Mechanical modelling with FEniCS

A wish list

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Outline

Interests

Example applications of FEniCS components

Wish list

Issues

Interests and motivation

- Rapid development and efficient solution of mechanical models.
- Minimal simplicity versus computational speed compromise.
- Significant productivity increase.
- Open source.

Interest

Licensing: GPL or LGPL?

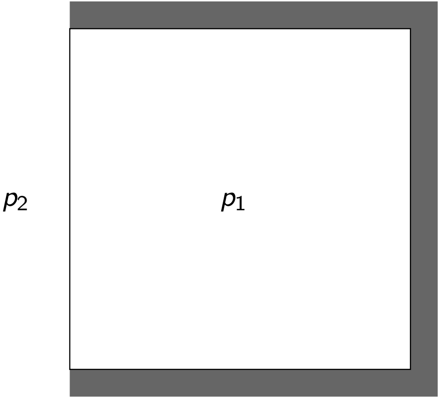
- GPL/LGPL protects *me* from my project sponsors.
- GPL might be too strong for some project sponsors.

Problem hallmarks

- Nonlinear.
- Multiple fields.

Porous media

Classical Biot theory + Darcy flow



Mechanical swelling due to fluid penetration

Porous media

```
PU = FiniteElement("Vector Lagrange", "triangle", 2)
PP = FiniteElement("Lagrange", "triangle", 1)

ME = PU + PP

(v, q)   = BasisFunctions(ME) # test functions
(u, p)   = BasisFunctions(ME) # trial functions
.
.
# Bilinear and linear form for solid component
aSolid    = dt*theta*dot(grad(v), stress(symgrad(u), p, mu, . . .

LSolidInt = dt*theta*dot(grad(v), stress(symgrad(u0), p0, mu, . . .
LSolidExt = dt*theta*v[1]*(rho*g)*dx

# Bilinear and linear form for fluid component
aFluid    = q*comp*p*dx + q*alpha*Sw*div(u)*dx + . . .

LFluidInt = dt*theta*q*comp*pr*dx + dt*theta*q*alpha*Sw* . . .
LFluidExt = dt*theta*q*f*dx + dt*theta*perm*rhow*q.dx(1)*g*dx
```

Mechanical response

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0}$$
$$\boldsymbol{\sigma} = \mathcal{C} : \nabla^{\mathsf{s}}\mathbf{u} - \beta \mathbf{I} c$$
$$+ B.C.$$

Steady-state diffusion

$$\nabla \cdot \mathbf{q} = 0$$
$$\mathbf{q} = -\kappa \nabla c + M \nabla \left(\nabla \cdot \mathbf{u} \right)$$
$$+ B.C.$$

Mechanically-driven diffusion in elastic solids

Find $\mathbf{u}^h \in V^h$, $e^h \in S^h$, $c^h \in X^h$ such that:

$$\left(\nabla \mathbf{w}^h, C : \nabla^s \mathbf{u}^h\right)_\Omega - \left(\nabla \mathbf{w}^h, \beta \mathbf{I} c^h\right)_\Omega = \left(\mathbf{w}^h, \mathbf{f}\right) \quad \forall\ \mathbf{w}^h \in V^h,$$

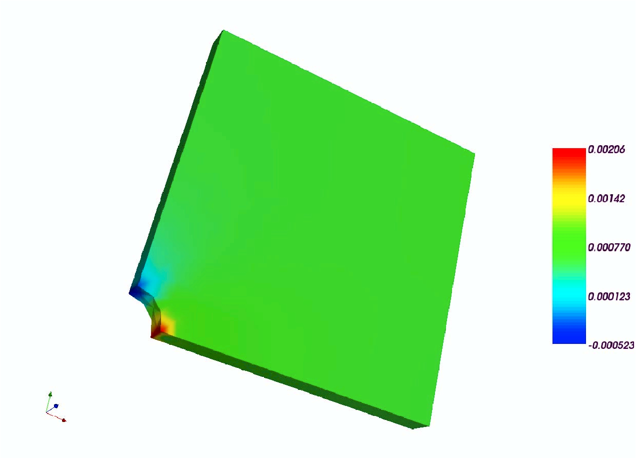
$$\left(v^h, e^h\right)_\Omega - \left(v^h, \nabla \cdot \mathbf{u}^h\right)_\Omega = 0 \quad \forall\ v^h \in S^h,$$

$$\left(\nabla q^h, \kappa \nabla c^h\right)_\Omega - \left(\nabla v^h, M \nabla e^h\right)_\Omega = 0 \quad \forall\ q^h \in X^h.$$

Mechanically-driven diffusion in elastic solids

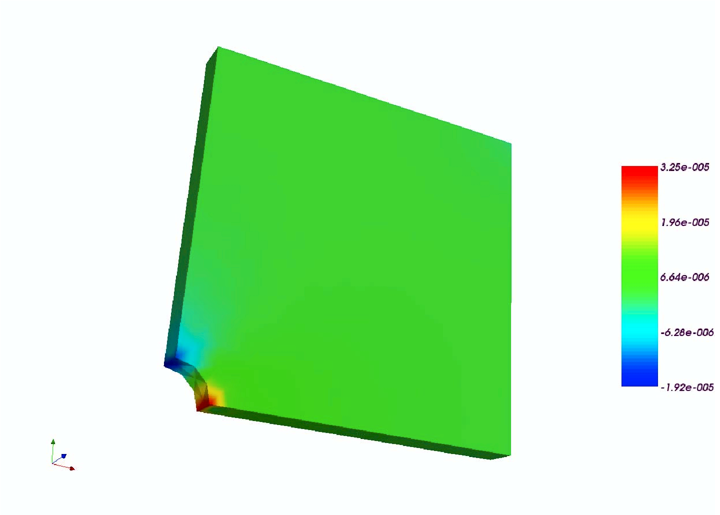
```
E1 = FiniteElement("Vector Lagrange", "tetrahedron", 2)
E2 = FiniteElement("Lagrange", "tetrahedron", 1)
E3 = FiniteElement("Lagrange", "tetrahedron", 1)

element = E1 + E2 + E3
.
.
# Elasticity
au = . . .

# Divergence of u
ae = . . .

# Diffusion
ac = . . .
.
.
```

Mechanically-driven diffusion in elastic solids



dilation

Mechanically-driven diffusion in elastic solids



concentration

Cahn-Hilliard equation

Model for phase separation

- Important in material science and other fields.
- Diffuse interface model.
- Fourth-order in space nonlinear parabolic equation.

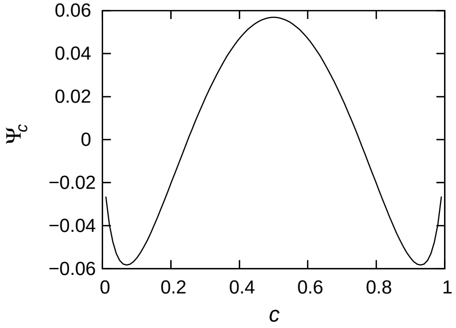
$$\dot{c} = \nabla \cdot M(c) \nabla \left(\mu_c(c) - \lambda \nabla^2 c \right) \quad \text{in } \Omega$$

$$M \lambda \nabla c \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega$$

$$M \nabla \left(\mu_c - \lambda \nabla^2 c \right) \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega$$

- c: concentration $0 < c < 1$
- M: mobility
- μ_c: chemical potential $(= d\Psi_c/dc)$
- λ: surface energy term

Chemical free-energy Ψ^c



Surface free-energy Ψ^s

$$\Psi^s = \frac{1}{2}\lambda \nabla c : \nabla c$$

Cahn-Hilliard equation

Mixed formulation:

$$\dot{c} = \nabla \cdot \left(M \nabla \left(\mu_c - \kappa \right) \right),$$

$$\kappa = \lambda \nabla^2 c.$$

Find $c^h \in S^h \times [0, T]$ and $\kappa^h \in P^h$ such that

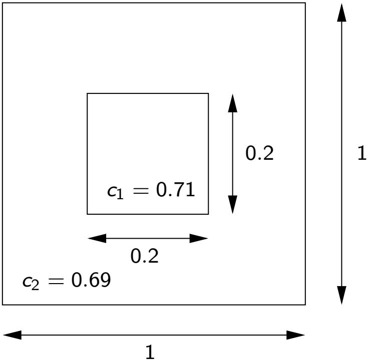
$$\left(w^h, \dot{c}^h \right)_\Omega + \left(\nabla w^h, M^h \nabla \left(\mu_c^h - \kappa^h \right) \right)_\Omega = 0 \quad \forall w^h \in V^h,$$

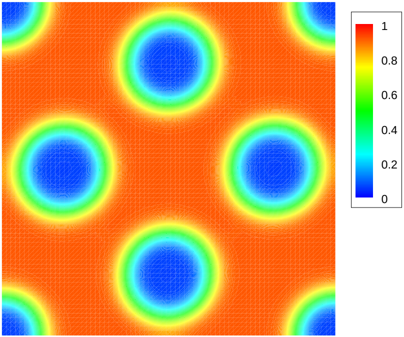
$$\left(v^h, \kappa^h \right)_\Omega + \left(\nabla v^h, \lambda \nabla c^h \right)_\Omega = 0 \quad \forall v^h \in Q^h,$$

$$\left(w^h, c\left(\mathbf{x}, 0 \right) \right)_\Omega = \left(w^h, c_0\left(\mathbf{x} \right) \right)_\Omega \quad \forall w^h \in V^h.$$

Cahn-Hilliard equation

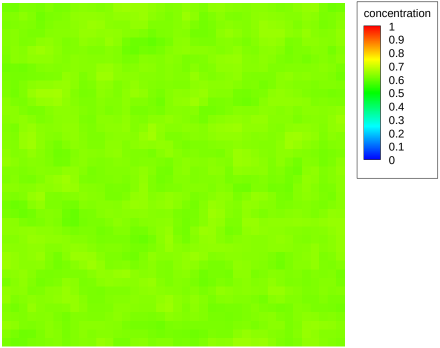
Benchmark





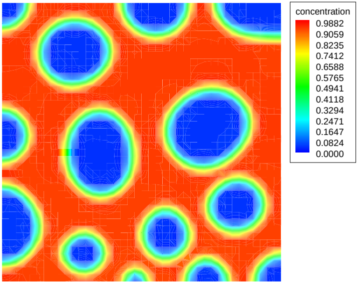
Cahn-Hilliard equation

Randomly perturbed initial conditions.

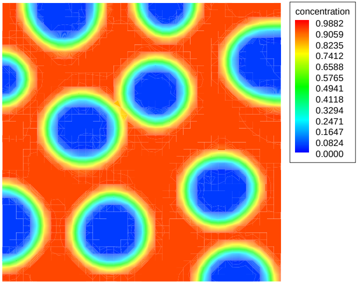


Initial condition $c = 0.63 +$ small random fluctuation.

Cahn-Hilliard equation

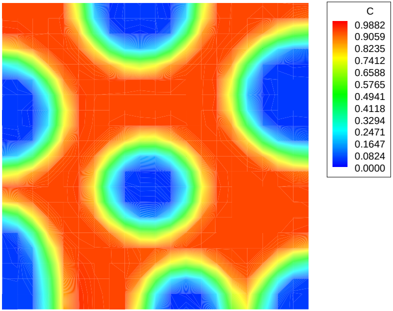


low surface energy



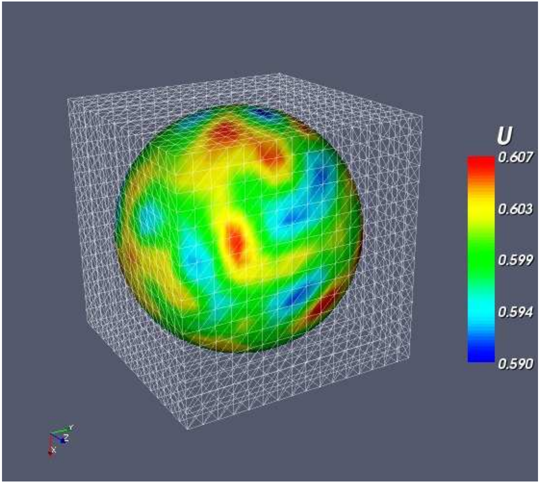
higher surface energy

Cahn-Hilliard equation



. . . even higher surface energy

Cahn-Hilliard equation



3D plane DOLFIN

Cahn-Hilliard equation

Problem: cannot find an iterative solver that works.

Cahn-Hilliard primal formulation

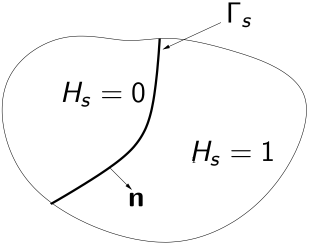
Find $c^h \in \mathcal{V}^h \times [0, T]$ such that

$$
\begin{aligned}
&\left(w^h, \dot{c}^h\right)_\Omega + \left(\nabla w^h, M^h \nabla \mu_c^h\right)_\Omega + \left(\nabla^2 w^h, M^h \lambda \nabla^2 c^h\right)_{\tilde{\Omega}} \\
&+ \left(\nabla w^h, \nabla M^h \lambda \nabla^2 c^h\right)_{\tilde{\Omega}} - \left(\left[\!\left[\nabla w^h\right]\!\right], \left\langle M^h \lambda \nabla^2 c^h \right\rangle\right)_{\tilde{\Gamma}} \\
&- \left(\left\langle M^h \lambda \nabla^2 w^h \right\rangle, \left[\!\left[\nabla c^h\right]\!\right]\right)_{\tilde{\Gamma}} - \left(\nabla w^h \cdot \mathbf{n}, M^h \lambda \nabla^2 c^h\right)_\Gamma \\
&- \left(M^h \lambda \nabla^2 w^h, \nabla c^h \cdot \mathbf{n}\right)_\Gamma + \left(\beta \nabla w^h \cdot \mathbf{n}, \nabla c^h \cdot \mathbf{n}\right)_\Gamma \\
&\qquad + \left(\beta \left[\!\left[\nabla w^h\right]\!\right], \left[\!\left[\nabla c^h\right]\!\right]\right)_{\tilde{\Gamma}} = 0 \quad \forall\, w^h \in \mathcal{V}^h
\end{aligned}
$$

Modelling discontinuities

Approach:

$$\mathbf{u}^h = \bar{\mathbf{u}}^h + H_s \tilde{\mathbf{u}}^h$$

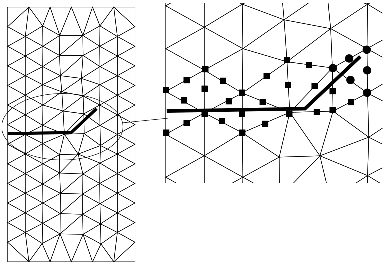


Discontinuity surface evolves.

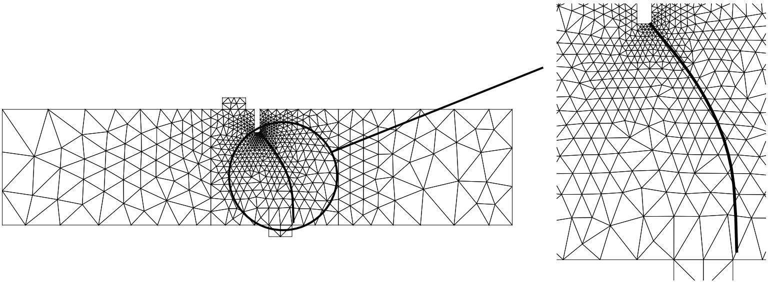
Modelling discontinuities

Exploit partition of unity property (Melenk & Babuska, Duarte & Oden, Belytschko & Black)

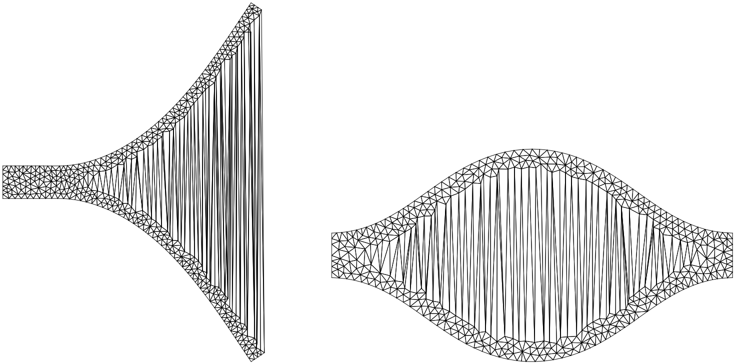
$$u^h = \sum_{i=1}^{n} \phi_i a_i + \sum_{j=1}^{m} H_s \phi_j b_i$$



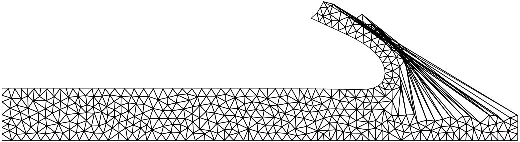
Crack propagation



Delamination



Delamination



Requirements

- Abstract evolving surface representation.
- Integration on an evolving surface.

Find . . .

$$\left(\nabla \bar{\mathbf{w}}^h, C : \nabla^s \left(\bar{\mathbf{u}}^h + H_s \tilde{\mathbf{u}}^h\right)\right)_\Omega + \left(\nabla \tilde{\mathbf{w}}^h, C : \nabla^s \left(\bar{\mathbf{u}}^h + H_s \tilde{\mathbf{u}}^h\right)\right)_{\Omega^+} + \left(\tilde{\mathbf{w}}^h, \mathbf{t}\left(\tilde{\mathbf{u}}^h\right)\right)_{\Gamma_s} = \left(\mathbf{w}^h, \mathbf{f}\right)_\Omega \quad \forall\ \bar{\mathbf{w}}^h \in \bar{V}^h, \tilde{\mathbf{w}}^h \in \tilde{V}^h$$

General wishes (FFC)

- Complex numbers.
- Inter-element boundary integrals.
- Simple polar coordinates.

Compact notation for nonlinear problems

- Variational problem compact.
- Linearised and time-dependent form very large (decrease in readability).

Issues

- Students
  - Loss of transparency.
  - Don't develop skills to implement models going beyond the current capabilities of FIAT/FFC/DOLFIN.
- Penetration
  - Level of abstraction too high for old-style FE users.
  - Quadrilateral and brick elements.
- Developers ready for users?
  - Preparedness/time to help novice users with trivial questions?
  - 0800-Anders-and-JohanJansson-help-desk (24 hour).

DOLFIN needs . . .

Most important aspect for dragging people over the threshold: simple, accessible demos with immediate postprocessing.

Solver demos to key mechanical problems:

- Linear-elasticity.
- Classical plasticity.
- Advection-diffusion.
- Stokes flow / incompressible elasticity.
- Incompressible Navier-Stokes.

'Extras' section outside of DOLFIN `src` tree.

Packaging and distribution

- Bloat in number of required components.
- Version dependencies becoming an issue.
- Bundle components?

Supporting FEniCS

Details

- Sufficient financial structure to make contributions possible.

How to spend it?

- Meetings
- Hardware, network
- ???