Capturing Interfaces in Multi-Phase Problems

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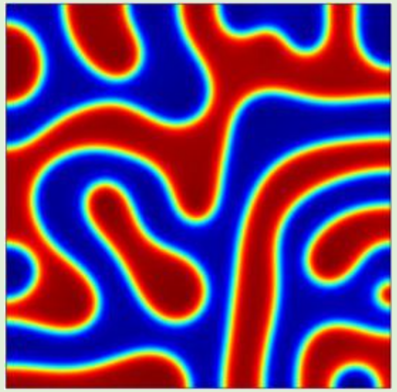
24658: Image-Based Computational Modeling and Analysis

Interface problems arise across many fields of physics and engineering.

Fluid-Fluid Interfaces

Multi-phase fluid flow

Convective Heat Flow

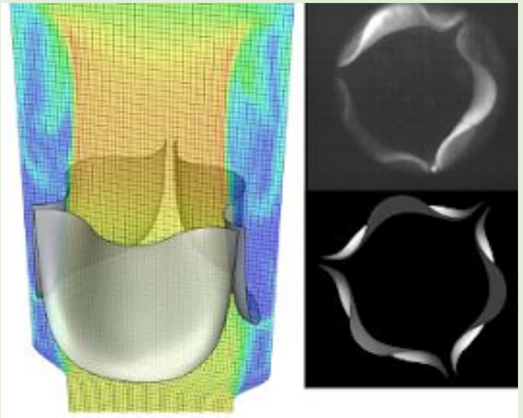


COMSOL

Fluid-Solid Interfaces

Fluid-structure interactions

Cardiovascular mechanics

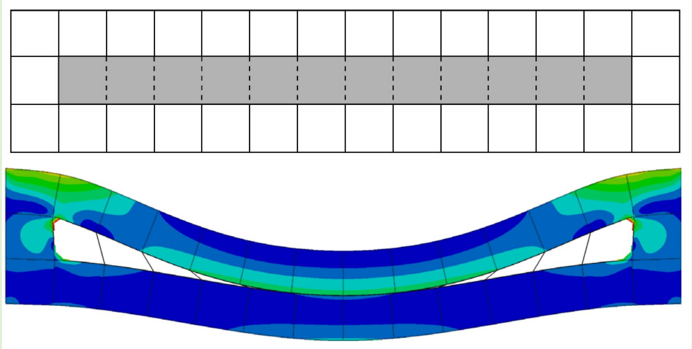


Kamensky, et al. 2017.

Solid-Solid Interfaces

Contact mechanics

Fracture mechanics

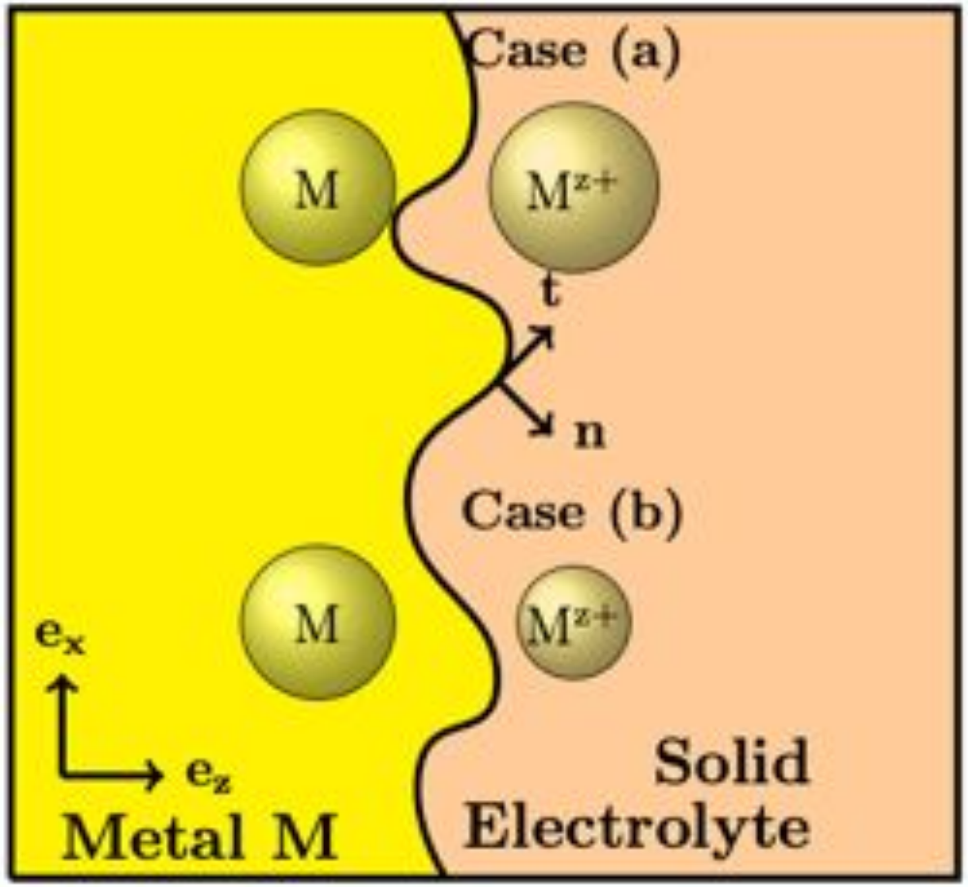


Bog, et al. 2015.

Tracking of the interface takes significant computational expense.

We are interested in moving-boundary problems

- Stefan problem - evolving boundary between phases
- Challenges:
  - discontinuous material properties
  - complex mesh generation
  - remeshing/ mesh evolution
  - mesh topology management



Ahmad, et al. 2017

Many computational approaches have been developed to captures these interfaces.

Explicit Interface Representations

Location of the interface is explicitly tracked, and interactions are captured at those interface points.

- Immersed Boundary Method
- Penetration Penalty Methods
- Lagrange Multiplier Methods

Implicit Interface Representations

Location of interface is captured with an auxiliary function/field, and interactions are incorporated into the energy functionals.

- Level Set Method
- Finite Cell Method
- Phase Field Method

Explicit Interface Representations

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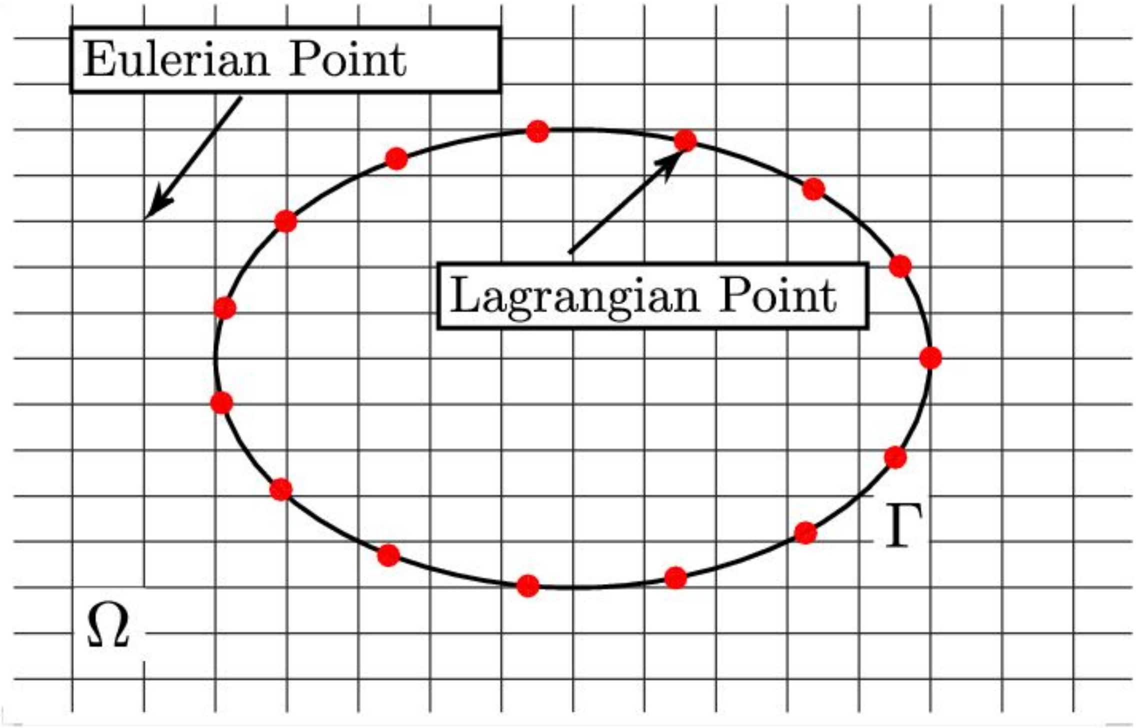
- Immersed Boundary Method



Cai, et al. 2017.

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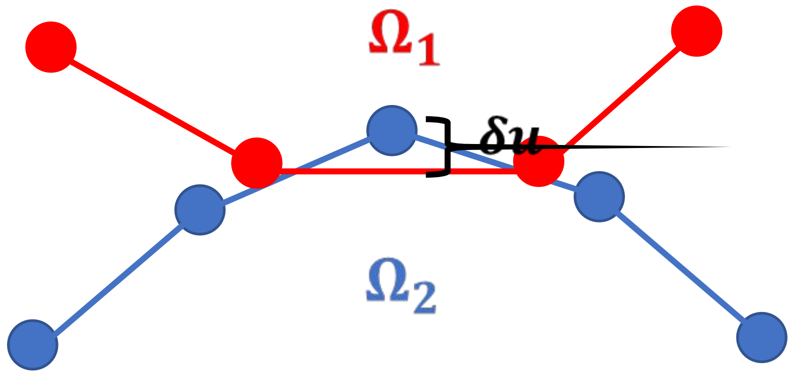

$$\underbrace{\int_{\Omega_1} \operatorname{div} \frac{\partial \Psi(\boldsymbol{u})}{\partial \boldsymbol{u}} \cdot \boldsymbol{v} \, d\Omega - \int_{\Omega_1} \boldsymbol{b} \cdot \boldsymbol{v} \, d\Omega - \int_{\partial\Omega_1} \boldsymbol{t} \cdot \boldsymbol{v} \, d\partial\Omega}_{\text{Standard Force Balance}} - \underbrace{\int_{\partial\Omega_1} f(\max(0, \delta u)) \cdot \boldsymbol{v} \, d\partial\Omega}_{\text{Penalty Force}} = 0$$

Aldakheel, et al. 2022

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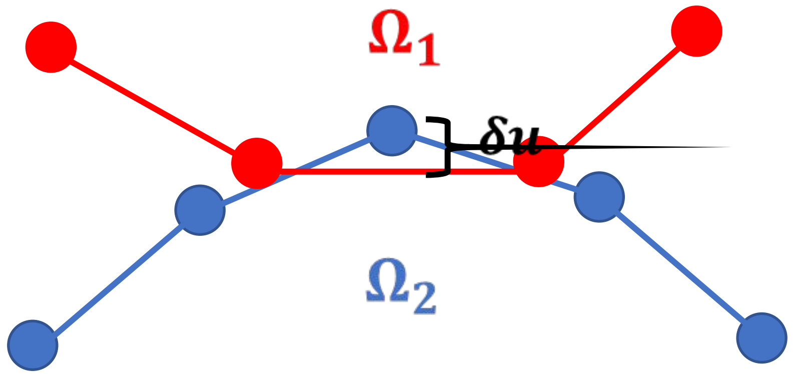

$$\underbrace{\int_{\Omega_1} \operatorname{div} \frac{\partial \Psi(\boldsymbol{u})}{\partial \boldsymbol{u}} \cdot \boldsymbol{v}\, d\Omega - \int_{\Omega_1} \boldsymbol{b} \cdot \boldsymbol{v}\, d\Omega - \int_{\partial\Omega_1} \boldsymbol{t} \cdot \boldsymbol{v}\, d\partial\Omega}_{\text{Standard Force Balance}} - \underbrace{\int_{\partial\Omega_1} \boldsymbol{\lambda}\, G(\delta u) \cdot \boldsymbol{v}\, d\partial\Omega}_{\text{Lagrange Multiplier}} = 0$$

Aldakheel, et al. 2022

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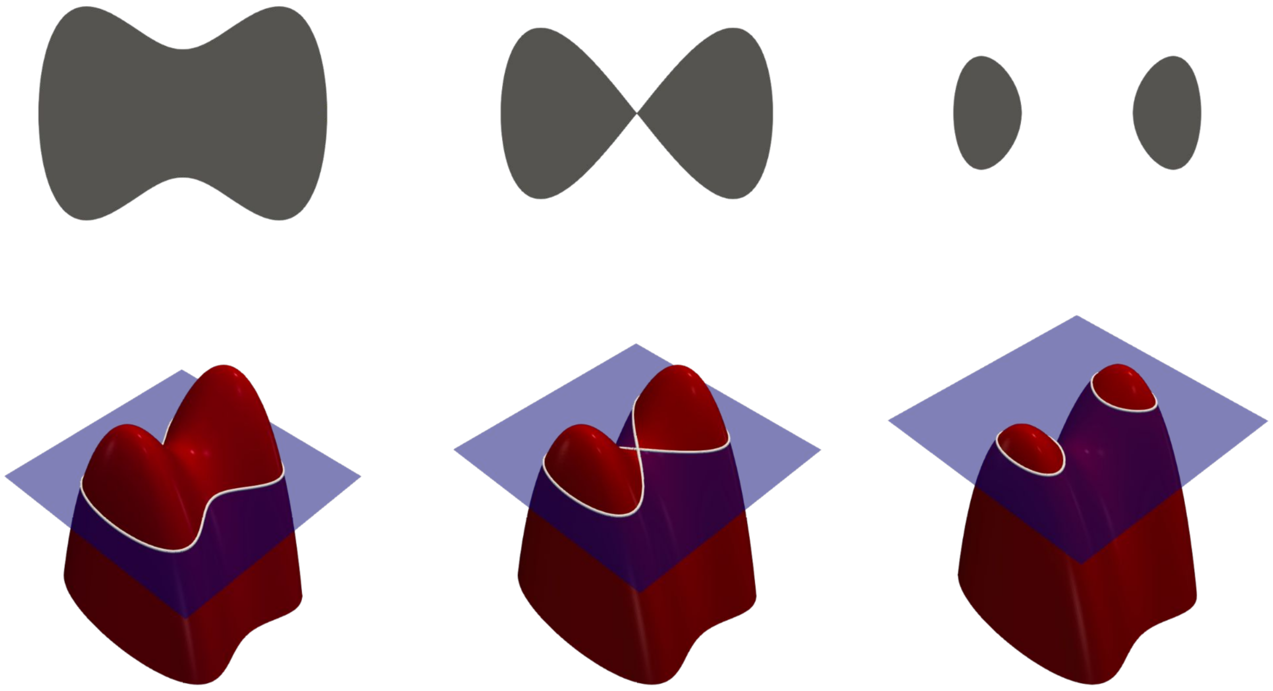

Wikipedia. *Phase Field Method.*

Implicit Interface Representations

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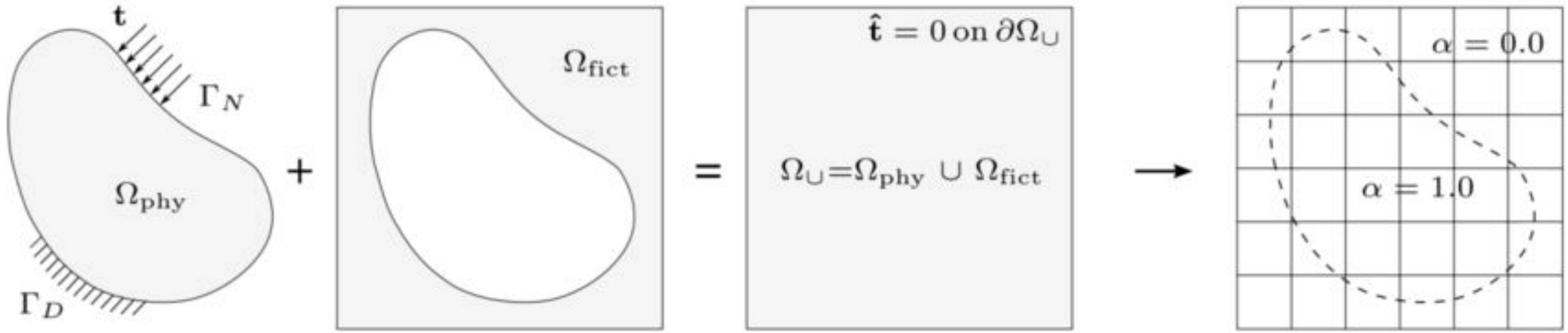
- Level Set Method
- Finite Cell Method



Elhaddad, et al. 2015

Implicit Interface Representations

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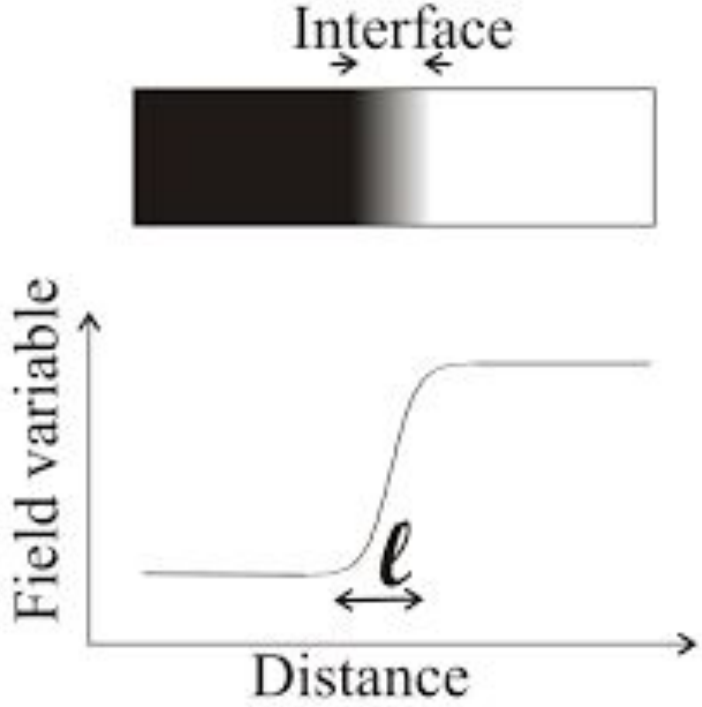
- Level Set Method
- Finite Cell Method
- Phase Field Model



Moelans, et al. 2008

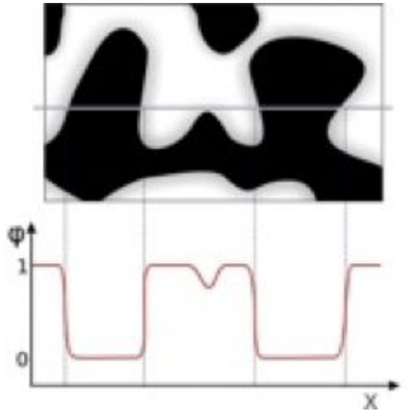
PFM boundary evolution is governed by energy minimization principles.

- Order parameter describes phase as a continuous variable

$$\phi : x \to [\phi_\alpha, \phi_\beta]$$

- Time-evolution of order parameter is due to gradient flows free-energy function

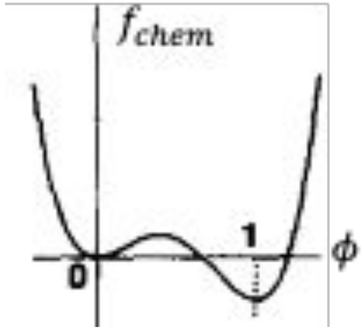
$$\frac{\partial \phi}{\partial t} = -M \frac{\delta F(\phi)}{\delta \phi}$$



Wikipedia. *Phase Field Method.*

- Double-well potential keeps material in either phase

$$F = \int_\Omega f_{chem} + \frac{1}{2}\kappa |\nabla \phi|^2 + \cdots \; dx \qquad f_{chem} = \varrho(\phi - \phi_\alpha)^2(\phi - \phi_\beta)^2$$



Wikipedia. *Phase Field Method.*

- Relevant physics is embedded in free-energy functional

Phase field methods can be applied for fracture mechanics problems.

- Standard field variable (ϕ) – indicator of material health

$$E[\boldsymbol{u}, \phi] = \int_{\Omega_c} [(1-\phi)W(\nabla\boldsymbol{u}) + G_c f(\phi)] d\Omega$$

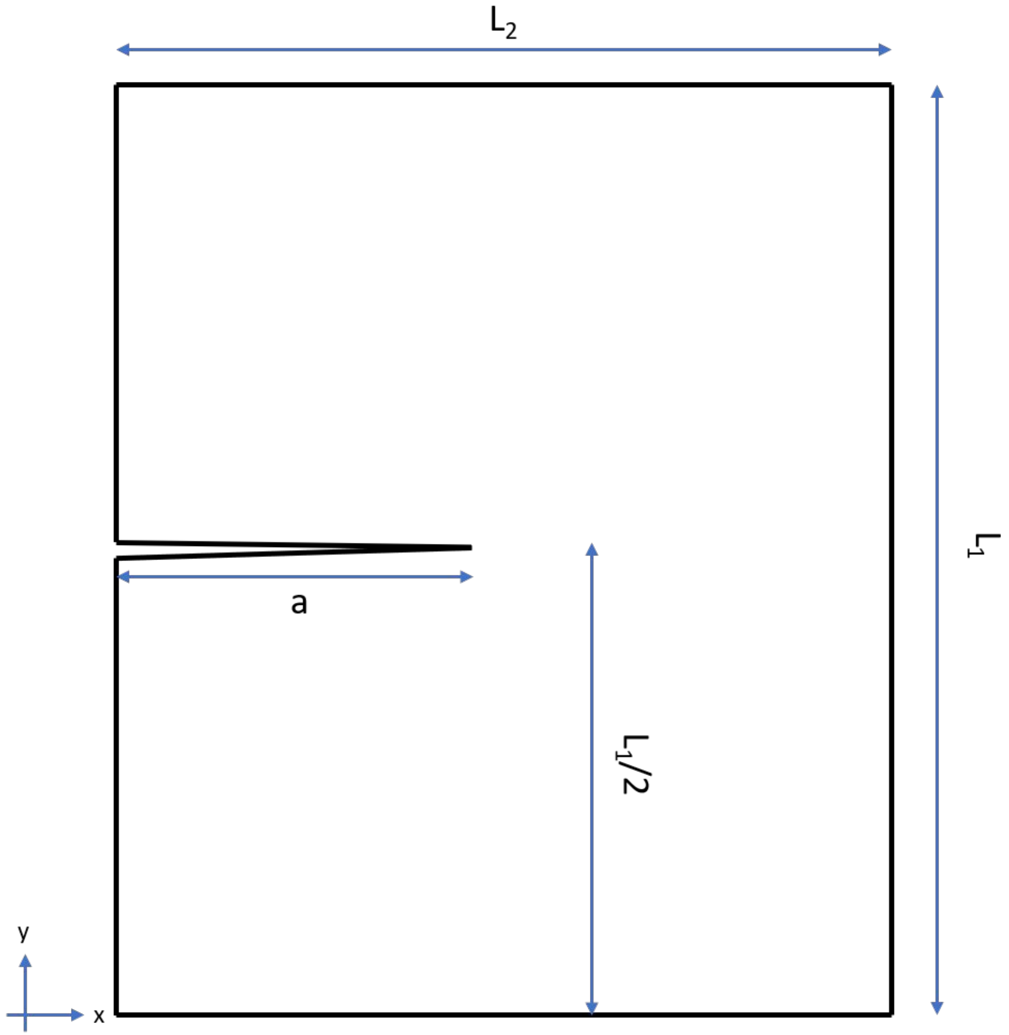
- Modified field variable ($\boldsymbol{d}$) – normal vector of crack face
  - Hakimzadeh et al. 2022

$$E[\boldsymbol{u}, \boldsymbol{d}] = \int_{\Omega_c} \left[\left((1-|\boldsymbol{d}|)^2\right)W(\nabla\boldsymbol{u}) + \left(1-(1-|\boldsymbol{d}|)^2\right)W_d(\nabla\boldsymbol{u}, \boldsymbol{d}) + G_c f(\boldsymbol{d})\right] d\Omega$$

By applying displacements to cracked, materials we can observe crack growth

- Material Properties (PMMA)
- $L_1 = L_2 = 1$
- $a = 0.5$

- Boundary Conditions:
  - Fixed displacement at base
  - Ramped vertical displacement at top



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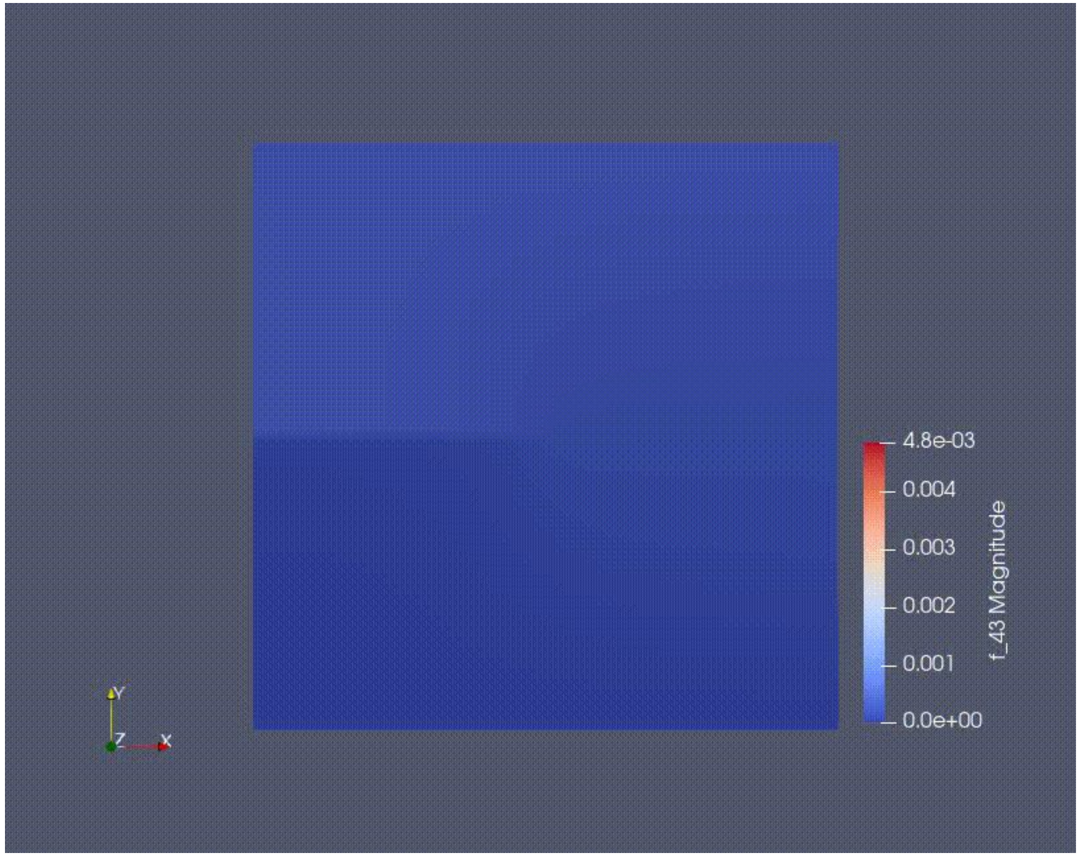

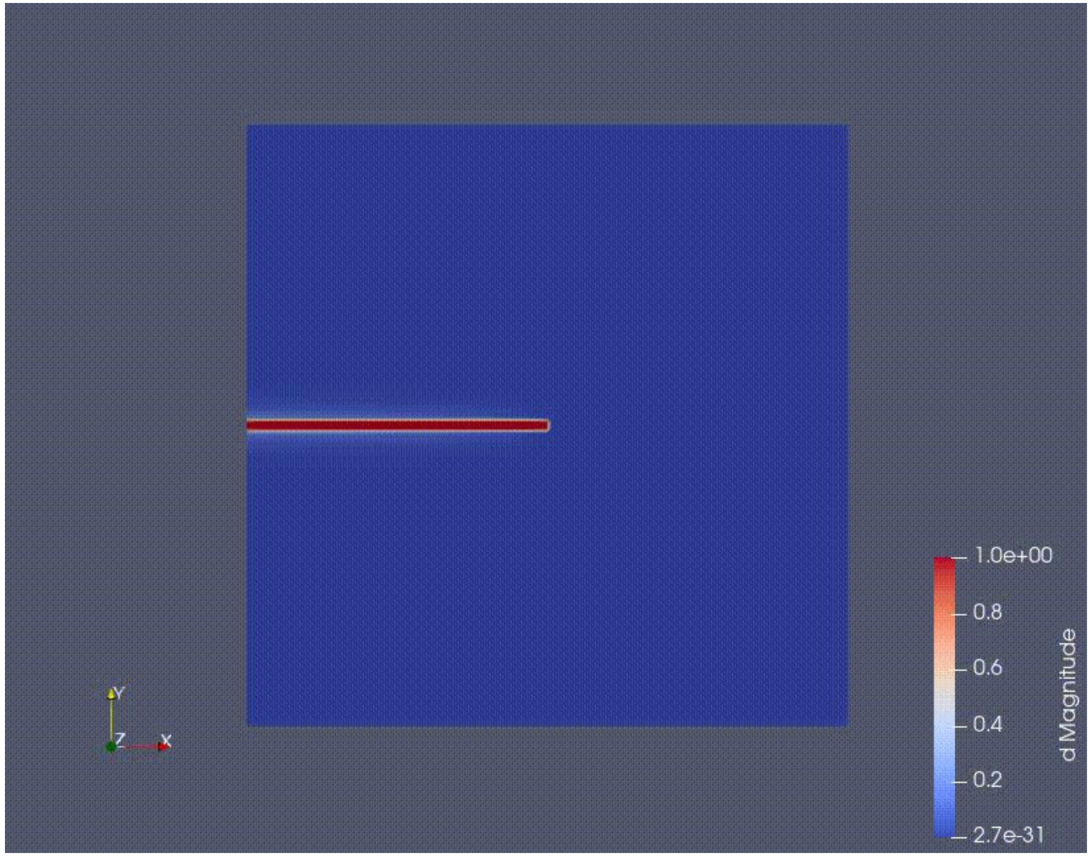

Future Directions

- Testing crack growth with:
  - Additional loading conditions
  - Varying initial crack lengths
- Comparisons with analytical modeling of crack energy

Questions?