3D03_fixed_end_torsion_v0p8_A.Flowers_Comments

June 9, 2025

1 Torsion of a 3D cylinder

1.0.1 Units

- Length: mm
- Mass: kg
- Time: s
- Force: milliNewtons
- Stress: kPa

1.0.2 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/

2 Import modules

[1]:
```
# 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)

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

3 Define geometry

[2]:
```
L = 25.4  # Length mm
R = 12.7  # Radius mm

with XDMFFile(MPI.COMM_WORLD,"meshes/cylinder.xdmf",'r') as infile:
    domain = infile.read_mesh(name="Grid",xpath="/Xdmf/Domain")
    cell_tags = infile.read_meshtags(domain,name="Grid")
domain.topology.create_connectivity(domain.topology.dim, domain.topology.dim-1)
```

```
with XDMFFile(MPI.COMM_WORLD, "meshes/facet_cylinder.xdmf", "r") as xdmf:
    facet_tags = xdmf.read_meshtags(domain, name="Grid")

x = ufl.SpatialCoordinate(domain)
```

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

L = 25.4  # Length mm
R = 12.7  # Radius mm
##Geometry parameter of cylinder defined

with XDMFFile(MPI.COMM_WORLD,"meshes/cylinder.xdmf",'r') as infile:
    domain = infile.read_mesh(name="Grid",xpath="/Xdmf/Domain")
    cell_tags = infile.read_meshtags(domain,name="Grid")
##Mesh created of geometry. MPI used as default communicator; includes all␣
↪processes used in parallel computation of command
##Reads mesh geometry and topology; Reads cell markers / subdomains

domain.topology.create_connectivity(domain.topology.dim, domain.topology.dim-1)
##Connectivity created between mesh cells and facets

with XDMFFile(MPI.COMM_WORLD, "meshes/facet_cylinder.xdmf", "r") as xdmf:
    facet_tags = xdmf.read_meshtags(domain, name="Grid")
##Reads mesh facets, mapping to integer IDs for boundary conditions

x = ufl.SpatialCoordinate(domain)
##x,y,z spatial coordinates used from boundary conditions
```

Print out the unique facet index numbers

[3]:
```
top_imap = domain.topology.index_map(2)      # index map of 2D entities in␣
↪domain (facets)
values = np.zeros(top_imap.size_global)      # an array of zeros of the same␣
↪size as number of 2D entities
values[facet_tags.indices]=facet_tags.values # populating the array with facet␣
↪tag index numbers
print(np.unique(facet_tags.values))          # printing the unique indices

# Surface labels from gmsh:
# Physical Surface("xBot", 101)
# Physical Surface("xTop", 102)
# The "side" is automatically assigned index 7.
```

```
[  7 101 102]
```

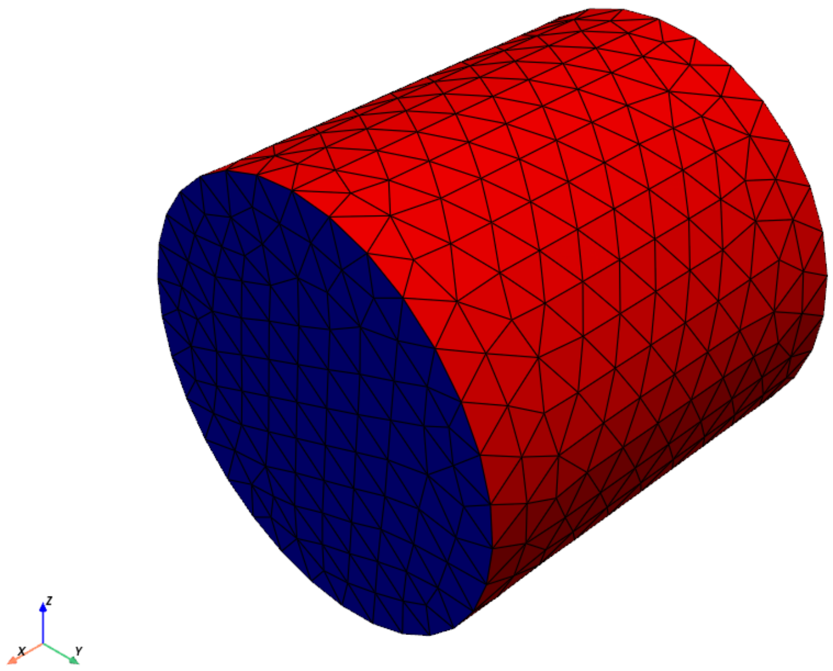
[ ]:
```
##A.Flowers Comments
```

```
top_imap = domain.topology.index_map(2)      # index map of 2D entities in␣
 ↪domain (facets)
##Refers to topological dimension of facets; 0=vertices, 1=edges, 2=facets␣
 ↪(triangle or quadrilateral), 3=cells (tetrahedra or hexahedra)
##Helps relate indexing of facets for parallel computing; how many facets exist␣
 ↪and how they are indexed

values = np.zeros(top_imap.size_global)      # an array of zeros of the same␣
 ↪size as number of 2D entities
##How many facets (2D entities); Used to assign tag values for specific␣
 ↪boundary conditions to each facet

values[facet_tags.indices]=facet_tags.values # populating the array with facet␣
 ↪tag index numbers
##Populates array of facets with the indicies and values (boundary conditions)

print(np.unique(facet_tags.values))          # printing the unique indices
##Displays the unique facet tag values (representing boundary coniditions given)
```

Visualize reference configuration and boundary facets

[4]:
```
import pyvista
pyvista.set_jupyter_backend('html')
from dolfinx.plot import vtk_mesh
pyvista.start_xvfb()

plotter = pyvista.Plotter()

top = pyvista.UnstructuredGrid(*vtk_mesh(domain, domain.topology.
 ↪dim-1,facet_tags.indices[facet_tags.values==102]) )
sides = pyvista.UnstructuredGrid(*vtk_mesh(domain, domain.topology.
 ↪dim-1,facet_tags.indices[facet_tags.values==7]) )
bottom = pyvista.UnstructuredGrid(*vtk_mesh(domain, domain.topology.
 ↪dim-1,facet_tags.indices[facet_tags.values==101]) )

actor = plotter.add_mesh(top, show_edges=True,color="blue") # top face is blue
actor2 = plotter.add_mesh(sides, show_edges=True,color="red") # sides are red
actor3 = plotter.add_mesh(bottom, show_edges=True,color="green") # bottom face␣
 ↪is green

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

plotter.screenshot("mesh.png")

from IPython.display import Image
Image(filename='mesh.png')
```

[4]:



[ ]:

```
##A.Flowers Comments

import pyvista
pyvista.set_jupyter_backend('html')
from dolfinx.plot import vtk_mesh
pyvista.start_xvfb()
##Jupyter notebook display of FE meshes (non-GUI format)

plotter = pyvista.Plotter()
##Creates 3D renderings

top = pyvista.UnstructuredGrid(*vtk_mesh(domain, domain.topology.
 ↪dim-1,facet_tags.indices[facet_tags.values==102]) )
sides = pyvista.UnstructuredGrid(*vtk_mesh(domain, domain.topology.
 ↪dim-1,facet_tags.indices[facet_tags.values==7]) )
bottom = pyvista.UnstructuredGrid(*vtk_mesh(domain, domain.topology.
 ↪dim-1,facet_tags.indices[facet_tags.values==101]) )
##Extracts specified facets from mesh

actor = plotter.add_mesh(top, show_edges=True,color="blue") # top face is blue
```

```
actor2 = plotter.add_mesh(sides, show_edges=True,color="red") # sides are red
actor3 = plotter.add_mesh(bottom, show_edges=True,color="green") # bottom face␣
 ↪is green
##Visualization aspects implemented (color, animation, opacity, etc.)

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

plotter.screenshot("mesh.png")
##Saves images to path

from IPython.display import Image
Image(filename='mesh.png')
##Displays images within Jupyter notebook
```

3.1 Define boundary and volume integration measure

[5]:
```
# Surface labels from gmsh:
# Physical Surface("xBot", 101)
# Physical Surface("xTop", 102)

# 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': 4})

# Define the volume integration measure "dx"
# also specify the number of volume quadrature points.
dx = ufl.Measure('dx', domain=domain, metadata={'quadrature_degree': 4})

#  Define facet normal
n = ufl.FacetNormal(domain)
```

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

# Surface labels from gmsh:
# Physical Surface("xBot", 101)
# Physical Surface("xTop", 102)

# 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': 4})
##UFL used in DolfinX and FEniCS to define symbolic integral measures; tells␣
 ↪solver how and where to integrate expressions in weak forms
##ds= defining boundary measure integration over facets
```

```
##quadrature= accuracy of numerical integration; high degree= more accurate and␣
↪more computation

# Define the volume integration measure "dx"
# also specify the number of volume quadrature points.
dx = ufl.Measure('dx', domain=domain, metadata={'quadrature_degree': 4})
##dx=volume domain

#  Define facet normal
n = ufl.FacetNormal(domain)
##Expression for outward unit normal vector on boundary facets; vector shape is␣
↪same as mesh dimension. Used for Neumann boundary conditions
```

4 Material parameters

-Arruda-Boyce model

[6]:
```
Gshear_0 = Constant(domain,PETSc.ScalarType(280.0))            # Ground state␣
↪shear modulus
lambdaL  = Constant(domain,PETSc.ScalarType(5.12))             # Locking stretch
Kbulk    = Constant(domain,PETSc.ScalarType(1000.0*Gshear_0))
```

5 Simulation time-control related params

[7]:
```
t         = 0.0          # start time
theta_tot = 2.5 # 3/4*np.pi          # total rotation of end-face in radians
Ttot      = 20           # total simulation time
numSteps  = 20
dt        = Ttot/numSteps       # (fixed) step size
```

6 Function spaces

[8]:
```
# dolfinx v0.8.0 syntax:
U2 = element("Lagrange", domain.basix_cell(), 2, shape=(3,)) # For displacement
P1 = element("Lagrange", domain.basix_cell(), 1)  # For  pressure              ␣
↪
#
TH = mixed_element([U2, 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 = split(w)  # displacement u, pressure p

# A copy of functions to store values in the previous step
```

```
w_old          = Function(ME)
u_old,  p_old = split(w_old)

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

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

7 Initial conditions

- The initial conditions for degrees of freedom u and p are zero everywhere
- These are imposed automatically, since we have not specified any non-zero initial conditions.

8 Subroutines for kinematics and constitutive equations

[10]:
```
# Deformation gradient
def F_calc(u):
    Id = Identity(3)
    F  = Id + grad(u)
    return F

def lambdaBar_calc(u):
    F = F_calc(u)
    C = F.T*F
    Cdis = J**(-2/3)*C
    I1 = tr(Cdis)
    lambdaBar = sqrt(I1/3.0)
    return lambdaBar

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

# Generalized shear modulus for Arruda-Boyce model
def Gshear_AB_calc(u):
    zeta    = zeta_calc(u)
    Gshear  = Gshear_0 * zeta
    return Gshear

#---------------------------------------------
```

```
# Subroutine for calculating the Cauchy stress
#---------------------------------------------
def T_calc(u,p):
    Id = Identity(3)
    F   = F_calc(u)
    J = det(F)
    B = F*F.T
    Bdis = J**(-2/3)*B
    Gshear  = Gshear_AB_calc(u)
    T = (1/J)* Gshear * dev(Bdis) - p * Id
    return T

#----------------------------------------------
# Subroutine for calculating the Piola  stress
#----------------------------------------------
def Piola_calc(u, p):
    Id = Identity(3)
    F   = F_calc(u)
    J = det(F)
    #
    T   = T_calc(u,p)
    #
    Tmat   = J * T * inv(F.T)
    return Tmat
```

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

# Deformation gradient
def F_calc(u):
    Id = Identity(3)
    F  = Id + grad(u)
    return F
##Calculation for deformation gradient tensor F

def lambdaBar_calc(u):
    F = F_calc(u)
    C = F.T*F
    Cdis = J**(-2/3)*C
    I1 = tr(Cdis)
    lambdaBar = sqrt(I1/3.0)
    return lambdaBar
##Scalar stretch measure used in hyperelasticity models

def zeta_calc(u):
    lambdaBar = lambdaBar_calc(u)
##Isochoric stretch from deformation
    # Use Pade approximation of Langevin inverse
    z    = lambdaBar/lambdaL
##Normalizes stretch from polymer network
    z    = conditional(gt(z,0.95), 0.95, z) # Keep simulation from blowing up
##Prevents numeric instability; Langevin function because singular
    beta = z*(3.0 - z**2.0)/(1.0 - z**2.0)
##Pade approximation; used for stability
    zeta = (lambdaL/(3*lambdaBar))*beta
    return zeta
##Stress scalar from statistical mechanics model for polymers; accounts for␣
 ↪finite chain extensibility. Stress tensors for nonlinear chain elasticity

# Generalized shear modulus for Arruda-Boyce model
def Gshear_AB_calc(u):
##Effective shear for nonlinear hyperelastic material
    zeta    = zeta_calc(u)
##Stretch dependent factor using inverse Langevin. Increasing of stretch=␣
 ↪polymers stiffen
    Gshear  = Gshear_0 * zeta
    return Gshear
##Shear module grows due to deformation
##This is important due to modeling with biological materials (i.e. tissue);␣
 ↪nonlinear and stretch sensitive

#---------------------------------------------
# Subroutine for calculating the Cauchy stress
#---------------------------------------------
def T_calc(u,p):
    Id = Identity(3)
    F   = F_calc(u)
##Deformation gradient
    J = det(F)
##Jacobian (volume change due to deformation)
    B = F*F.T
##Cauchy-Green tensor
    Bdis = J**(-2/3)*B
##Removes volumetric part to get isochoric (volume perserving aspect)
    Gshear  = Gshear_AB_calc(u)
##Stretch dependent shear
    T = (1/J)* Gshear * dev(Bdis) - p * Id
    return T
##Cauchy stress calculation; shape change and pressure separated to obtain␣
 ↪deformed configuration

#----------------------------------------------
# Subroutine for calculating the Piola  stress
#----------------------------------------------
def Piola_calc(u, p):
    Id = Identity(3)
    F    = F_calc(u)
    J = det(F)
    T    = T_calc(u,p)
    Tmat    = J * T * inv(F.T)
    return Tmat
##Piola stress used in weak form of balance equation, with displacement␣
↪gradient; defined in terms of reference coordinates
```

9 Evaluate kinematics and constitutive relations

[11]:
```
F =  F_calc(u)
J = det(F)
lambdaBar = lambdaBar_calc(u)

# Piola stress
Tmat = Piola_calc(u, p)
```

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

F =  F_calc(u)
##F= deformation gradient tensor; u= displacement (unkown and solving for)
J = det(F)
##J= Jacobian determinant. Volume change during deformation
lambdaBar = lambdaBar_calc(u)
##incompressible hyperelasticity; seperates volumetric deviatoric, shape␣
↪changing parts of deformation. Volume corrected stretch is calculated for␣
↪use in isochoric strain energy

# Piola stress
Tmat = Piola_calc(u, p)
##Computes Piola stress tensor from displacement field (u) and pressure (p)
```

10 Weak forms

[12]:
```
# Residuals:
# Res_0: Balance of forces (test fxn: u)
# Res_1: Coupling pressure (test fxn: p)

# The weak form for the equilibrium equation. No body force
Res_0 = inner(Tmat , grad(u_test) )*dx

# The weak form for the pressure
fac_p = ln(J)/J
#
Res_1 = dot( (p/Kbulk + fac_p), p_test)*dx
```

```
# Total weak form
Res = Res_0 +  Res_1

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

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

# Residuals:
# Res_0: Balance of forces (test fxn: u)
# Res_1: Coupling pressure (test fxn: p)

# The weak form for the equilibrium equation. No body force
Res_0 = inner(Tmat , grad(u_test) )*dx
##Mechanical residual of weak form for nonlinear elasticity; used to build the␣
 ↪residual vector. Used in FE for a deforming solid

# The weak form for the pressure
fac_p = ln(J)/J
##Scalar factor used for compressible / incompressible materials due to␣
 ↪pressure / energy in nonlinear elasticity

Res_1 = dot( (p/Kbulk + fac_p), p_test)*dx
##Residual defined for pressure field in FE due to incompressible materials.␣
 ↪Differentiates volumetric strain energy

# Total weak form
Res = Res_0 +  Res_1
##Defines total residual of weak form; from force balance (linear momentum /␣
 ↪mechanical equillibrium) and incompressibility (pressure equation)

# Automatic differentiation tangent:
a = derivative(Res, w, dw)
##Jacobian form to solve for nonlinear PDE
```

11 Set-up output files

[13]:
```
# results file name
results_name = "3D_torsion"

# v0.8.0 syntax:
U1 = element("DG", domain.basix_cell(), 1, shape=(3,)) # For displacement
P0 = element("DG", domain.basix_cell(), 1)             # For  pressure

V2 = fem.functionspace(domain, U1) #Vector function space
```

```
V1 = fem.functionspace(domain, P0) #Scalar function space, must be␣
↪discontinuous here since materials are discontinuous.


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

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

J_vis = Function(V1)
J_vis.name = "J"
J_expr = Expression(J,V1.element.interpolation_points())

lambdaBar_vis = Function(V1)
lambdaBar_vis.name = "lambdaBar"
lambdaBar_expr = Expression(lambdaBar,V1.element.interpolation_points())

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

T   = Tmat*F.T/J
T0   = T - (1/3)*tr(T)*Identity(3)
Mises = sqrt((3/2)*inner(T0, T0))
Mises_vis= Function(V1,name="Mises")
Mises_expr = Expression(Mises,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, J_vis, P11, P22, P33, lambdaBar_vis,
        Mises_vis,
    ],
    engine="BP4",
)

def writeResults(t):
       # Output field interpolation
       u_vis.interpolate(w.sub(0))
       p_vis.interpolate(w.sub(1))
       J_vis.interpolate(J_expr)
       P11.interpolate(P11_expr)
       P22.interpolate(P22_expr)
       P33.interpolate(P33_expr)
       lambdaBar_vis.interpolate(lambdaBar_expr)
       Mises_vis.interpolate(Mises_expr)

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

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

[14]:
```
# infrastructure for evaluating functions at a certain point efficiently
# (not actually used in this code)
pointForStress = np.array([L, 0, 0])

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

# Define functions (UFL forms) for evaluating the torque and normal traction on␣
 ↪the top surface
origin = ufl.as_vector([0.0,0.0,0.0])
traction = dot(Tmat,n)
#
vec = ufl.cross((x-origin),traction)
Torque = fem.form(dot(vec,n)*ds(101))
#
Force = fem.form(dot(traction,n)*ds(101))

# Surface labels from gmsh:
# Physical Surface("xBot", 101)
# Physical Surface("xTop", 102)
```

13 Name the analysis step

[15]:
```
# Give the step a descriptive name
step = "Twist"
```

13.1 Boundary condtions

[16]:
```
# Setting up the expressions for rotation of the top surface.
scale = 1.0
y0 = 0.0
z0 = 0.0
Time_cons = Constant(domain,PETSc.ScalarType(0))

V_y, V_y_to_ME =  ME.sub(0).sub(1).collapse() #Scalar function space␣
 ↪corresponding to u2 / y-displacement
V_z, V_z_to_ME =  ME.sub(0).sub(2).collapse() #Scalar function space␣
 ↪corresponding to u3 / z-displacement

boundary_twist_y = scale*(y0 + (x[1] - y0)*ufl.cos(theta_tot*(Time_cons/Ttot))␣
 ↪- (x[2] - z0)*ufl.sin(theta_tot*(Time_cons/Ttot)) - x[1])

exp_y    = Expression(boundary_twist_y,V_y.element.interpolation_points())
func_y   = Function(V_y)
func_y.interpolate(exp_y)

boundary_twist_z = scale*(z0 + (x[1] - y0)*ufl.sin(theta_tot*(Time_cons/Ttot))␣
 ↪+ (x[2] - z0)*ufl.cos(theta_tot*(Time_cons/Ttot)) - x[2])

exp_z    = Expression(boundary_twist_z,V_z.element.interpolation_points())
func_z   = Function(V_z)
func_z.interpolate(exp_z)
```

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

# Setting up the expressions for rotation of the top surface.
scale = 1.0
y0 = 0.0
z0 = 0.0
##Scalar given; Center of rotation in the y-z plane

Time_cons = Constant(domain,PETSc.ScalarType(0))
##Time parameter; simulating time-dependent twisting over a total time

V_y, V_y_to_ME =  ME.sub(0).sub(1).collapse() #Scalar function space␣
 ↪corresponding to u2 / y-displacement
V_z, V_z_to_ME =  ME.sub(0).sub(2).collapse() #Scalar function space␣
 ↪corresponding to u3 / z-displacement
```

```
##Mechanical displacement vector field=sub(0); y-z components=sub(1) and sub(2)
##Extracts scalar Lagrange space

boundary_twist_y = scale*(y0 + (x[1] - y0)*ufl.cos(theta_tot*(Time_cons/Ttot))␣
 ↪- (x[2] - z0)*ufl.sin(theta_tot*(Time_cons/Ttot)) - x[1])
##Y-displacement of a point of top face under rotation about the x-axis by an␣
 ↪angle that is increasing linearly with time
##Subtracts x[1] to give actual displacement, not the new position

exp_y    = Expression(boundary_twist_y,V_y.element.interpolation_points())
func_y   = Function(V_y)
func_y.interpolate(exp_y)
##Interpolated displacement field for the y-direction twist
##Correct time-dependent y-displacement to apply to the boundary

boundary_twist_z = scale*(z0 + (x[1] - y0)*ufl.sin(theta_tot*(Time_cons/Ttot))␣
 ↪+ (x[2] - z0)*ufl.cos(theta_tot*(Time_cons/Ttot)) - x[2])
##Analogues but for z-displacement due to same rotation; Total angle rotation
##Subtracts x[2] to express displacement, not position

exp_z    = Expression(boundary_twist_z,V_z.element.interpolation_points())
func_z   = Function(V_z)
func_z.interpolate(exp_z)
##z-displacement for use as Dirichlet boundary condition
```

[17]:
```
# Surface labels from gmsh:
# Physical Surface("xBot", 101)
# Physical Surface("xTop", 102)

# Find the specific DOFs which will be constrained.
#
# Bottom surface displacement degrees of freedom
Btm_dofs_u1 = fem.locate_dofs_topological(ME.sub(0).sub(0), facet_tags.dim,␣
 ↪facet_tags.find(101))
Btm_dofs_u2 = fem.locate_dofs_topological(ME.sub(0).sub(1), facet_tags.dim,␣
 ↪facet_tags.find(101))
Btm_dofs_u3 = fem.locate_dofs_topological(ME.sub(0).sub(2), facet_tags.dim,␣
 ↪facet_tags.find(101))
# Top surface displacement degrees of freedom
Top_dofs_u1 = fem.locate_dofs_topological(ME.sub(0).sub(0), facet_tags.dim,␣
 ↪facet_tags.find(102))
Top_dofs_u2 = fem.locate_dofs_topological((ME.sub(0).sub(1), V_y), facet_tags.
 ↪dim, facet_tags.find(102))
Top_dofs_u3 = fem.locate_dofs_topological((ME.sub(0).sub(2), V_z), facet_tags.
 ↪dim, facet_tags.find(102))
```

```
# Build the Dirichlet BCs
bcs_0 = dirichletbc(0.0, Btm_dofs_u1, ME.sub(0).sub(0))  # u1 fix    - xBtm
bcs_1 = dirichletbc(0.0, Btm_dofs_u2, ME.sub(0).sub(1))  # u2 fix    - xBtm
bcs_2 = dirichletbc(0.0, Btm_dofs_u3, ME.sub(0).sub(2))  # u3 fix    - xBtm
#
bcs_3 = dirichletbc(0.0, Top_dofs_u1, ME.sub(0).sub(0))     # u1 fix    - xTop
bcs_4 = dirichletbc(func_y, Top_dofs_u2, ME.sub(0).sub(1))  # u2 rotate - xTop
bcs_5 = dirichletbc(func_z, Top_dofs_u3, ME.sub(0).sub(2))  # u3 rotate - xTop

# collect all BCs in one object.
bcs = [bcs_0, bcs_1, bcs_2, bcs_3, bcs_4, bcs_5]
```

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

# Surface labels from gmsh:
# Physical Surface("xBot", 101)
# Physical Surface("xTop", 102)

# Find the specific DOFs which will be constrained.

# Bottom surface displacement degrees of freedom
Btm_dofs_u1 = fem.locate_dofs_topological(ME.sub(0).sub(0), facet_tags.dim,␣
 ↪facet_tags.find(101))
Btm_dofs_u2 = fem.locate_dofs_topological(ME.sub(0).sub(1), facet_tags.dim,␣
 ↪facet_tags.find(101))
Btm_dofs_u3 = fem.locate_dofs_topological(ME.sub(0).sub(2), facet_tags.dim,␣
 ↪facet_tags.find(101))
##Find DOFs on bottom surface of mesh boundary

# Top surface displacement degrees of freedom
Top_dofs_u1 = fem.locate_dofs_topological(ME.sub(0).sub(0), facet_tags.dim,␣
 ↪facet_tags.find(102))
Top_dofs_u2 = fem.locate_dofs_topological((ME.sub(0).sub(1), V_y), facet_tags.
 ↪dim, facet_tags.find(102))
Top_dofs_u3 = fem.locate_dofs_topological((ME.sub(0).sub(2), V_z), facet_tags.
 ↪dim, facet_tags.find(102))
##Find DOFs on top surface of mesh boundary

# Build the Dirichlet BCs
bcs_0 = dirichletbc(0.0, Btm_dofs_u1, ME.sub(0).sub(0))  # u1 fix    - xBtm
bcs_1 = dirichletbc(0.0, Btm_dofs_u2, ME.sub(0).sub(1))  # u2 fix    - xBtm
bcs_2 = dirichletbc(0.0, Btm_dofs_u3, ME.sub(0).sub(2))  # u3 fix    - xBtm
##Bottom surface is fully fixed, with no displacement in any direction

bcs_3 = dirichletbc(0.0, Top_dofs_u1, ME.sub(0).sub(0))     # u1 fix    - xTop
bcs_4 = dirichletbc(func_y, Top_dofs_u2, ME.sub(0).sub(1))  # u2 rotate - xTop
bcs_5 = dirichletbc(func_z, Top_dofs_u3, ME.sub(0).sub(2))  # u3 rotate - xTop
```

```
##Top surface is fixed at x-axial displacement
##Rotation in y and z-direction defined; Giving rotation about the x-axis␣
↪creating torsion

# collect all BCs in one object.
bcs = [bcs_0, bcs_1, bcs_2, bcs_3, bcs_4, bcs_5]
##Applies boundary conditions to the nonlinear solver
```

13.2 Define the nonlinear variational problem

[18]:
```
# # Optimization options for the form compiler

# 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()
```

13.3 Start calculation loop

[19]:
```
# Variables for storing time history
totSteps = numSteps+1
timeHist0 = np.zeros(shape=[totSteps])
timeHist1 = np.zeros(shape=[totSteps])
timeHist2 = np.zeros(shape=[totSteps])

#Iinitialize a counter for reporting data
ii=0

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

```
# Print out 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
    Time_cons.value = t
    func_y.interpolate(exp_y)
    func_z.interpolate(exp_z)

    # 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

    # Store time history variables at this time
    timeHist0[ii] = theta_tot*(t/Ttot) # Current twist angle
    timeHist1[ii] = domain.comm.gather(fem.assemble_scalar(Torque))[0] # time␣
 ↪history of reaction torque
    timeHist2[ii] = domain.comm.gather(fem.assemble_scalar(Force))[0]  # time␣
 ↪history of axial force

    # 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("-------------------------------------------")
```

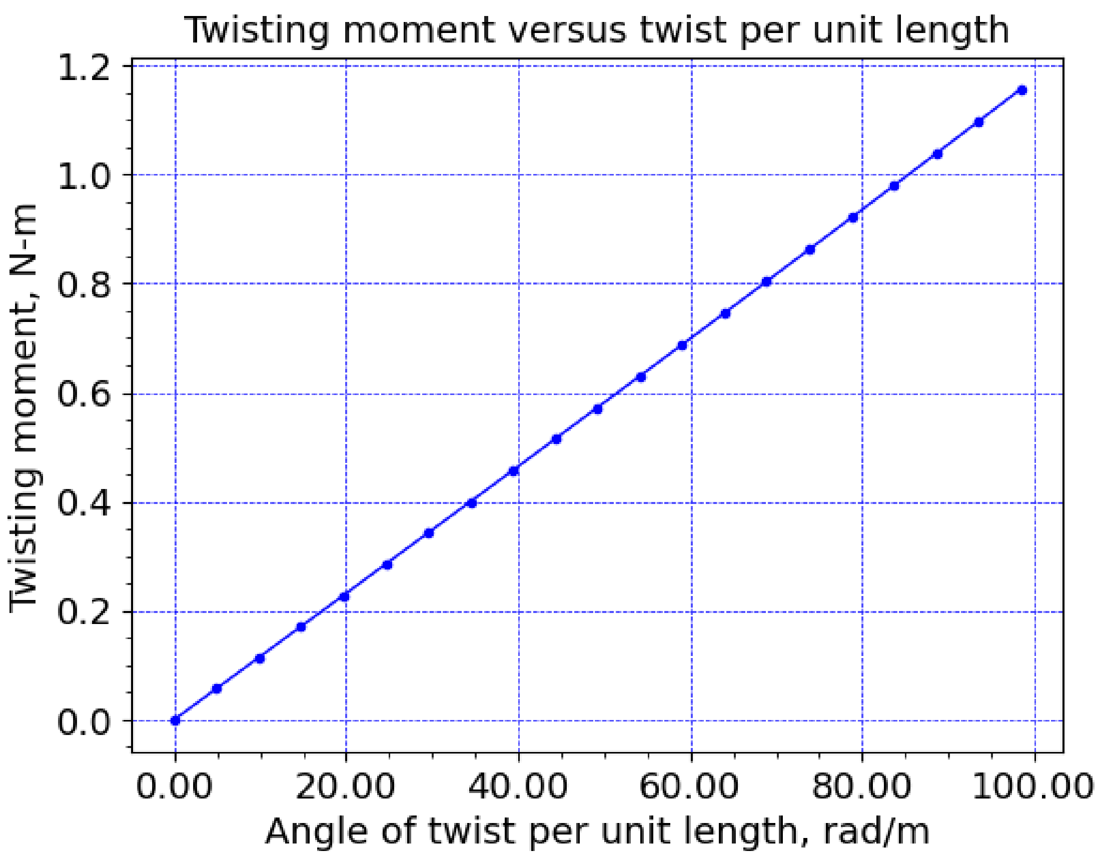
```
------------------------------------
Simulation Start
------------------------------------

Step: Twist | Increment: 1, Iterations: 5
      Simulation Time: 1.0 s  of  20 s

Step: Twist | Increment: 2, Iterations: 5
      Simulation Time: 2.0 s  of  20 s

Step: Twist | Increment: 3, Iterations: 5
      Simulation Time: 3.0 s  of  20 s

Step: Twist | Increment: 4, Iterations: 5
      Simulation Time: 4.0 s  of  20 s

Step: Twist | Increment: 5, Iterations: 5
      Simulation Time: 5.0 s  of  20 s

Step: Twist | Increment: 6, Iterations: 5
      Simulation Time: 6.0 s  of  20 s

Step: Twist | Increment: 7, Iterations: 5
      Simulation Time: 7.0 s  of  20 s

Step: Twist | Increment: 8, Iterations: 5
      Simulation Time: 8.0 s  of  20 s
```

```
Step: Twist | Increment: 9, Iterations: 5
      Simulation Time: 9.0 s  of  20 s

Step: Twist | Increment: 10, Iterations: 5
      Simulation Time: 10.0 s  of  20 s

Step: Twist | Increment: 11, Iterations: 5
      Simulation Time: 11.0 s  of  20 s

Step: Twist | Increment: 12, Iterations: 5
      Simulation Time: 12.0 s  of  20 s

Step: Twist | Increment: 13, Iterations: 5
      Simulation Time: 13.0 s  of  20 s

Step: Twist | Increment: 14, Iterations: 5
      Simulation Time: 14.0 s  of  20 s

Step: Twist | Increment: 15, Iterations: 5
      Simulation Time: 15.0 s  of  20 s

Step: Twist | Increment: 16, Iterations: 5
      Simulation Time: 16.0 s  of  20 s

Step: Twist | Increment: 17, Iterations: 5
      Simulation Time: 17.0 s  of  20 s

Step: Twist | Increment: 18, Iterations: 5
      Simulation Time: 18.0 s  of  20 s

Step: Twist | Increment: 19, Iterations: 5
      Simulation Time: 19.0 s  of  20 s

Step: Twist | Increment: 20, Iterations: 5
      Simulation Time: 20.0 s  of  20 s

-----------------------------------------
End computation
------------------------------------------
Elapsed real time:  0:02:18.379461
------------------------------------------
```

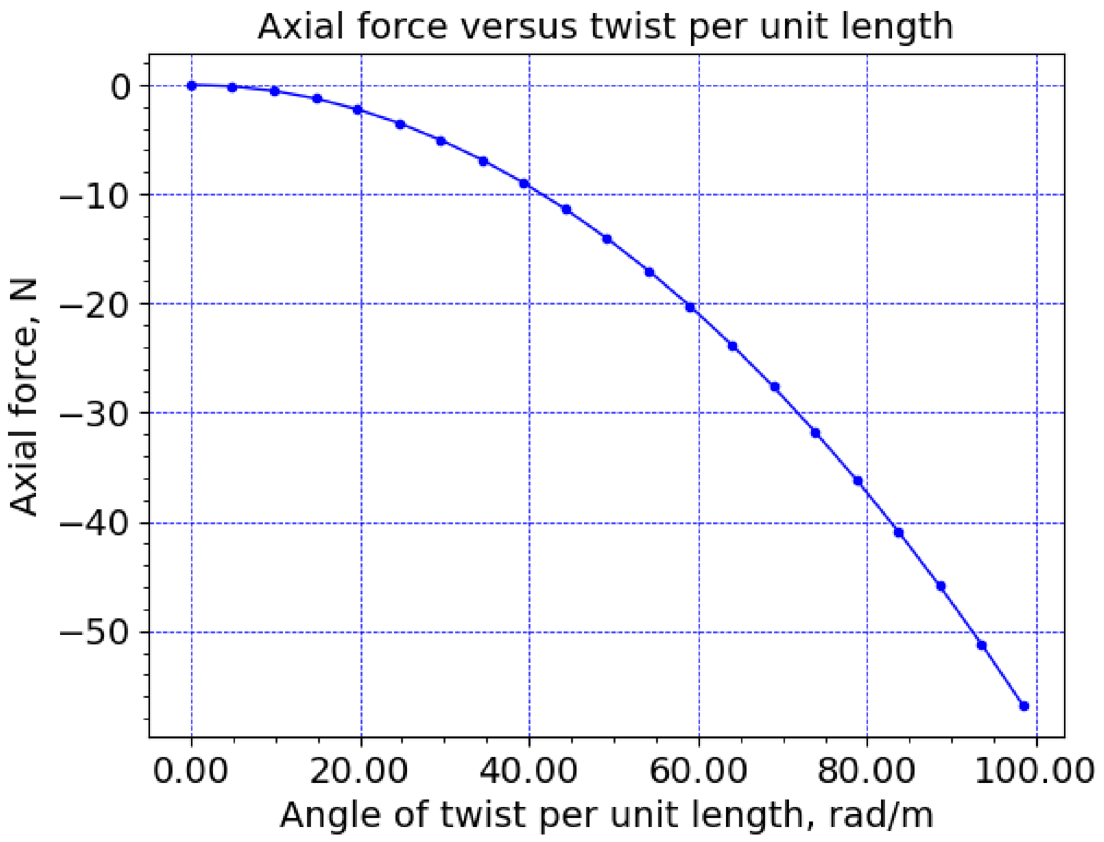
14 Plot results

[20]:
```
# set plot font to size 14
font = {'size'   : 14}
plt.rc('font', **font)

# Get array of default plot colors
prop_cycle = plt.rcParams['axes.prop_cycle']
colors = prop_cycle.by_key()['color']

#  Torque versus twist curve:
#
fig = plt.figure()
#fig.set_size_inches(7,4)
ax=fig.gca()
plt.plot(timeHist0/25.4E-3, timeHist1/1.E6 , c='b', linewidth=1.0, marker='.')
#-------------------------------------------------------------
#ax.set.xlim(-0.01,0.01)
#ax.set.ylim(-0.03,0.03)
#plt.axis('tight')
plt.grid(linestyle="--", linewidth=0.5, color='b')
ax.set_xlabel("Angle of twist per unit length, rad/m",size=14)
ax.set_ylabel("Twisting moment, N-m",size=14)
ax.set_title("Twisting moment versus twist per unit length", size=14,␣
 ↪weight='normal')
from matplotlib.ticker import AutoMinorLocator,FormatStrFormatter
ax.xaxis.set_minor_locator(AutoMinorLocator())
ax.yaxis.set_minor_locator(AutoMinorLocator())
import matplotlib.ticker as ticker
ax.xaxis.set_major_formatter(ticker.FormatStrFormatter('%0.2f'))
plt.show()

fig = plt.gcf()
fig.set_size_inches(7,5)
plt.tight_layout()
plt.savefig("results/3D_torsion_torque_twist.png", dpi=600)


#  Normal force versus twist curve:
#
fig = plt.figure()
#fig.set_size_inches(7,4)
ax=fig.gca()
plt.plot(timeHist0/25.4E-3, timeHist2/1.E3, c='b', linewidth=1.0, marker='.')
#-------------------------------------------------------------
#ax.set.xlim(-0.01,0.01)
#ax.set.ylim(-0.03,0.03)
```

```
#plt.axis('tight')
plt.grid(linestyle="--", linewidth=0.5, color='b')
ax.set_xlabel("Angle of twist per unit length, rad/m",size=14)
ax.set_ylabel("Axial force, N",size=14)
ax.set_title("Axial force versus twist per unit length", size=14,␣
  ↪weight='normal')
from matplotlib.ticker import AutoMinorLocator,FormatStrFormatter
ax.xaxis.set_minor_locator(AutoMinorLocator())
ax.yaxis.set_minor_locator(AutoMinorLocator())
import matplotlib.ticker as ticker
ax.xaxis.set_major_formatter(ticker.FormatStrFormatter('%0.2f'))
plt.show()

fig = plt.gcf()
fig.set_size_inches(7,5)
plt.tight_layout()
plt.savefig("results/3D_torsion_axial_force_twist.png", dpi=600)
```



```
<Figure size 700x500 with 0 Axes>
```


Axial force versus twist per unit length
Axial force, N
0
−10
−20
−30
−40
−50
0.00
20.00
40.00
60.00
80.00
100.00
Angle of twist per unit length, rad/m

```
<Figure size 700x500 with 0 Axes>
```