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Arbitrary order virtual element methods for high-order phase-field modeling of dynamic fracture

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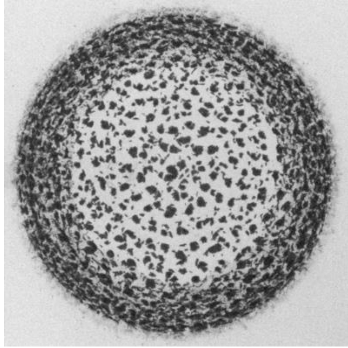
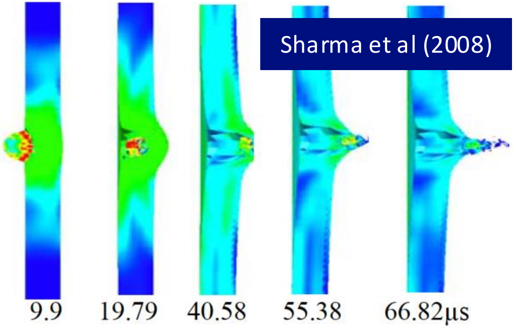
Outline

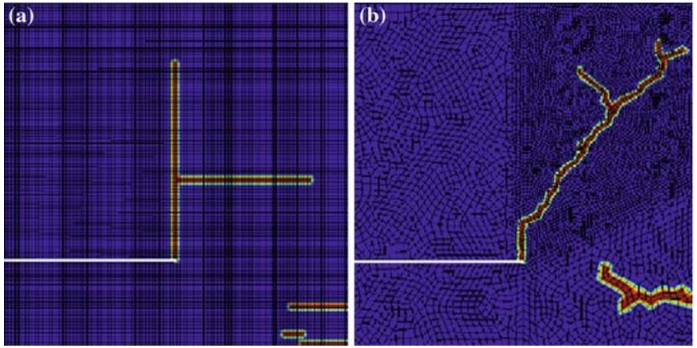
- **Motivation and high-order phase-field fracture model**
- **Virtual element method**
  - Motivation
  - Virtual element method is a finite element method.
- **Numerical experiments**
  - Dynamic crack branching using different elements
  - Quasi-static benchmark test
- **Summary**

Motivation





Sharma et al (2008)



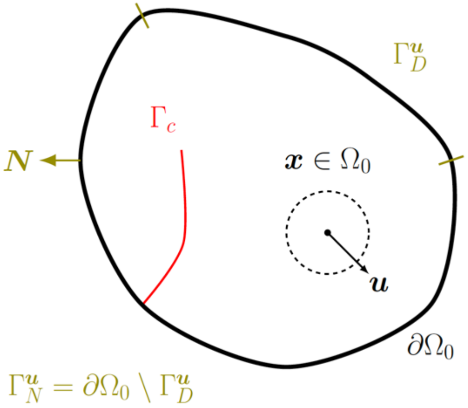
- The physical processes that culminate in fracture (and the interplay between them) are complex, and dependent on the material and the applied loading
- This complexity is most pronounced in problems which involve extreme conditions, multi-physics and multi-scale aspects
- Predictive computational treatments, that are practical and amenable to implementation, are currently unavailable

Modeling of material failure (damage and fracture)

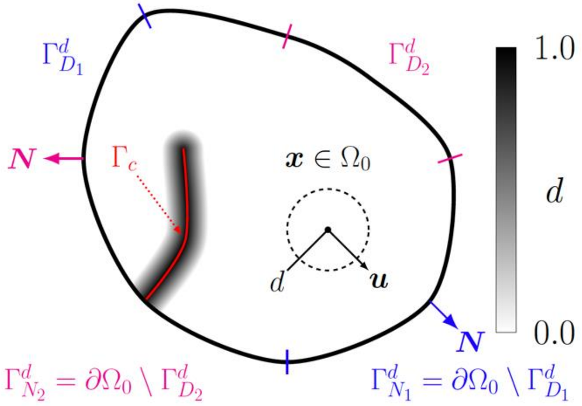
- Still, *predictive* modelling of crack initiation and propagation in materials and structures remains *one of the most significant challenges in solid mechanics* (Wu et al, 2019)
- Two general approaches to the representation of material failure in a computational setting:
  - The discrete approach: representing failure as a discontinuity
  - The continuous approach: representing failure using damage variables
- Examples of the discrete approach include Cohesive Zone Models (CZM) and Sub-grid Embedded / eXtended Finite Element Methods (EFEM/XFEM)
- Examples of the continuous approach include Continuum Damage Mechanics (CDM), Peridynamics, and Phase-field Fracture Models (PFM).

The phase-field method for brittle fracture

Sharp Crack Representation



Diffusive Crack Representation



Approximation based on the introduction of a crack phase field
$d \in [0,1]$

$d = 0$: undamaged
$d = 1$: broken

- Based on the variational formulation of Bourdin et al (2008), crack propagation can be expressed as an energy minimization problem:

Crack density function

$$\mathcal{E} = \int_{\Omega_0 \setminus \Gamma_c} W_e(\boldsymbol{F})\,\mathrm{d}V + \int_{\Gamma_c} G_c\,\mathrm{d}A \;\xleftarrow[\text{Gamma convergence}]{\ell_0 \to 0}\; \mathcal{E} \approx \underbrace{\int_{\Omega_0} \hat{W}_e(\boldsymbol{F}, d)\,\mathrm{d}V}_{\text{Elastic energy functional}} + \underbrace{\int_{\Omega_0} G_c \boxed{\gamma_{\ell_0}(d, \nabla d, \Delta d)}\,\mathrm{d}V}_{\text{Surface energy functional}}$$

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High-order phase-field fracture model

High-order term

$$\rho \ddot{\boldsymbol{u}} - \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}, d) - \boldsymbol{f} = \mathbf{0}, \quad \text{on } \Omega \times (0, T],$$

$$\boxed{\alpha_2 \Delta^2 d} - \alpha_1 \Delta d + \alpha_0 d + g'(d)\mathcal{H}_t = 0, \quad \text{on } \Omega \times (0, T],$$

Stress: $\boldsymbol{\sigma}(\boldsymbol{u}, d) = g(d)\left[\lambda \operatorname{tr}(\boldsymbol{\varepsilon}) \boldsymbol{I} + 2\mu \boldsymbol{\varepsilon}\right].$

Strain (small deformation): $\boldsymbol{\varepsilon}(\boldsymbol{u}) = \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)/2$

Strain decomposition: $\boldsymbol{\varepsilon}_{\pm} = \sum_I \langle \varepsilon_I \rangle_{\pm} \boldsymbol{n}_I \otimes \boldsymbol{n}_I,$

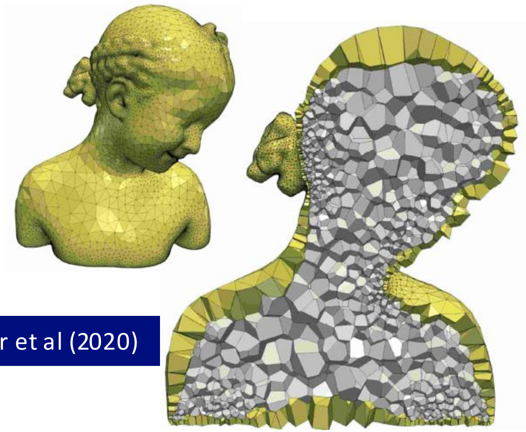
History variable: $\mathcal{H}_t = \max\limits_{t \in (0,T]} \Psi^+(\boldsymbol{\varepsilon}).$

Staggered scheme for solving the two equations

Generalized-alpha method for time integration

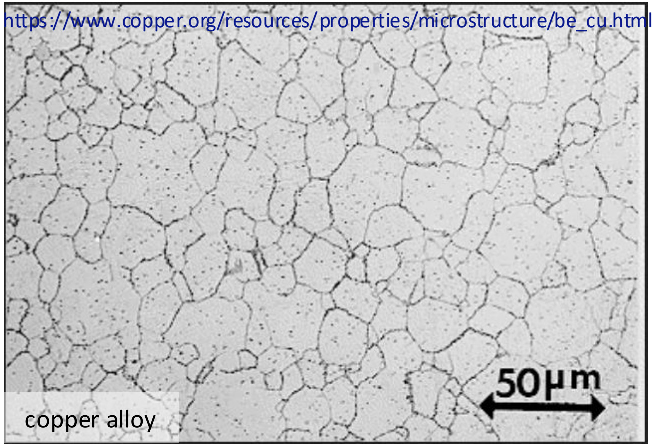
Motivation: Polytopal elements

- Polytopal (2D polygonal / 3D polyhedral) elements greatly reduce the difficulty of meshing geometrically complex domains
- This allows overly-stiff triangular/tetrahedral elements to be avoided in such applications
- Microstructure of the materials



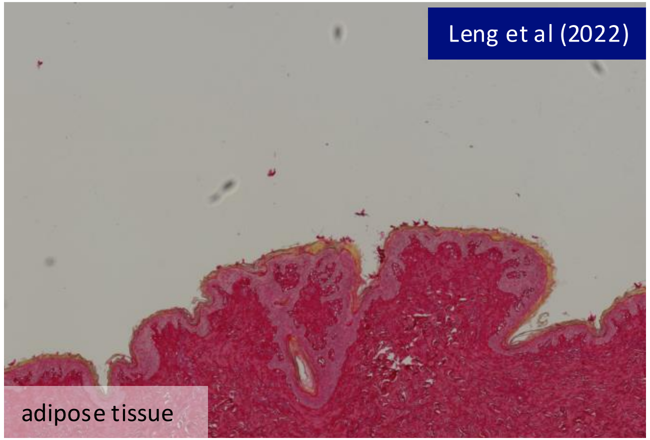
Abdelkader et al (2020)

https://www.copper.org/resources/properties/microstructure/be_cu.html



copper alloy

Leng et al (2022)



adipose tissue

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Finite element method

$$-\Delta u = f \quad \text{in } \Omega \qquad \text{with} \quad u = 0 \quad \text{on } \partial\Omega$$

Find $u \in H_0^1(\Omega)$ *such that*

$$\int_\Omega \nabla u \cdot \nabla v \, dV = \int_\Omega f v \, dV \quad \forall v \in H_0^1(\Omega)$$

Find $u_h \in \mathcal{V}_0^{h,k} \subset H_0^1(\Omega)$ *such that*

$$\int_\Omega \nabla u_h \cdot \nabla v_h \, dV = \int_\Omega f v_h \, dV \qquad \forall v_h \in \mathcal{V}_0^{h,k}$$

where $\mathcal{V}_0^{h,k} \subset H_0^1(\Omega)$ is the **(conforming) finite element space**.

Finite element method

We introduce a set of **basis functions**: $\mathcal{V}_0^{h,k} = \mathrm{span}\{\psi_1, \psi_2, \ldots, \psi_N\}$

We consider the expansion of the solution u_h on the basis functions ψ_j

$$u_h(\mathbf{x}) = \sum_{j=1}^{N} u_j \psi_j(\mathbf{x}), \qquad u_j = \textbf{degrees of freedom}$$

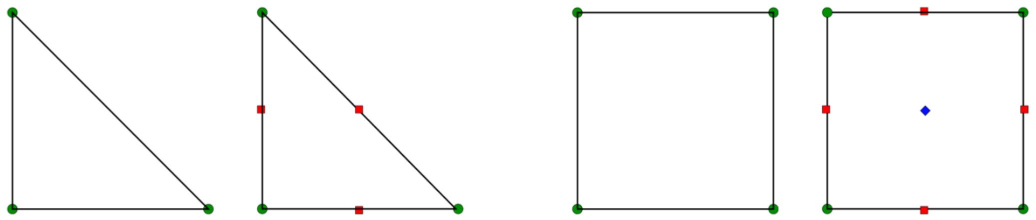
Solving the linear system

$$\mathbf{Au} = \mathbf{b} \qquad \equiv \qquad \sum_{j=1}^{N} \underbrace{\left(\int_\Omega \nabla\psi_i \cdot \nabla\psi_j \, dV \right)}_{\textbf{A: STIFFNESS MATRIX}} u_j = \underbrace{\int_\Omega f \psi_i \, dV}_{\textbf{b: R.H.S.}} \quad \forall i$$

gives us the **degrees of freedom** $\{u_j\}$ of u_h

VEM follows the same procedure – VEM is a finite element method

Basis functions in simple geometric shapes



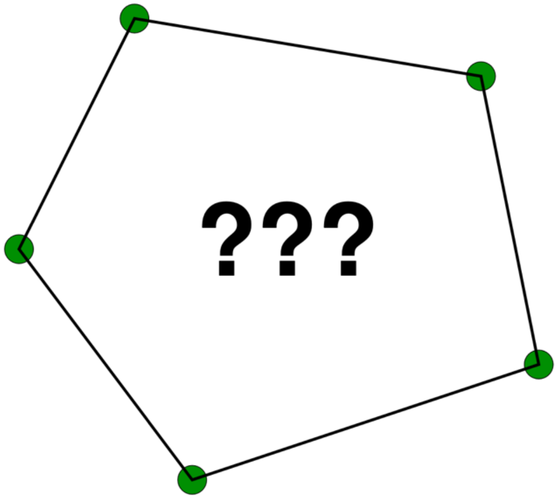
Polynomials basis functions supporting **Lagrange interpolation**: $\psi_j(\mathbf{x}_i) = \delta_{i,j}$
and reproducing polynomial functions exactly

$$\text{for } k = 1: \qquad 1 = \sum_j \psi_j(\mathbf{x}), \quad \mathbf{x} = \sum_j \mathbf{x}_j \psi_j(\mathbf{x}),$$

$$\text{for } k = 2: \qquad x^2 = \sum_j x_j \psi_j(\mathbf{x}), \ldots$$

Finite element spaces are built on **simple geometric shapes**, e.g., triangles, quadrilaterals, tetrahedra, hexahedra.

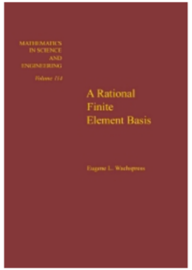
Basis functions for polygons



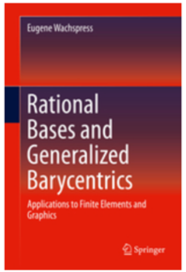
Lagrange basis functions are not polynomials!

On polygons/polyhedra, the basis functions are not polynomials

In 1975 (and 2016), **Eugene Wachspress** proposed to use of **rational basis functions**



(1975)



(2016)

Linear basis functions on triangles are **linear Lagrange interpolants** $\longrightarrow$ **non-linear Lagrange interpolants** on polygons reproducing linear polynomials (*Wachspress*)

(direct) solution of a local elliptic PDE (harmonic lifting)

$$\Delta v_h = 0 \quad \text{on E}$$

In VEM we do not build or try to evaluate the basis functions or their gradients directly, but we approximate them by polynomial projections.

The virtual element method: three basic concepts

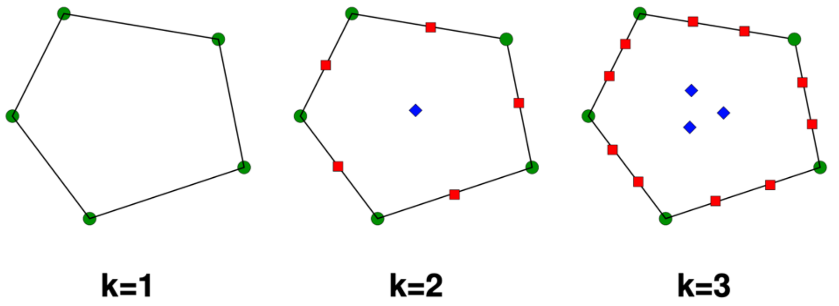
(1) ***The Virtual Element Method is a Finite Element Method***
We have all typical FEM ingredients:

- functional spaces and variational formulations
- convergence analysis to have error estimates
- basis functions to compute stiffness and mass matrices
- local construction and global assembly of matrix operators

(2) *The finite element space is “**virtual**”: we never compute the basis functions! Instead, we use their **polynomial projections***

(3) *We choose the degrees of freedom “smartly” so that these projections are always computable without any approximation*

The conforming virtual element space



- The **conforming virtual element space** on E:

$$V_k^h(\mathrm{E}) := \Big\{ v_h \in H^1(\mathrm{E}) \ : v_{h|\partial E} \text{ is continuous on } \partial E \text{ and}$$
$$\Delta v_h \in \mathcal{P}_{k-2}(\mathrm{E}) \quad \text{in } E$$
$$v_{h|\mathrm{e}} \in \mathcal{P}_k(\mathrm{e}) \quad \text{on every } \mathrm{e} \in \partial E \Big\}$$

- the degrees of freedom are unisolvent
- polynomials of degree up to k form a subspace
- the elliptic projection operator is computable

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The elliptic projector Π_k^∇

Elliptic projection: $\Pi_k^\nabla v_h \in \mathcal{P}_k(\mathrm{E})$ of a virtual element function v_h:

$$\int_{\mathrm{E}} \nabla \Pi_k^\nabla v_h \cdot \nabla q_k \, dV = \int_{\mathrm{E}} \nabla v_h \cdot \nabla q_k \, dV \qquad \forall q_k \in \mathcal{P}_k(\mathrm{E}),$$

which defines $\Pi_k^\nabla v_h$ on each element E up to an additive constant

To fix the **constant factor**:

$$\text{for } k = 1: \quad \int_{\partial \mathrm{E}} \Pi_1^\nabla v_h \, dS = \int_{\partial \mathrm{E}} v_h \, dS$$

$$\text{for } k > 1: \quad \int_{\mathrm{E}} \Pi_k^\nabla v_h \, dV = \int_{\mathrm{E}} v_h \, dV$$

*The breakthrough is that we can always choose the **degrees of freedom** of v_h so that its **elliptic projection** is computable*

$$\int_{\mathrm{E}} \nabla \Pi_k^\nabla v_h \cdot \nabla q_k \, dV = \int_{\mathrm{E}} \nabla v_h \cdot \nabla q_k \, dV$$

$$= - \int_{\mathrm{E}} \Delta q_k \, v_h \, dV + \int_{\partial \mathrm{E}} (\nabla q_k \cdot \mathbf{n}_{\mathrm{E}}) \, v_h \, dS \qquad \forall q_k \in \mathcal{P}_k(\mathrm{E})$$

A useful decomposition

- $\{\psi_i\}$: "canonical" basis functions on element E
  $\longrightarrow$ the *i*-th degree of freedom is 1, the others are zero;

- Π_k^∇: elliptic projection onto polynomials of degree k on element E;
  $\longrightarrow$ computable from the degrees of freedom;

- Hence, $\psi_i = \Pi_k^\nabla \psi_i + (1-\Pi_k^\nabla)\psi_i, \qquad \nabla\psi_i = \underbrace{\nabla\Pi_k^\nabla \psi_i}_{\textbf{computable}} + \underbrace{\nabla(1-\Pi_k^\nabla)\psi_i}_{\textbf{non-computable}}$

- The integral of "mixed" terms is zero (by definition):

$$\int_E \nabla\Pi_k^\nabla \psi_i \cdot \nabla(1-\Pi_k^\nabla)\psi_j \, dV = 0$$

$$\boxed{\int_E \nabla\Pi_k^\nabla v_h \cdot \nabla q_k \, dV = \int_E \nabla v_h \cdot \nabla q_k \, dV \qquad \forall q_k \in \mathcal{P}_k(E),}$$

Local stiffness matrix

$$\boxed{\nabla\psi_i = \nabla\Pi_k^{\nabla}\psi_i + \nabla(1-\Pi_k^{\nabla})\psi_i}$$

$$\int_E \nabla\psi_i\cdot\nabla\psi_j\,dV = \underbrace{\int_E \nabla\Pi_k^{\nabla}\psi_i\cdot\nabla\Pi_k^{\nabla}\psi_j\,dV}_{\text{computable using DOFs}} + \underbrace{\int_E \nabla(1-\Pi_k^{\nabla})\psi_i\cdot\nabla(1-\Pi_k^{\nabla})\psi_j\,dV}_{\cancel{\text{non-computable (unless we know } \psi_i,\psi_j)}} \;\; \text{+STABILIZATION}$$

$$+\underbrace{\int_E \nabla\Pi_k^{\nabla}\psi_i\cdot\nabla(1-\Pi_k^{\nabla})\psi_j\,dV + \int_E \nabla(1-\Pi_k^{\nabla})\psi_i\cdot\nabla\Pi_k^{\nabla}\psi_j\,dV}_{\text{mixed terms are zero}}$$

substitute $\int_E \nabla(1-\Pi_k^{\nabla})\psi_i\cdot\nabla(1-\Pi_k^{\nabla})\psi_j\,dV$ with $\mathcal{S}_E\big((1-\Pi_k^{\nabla})\psi_i,\,(1-\Pi_k^{\nabla})\psi_j\big)$,

where $\mathcal{S}_E$ can be **any** continuous bilinear form that is

- symmetric and positive definite (SPD) on the kernel of Π_k^{∇}
- computable from the degrees of freedom of its arguments

Beirao, Brezzi, et al (2013)

Convergence theorem

Theorem

Beirao, Brezzi, et al (2013)

- *Under a few assumptions on the regularity of the mesh (which imply standard approximation properties for interpolation and projection operators),*
- *for each polygonal cell* E*, we are given*
  - \+ *the virtual element bilinear form* $\mathcal{A}_{h,\mathrm{E}}(\cdot,\cdot)$ *built using* $\Pi_k^{\nabla,\mathrm{E}}$
  - \+ *the virtual RHS* $\langle f_h,\cdot\rangle_{\mathrm{E}}$ *built using* $\Pi_{k-2}^{0,\mathrm{E}}$
- *then, the solution of the variational problem: Find* $u_h \in \mathcal{V}^{h,k}$ *such that*

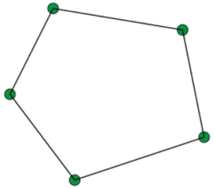
$$\mathcal{A}_h(u_h, v_h) = \langle f, v_h\rangle \qquad \forall v_h \in \mathcal{V}^{h,k}$$

exists and is unique with the following convergence estimate of the approximation error:

$$\boxed{\|u - u_h\|_{H^1(\Omega)} \leq Ch^k \|u\|_{H^{k+1}(\Omega)}}$$

H¹-conforming VEM degrees of freedom - displacement

Each function $v_h \in V_k^h(\mathsf{E})$ is uniquely characterized by the following DOFs:

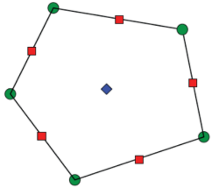


(k=1)

(D1) the values of v_h at the vertices of E

(D2) the moments of v_h of order up to $k-2$ on each one-dimensional edge $\mathsf{e} \in \partial\mathsf{E}$:

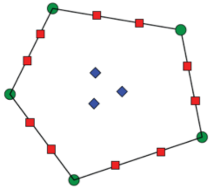
$$\frac{1}{|\mathsf{e}|}\int_{\mathsf{e}} v_h\, m\, ds, \;\; \forall m \in \mathcal{M}_{k-2}(\mathsf{e}),\, \forall \mathsf{e} \in \partial\mathsf{E}$$



(k=2)

(D3) the moments of v_h of order up to $k-2$ on E:

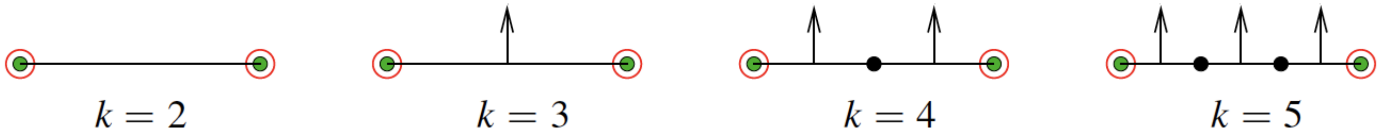
$$\frac{1}{|\mathsf{E}|}\int_{\mathsf{E}} v_h\, m\, ds, \;\; \forall m \in \mathcal{M}_{k-2}(\mathsf{E})$$



(k=3)

$$\boxed{\begin{aligned} \rho\ddot{\boldsymbol{u}} - \nabla\cdot\boldsymbol{\sigma}(\boldsymbol{u},d) - \boldsymbol{f} &= \boldsymbol{0}, \quad \text{on } \Omega\times(0,T], \\ \alpha_2\Delta^2 d - \alpha_1\Delta d + \alpha_0 d + g'(d)\mathcal{H}_t &= 0, \quad \text{on } \Omega\times(0,T], \end{aligned}}$$

H^2-conforming VEM degrees of freedom – phase field



(**D1**): for $k \geq 2$, $v(\mathbf{x}_{\mathsf{v}})$, $\partial_x v(\mathbf{x}_{\mathsf{v}})$, $\partial_y v(\mathbf{x}_{\mathsf{v}})$ for any vertex v of $\partial\mathsf{E}$

(**D2**): for $k \geq 4$, $\dfrac{1}{h_{\mathsf{e}}}\displaystyle\int_{\mathsf{e}} qv\, ds$ for any $q \in \mathbb{P}_{k-4}(\mathsf{e})$, and any edge $\mathsf{e} \in \partial\mathsf{E}$

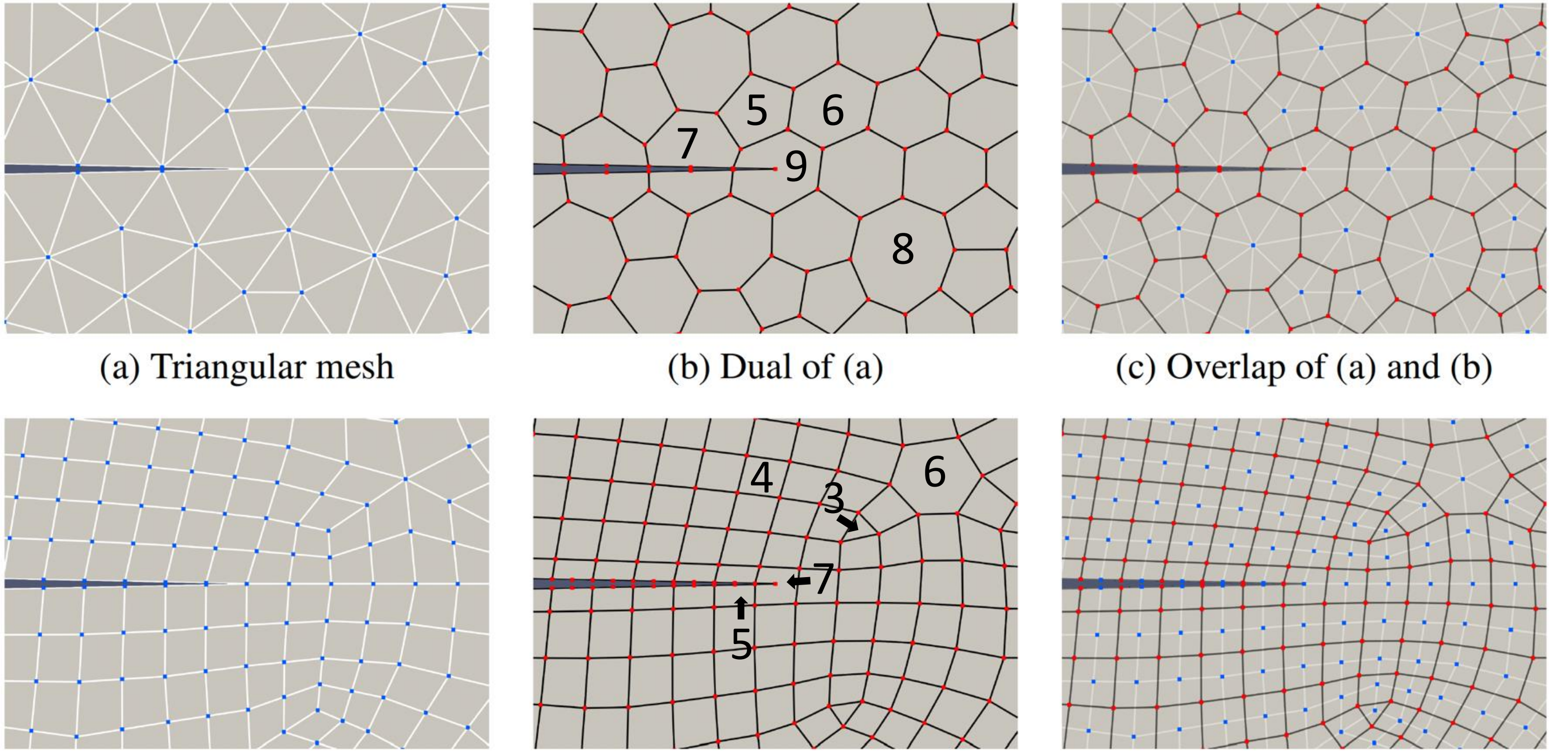
(**D3**): for $k \geq 3$, $\displaystyle\int_{\mathsf{e}} q\partial_n v\, ds$ for any $q \in \mathbb{P}_{k-3}(\mathsf{e})$, and any edge $\mathsf{e} \in \partial\mathsf{E}$

and

(**D4**): for $k \geq 2$, $\dfrac{1}{|\mathsf{E}|}\displaystyle\int_{\mathsf{E}} qv\, dV$ for any $q \in \mathbb{P}_{k-2}(\mathsf{E})$

$$\boxed{\begin{aligned} \rho\ddot{\boldsymbol{u}} - \nabla\cdot\boldsymbol{\sigma}(\boldsymbol{u}, d) - \boldsymbol{f} &= \boldsymbol{0}, \quad \text{on } \Omega\times(0,T], \\ \alpha_2\Delta^2 d - \alpha_1\Delta d + \alpha_0 d + g'(d)\mathcal{H}_t &= 0, \quad \text{on } \Omega\times(0,T], \end{aligned}}$$

Meshes Implemented in MFEM

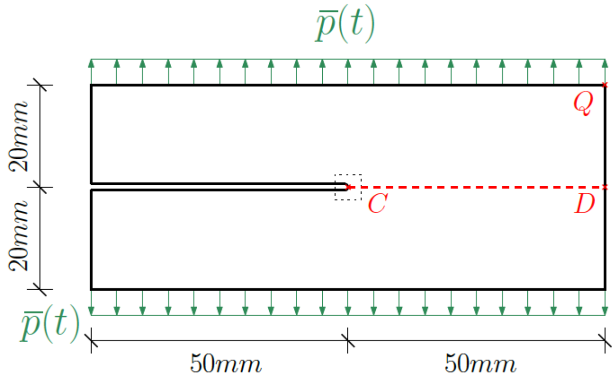


(a) Triangular mesh (b) Dual of (a) (c) Overlap of (a) and (b)

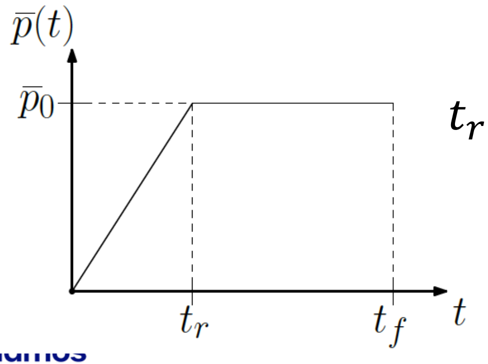
(d) Quadrilateral mesh (e) Dual of (b) (f) Overlap of (d) and (e)

Double cantilever beam experiment

Geometry, boundary conditions, and loading



$$\boxed{\begin{aligned} \rho\ddot{\boldsymbol{u}} - \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}, d) - \boldsymbol{f} = \boldsymbol{0}, &\quad \text{on } \Omega \times (0, T], \\ \alpha_2 \Delta^2 d - \alpha_1 \Delta d + \alpha_0 d + g'(d)\mathcal{H}_t = 0, &\quad \text{on } \Omega \times (0, T], \end{aligned}}$$

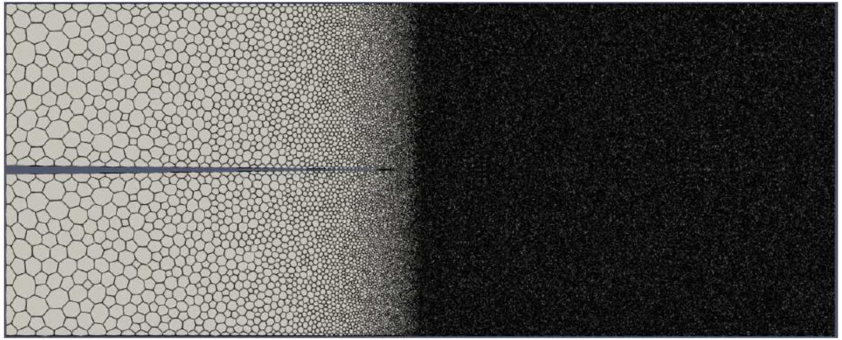


$t_r = 1\ \mu s$

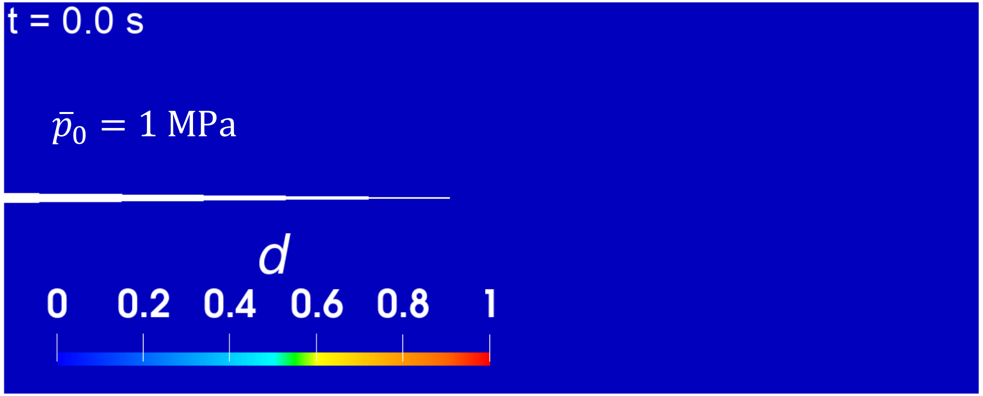
Depending on the magnitude of the loading

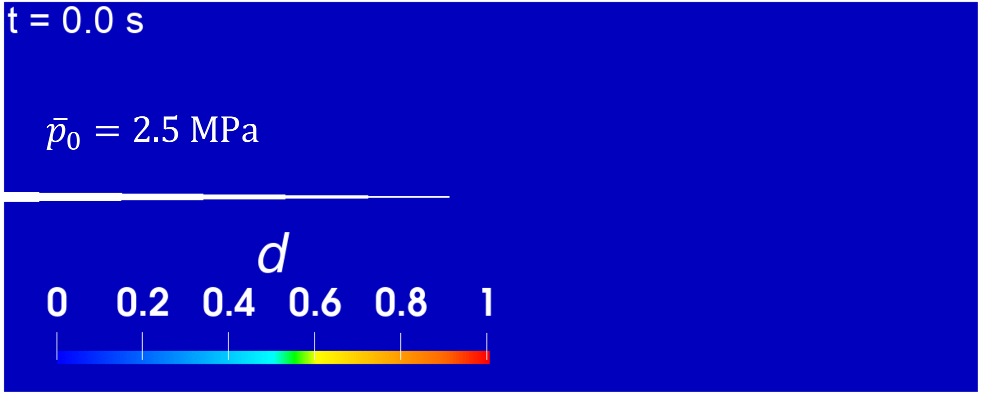
- Single crack branching
- Multiple crack branching

Dynamic crack branching

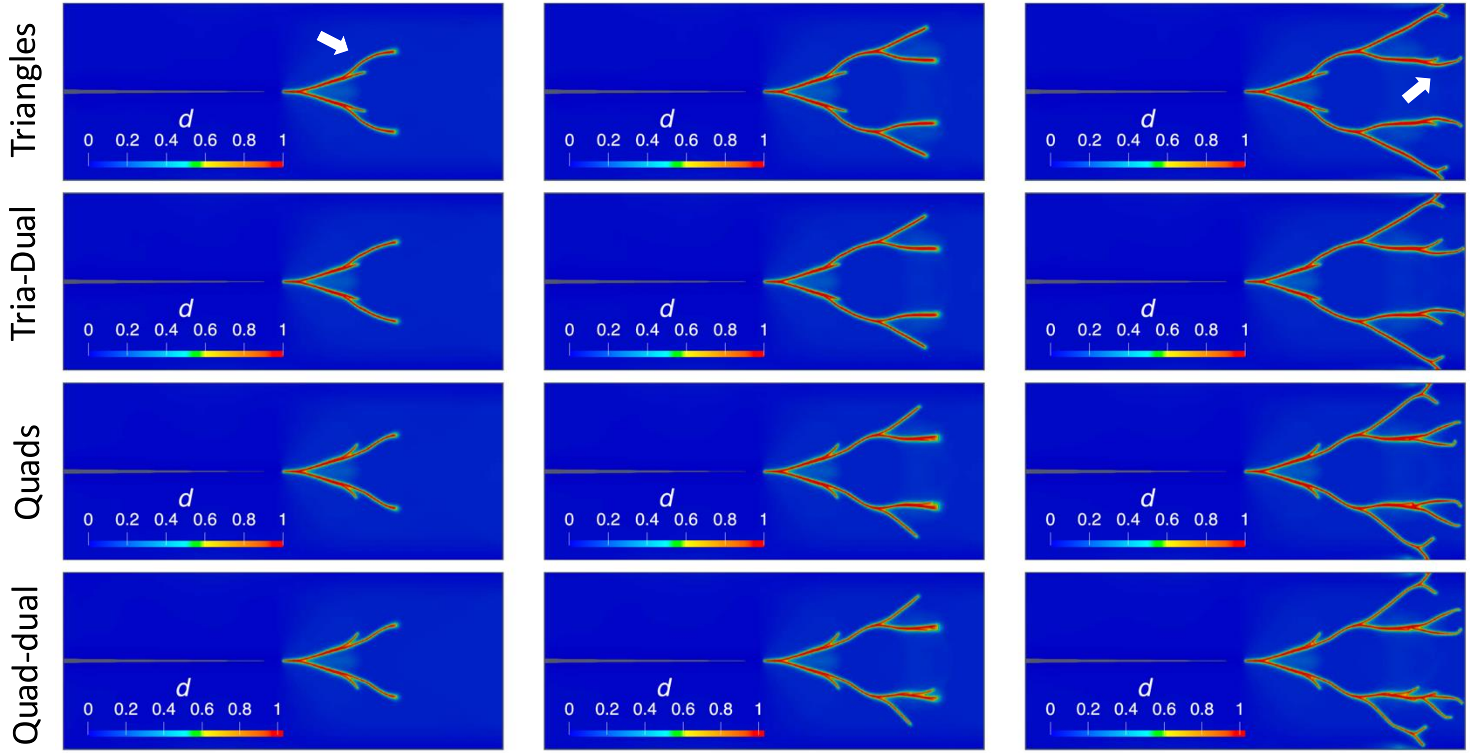


695,210 elements



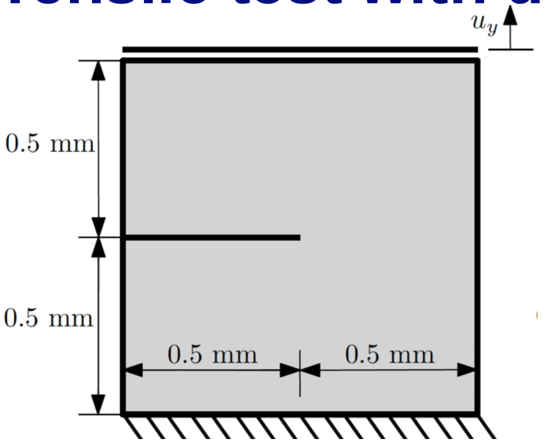


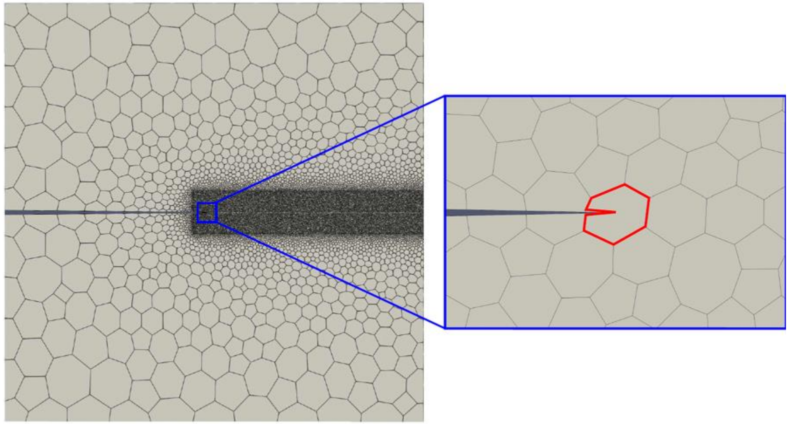
Multiple crack branching with different elements types

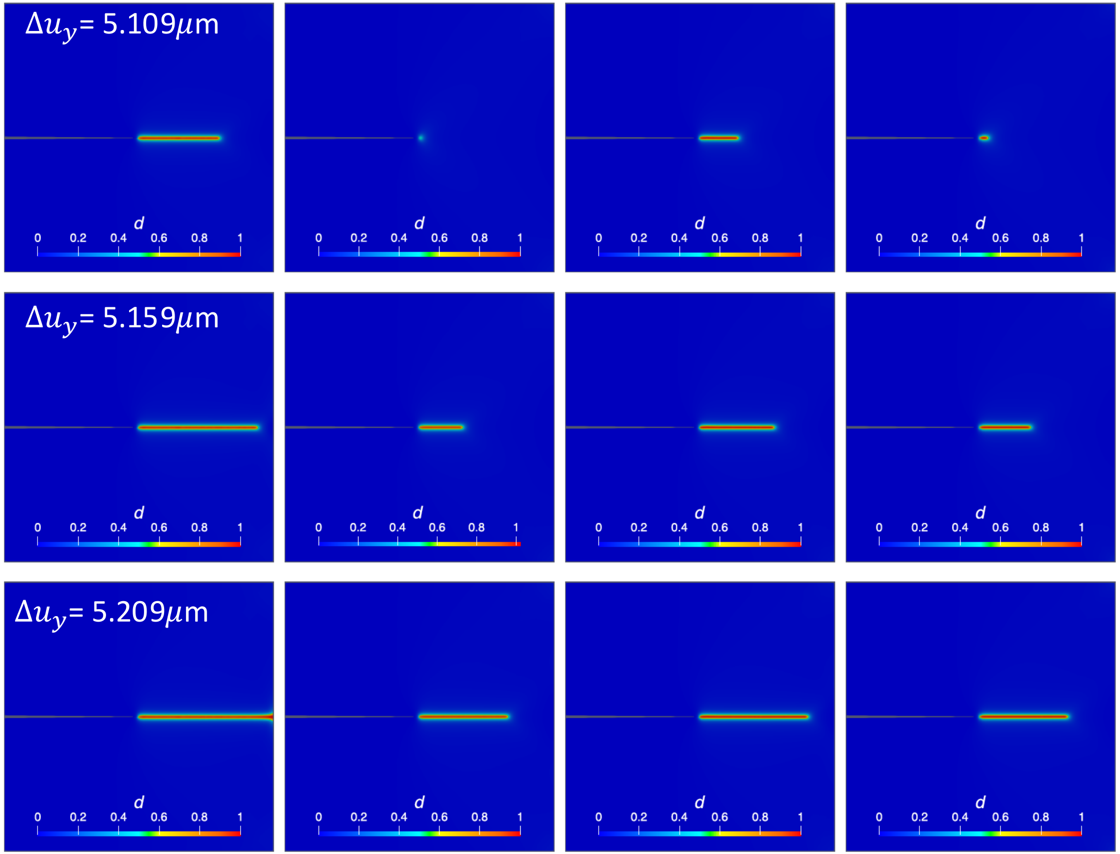


(a) $t = 30\mu s$ (b) $t = 40\mu s$ (c) $t = 50\mu s$

Tensile test with different elements types







(a) Triangular mesh (b) Dual of (a) (c) Quadrilateral mesh (d) Dual of (c)

Summary

- We have developed a virtual element framework in MFEM to solve dynamic fracture problems governed by the high-order phase-field model on polygonal meshes.
- We have verified our numerical framework by simulating benchmark quasi-static tensile and shear tests and applied it to dynamic fracture.
- For fast crack propagation, the details of the crack path is sensitive to element types

Y. Leng, L. Svolos, I. Boureima, G. Manzini, JY. N. Plohr, and H. Mourad. Arbitrary order virtual element methods for high-order phase-field modeling of dynamic fracture. *International Journal for Numerical Methods in Engineering*, page e7605, 2024. doi:https://doi.org/10.1002/nme.7605.

```
// 5. Define a finite element space on the mesh. Here we use H1 continuous
//    high-order Lagrange finite elements of the given order.
H1_VEMCollection  *fec = new H1_VEMCollection(order);
ParFiniteElementSpace *fes = new ParFiniteElementSpace(&mesh, fec);
HYPRE_BigInt total_num_dofs = fes->GlobalTrueVSize();
if (Mpi::Root())
{
   cout << "VEM Number of unknowns: " << total_num_dofs << endl;
}
```