Virtual Elements For Computational Fracture Mechanics

Fadi Aldakheel
Blaž Hudobivnik & Peter Wriggers

Institute of Continuum Mechanics

May 18, 2021

Polygonal methods for PDEs: theory and applications, Online Conference 2021
Outline

- Motivation and overview

- Phase-field modeling of brittle and ductile fracture
  - Basic kinematics
  - Phase field approximation of crack topology
  - Constitutive work density function
  - Governing equations

- Virtual Element Method (VEM)
  - Basic introduction
  - Defining of physical fields quantities and gradients
  - Construction of the potential function
  - Stabilization

- Representative numerical examples

- Summary and conclusion
Computational Fracture Mechanics

- Discontinuous Approaches:
  - CZM
  - XFEM
  - Remeshing

- Continuous Approaches: **Phase-field**
Phase field approach is a very powerful technique to simulate complex crack phenomena in multiphysical environments.

- **Advantages:**
  - Simplicity and Generality
  - Solving mechanics problems with PDEs
  - No need for ad-hoc criteria (initiation, propagation, merging, branching)

- **Disadvantages:**
  - Requires very fine meshes
Motivation and Overview
Virtual element method (VEM)

- Basic principles of virtual element methods: Da Veiga & Brezzi et al. 2013
- Today’s Focus: Extension of VEM towards phase-field modeling of fracture
Outline

• Motivation and overview

• Phase-field modeling of brittle and ductile fracture
  ◦ Basic kinematics
  ◦ Phase field approximation of crack topology
  ◦ Constitutive work density function
  ◦ Governing equations

• Virtual element method (VEM)
  ◦ Basic introduction
  ◦ Definition of physical field quantities and gradients
  ◦ Construction of the potential function
  ◦ Stabilisation

• Representative numerical examples

• Summary and Conclusion
Phase-field modeling of fracture

Basic kinematics

The response of fracturing solid is described by deformation map and crack phase field

Primary Fields: $\mathcal{U} := \{\varphi, d\}$

A regularized crack functional that governs uniquely diffusive crack phase field inside $\Omega$

$$\Gamma_l(d) = \int_\Omega \gamma_l(d, \nabla d) \, d\Omega \quad \text{with} \quad \gamma_l(d, \nabla d) = \frac{1}{2l} d^2 + \frac{l}{2} |\nabla d|^2$$

in terms of the crack surface density function $\gamma_l(d, \nabla d)$ per unit volume
Phase Field modeling of fracture

Phase field approximation of crack topology

Diffusive approximation of crack topology $\Gamma_l(d)$ for different $l$ embedded into $\Omega \subset \mathbb{R}^3$

Minimization Principle allows to determine the regularized crack phase field $d(x, t)$ in $\Omega$

$$d(x, t) = \text{Arg}\left\{ \inf_{d \in W_{\Gamma(t)}} \Gamma_l(d) \right\}$$

subject to the Dirichlet-type constraints $W_{\Gamma(t)} = \{d \mid d(x, t) = 1 \text{ at } x \in \Gamma(t)\}$ yielding

$$d - l^2 \Delta d = 0 \text{ in } \Omega \quad \text{and} \quad \nabla d \cdot n = 0 \text{ on } \partial \Omega$$

where $\Delta d$ is the Laplacian of the crack phase field and $n$ the outward normal on $\partial \Omega$. 
Phase Field modeling of fracture

Phase field approximation of crack topology
Phase-field modeling of fracture

Phase Field modelling of brittle and ductile fracture (Aldakheel et al. CMAME 2018)

- Global fields: \( \mathbf{U} = \{\varphi, d\} \), Constitutive state variables: \( \mathbf{C} = \{b_e, \alpha, \mathcal{H}, d, \nabla d\} \)
- Deformation gradient: \( \mathbf{F} = \nabla \mathbf{u} + \mathbf{1} = \mathbf{F}^e \mathbf{F}^p \)
- Elastic strain tensor: \( b_e = \mathbf{F}^e \mathbf{F}^{eT} = \mathbf{F} \mathbf{C}_p^{-1} \mathbf{F}^T \) with \( \mathbf{C}_p = \mathbf{F}^p \mathbf{F}^p \)
- Total pseudo-energy density per unit volume:

\[
W(\mathbf{C}) = W_{elas}(b_e, d) + W_{plas}(\alpha, d) + W_{frac}(\mathcal{H}, d, \nabla d)
\]

- The elastic contribution with crack evolution only in tension

\[
W_{elas}(b_e, d) = g(d) \left[ \psi_{vol}^+(b_e) + \psi_{iso}(b_e) \right] + \psi_{vol}^-(b_e) \quad \text{with} \quad g(d) = (1 - d)^2
\]

- The volumetric and isochoric parts of the elastic energy are defined as

\[
\psi_{vol}^\pm = \frac{\kappa}{4} (I_3^\pm - 1 - \ln I_3^\pm) \quad \text{and} \quad \psi_{iso} = \frac{\mu}{2} (I_3^{-1/3} I_1 - 3) \quad \text{with} \quad I_1 = \text{tr} b_e
\]

in terms of the positive and the negative third invariant \( I_3 = \det b_e \) defined as

\[
I_3^+ := \max\{I_3, 1\} = \langle I_3 - 1 \rangle_+ + 1 = \frac{1}{2} \left[ (I_3 - 1) + |I_3 - 1| \right] + 1
\]

\[
I_3^- := \min\{I_3, 1\} = \langle I_3 - 1 \rangle_- + 1 = \frac{1}{2} \left[ (I_3 - 1) - |I_3 - 1| \right] + 1
\]
Phase-field modeling of fracture
Phase Field modelling of brittle and ductile fracture (Aldakheel et al. CMAME 2018)

- Global fields: $\mathcal{U} = \{\varphi, d\}$, Constitutive state variables: $\mathcal{C} = \{b_e, \alpha, \mathcal{H}, d, \nabla d\}$
- Total pseudo-energy density per unit volume:
  \[ W(\mathcal{C}) = W_{elas}(b_e, d) + W_{plas}(\alpha, d) + W_{frac}(\mathcal{H}, d, \nabla d) \]
- The elastic contribution with crack evolution only in tension
  \[ W_{elas}(b_e, d) = g(d) \left[ \psi_{vol}^+(b_e) + \psi_{iso}(b_e) \right] + \psi_{vol}^-(b_e) \]
  with \( g(d) = (1 - d)^2 \)
- The plastic contribution is assumed to have the form
  \[ W_{plas}(\alpha, d) = g(d) \psi_p(\alpha) \]
  with \( \psi_p = Y_0 \alpha + \frac{H}{2} \alpha^2 + (Y_\infty - Y_0)(\alpha + \exp[-\delta \alpha]/\delta) \)
- The fracture part of pseudo-energy density
  \[ W_{frac}(d, \nabla d) = 2\frac{\psi_c}{\zeta} l \gamma_l(d, \nabla d) + \frac{\eta}{2 \Delta t} (d - d_n)^2 + g(d) \mathcal{H} \]
Phase-field modeling of fracture

Phase Field modelling of brittle and ductile fracture (Aldakheel et al. IJMCE 2018)

- Global fields: $\mathbf{U} = \{\varphi, d\}$, Constitutive state variables: $\mathbf{C} = \{b_e, \alpha, \mathcal{H}, d, \nabla d\}$
- Local history variables: $\mathbf{h} = \{\mathbf{C}^{-1}_p, \alpha\}$ at one Gauss point of an element
- Elastic strain tensor: $b_e = \mathbf{F}^e \mathbf{F}^{eT} = \mathbf{F} \mathbf{C}^{-1}_p \mathbf{F}^T$ with $\mathbf{C} = \mathbf{F}^p T \mathbf{F}^p$
- Kirchoff stress tensor: $\tau = 2 b_e \frac{\partial \Psi}{\partial b_e}, \quad s = \tau - \frac{1}{3} \text{tr} \tau$
- Yield function: $\Phi = \sigma_{VM} - [Y_\infty - (Y_\infty - Y_0) e^{-\delta \alpha} + H \alpha], \sigma_{VM} = \sqrt{\frac{3}{2}} \|s\|$
- Check yielding: IF $\Phi < 0$ then elastic $\mathbf{h} \leftarrow \mathbf{h}^n$ else plastic
- Plastic evolution: $\mathbf{Q} = \mathbf{F} \mathbf{C}^{-1}_p - \exp[-2(\alpha - \alpha_n) \mathcal{N}] \mathbf{F} \mathbf{C}^{-1}_p, \quad \mathcal{N} = \frac{\partial \Phi}{\partial \mathbf{s}}$
- Local residual: $\mathbf{Q} = \{\mathbf{Q}, \Phi\} \rightarrow 0 \quad \Rightarrow \quad$ Solve for $\mathbf{h}$
Phase-field modeling of fracture

Governing equations (Aldakheel et al. CMAME 2018 + IJMCE 2018)

- Balance of linear momentum

\[ \text{Div} [P] + \bar{f} = 0 \]

- Incremental evolution of the crack phase-field

\[ \eta (d - d_n) / \tau = (1 - d) \mathcal{H} - [d - l^2 \Delta d] \]

with the crack driving force \( \mathcal{H} \) that accounts on irreversibility of phase-field evolution by filtering out a maximum value of the crack driving state function \( D \)

\[ \mathcal{H} = \max_{s \in [0,t]} D(X, s) \geq 0 \quad \text{with} \quad D := \left( \psi^{+}_{vol} + \psi_{iso} + \psi_{p} - \psi_{c} \right)_{+} \]

with Macaulay bracket \( \langle x \rangle_{+} := (x + |x|)/2 \) to ensures irreversibility of crack evolution
Outline

• Motivation and overview

• Phase-field modeling of brittle and ductile fracture
  ○ Basic kinematics
  ○ Phase field approximation of crack topology
  ○ Constitutive work density function
  ○ Governing equations

• Virtual element method (VEM)
  ○ Basic introduction
  ○ Definition of physical field quantities and gradients
  ○ Construction of the potential function
  ○ Stabilisation

• SPP2020: Water-induced failure mechanics for concrete

• Summary and Conclusion
Virtual element method (VEM)

Basic introduction

VEM ansatz

- The field variables are split into a projection part $\mathbf{U}_\Pi$ and a reminder as

$$\mathbf{U} = \mathbf{U}_\Pi + (\mathbf{U} - \mathbf{U}_\Pi), \quad \text{with} \quad \mathbf{U}_\Pi = \mathbf{N}_\Pi \cdot \mathbf{A}, \quad \text{and} \quad \mathbf{U} = (\mathbf{N}_{\text{FEM}} \cdot \mathbf{U}_e)$$

$\mathbf{U}$ is a list of physical fields, e.g. displacements: $\mathbf{u}$, phase-field: $\mathbf{d}$, ...

- The polynomial projection function of 1st order VEM is $\mathbf{N}_\Pi = (1, X, Y, Z)$

FEM ansatz
Virtual element method (VEM)

Defining of physical fields quantities and gradients

- A direct evaluation of $\nabla \mathbf{U}_\Pi$ (constant) is possible: (Wriggers et al. 2016)

$$\int_{\Omega_e} \nabla \mathbf{U}_\Pi \, dV = \int_{\Omega_e} \nabla \mathbf{U} \, d\Omega \quad \text{and} \quad \frac{1}{n_V} \sum_{I=1}^{n_V} \mathbf{U}_\Pi I = \frac{1}{n_V} \sum_{I=1}^{n_V} \mathbf{U}_I$$

- The parameters of coefficient matrix $\mathbf{A}$ follow as:

$$A_{ij, j \geq 2} = \nabla \mathbf{U}_\Pi^e = \frac{1}{\Omega_e} \int_{\Gamma_e} \mathbf{U} \otimes \mathbf{N} \, d\Gamma \quad \text{and} \quad A_{i1} = \frac{1}{n_V} \sum_{I=1}^{n_V} [\mathbf{U}_I - \nabla \mathbf{U}_\Pi I \cdot \mathbf{X}_I]$$
Virtual element method (VEM)

Construction of the potential function

- The total potential functional of VEM is defined as:
  \[ \Pi(\mathbf{u}) = \sum_{e=1}^{N_e} \Pi_e, \quad \Pi_e = [\Pi_c(\mathbf{u}_\Pi) + \Pi_{stab}(\mathbf{u} - \mathbf{u}_\Pi)] , \]

  \[ \Pi_c(\mathbf{u}_\Pi) = \int_{\Omega_e} W(\mathbf{C}_\Pi) \, d\Omega - \int_{\Omega_e} \mathbf{f} \cdot \mathbf{C}_\Pi \, d\Omega - \int_{\Gamma_e} \mathbf{t} \cdot \mathbf{C}_\Pi \, d\Gamma \ldots \]

- The constitutive state variables are defined as
  \[ \mathbf{C}_\Pi = \{\mathbf{u}_\Pi, \nabla \mathbf{u}_\Pi\}, \quad \text{such as} \quad \mathbf{C}_\Pi = \{\nabla \mathbf{u}_\Pi, \mathbf{d}_\Pi, \nabla \mathbf{d}_\Pi \ldots\} \]

- The compatibility term \( \Pi_c(\mathbf{u}_\Pi) \) alone will result in rank deficient tangent

- The stabilization term \( \Pi_{Stab} \) is needed for completeness

- Element residual and tangent follows automatically by employing AceGen:
  \[ \mathbf{R}_e = \left. \frac{\partial \Pi_e}{\partial \mathbf{u}_e} \right|_{\text{const}}, \quad \mathbf{K}_e = \left. \frac{\partial \mathbf{R}_e}{\partial \mathbf{u}_e} \right|_{\text{const}} \]

- \( \mathbf{u}_e \) are all nodal DOF, \( \text{const} \) are derivation constants
Virtual element method (VEM)

Construction of the potential function

• The compatibility part of 1st order VEM can be evaluated directly as:

\[
\Pi_c(\mathbf{u}_\Pi) = \int_{\Omega_e} W(\mathbf{C}_\Pi) \, d\Omega = \Omega_e W(\mathbf{C}_\Pi(\mathbf{x}_C))
\]
Virtual element method (VEM)

Stabilization

- Difference between potentials: $\Pi_{stab} = \hat{\Pi}(\mathbf{u}) - \hat{\Pi}(\mathbf{u}_\Pi)$ with $\hat{\Pi} = \beta \Pi_c$
- $\hat{\Pi}(\mathbf{u}_\Pi)$ is integrated analogous to $\Pi_c(\mathbf{u}_\Pi)$
- $\hat{\Pi}(\mathbf{u})$ by standard FEM shape functions on triangle sub-mesh
- The potential is then
  $\Pi_e = \Pi_c(\mathbf{u}_\Pi) + \hat{\Pi}(\mathbf{u}) - \hat{\Pi}(\mathbf{u}_\Pi) = (1 - \beta)\Pi_c(\mathbf{u}_\Pi) + \beta \Pi_c(\mathbf{u})$
- $\beta = 1 \rightarrow$ FEM, $\beta = 0 \rightarrow$ only rank deficient projection
**VEM + Phase Field**

Stabilization parameter (Aldakheel et al. *CMAME 2018*)

- The choice of $\beta \in (0, 1)$
- If element size limits towards 0, stability term will disappear
- Any choice larger than 0 is sufficient. The optimal ratio extrapolated from the $\beta$ of hyperelastic case and various cases is around $\beta = 0.4$:

![Graph](image)

- a) phase field $\beta$ study (notched block)
- b) hyperelastic $\beta$ study (cooke)
Outline

• Motivation and overview

• Phase-field modeling of brittle and ductile fracture
  ○ Basic kinematics
  ○ Phase field approximation of crack topology
  ○ Constitutive work density function
  ○ Governing equations

• Virtual element method (VEM)
  ○ Basic introduction
  ○ Definition of physical field quantities and gradients
  ○ Construction of the potential function
  ○ Stabilisation

• Representative numerical examples

• Summary and Conclusion
Representative numerical examples

Tensile test of block with two holes or notches:

- Dimensions: $L = 20\text{mm}$, $H = 10\text{mm}$, $R = 2\text{mm}$ and $A = 3\text{mm}$
Representative numerical examples

- Phase field evolution of block with two holes:
Representative numerical examples

Virtual element formulation for phase-field modeling of ductile fracture

Axial stretch of a bar

\[ \text{Aldakheel+Hudobivnik+Wriggers [IJMCE 2018]} \]
Representative numerical examples

Virtual element formulation for phase-field modeling of ductile fracture

Equivalent plastic strain $\alpha$ and crack phase-field $d$ evolution
Adaptive VEM for Large-Strain Phase-Field Fracture
VEM for crack propagation and cutting techniques

Modeling crack propagation using VEM

- A prescribed crack evolution during a tensile load condition
- Crack path has the possibility to change its direction within a virtual element
- A kinked crack can be modeled using VEM without any restriction
VEM for crack propagation and cutting techniques
Wall mounting of a bolt: Adaptive VEM + Fracture + Contact
Summary and Conclusion

- The virtual element method is a generalization of the finite element method, which has inspired from modern mimetic finite difference schemes.
- It can simulate various range of problems, from linear to highly nonlinear and multi-field problems.
- Solving of certain geometrical problems is greatly simplified, e.g. contact and cutting.
- Phase field approach is a very powerful technique to simulate complex crack phenomena in multi-physical environments.