Deep Ritz Method for the Phase Field Model of Fracture

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Motivation

- Phase field models are a popular technique to model damage and cracks
- Require refined and/or adaptive meshes when solved with the finite element method
- Investigate using neural networks as discretization
- *Find that a comparatively small number of degrees of freedom are required to represent localized solutions*

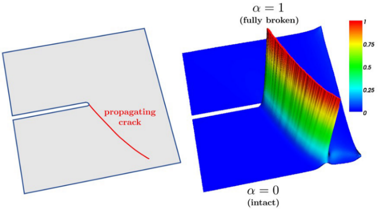


Figure: Sharp crack represented by scalar phase field [1]

Neural Networks and PDE's

- Karniadakis et al [3] introduce Physics-informed Neural Networks (PINN's)
- Solution represented with a feed-forward network
- "Trained" by minimizing the strong form residual at discrete points
- No data!

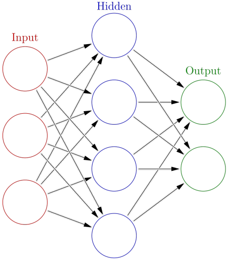


Figure: A single hidden-layer feed-forward neural network [2]

Neural Networks and PDE's

- Various techniques available to enforce boundary conditions
- Inspired many related investigations

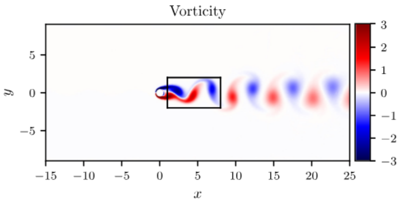
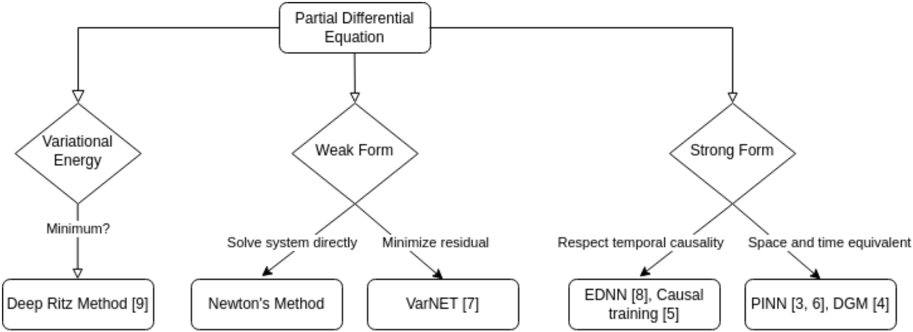


Figure: Incompressible Navier-Stokes simulation from [3]

Overview of Methods



- Different methods correspond to different perspectives on PDE solution
- Can be further categorized by method of BC enforcement
- *When possible, minimizing the variational energy is appealing*

Why Neural Networks?

- Global basis, no mesh
- Continuous and differentiable
- Easy to implement and prototype
- Convenience of automatic differentiation
- Neural networks very expressive
- Handle parametric problems easily

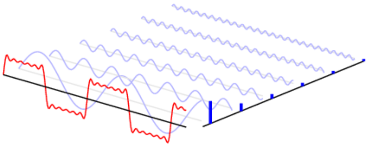
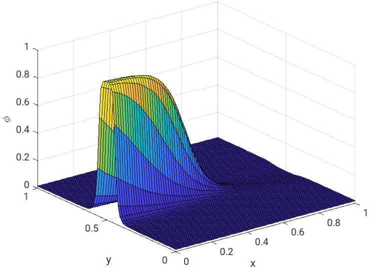


Figure: Spectral basis [10]



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The Deep Ritz Method

Principle of Minimum Potential Energy

If $\Pi\Big(u(x)\Big)$ is an energy functional and the PDE solution $u(x)$ is parameterized by θ, then the Galerkin optimal parameters can be determined by computing $\theta^* = \underset{\theta}{\text{argmin}}\ \Pi\Big(u(x;\theta)\Big)$

- Weights, biases, and architecture of network define discretization
- Solution is a nonlinear function of the parameters
- Variants of gradient descent or Newton-type optimization strategies used for minimization

Simple Example: 1D Boundary Value Problem

$$\frac{\partial^2 u}{\partial x^2} + 1 = 0, \quad u(0) = u(1) = 0$$

$$\Pi\Big(u(x)\Big) = \int_0^1 \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 - u dx$$

The solution is discretized with parameters $\theta = [w_1, b_1, w_2]$:

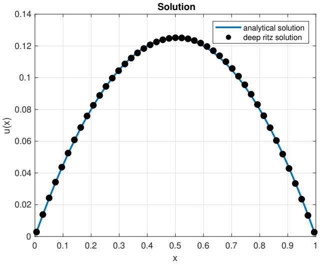
$$u(x) = w_2^T \sin(\pi x)\sigma(w_1 x + b_1)$$

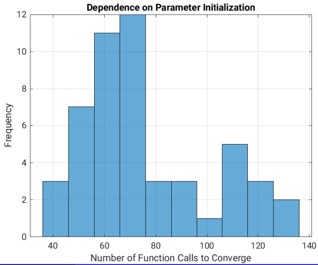
where $\sigma(\cdot)$ is a nonlinear activation function and $\sin(\pi x)$ enforces boundary conditions. The condition for a minimum of the energy is:

$$\frac{\partial \Pi}{\partial \theta} = \int_0^1 \frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial x \partial \theta} - \frac{\partial u}{\partial \theta} dx = 0$$

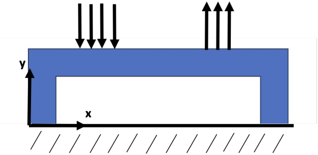
Simple Example: 1D Boundary Value Problem

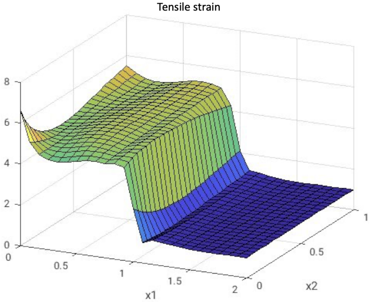
- Compute number of steps to obtain 1% relative ℓ_1 error with analytical solution
- Sequential Quadratic Programming (SQP) with line search sensitive to initialization
- Stochastic gradient descent slower to converge, but useful for complex objectives

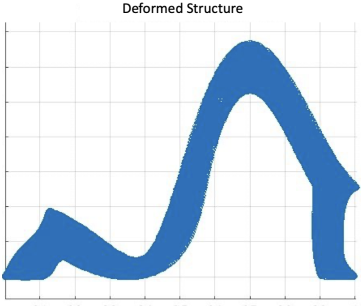




Other Examples







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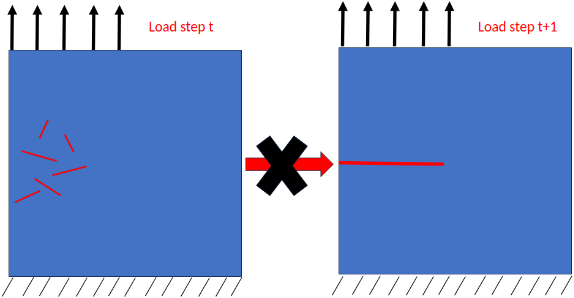
Energy Formulation of Isotropic Phase Field Fracture

Introduce the phase field $\phi \in [0, 1]$. The elastic potential energy is modified to account for energy associated with crack formation:

$$\Pi = \int_\Omega \frac{1}{2}(\phi - 1)^2 \epsilon_{ij} C_{ijk\ell} \epsilon_{k\ell} d\Omega + \int_\Omega \frac{G}{2\ell}\left(\phi^2 + \ell^2 \frac{\partial \phi}{\partial x_i}\frac{\partial \phi}{\partial x_i}\right) d\Omega - \int_{\partial\Omega} t_i u_i dS$$

Cracks release strain energy through softening the material, but also take energy to form. *The displacement and phase field are such that the total energy is minimized.*

Additional Considerations



- Load application is quasi-static process
- Cracks cannot "heal" $\implies \phi^{t+1}(x) \geq \phi^{t}(x)$
- Phase field model needs to be load-stepped, meaning that forces and/or displacements are applied incrementally

Remarks on Implementation

Penalty formulation used for the crack irreversibility condition:

$$\Pi^t = \int_\Omega \frac{1}{2}(\phi^t - 1)^2 \epsilon_i^t C_{ij} \epsilon_j^t d\Omega + \int_\Omega \frac{G}{2\ell}\left((\phi^t)^2 + \ell^2 \frac{\partial \phi^t}{\partial x_i}\frac{\partial \phi^t}{\partial x_i}\right) d\Omega + \lambda \int_\Omega max(0, \phi^{t-1} - \phi^t) d\Omega$$

Separate neural networks are used to discretize two displacement components and one phase field variable:

$$u_i(\underline{x}) = \mathcal{D}^{u_i}(\underline{x}) + \mathcal{B}^{u_i}(\underline{x})\underline{w}_2^{u_i} \cdot \sigma(\underline{\underline{w}}_1^{u_i}\underline{x} + \underline{b}_1^{u_i})$$

$$\phi(\underline{x}) = \frac{1}{2}\left(1 + \tanh\left(p\underline{w}_2^{\phi} \cdot \sigma(\underline{\underline{w}}_1^{\phi}\underline{x} + \underline{b}_1^{\phi})\right)\right)$$

$$\sigma(x) = \tanh(x)$$

Combination of ADAM and SQP with line-search used for optimization

Previous Work

- Lian et al. [11] and Goswami et al. [12, 13, 14] use energy formulation with hard BC enforcement and history variable
- Manav et al. [16] use energy formulation with hard BC enforcement and penalty
- *In this work, we follow Manav et al. in using the penalty method and take steps towards uncertainty quantification*

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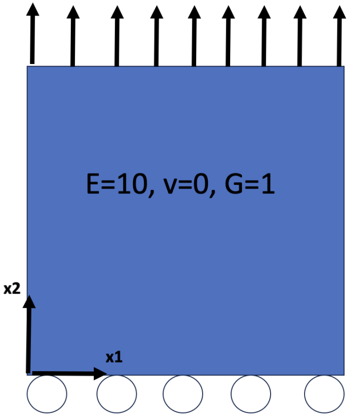
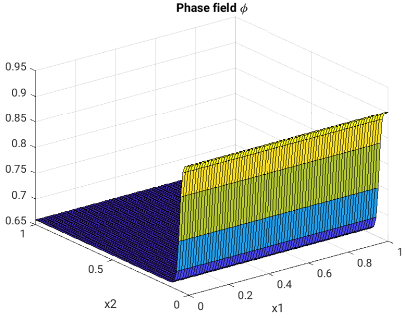
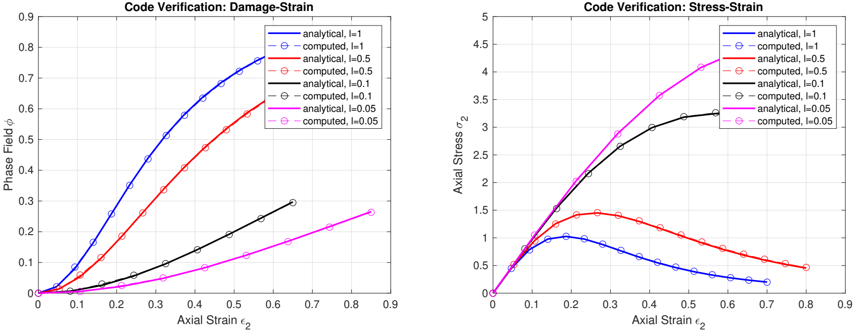
Code Verification





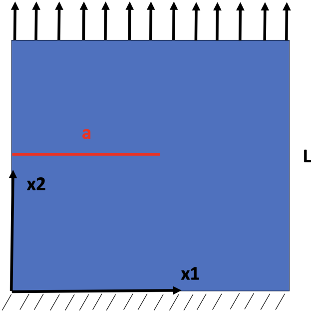
- Verify code against 1D analytical solution for displacement control
- Comparison with analytical solution breaks down when damage localizes along x_1 direction

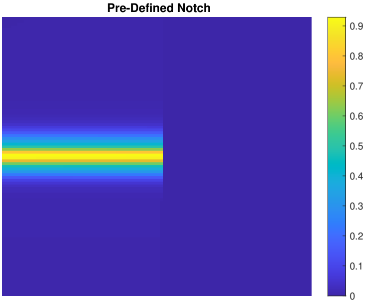
Code Verification



- Verify that 2D code finds 1D stress state and correct damage-strain relation
- Stop generating data when damage localizes
- Very good agreement in this regime

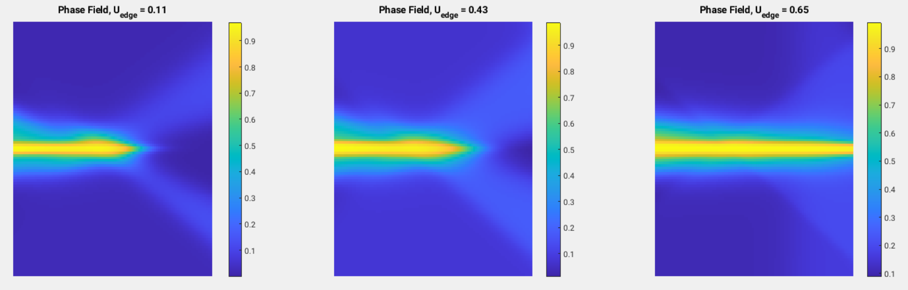
Displacement-driven Notched Plate (Plane Stress)





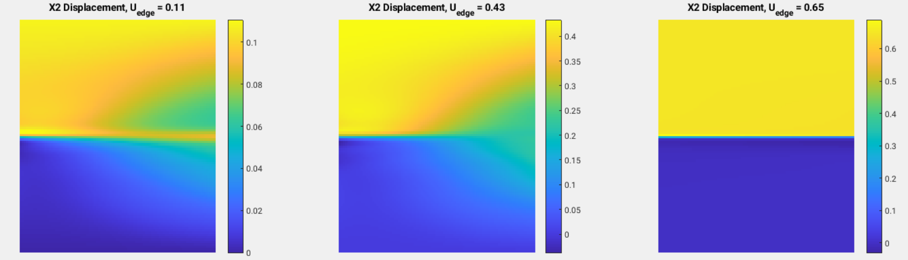
- Fit an initial crack in square plate by minimizing crack energy functional s.t. $\phi = 1$ along notch
- Displacement applied along top surface
- Problem parameters: $E = 10$, $\nu = 0.2$, $G = 1$, $\ell = 0.05$, $L = 1$, $a = 1/2$, $\sim$ 4000 integration points, 140 total neural network parameters

Results: Phase Field



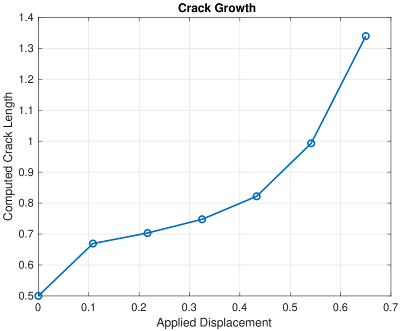
- Damage widens slightly when coupled with elasticity problem
- Crack follows expected path for notched tension specimen
- Fully-fractured at $U_{edge} = 0.65$

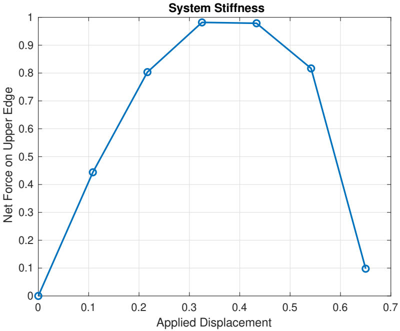
Results: Displacement Field



- Accurately captures displacement discontinuity across crack surface
- Nonlinear activation functions are well-suited for representing this kind of response

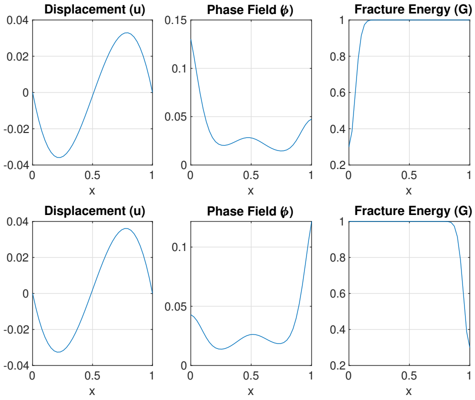
Results: Loading Curves

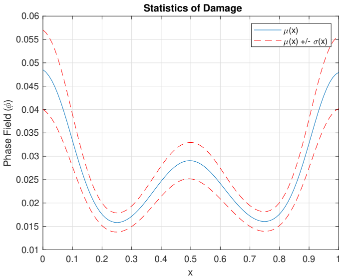




- Crack length can be computed by evaluating crack energy functional at the converged phase field $\implies \frac{1}{2\ell}\int_{\Omega}\phi^2 + \ell^2\nabla\phi\cdot\nabla\phi d\Omega$
- Rate of crack growth increases with the applied displacement; system exhibits softening behavior after the crack reaches a critical length

Work in Progress: Uncertainty Quantification





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Discussion

- Small networks sufficiently expressive to capture localized solution
- Penalty formulation is a simple approach to enforce irreversibility constraint
- Qualitative features of crack problem reliably captured; need to investigate "speed" of crack growth
- Changing optimization algorithm impacts the solution; ADAM widens damage but grows crack length, SQP sharpens damage profile but overly stiff
- Extending Deep Ritz Method to uncertainty quantification is promising

Future Work

- Verify rate of crack growth
- Better understand influence of the optimization algorithm
- Explore more sophisticated adaptive integration techniques
- Work on different fracture patterns
- Extend UQ efforts to more realistic problems

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