      Simulation Time: 4300.0 s  of  21600 s

Step: Swell | Increment: 44, Iterations: 4
      Simulation Time: 4400.0 s  of  21600 s

Step: Swell | Increment: 45, Iterations: 4
      Simulation Time: 4500.0 s  of  21600 s

Step: Swell | Increment: 46, Iterations: 4
      Simulation Time: 4600.0 s  of  21600 s

Step: Swell | Increment: 47, Iterations: 4
      Simulation Time: 4700.0 s  of  21600 s

Step: Swell | Increment: 48, Iterations: 4
      Simulation Time: 4800.0 s  of  21600 s

Step: Swell | Increment: 49, Iterations: 4
      Simulation Time: 4900.0 s  of  21600 s

Step: Swell | Increment: 50, Iterations: 4
      Simulation Time: 5000.0 s  of  21600 s

Step: Swell | Increment: 51, Iterations: 4
      Simulation Time: 5100.0 s  of  21600 s

Step: Swell | Increment: 52, Iterations: 4
      Simulation Time: 5200.0 s  of  21600 s

Step: Swell | Increment: 53, Iterations: 4
      Simulation Time: 5300.0 s  of  21600 s

Step: Swell | Increment: 54, Iterations: 4
```

```
      Simulation Time: 5400.0 s  of  21600 s

Step: Swell | Increment: 55, Iterations: 4
      Simulation Time: 5500.0 s  of  21600 s

Step: Swell | Increment: 56, Iterations: 4
      Simulation Time: 5600.0 s  of  21600 s

Step: Swell | Increment: 57, Iterations: 4
      Simulation Time: 5700.0 s  of  21600 s

Step: Swell | Increment: 58, Iterations: 4
      Simulation Time: 5800.0 s  of  21600 s

Step: Swell | Increment: 59, Iterations: 4
      Simulation Time: 5900.0 s  of  21600 s

Step: Swell | Increment: 60, Iterations: 4
      Simulation Time: 6000.0 s  of  21600 s

Step: Swell | Increment: 61, Iterations: 4
      Simulation Time: 6100.0 s  of  21600 s

Step: Swell | Increment: 62, Iterations: 4
      Simulation Time: 6200.0 s  of  21600 s

Step: Swell | Increment: 63, Iterations: 4
      Simulation Time: 6300.0 s  of  21600 s

Step: Swell | Increment: 64, Iterations: 4
      Simulation Time: 6400.0 s  of  21600 s

Step: Swell | Increment: 65, Iterations: 4
      Simulation Time: 6500.0 s  of  21600 s

Step: Swell | Increment: 66, Iterations: 4
      Simulation Time: 6600.0 s  of  21600 s

Step: Swell | Increment: 67, Iterations: 4
      Simulation Time: 6700.0 s  of  21600 s

Step: Swell | Increment: 68, Iterations: 4
      Simulation Time: 6800.0 s  of  21600 s

Step: Swell | Increment: 69, Iterations: 4
      Simulation Time: 6900.0 s  of  21600 s

Step: Swell | Increment: 70, Iterations: 4
```

```
      Simulation Time: 7000.0 s  of  21600 s

Step: Swell | Increment: 71, Iterations: 4
      Simulation Time: 7100.0 s  of  21600 s

Step: Swell | Increment: 72, Iterations: 4
      Simulation Time: 7200.0 s  of  21600 s

Step: Swell | Increment: 73, Iterations: 4
      Simulation Time: 7300.0 s  of  21600 s

Step: Swell | Increment: 74, Iterations: 4
      Simulation Time: 7400.0 s  of  21600 s

Step: Swell | Increment: 75, Iterations: 4
      Simulation Time: 7500.0 s  of  21600 s

Step: Swell | Increment: 76, Iterations: 4
      Simulation Time: 7600.0 s  of  21600 s

Step: Swell | Increment: 77, Iterations: 4
      Simulation Time: 7700.0 s  of  21600 s

Step: Swell | Increment: 78, Iterations: 4
      Simulation Time: 7800.0 s  of  21600 s

Step: Swell | Increment: 79, Iterations: 4
      Simulation Time: 7900.0 s  of  21600 s

Step: Swell | Increment: 80, Iterations: 4
      Simulation Time: 8000.0 s  of  21600 s

Step: Swell | Increment: 81, Iterations: 4
      Simulation Time: 8100.0 s  of  21600 s

Step: Swell | Increment: 82, Iterations: 4
      Simulation Time: 8200.0 s  of  21600 s

Step: Swell | Increment: 83, Iterations: 4
      Simulation Time: 8300.0 s  of  21600 s

Step: Swell | Increment: 84, Iterations: 4
      Simulation Time: 8400.0 s  of  21600 s

Step: Swell | Increment: 85, Iterations: 4
      Simulation Time: 8500.0 s  of  21600 s

Step: Swell | Increment: 86, Iterations: 4
```

```
      Simulation Time: 8600.0 s  of  21600 s

Step: Swell | Increment: 87, Iterations: 4
      Simulation Time: 8700.0 s  of  21600 s

Step: Swell | Increment: 88, Iterations: 4
      Simulation Time: 8800.0 s  of  21600 s

Step: Swell | Increment: 89, Iterations: 4
      Simulation Time: 8900.0 s  of  21600 s

Step: Swell | Increment: 90, Iterations: 4
      Simulation Time: 9000.0 s  of  21600 s

Step: Swell | Increment: 91, Iterations: 4
      Simulation Time: 9100.0 s  of  21600 s

Step: Swell | Increment: 92, Iterations: 4
      Simulation Time: 9200.0 s  of  21600 s

Step: Swell | Increment: 93, Iterations: 4
      Simulation Time: 9300.0 s  of  21600 s

Step: Swell | Increment: 94, Iterations: 4
      Simulation Time: 9400.0 s  of  21600 s

Step: Swell | Increment: 95, Iterations: 4
      Simulation Time: 9500.0 s  of  21600 s

Step: Swell | Increment: 96, Iterations: 3
      Simulation Time: 9600.0 s  of  21600 s

Step: Swell | Increment: 97, Iterations: 3
      Simulation Time: 9700.0 s  of  21600 s

Step: Swell | Increment: 98, Iterations: 3
      Simulation Time: 9800.0 s  of  21600 s

Step: Swell | Increment: 99, Iterations: 3
      Simulation Time: 9900.0 s  of  21600 s

Step: Swell | Increment: 100, Iterations: 3
      Simulation Time: 10000.0 s  of  21600 s

Step: Swell | Increment: 101, Iterations: 3
      Simulation Time: 10100.0 s  of  21600 s

Step: Swell | Increment: 102, Iterations: 3
```

```
      Simulation Time: 10200.0 s  of  21600 s

Step: Swell | Increment: 103, Iterations: 3
      Simulation Time: 10300.0 s  of  21600 s

Step: Swell | Increment: 104, Iterations: 3
      Simulation Time: 10400.0 s  of  21600 s

Step: Swell | Increment: 105, Iterations: 3
      Simulation Time: 10500.0 s  of  21600 s

Step: Swell | Increment: 106, Iterations: 3
      Simulation Time: 10600.0 s  of  21600 s

Step: Swell | Increment: 107, Iterations: 3
      Simulation Time: 10700.0 s  of  21600 s

Step: Swell | Increment: 108, Iterations: 3
      Simulation Time: 10800.0 s  of  21600 s

Step: Swell | Increment: 109, Iterations: 3
      Simulation Time: 10900.0 s  of  21600 s

Step: Swell | Increment: 110, Iterations: 3
      Simulation Time: 11000.0 s  of  21600 s

Step: Swell | Increment: 111, Iterations: 3
      Simulation Time: 11100.0 s  of  21600 s

Step: Swell | Increment: 112, Iterations: 3
      Simulation Time: 11200.0 s  of  21600 s

Step: Swell | Increment: 113, Iterations: 3
      Simulation Time: 11300.0 s  of  21600 s

Step: Swell | Increment: 114, Iterations: 3
      Simulation Time: 11400.0 s  of  21600 s

Step: Swell | Increment: 115, Iterations: 3
      Simulation Time: 11500.0 s  of  21600 s

Step: Swell | Increment: 116, Iterations: 3
      Simulation Time: 11600.0 s  of  21600 s

Step: Swell | Increment: 117, Iterations: 3
      Simulation Time: 11700.0 s  of  21600 s

Step: Swell | Increment: 118, Iterations: 3
```

```
      Simulation Time: 11800.0 s  of  21600 s

Step: Swell | Increment: 119, Iterations: 3
      Simulation Time: 11900.0 s  of  21600 s

Step: Swell | Increment: 120, Iterations: 3
      Simulation Time: 12000.0 s  of  21600 s

Step: Swell | Increment: 121, Iterations: 3
      Simulation Time: 12100.0 s  of  21600 s

Step: Swell | Increment: 122, Iterations: 3
      Simulation Time: 12200.0 s  of  21600 s

Step: Swell | Increment: 123, Iterations: 3
      Simulation Time: 12300.0 s  of  21600 s

Step: Swell | Increment: 124, Iterations: 3
      Simulation Time: 12400.0 s  of  21600 s

Step: Swell | Increment: 125, Iterations: 3
      Simulation Time: 12500.0 s  of  21600 s

Step: Swell | Increment: 126, Iterations: 3
      Simulation Time: 12600.0 s  of  21600 s

Step: Swell | Increment: 127, Iterations: 3
      Simulation Time: 12700.0 s  of  21600 s

Step: Swell | Increment: 128, Iterations: 3
      Simulation Time: 12800.0 s  of  21600 s

Step: Swell | Increment: 129, Iterations: 3
      Simulation Time: 12900.0 s  of  21600 s

Step: Swell | Increment: 130, Iterations: 3
      Simulation Time: 13000.0 s  of  21600 s

Step: Swell | Increment: 131, Iterations: 3
      Simulation Time: 13100.0 s  of  21600 s

Step: Swell | Increment: 132, Iterations: 3
      Simulation Time: 13200.0 s  of  21600 s

Step: Swell | Increment: 133, Iterations: 3
      Simulation Time: 13300.0 s  of  21600 s

Step: Swell | Increment: 134, Iterations: 3
```

```
      Simulation Time: 13400.0 s  of  21600 s

Step: Swell | Increment: 135, Iterations: 3
      Simulation Time: 13500.0 s  of  21600 s

Step: Swell | Increment: 136, Iterations: 3
      Simulation Time: 13600.0 s  of  21600 s

Step: Swell | Increment: 137, Iterations: 3
      Simulation Time: 13700.0 s  of  21600 s

Step: Swell | Increment: 138, Iterations: 3
      Simulation Time: 13800.0 s  of  21600 s

Step: Swell | Increment: 139, Iterations: 3
      Simulation Time: 13900.0 s  of  21600 s

Step: Swell | Increment: 140, Iterations: 3
      Simulation Time: 14000.0 s  of  21600 s

Step: Swell | Increment: 141, Iterations: 3
      Simulation Time: 14100.0 s  of  21600 s

Step: Swell | Increment: 142, Iterations: 3
      Simulation Time: 14200.0 s  of  21600 s

Step: Swell | Increment: 143, Iterations: 3
      Simulation Time: 14300.0 s  of  21600 s

Step: Swell | Increment: 144, Iterations: 3
      Simulation Time: 14400.0 s  of  21600 s

Step: Swell | Increment: 145, Iterations: 3
      Simulation Time: 14500.0 s  of  21600 s

Step: Swell | Increment: 146, Iterations: 3
      Simulation Time: 14600.0 s  of  21600 s

Step: Swell | Increment: 147, Iterations: 3
      Simulation Time: 14700.0 s  of  21600 s

Step: Swell | Increment: 148, Iterations: 3
      Simulation Time: 14800.0 s  of  21600 s

Step: Swell | Increment: 149, Iterations: 3
      Simulation Time: 14900.0 s  of  21600 s

Step: Swell | Increment: 150, Iterations: 3
```

```
      Simulation Time: 15000.0 s  of  21600 s

Step: Swell | Increment: 151, Iterations: 3
      Simulation Time: 15100.0 s  of  21600 s

Step: Swell | Increment: 152, Iterations: 3
      Simulation Time: 15200.0 s  of  21600 s

Step: Swell | Increment: 153, Iterations: 3
      Simulation Time: 15300.0 s  of  21600 s

Step: Swell | Increment: 154, Iterations: 3
      Simulation Time: 15400.0 s  of  21600 s

Step: Swell | Increment: 155, Iterations: 3
      Simulation Time: 15500.0 s  of  21600 s

Step: Swell | Increment: 156, Iterations: 3
      Simulation Time: 15600.0 s  of  21600 s

Step: Swell | Increment: 157, Iterations: 3
      Simulation Time: 15700.0 s  of  21600 s

Step: Swell | Increment: 158, Iterations: 3
      Simulation Time: 15800.0 s  of  21600 s

Step: Swell | Increment: 159, Iterations: 3
      Simulation Time: 15900.0 s  of  21600 s

Step: Swell | Increment: 160, Iterations: 3
      Simulation Time: 16000.0 s  of  21600 s

Step: Swell | Increment: 161, Iterations: 3
      Simulation Time: 16100.0 s  of  21600 s

Step: Swell | Increment: 162, Iterations: 3
      Simulation Time: 16200.0 s  of  21600 s

Step: Swell | Increment: 163, Iterations: 3
      Simulation Time: 16300.0 s  of  21600 s

Step: Swell | Increment: 164, Iterations: 3
      Simulation Time: 16400.0 s  of  21600 s

Step: Swell | Increment: 165, Iterations: 3
      Simulation Time: 16500.0 s  of  21600 s

Step: Swell | Increment: 166, Iterations: 3
```

```
      Simulation Time: 16600.0 s  of  21600 s

Step: Swell | Increment: 167, Iterations: 3
      Simulation Time: 16700.0 s  of  21600 s

Step: Swell | Increment: 168, Iterations: 3
      Simulation Time: 16800.0 s  of  21600 s

Step: Swell | Increment: 169, Iterations: 3
      Simulation Time: 16900.0 s  of  21600 s

Step: Swell | Increment: 170, Iterations: 3
      Simulation Time: 17000.0 s  of  21600 s

Step: Swell | Increment: 171, Iterations: 3
      Simulation Time: 17100.0 s  of  21600 s

Step: Swell | Increment: 172, Iterations: 3
      Simulation Time: 17200.0 s  of  21600 s

Step: Swell | Increment: 173, Iterations: 3
      Simulation Time: 17300.0 s  of  21600 s

Step: Swell | Increment: 174, Iterations: 3
      Simulation Time: 17400.0 s  of  21600 s

Step: Swell | Increment: 175, Iterations: 3
      Simulation Time: 17500.0 s  of  21600 s

Step: Swell | Increment: 176, Iterations: 3
      Simulation Time: 17600.0 s  of  21600 s

Step: Swell | Increment: 177, Iterations: 3
      Simulation Time: 17700.0 s  of  21600 s

Step: Swell | Increment: 178, Iterations: 3
      Simulation Time: 17800.0 s  of  21600 s

Step: Swell | Increment: 179, Iterations: 3
      Simulation Time: 17900.0 s  of  21600 s

Step: Swell | Increment: 180, Iterations: 3
      Simulation Time: 18000.0 s  of  21600 s

Step: Swell | Increment: 181, Iterations: 3
      Simulation Time: 18100.0 s  of  21600 s

Step: Swell | Increment: 182, Iterations: 3
```

```
      Simulation Time: 18200.0 s  of  21600 s

Step: Swell | Increment: 183, Iterations: 3
      Simulation Time: 18300.0 s  of  21600 s

Step: Swell | Increment: 184, Iterations: 3
      Simulation Time: 18400.0 s  of  21600 s

Step: Swell | Increment: 185, Iterations: 3
      Simulation Time: 18500.0 s  of  21600 s

Step: Swell | Increment: 186, Iterations: 3
      Simulation Time: 18600.0 s  of  21600 s

Step: Swell | Increment: 187, Iterations: 3
      Simulation Time: 18700.0 s  of  21600 s

Step: Swell | Increment: 188, Iterations: 3
      Simulation Time: 18800.0 s  of  21600 s

Step: Swell | Increment: 189, Iterations: 3
      Simulation Time: 18900.0 s  of  21600 s

Step: Swell | Increment: 190, Iterations: 3
      Simulation Time: 19000.0 s  of  21600 s

Step: Swell | Increment: 191, Iterations: 3
      Simulation Time: 19100.0 s  of  21600 s

Step: Swell | Increment: 192, Iterations: 3
      Simulation Time: 19200.0 s  of  21600 s

Step: Swell | Increment: 193, Iterations: 3
      Simulation Time: 19300.0 s  of  21600 s

Step: Swell | Increment: 194, Iterations: 3
      Simulation Time: 19400.0 s  of  21600 s

Step: Swell | Increment: 195, Iterations: 3
      Simulation Time: 19500.0 s  of  21600 s

Step: Swell | Increment: 196, Iterations: 3
      Simulation Time: 19600.0 s  of  21600 s

Step: Swell | Increment: 197, Iterations: 3
      Simulation Time: 19700.0 s  of  21600 s

Step: Swell | Increment: 198, Iterations: 3
```

```
      Simulation Time: 19800.0 s  of  21600 s

Step: Swell | Increment: 199, Iterations: 3
      Simulation Time: 19900.0 s  of  21600 s

Step: Swell | Increment: 200, Iterations: 3
      Simulation Time: 20000.0 s  of  21600 s

Step: Swell | Increment: 201, Iterations: 3
      Simulation Time: 20100.0 s  of  21600 s

Step: Swell | Increment: 202, Iterations: 3
      Simulation Time: 20200.0 s  of  21600 s

Step: Swell | Increment: 203, Iterations: 3
      Simulation Time: 20300.0 s  of  21600 s

Step: Swell | Increment: 204, Iterations: 3
      Simulation Time: 20400.0 s  of  21600 s

Step: Swell | Increment: 205, Iterations: 3
      Simulation Time: 20500.0 s  of  21600 s

Step: Swell | Increment: 206, Iterations: 3
      Simulation Time: 20600.0 s  of  21600 s

Step: Swell | Increment: 207, Iterations: 3
      Simulation Time: 20700.0 s  of  21600 s

Step: Swell | Increment: 208, Iterations: 3
      Simulation Time: 20800.0 s  of  21600 s

Step: Swell | Increment: 209, Iterations: 3
      Simulation Time: 20900.0 s  of  21600 s

Step: Swell | Increment: 210, Iterations: 3
      Simulation Time: 21000.0 s  of  21600 s

Step: Swell | Increment: 211, Iterations: 3
      Simulation Time: 21100.0 s  of  21600 s

Step: Swell | Increment: 212, Iterations: 3
      Simulation Time: 21200.0 s  of  21600 s

Step: Swell | Increment: 213, Iterations: 3
      Simulation Time: 21300.0 s  of  21600 s

Step: Swell | Increment: 214, Iterations: 3
```

```
      Simulation Time: 21400.0 s  of  21600 s

Step: Swell | Increment: 215, Iterations: 3
      Simulation Time: 21500.0 s  of  21600 s

Step: Swell | Increment: 216, Iterations: 3
      Simulation Time: 21600.0 s  of  21600 s

----------------------------------------
End computation
----------------------------------------
Elapsed real time:  0:00:03.677260
----------------------------------------
```