An automated computational framework for hyperelasticity

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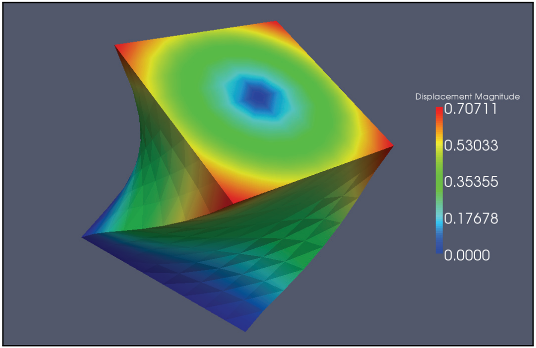
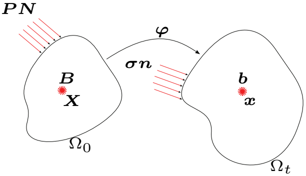


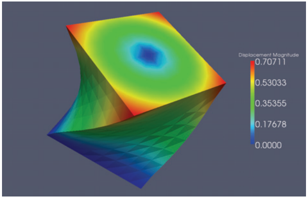
This talk will examine the motivation, design and use of our general framework for hyperelasticity



A review of relevant topics from continuum mechanics

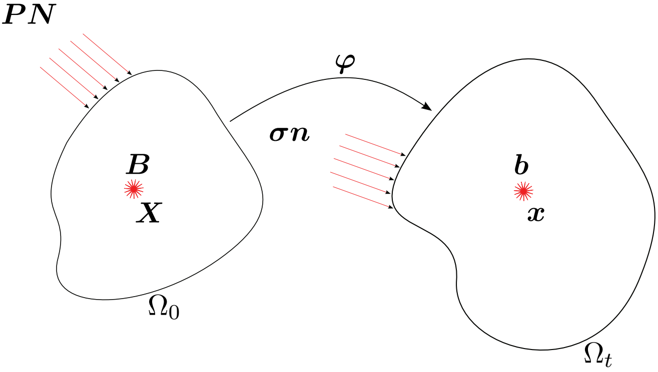
```
def SecondPiolaKirchhoffStress(self, u):
    self._construct_local_kinematics(u)
    psi = self.strain_energy(MaterialModel._parameters_as_fu

    if self.kinematic_measure == "InfinitesimalStrain":
        epsilon = self.epsilon
        S = diff(psi, epsilon)
    elif self.kinematic_measure == "RightCauchyGreen":
        C = self.C
        S = 2*diff(psi, C)
    elif self.kinematic_measure ==  "GreenLagrangeStrain":
        E = self.E
        S = diff(psi, E)
```

A brief look at numerical and computational aspects



Examples demonstrating the use of the framework

Recall, from elementary continuum mechanics . . .



The body idealised as a continuous medium

Reference and current configurations, body forces and tractions

. . . that the motion of solid bodies can be described using different strain measures

- Infinitesimal strain: $\boldsymbol{\epsilon} = \frac{1}{2}\left(\mathrm{Grad}(\boldsymbol{u}) + \mathrm{Grad}(\boldsymbol{u})^{\mathrm{T}}\right)$
- Deformation gradient: $\boldsymbol{F} = \mathbf{1} + \mathrm{Grad}(\boldsymbol{u})$
- Right Cauchy-Green: $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}$
- Green-Lagrange: $\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{C} - \mathbf{1}\right)$
- Left Cauchy-Green: $\boldsymbol{b} = \boldsymbol{F}\boldsymbol{F}^{\mathrm{T}}$
- Euler-Almansi: $\boldsymbol{e} = \frac{1}{2}\left(\mathbf{1} - \boldsymbol{b}^{-1}\right)$
- Volumetric and isochoric splits: e.g.
  $J = \mathrm{Det}(\boldsymbol{F}), \quad \bar{\boldsymbol{C}} = J^{-\frac{2}{3}}\boldsymbol{C}$
- Invariants of the tensors: I_1, I_2, I_3
- Principal stretches and directions: λ_1, λ_2, λ_3; $\quad \hat{\boldsymbol{N}}_1, \hat{\boldsymbol{N}}_2, \hat{\boldsymbol{N}}_3$

And the UFL syntax for defining these measures is almost identical to the mathematical notation

```
# Infinitesimal strain tensor
def InfinitesimalStrain(u):
    return variable(0.5*(Grad(u) + Grad(u).T))

# Second order identity tensor
def SecondOrderIdentity(u):
    return variable(Identity(u.cell().d))

# Deformation gradient
def DeformationGradient(u):
    I = SecondOrderIdentity(u)
    return variable(I + Grad(u))

# Determinant of the deformation gradient
def Jacobian(u):
    F = DeformationGradient(u)
    return variable(det(F))

# Right Cauchy-Green tensor
def RightCauchyGreen(u):
    F = DeformationGradient(u)
    return variable(F.T*F)

# Green-Lagrange strain tensor
def GreenLagrangeStrain(u):
    I = SecondOrderIdentity(u)
    C = RightCauchyGreen(u)
    return variable(0.5*(C - I))
```

```
# Left Cauchy-Green tensor
def LeftCauchyGreen(u):
    F = DeformationGradient(u)
    return variable(F*F.T)

# Euler-Almansi strain tensor
def EulerAlmansiStrain(u):
    I = SecondOrderIdentity(u)
    b = LeftCauchyGreen(u)
    return variable(0.5*(I - inv(b)))

# Invariants of an arbitrary tensor, A
def Invariants(A):
    I1 = tr(A)
    I2 = 0.5*(tr(A)**2 - tr(A*A))
    I3 = det(A)
    return [I1, I2, I3]

# Invariants of the (right/left) Cauchy-Green tensor
def CauchyGreenInvariants(u):
    C = RightCauchyGreen(u)
    [I1, I2, I3] = Invariants(C)
    return [variable(I1), variable(I2), variable(I3)]

# Isochoric part of the deformation gradient
def IsochoricDeformationGradient(u):
    F = DeformationGradient(u)
    J = Jacobian(u)
    return variable(J**(-1.0/3.0)*F)
```

Stress responses of hyperelastic materials are specified using constitutive relationships involving strain energy functions

- Strain energy functions: $\Psi(\boldsymbol{F}), \Psi(\boldsymbol{C}), \Psi(\boldsymbol{E}), \ldots$
- First Piola Kirchhoff: $\boldsymbol{P} = \frac{\partial \Psi(\boldsymbol{F})}{\partial \boldsymbol{F}} = 2\boldsymbol{F}\frac{\partial \Psi(\boldsymbol{C})}{\partial \boldsymbol{C}} = \ldots$
- Second Piola Kirchhoff: $\boldsymbol{S} = 2\frac{\partial \Psi(\boldsymbol{C})}{\partial \boldsymbol{C}} = \frac{\partial \Psi(\boldsymbol{E})}{\partial \boldsymbol{E}} = 2\left[\left(\frac{\partial \Psi}{\partial I_1} + I_1\frac{\partial \Psi}{\partial I_2}\right)\boldsymbol{1} - \frac{\partial \Psi}{\partial I_2}\boldsymbol{C} + I_3\frac{\partial \Psi}{\partial I_3}\boldsymbol{C}^{-1}\right] = \sum_{a=1}^{3}\frac{1}{\lambda_a}\frac{\partial \Psi}{\partial \lambda_a}\hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_a = \ldots$
- e.g. $\Psi_{\mathrm{St.Venant-Kirchhoff}} = \frac{\lambda}{2}\mathrm{tr}(\boldsymbol{E})^2 + \mu\mathrm{tr}(\boldsymbol{E}^2)$
  $\Psi_{\mathrm{Ogden}} = \sum_{p=1}^{N}\frac{\mu_p}{\alpha_p}\left(\lambda_1^{\alpha_p} + \lambda_2^{\alpha_p} + \lambda_3^{\alpha_p} - 3\right)$
  $\Psi_{\mathrm{Mooney-Rivlin}} = c_1(I_1 - 3) + c_2(I_2 - 3)$
  $\Psi_{\mathrm{Arruda-Boyce}} = \mu\left[\frac{1}{2}(I_1 - 3) + \frac{1}{20n}(I_1^2 - 9) + \frac{11}{1050n^2}(I_1^3 - 27) + \ldots\right]$
  $\Psi_{\mathrm{Yeoh}}, \Psi_{\mathrm{Gent-Thomas}}, \Psi_{\mathrm{neo-Hookean}}, \Psi_{\mathrm{Ishihara}}, \Psi_{\mathrm{Blatz-Ko}}, \ldots$

Again, the UFL syntax for defining different materials is almost identical to the mathematical notation

```
class StVenantKirchhoff(MaterialModel):
    """Defines the strain energy function for a St. Venant-Kirchhoff
    material"""

    def model_info(self):
        self.num_parameters = 2
        self.kinematic_measure = "GreenLagrangeStrain"

    def strain_energy(self, parameters):
        E = self.E
        [mu, lmbda] = parameters
        return lmbda/2*(tr(E)**2) + mu*tr(E*E)


class MooneyRivlin(MaterialModel):
    """Defines the strain energy function for a (two term)
    Mooney-Rivlin material"""

    def model_info(self):
        self.num_parameters = 2
        self.kinematic_measure = "CauchyGreenInvariants"

    def strain_energy(self, parameters):
        I1 = self.I1
        I2 = self.I2

        [C1, C2] = parameters
        return C1*(I1 - 3) + C2*(I2 - 3)
```

Again, the UFL syntax for defining different materials is almost identical to the mathematical notation

```
def SecondPiolaKirchhoffStress(self, u):
    self._construct_local_kinematics(u)
    psi = self.strain_energy(MaterialModel._parameters_as_functions(self, u))

    if self.kinematic_measure == "InfinitesimalStrain":
        epsilon = self.epsilon
        S = diff(psi, epsilon)
    elif self.kinematic_measure == "RightCauchyGreen":
        C = self.C
        S = 2*diff(psi, C)
    elif self.kinematic_measure ==  "GreenLagrangeStrain":
        E = self.E
        S = diff(psi, E)
    elif self.kinematic_measure == "CauchyGreenInvariants":
        I = self.I; C = self.C
        I1 = self.I1; I2 = self.I2; I3 = self.I3
        gamma1 = diff(psi, I1) + I1*diff(psi, I2)
        gamma2 = -diff(psi, I2)
        gamma3 = I3*diff(psi, I3)
        S = 2*(gamma1*I + gamma2*C + gamma3*inv(C))
    elif self.kinematic_measure == "IsochoricCauchyGreenInvariants":
        I = self.I; Cbar = self.Cbar
        I1bar = self.I1bar; I2bar = self.I2bar; J = self.J
        gamma1bar = diff(psibar, I1bar) + I1bar*diff(psibar, I2bar)
        gamma2bar = -diff(psibar, I2bar)
        Sbar = 2*(gamma1bar*I + gamma2bar*C_bar)
        ...
```

The equations that need to be solved are the balance laws in the reference configuration

- Balance of mass: $\frac{\partial \rho_0}{\partial t} = 0$
- Balance of linear momentum: $\rho_0 \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \mathrm{Div}(\boldsymbol{P}) + \boldsymbol{B}$
- Balance of angular momentum: $\boldsymbol{P}\boldsymbol{F}^{\mathrm{T}} = \boldsymbol{F}\boldsymbol{P}^{\mathrm{T}}$

The weak form thus reads: Find $\boldsymbol{u} \in \mathrm{V}$, such that $\forall\ \boldsymbol{v} \in \hat{\mathrm{V}}$:

$$\int_{\Omega_0} \rho_0 \frac{\partial^2 \boldsymbol{u}}{\partial t^2} \cdot \boldsymbol{v}\, dx + \int_{\Omega_0} \boldsymbol{P} : \mathrm{Grad}(\boldsymbol{v})\, dx \ = \int_{\Omega_0} \boldsymbol{B} \cdot \boldsymbol{v}\, dx + \int_{\Gamma_{\mathrm{N}}} \boldsymbol{P}\boldsymbol{N} \cdot \boldsymbol{v}\, dx$$

with suitable initial conditions, and Dirichlet and Neumann boundary conditions.

UFL's automatic differentiation capabilities allows for easy specification of such a problem

```
# Get the problem mesh
mesh = problem.mesh()

# Define the function space
vector = VectorFunctionSpace(mesh, "CG", 1)

# Test and trial functions
v = TestFunction(vector)
u = Function(vector)
du = TrialFunction(vector)

# Get forces and boundary conditions
B = problem.body_force()
PN = problem.surface_traction()
bcu = problem.boundary_conditions()

# First Piola-Kirchhoff stress tensor based on the material
# model
P = problem.first_pk_stress(u)

# The variational form corresponding to static hyperelasticity
L = inner(P, Grad(v))*dx - inner(B, v)*dx - inner(PN, v)*ds
a = derivative(L, u, du)

# Setup and solve problem
equation = VariationalProblem(a, L, bcu, nonlinear = True)
equation.solve(u)
```

UFL's automatic differentiation capabilities allows for easy specification of such a problem

- Spatial derivatives:
```
df_i = Dx(f, i)
```
- With respect to user-defined variables:
```
g = variable(cos(cell.x[0]))
f = exp(g**2)
h = diff(f, g)
```
- Forms with respect to coefficients of a discrete function:
```
a = derivative(L, w, u)
```
- Computing expressions and automatic differentiation:

  for $i = 1, \ldots, m$:

  $$y_i = t_i = \text{terminal expression}$$
  $$\frac{dy_i}{dv} = \frac{dt_i}{dv} = \text{terminal differentiation rule}$$

  for $i = m+1, \ldots, n$:

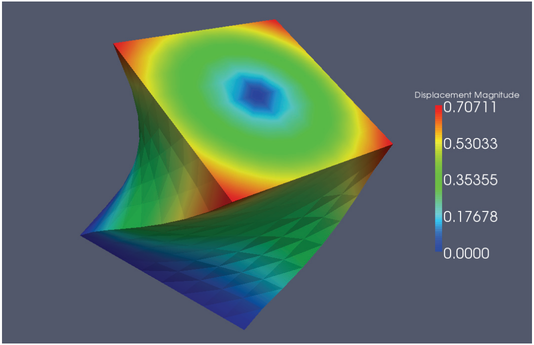
  $$y_i = f_i(<y_j>_{j \in \mathcal{J}_i})$$
  $$\frac{dy_i}{dv} = \sum_{k \in \mathcal{J}_i} \frac{\partial f_i}{\partial y_k} \frac{dy_k}{dv}$$

  $$z = y_n$$
  $$\frac{dz}{dv} = \frac{dy_n}{dv}$$

A simple static calculation involving a twisted block

```
class Twist(StaticHyperelasticity):

    def mesh(self):
        n = 8
        return UnitCube(n, n, n)

    def dirichlet_conditions(self):
        clamp = Expression(("0.0", "0.0", "0.0"))
        twist = Expression(("0.0",
                            "y0 + (x[1] - y0) * cos(theta) - (x[2] - z0) * sin(theta) - x[1]",
                            "z0 + (x[1] - y0) * sin(theta) + (x[2] - z0) * cos(theta) - x[2]"))
        twist.y0 = 0.5
        twist.z0 = 0.5
        twist.theta = pi/3
        return [clamp, twist]

    def dirichlet_boundaries(self):
        return ["x[0] == 0.0", "x[0] == 1.0"]

    def material_model(self):
        # Material parameters can either be numbers or spatially
        # varying fields. For example,
        mu       = 3.8461
        lmbda    = Expression("x[0]*5.8 + (1 - x[0])*5.7")
        C10 = 0.171; C01 = 4.89e-3; C20 = -2.4e-4; C30 = 5.e-4

        #material = MooneyRivlin([mu/2, mu/2])
        material = StVenantKirchhoff([mu, lmbda])
        #material = Isihara([C10, C01, C20])
        #material = Biderman([C10, C01, C20, C30])
        return material

# Setup and solve the problem
twist = Twist()
u = twist.solve()
```

A simple static calculation involving a twisted block



A solid block twisted by 60 degrees

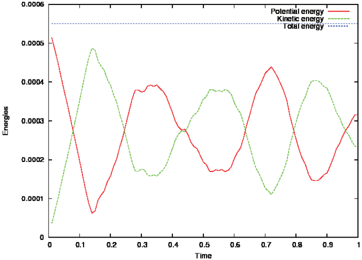
Iteration	Res. Norm
1	2.397e+00
2	6.306e-01
3	1.495e-01
4	4.122e-02
5	4.587e-03
6	8.198e-05
7	4.081e-08
8	1.579e-14

Newton scheme convergence

The dynamic release of the twisted block

```
class Release(Hyperelasticity):

        ...

    def end_time(self):
        return 10.0

    def time_step(self):
        return 2.e-3

    def reference_density(self):
        return 1.0

    def initial_conditions(self):
        """Return initial conditions for displacement field, u0, and
        velocity field, v0"""
        u0 = "twisty.txt"
        v0 = Expression(("0.0", "0.0", "0.0"))
        return u0, v0

    def dirichlet_conditions(self):
        clamp = Expression(("0.0", "0.0", "0.0"))
        return [clamp]

    def dirichlet_boundaries(self):
        return ["x[0] == 0.0"]

    def material_model(self):
        material = StVenantKirchhoff([3.8461, 5.76])
        return material

# Setup and solve the problem
release = Release()
u = release.solve()
```

The dynamic release of the twisted block



The relaxation of the released block

Conservation of energy

A silly hyperelastic fish being forced by a “flow”

```
class FishyFlow(Hyperelasticity):

    def mesh(self):
        mesh = Mesh("dolphin.xml.gz")
        return mesh

    def end_time(self):
        return 10.0

    def time_step(self):
        return 0.1

    def neumann_conditions(self):
        flow_push = Expression(("force", "0.0"))
        flow_push.force = 0.05
        return [flow_push]

    def neumann_boundaries(self):
        everywhere = "on_boundary"
        return [everywhere]

    def material_model(self):

        material = MooneyRivlin([6.169, 10.15])
        return material

# Setup and solve the problem
fishy = FishyFlow()
u = fishy.solve()
```

A silly hyperelastic fish being forced by a “flow”

The tumbling of the hyperelastic fish!

Concluding remarks, and where you can obtain the code

- We have a general framework for isotropic, dynamic hyperelasticity
- The following extensions are being worked on:
  - Implementing other specific material models
  - Allow for multiple materials and anisotropy
  - Goal-oriented adaptivity
  - Introducing coupling with other physics (including FSI)

- FEniCS Project: `http://fenics.org/`
- FEniCS Project Installer: `https://launchpad.net/dorsal/`
  `bzr get lp:dorsal`
- cbc.solve: `https://launchpad.net/cbc.solve/`
  `bzr get lp:cbc.solve`