Introduction to FEniCS

Vahid Ziaei-Rad

University of Michigan-Shanghai Jiao Tong University Joint Institute

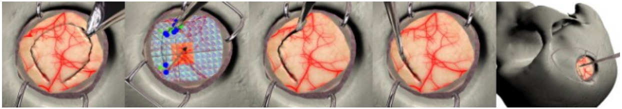
November 20, 2019

Prelude: Medical Simulations

Phase Field Approaches to Fracture

- The aim of "RealTCut" is to devise real-time numerical methods for the simulation of cutting. (Courtecuisse et al., 2014)

- These methods are aimed at surgical training, which has the potential to help surgeons improve their skills without endangering patients.

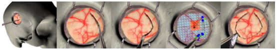


- Here, we are more interested in predictive and accurate simulations. . .

- We have some thoughts on phase field approaches to model fracture of "incompressible" soft tissues. (Gültekin et al., 2016)

Towards Real-Time Multi-Scale Simulation of Cutting

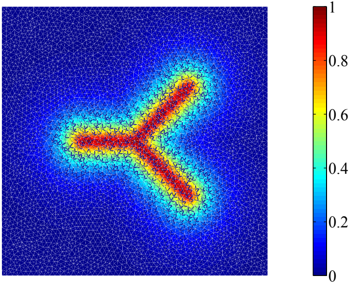
Phase Field Approaches to Fracture



Prelude: Smeared Crack Approaches

Phase Field Approaches to Fracture

- The phase field approaches to fracture
  - Based on energy minimization with both displacement and crack path (Francfort & Marigo, 1998)
  - Use a **continuous** scalar field to denote the crack (Bourdin et al., 2008)
  - Able to predict crack nucleation/branching without extra input



- **Cons:**
  - High computational cost
  - Polyconvexity of the functional

Outline

- **Phase Field Formulation in General Context**
- Phase Field Formulation with Incompressibility
- Impelementation on FEniCs

Small Strain Measures

Phase Field Formulation in General Context

- Let $\psi[\boldsymbol{\varepsilon}(\boldsymbol{u})]$ be the strain energy density which depends on the strain

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) := \frac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)$$

  as

$$\psi(\boldsymbol{\varepsilon}) := \frac{\lambda}{2}(\operatorname{tr} \boldsymbol{\varepsilon})^2 + \mu \|\boldsymbol{\varepsilon}\|^2$$

- Note that we exclude large strain measure, although most phenomenological models are based on hyperelastic formulation.

Variational Formulation of Fracture

Phase Field Formulation in General Context

- The variational formulation for fracture of the solid consists in finding the minimizer of the following potential:

$$\Pi[\boldsymbol{u},\Gamma] := \int_{\Omega\setminus\Gamma} \psi[\varepsilon(\boldsymbol{u})]\, d\Omega - \int_{\Omega} \boldsymbol{b}\cdot\boldsymbol{u}\, d\Omega - \int_{\partial_N\Omega} \boldsymbol{t}_N\cdot\boldsymbol{u}\, d\Gamma + g_c|\Gamma|$$

  among all $\boldsymbol{u}:\mathbb{R}^2\to\mathbb{R}^2$ that are bounded deformation functions of Ω and that satisfy

$$\boldsymbol{u} = \boldsymbol{u}_D, \quad \text{on } \partial_D\Omega.$$

- $\Gamma = \Gamma(\boldsymbol{u}) \subset \Omega$ is the set of discontinuities of $\boldsymbol{u}$. $|\Gamma|$ denotes the length of Γ.

- But it is not easy to search among all possible Γ's for minimization...

Phase Field Regularization

Phase Field Formulation in General Context

- We define a **continuous scalar field** (d) to denote the crack.

- We introduce the crack length functional, which takes the following form:

$$\Gamma_\ell[d] := \int_\Omega \left(\frac{d^2}{2\ell} + \frac{\ell}{2} \nabla d \cdot \nabla d \right) d\Omega,$$

  where ℓ is a **length scale** such that when $\ell \to 0$, the regularized formulation Γ-converges to that with explicit crack representation. (Dal Maso et al., 2005)

- $d : \Omega \to [0, 1]$: In particular, regions with $d = 0$ and $d = 1$ correspond to "perfect" and "fully-broken" states of the material, respectively.

Regularized Variational Formulation of Fracture

Phase Field Formulation in General Context

- We regularize the functional by means of the phase field:

$$\Pi_\ell[\boldsymbol{u}, d] := \int_\Omega \psi[\varepsilon(\boldsymbol{u}), d]\, d\Omega - \int_\Omega \mathbf{b} \cdot \boldsymbol{u}\, d\Omega - \int_{\partial_N \Omega} \boldsymbol{t}_N \cdot \boldsymbol{u}\, d\Gamma$$
$$+ g_c \int_\Omega \left(\frac{d^2}{2\ell} + \frac{\ell}{2} |\nabla d|^2 \right) d\Omega.$$

- Here $\psi(\varepsilon, d)$ is the strain energy density degraded by the phase field such that $\psi(\varepsilon, 0) = \psi_0(\varepsilon)$ and that $\psi(\varepsilon, d_1) \geq \psi(\varepsilon, d_2)$ if $d_1 < d_2$.

- Now we look for various ways to degrade the strain energy density...

Popular Phase Field Models (A)

Phase Field Formulation in General Context

- **Model A:** This is the original model proposed for similar formulations. It is convenient in that ψ is analytic in both d and ε. (Bourdin et al., 2008)

$$
\begin{aligned}
\psi &= (1-d)^2\psi_+ + \psi_-, \quad \sigma = \frac{\partial \psi}{\partial \varepsilon},\\
\psi_+ &= \frac{\lambda}{2}(\operatorname{tr}\boldsymbol{\varepsilon})^2 + \mu\|\boldsymbol{\varepsilon}\|^2,\\
\psi_- &= 0.
\end{aligned}
$$

Popular Phase Field Models (B)

Phase Field Formulation in General Context

- **Model B:** This model assumes that both volumetric expansion and deviatoric deformation contribute to crack propagation but not volumetric compression. (Amor et al., 2009)

$$\psi = (1-d)^2\psi_+ + \psi_-, \quad \sigma = \frac{\partial\psi}{\partial\varepsilon},$$
$$\psi_+ = (\lambda + 2\mu/3)\langle \operatorname{tr}\boldsymbol{\varepsilon}\rangle_+ \mathbf{1} + 2\mu\,\operatorname{dev}\boldsymbol{\varepsilon},$$
$$\psi_- = (\lambda + 2\mu/3)\langle \operatorname{tr}\boldsymbol{\varepsilon}\rangle_- \mathbf{1}.$$

Popular Phase Field Models (C)

Phase Field Formulation in General Context

- **Model C:** This model postulates that the stress degradation is due to a combination of tensile loading and volumetric expansion. (Miehe et al., 2010)

$$\psi = (1-d)^2\psi_+ + \psi_-, \quad \sigma = \frac{\partial\psi}{\partial\varepsilon},$$

$$\psi_+ = \lambda\langle \operatorname{tr} \boldsymbol{\varepsilon}\rangle_+ \mathbf{1} + 2\mu\sum_{i=1}^{3}\langle\varepsilon_i\rangle_+ \mathbf{n}_i \otimes \mathbf{n}_i,$$

$$\psi_- = \lambda\langle \operatorname{tr} \boldsymbol{\varepsilon}\rangle_- \mathbf{1} + 2\mu\sum_{i=1}^{3}\langle\varepsilon_i\rangle_- \mathbf{n}_i \otimes \mathbf{n}_i.$$

Outline

- Phase Field Formulation in General Context
- **Phase Field Formulation with Incompressibility**
- Impelementation on FEniCs

Regularized Variational Formulation of Fracture

Phase Field Formulation with Incompressibility

- Let

$$\mathscr{S}_u := \left\{ \boldsymbol{u} \in H^1\left(\Omega; \mathbb{R}^2\right) \middle| \boldsymbol{u}(\cdot) = \boldsymbol{u}_D(\cdot) \text{ on } \partial_D\Omega \right\},$$
$$\mathscr{S}_p := L^2(\Omega),$$
$$\mathscr{S}_d := H^1(\Omega).$$

- We aim to minimize the following potential: (Wheeler et al., 2014)

$$\Pi_\ell[\boldsymbol{u}, p, d] := \int_\Omega \psi^{Dev}[\varepsilon(\boldsymbol{u}), d]\, d\Omega + \int_\Omega \left(-\frac{p^2}{2\lambda} + p \operatorname{div} \boldsymbol{u} \right) d\Omega$$
$$- \int_{\partial_N\Omega} \boldsymbol{t}_N \cdot \boldsymbol{u}\, d\Gamma - \int_\Omega \rho \mathbf{b} \cdot \boldsymbol{u}\, d\Omega + g_c \int_\Omega \left(\frac{d^2}{2\ell} + \frac{\ell}{2} |\nabla d|^2 \right) d\Omega.$$

supplemental

The Strong Form

Phase Field Formulation with Incompressibility

- The Euler-Lagrange equations read:

$$
\begin{aligned}
\operatorname{div} \boldsymbol{\sigma}^{Dev} + \nabla p + \mathbf{b} &= \mathbf{0}, && \text{in } \Omega,\\
\left(-\frac{1}{\lambda} p + \operatorname{div} \boldsymbol{u}\right) &= 0, && \text{in } \Omega,\\
-\frac{\partial \psi^{Dev}}{\partial d} - \frac{g_c}{\ell}\left(d - \ell^2 \Delta d\right) &= 0, && \text{in } \Omega,\\
\left(\boldsymbol{\sigma}^{Dev} \cdot \boldsymbol{n}\right) - \boldsymbol{t}_N &= \mathbf{0}, && \text{on } \partial_N \Omega,\\
\frac{\partial d}{\partial \boldsymbol{n}} &= 0, && \text{on } \partial \Omega,\\
\boldsymbol{u} &= \boldsymbol{u}_D, && \text{on } \partial_D \Omega.
\end{aligned}
$$

The Weak Form

Phase Field Formulation with Incompressibility

- The weak form can be stated as: Find $(\boldsymbol{u}, p, d) \in \mathscr{S}_u \times \mathscr{S}_p \times \mathscr{S}_d$ such that for all $\boldsymbol{w} \in \mathscr{V}_u$, $\tilde{p} \in \mathscr{V}_p$, and $q \in \mathscr{V}_d$:

$$
\begin{aligned}
&\int_\Omega \boldsymbol{\sigma}^{Dev}[\varepsilon(\boldsymbol{u}), d] : \varepsilon^{Dev}(\boldsymbol{w})\, d\Omega + \int_\Omega p \operatorname{div} \boldsymbol{w}\, d\Omega \\
&= \int_{\partial_N \Omega} \boldsymbol{t}_N \cdot \boldsymbol{w}\, d\Gamma + \int_\Omega \mathbf{b} \cdot \boldsymbol{w}\, d\Omega, \\
&\int_\Omega \left(-\frac{1}{\lambda} p + \operatorname{div} \boldsymbol{u} \right) \tilde{p}\, d\Omega = 0, \\
&\int_\Omega \left[2dq\psi_+^{Dev}(\varepsilon) + g_c \left(\frac{d\ q}{\ell} + \ell \nabla d \cdot \nabla q \right) \right] d\Omega = \int_\Omega 2q\psi_+^{Dev}(\varepsilon)\, d\Omega.
\end{aligned}
$$

Outline

- Phase Field Formulation in Dynamic Context
- Phase Field Formulation in General Context
- Phase Field Formulation with Incompressibility
- **Impelementation on FEniCs**

Impelementation on FEniCs

Features

- The **FEniCS Project** is a collection of free software with an extensive list of features for efficient solution of differential equations.

```
energy_elastic = psi(epsdev(u_), d_) * dx
...
Residual_u = derivative (energy_total, v_, v_t)
Jacobian_u = derivative (Residual_u, v_, v)
```

- We use the FEniCS project and PETSc software packages:
  - "Rigid Punch Incompressible Elasticity" by **Jack S. Hale**
  - "FEniCS Variational Damage and Fracture" by **Corrado Maurini** *Available online at https://bitbucket.org/cmaurini/*
  - "Phase Field Models with Incompressibility" by **Vahid Ziaei-Rad**

supplemental

Conclusion

- We used phase field approach toward the simulation of cutting soft tissues.
- We discussed pros and cons of some popular phase field models.
- We developed a model for incompressible materials in small strain measure.
- We introduced some features of our FEniCS implementation.

Amor, H., Marigo, J.-J., & Maurini, C. (2009). Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments. *Journal of the Mechanics and Physics of Solids*, *57*, 1209–1229.

Bourdin, B., Francfort, G. A., & Marigo, J.-J. (2008). The variational approach to fracture. *Journal of Elasticity*, *91*, 5–148.

Courtecuisse, H., Allard, J., Kerfriden, P., Bordas, S. P., Cotin, S., & Duriez, C. (2014). Real-time simulation of contact and cutting of heterogeneous soft-tissues. *Medical Image Analysis*, *18*(2), 394 - 410.

Dal Maso, G., Francfort, A. G., & Toader, R. (2005). Quasistatic crack growth in nonlinear elasticity. *Archive for Rational Mechanics and Analysis*, *176*(2), 165–225.

Francfort, G. A., & Marigo, J.-J. (1998). Revisiting brittle fracture as an energy minimization problem. *Journal of the Mechanics and Physics of Solids*, *46*(8), 1319–1342.

Gültekin, O., Dal, H., & Holzapfel, G. A. (2016). A phase-field approach to model fracture of arterial walls: Theory and finite element analysis. *Computer Methods in Applied Mechanics and Engineering*, -.

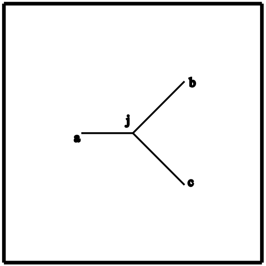
Miehe, C., Welschinger, F., & Hofacker, M. (2010). Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations. *International Journal for Numerical Methods in Engineering*, *83*, 1273–1311.

Wheeler, M. F., Wick, T., & Wollner, W. (2014). An augmented-Lagrangian method for the phase-field approach for pressurized fractures. *Computer Methods in Applied Mechanics and Engineering*, *271*, 69–85.

Prelude: Explicit Crack Approaches

Phase Field Approaches to Fracture

- The explicit crack approaches
  - **Family 1:** To regenerate/adjust the mesh
  - **Family 2:** To introduce enrichment for the displacement discontinuity



- **Cons:**
  - Need to track the complicated geometry of the evolving crack
  - Need extra input to predict complex phenomena

Phase Field Formulation in General Context

The first variation

- Taking the first variation yield:

$$
\begin{aligned}
\delta\Pi_\ell[(\boldsymbol{u}, d), (\boldsymbol{w}, q)] &:= \frac{d}{d\epsilon}\Pi_\ell[\boldsymbol{u} + \epsilon\boldsymbol{w}, d + \epsilon q]\Big|_{\epsilon=0} \\
&= \int_\Omega \boldsymbol{\sigma}[\varepsilon(\boldsymbol{u}), d] : \varepsilon(\boldsymbol{w})\ d\Omega - \int_{\Gamma_N} \boldsymbol{t}_N \cdot \boldsymbol{w}\ d\Gamma - \int_\Omega \mathbf{b} \cdot \boldsymbol{w}\ d\Omega \\
&\quad - \int_\Omega 2(1-d)q\psi_+(\varepsilon)\ d\Omega + g_c \int_\Omega \left(\frac{d\ q}{\ell} + \ell\nabla d \cdot \nabla q\right)\ d\Omega
\end{aligned}
$$

where

$$
\boldsymbol{\sigma} := \frac{\partial\psi}{\partial\varepsilon} = \left[(1-d)^2 + k\right]\frac{\partial\psi_+(\varepsilon)}{\partial\varepsilon} + \frac{\partial\psi_-(\varepsilon)}{\partial\varepsilon}
$$

is the Cauchy stress tensor.

The weak form

Phase Field Formulation in General Context

The residuals

- If we use $\{\mathbf{N}_P\}$ to denote the set of basis functions for $\boldsymbol{u}$ and $\boldsymbol{w}$, and $\{\phi_P\}$ that for d and q, then we can write the residuals as

$$R_P = \int_\Omega \boldsymbol{\sigma}[\varepsilon(\boldsymbol{u}), d] : \varepsilon(\mathbf{N}_P)\; d\Omega - \int_{\Gamma_N} \boldsymbol{t}_N \cdot \mathbf{N}_P\; d\Gamma - \int_\Omega \mathbf{b} \cdot \mathbf{N}_P\; d\Omega,$$

$$\overline{R}_P = -\int_\Omega 2(1-d)\phi_P \psi_+(\varepsilon)\; d\Omega + g_c \int_\Omega \left(\frac{d\; \phi_P}{\ell} + \ell \nabla d \cdot \nabla \phi_P \right)\; d\Omega.$$

FEniCS

Phase Field Formulation in General Context

The second variation

- To derive the expression of the tangent stiffness matrices, we take another variation:

$$
\begin{aligned}
\delta^2\Pi_\ell[(\boldsymbol{u},d),(\boldsymbol{w},q);(\delta\boldsymbol{u},\delta d)] &:= \frac{d}{d\epsilon}\delta\Pi_\ell[(\boldsymbol{u}+\epsilon\delta\boldsymbol{u},d+\epsilon\delta d),(\boldsymbol{w},q)]\Big|_{\epsilon=0} \\
&= \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{w}) : \mathbb{A}[\boldsymbol{\varepsilon}(\boldsymbol{u}),d] : \boldsymbol{\varepsilon}(\delta\boldsymbol{u})\ d\Omega \\
&\quad + \int_\Omega 2qd\ \frac{\partial\psi_+(\boldsymbol{\varepsilon})}{\partial\boldsymbol{\varepsilon}}\Big|_{\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}(\boldsymbol{u})} : \boldsymbol{\varepsilon}(\delta\boldsymbol{u})\ d\Omega \\
&\quad + \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{w}) : \frac{\partial\boldsymbol{\sigma}[\boldsymbol{\varepsilon}(\boldsymbol{u}),d]}{\partial d}\delta d\ d\Omega \\
&\quad - \int_\Omega 2q\psi_+(\boldsymbol{\varepsilon})\delta d\ d\Omega \\
&\quad + g_c\int_\Omega \left[\frac{q\delta d}{\ell} + \ell\nabla q\cdot\nabla(\delta d)\right]\ d\Omega.
\end{aligned}
$$

FEniCS

Popular Phase Field Models (B)

Phase Field Formulation in General Context

- **Model B:** This model assumes that both volumetric expansion and deviatoric deformation contribute to crack propagation but not volumetric compression. (Amor et al., 2009)

$$\psi = (1-d)^2\psi_+ + \psi_-, \quad \sigma = \frac{\partial\psi}{\partial\varepsilon},$$
$$\psi_+ = (\lambda + 2\mu/3)\langle \mathrm{tr}\,\boldsymbol{\varepsilon}\rangle_+ \mathbf{1} + 2\mu\,\mathrm{dev}\,\boldsymbol{\varepsilon},$$
$$\psi_- = (\lambda + 2\mu/3)\langle \mathrm{tr}\,\boldsymbol{\varepsilon}\rangle_- \mathbf{1}.$$

The incompressibility formulation