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

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: \( \epsilon = \frac{1}{2} (\text{Grad}(u) + \text{Grad}(u)^T) \)
- Deformation gradient: \( F = 1 + \text{Grad}(u) \)
- Right Cauchy-Green: \( C = F^T F \)
- Green-Lagrange: \( E = \frac{1}{2} (C - 1) \)
- Left Cauchy-Green: \( b = FF^T \)
- Euler-Almansi: \( e = \frac{1}{2} (1 - b^{-1}) \)
- Volumetric and isochoric splits: e.g. \( J = \text{Det}(F), \quad \tilde{C} = J^{-\frac{2}{3}} C \)
- Invariants of the tensors: \( I_1, I_2, I_3 \)
- Principal stretches and directions: \( \lambda_1, \lambda_2, \lambda_3; \quad \hat{N}_1, \hat{N}_2, \hat{N}_3 \)
And the UFL syntax for defining these measures is almost identical to the mathematical notation

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

Again, the UFL syntax for defining different materials is almost identical to the mathematical notation.
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:** \( \rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} = \text{Div}(\mathbf{P}) + \mathbf{B} \)
- **Balance of angular momentum:** \( \mathbf{P}^{\mathbf{F}} = \mathbf{F}^{\mathbf{P}} \)

The weak form thus reads: Find \( \mathbf{u} \in \mathbf{V} \), such that \( \forall \ \mathbf{v} \in \hat{\mathbf{V}} \):

\[
\int_{\Omega_0} \rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} \cdot \mathbf{v} \, dx + \int_{\Omega_0} \mathbf{P} : \text{Grad}(\mathbf{v}) \, dx = \int_{\Omega_0} \mathbf{B} \cdot \mathbf{v} \, dx + \int_{\Gamma_N} \mathbf{P} \mathbf{N} \cdot \mathbf{v} \, dx
\]

with suitable initial conditions, and Dirichlet and Neumann boundary conditions.
UFL’s automatic differentiation capabilities allows for easy specification of such a problem

```python
# 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:**
  \[ df_i = \text{Dx}(f, i) \]

- **With respect to user-defined variables:**
  \[ g = \text{variable} \left( \cos(\text{cell.x}[0]) \right) \]
  \[ f = \exp(g**2) \]
  \[ h = \text{diff}(f, g) \]

- **Forms with respect to coefficients of a discrete function:**
  \[ a = \text{derivative}(L, w, u) \]

- **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 \( i = m + 1, \ldots, n \):
  \[ y_i = f_i(\langle y_j \rangle_{j \in J_i}) \]
  \[ \frac{dy_i}{dv} = \sum_{k \in J_i} \frac{\partial f_i}{\partial y_k} \frac{dy_k}{dv} \]
  \[ z = y_n \]
  \[ \frac{dz}{dv} = \frac{dy_n}{dv} \]
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

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Res. Norm</th>
</tr>
</thead>
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<tr>
<td>1</td>
<td>2.397e+00</td>
</tr>
<tr>
<td>2</td>
<td>6.306e-01</td>
</tr>
<tr>
<td>3</td>
<td>1.495e-01</td>
</tr>
<tr>
<td>4</td>
<td>4.122e-02</td>
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<td>5</td>
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<td>6</td>
<td>8.198e-05</td>
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<tr>
<td>7</td>
<td>4.081e-08</td>
</tr>
<tr>
<td>8</td>
<td>1.579e-14</td>
</tr>
</tbody>
</table>

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”

```python
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