Computational & Multiscale Mechanics of Materials





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Content

- Introduction
 - Fracture modelling
- Hybrid discontinuous-Galerkin/ Extrinsic cohesive law framework
 - DG methods
 - Hybrid method
 - Parallel implementation
- Application to intra-laminar failure of composites
 - Numerical simulations
 - Micro-Meso fracture model
- Conclusions



Intra-laminar fracture challenges
Fracture can be

At fiber interfaces (debonding)
In matrix
Initially there is no crack
Cell size effect



- Intra-laminar fracture challenges
 - Fracture can be
 - At fiber interfaces (debonding)-
 - In matrix
 - Initially there is no crack
 - Cell size effect
- Numerical approach
 - Cohesive elements inserted between two
 bulk elements
 - They integrate the cohesive Traction Separation Laws
 - Characterized by
 - Strength σ_c &
 - Critical energy release rate G_C
 - Can be tailored for
 - Debonding
 - Matrix crack





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- Problems with cohesive elements
 - Intrinsic Cohesive Law (ICL)
 - Cohesive elements inserted from the beginning
 - Drawbacks:
 - Efficient if a priori knowledge of the crack path
 - Mesh dependency [Xu & Needelman, 1994]
 - Initial slope modifies the effective elastic modulus
 - This slope should tend to infinity [Klein et al. 2001]:
 - Alteration of a wave propagation
 - Critical time step is reduced





- Problems with cohesive elements
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 - Alteration of a wave propagation
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 - Extrinsic Cohesive Law (ECL)
 - Cohesive elements inserted on the fly when the failure criterion is verified [Ortiz & Pandolfi 1999]
 - Drawback
 - Complex implementation in 3D (parallelization)



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- Solution: Discontinuous Galerkin/Extrinsic Cohesive Law method
 - Embeds interface elements
 - Consistent
 - Highly scalable
- Successful applications
 - Ceramic fragmentation

Failure of blast loaded elasto-plastic thin structures



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- Discontinuous Galerkin (DG) methods
 - Finite-element discretization
 - Same discontinuous polynomial approximations for the
 - **Test** functions φ_h and
 - Trial functions $\delta \varphi$



- Definition of operators on the interface trace:
 - Jump operator: $\llbracket \cdot \rrbracket = \cdot^+ \cdot^-$
 - Mean operator: $\langle \cdot \rangle = \frac{\cdot^+ + \cdot^-}{2}$
- Continuity is weakly enforced, such that the method
 - Is consistent
 - Is stable
 - Has the optimal convergence rate





- Discontinuous Galerkin (DG) methods (2)
 - Formulation in terms of the first Piola-Kirchhoff stress tensor P

$$\nabla_{0} \cdot \mathbf{P}^{T} = 0 \text{ in } \Omega_{0} \qquad \& \qquad \begin{cases} \mathbf{P} \cdot \mathbf{N} = \overline{\mathbf{T}} \text{ on } \partial_{N} \Omega_{0} \\ \mathbf{\varphi} = \overline{\mathbf{\varphi}} \text{ on } \partial_{D} \Omega_{0} \end{cases}$$

• Weak formulation obtained by integration by parts on each element Ω^{e}



$$\sum_{e} \int_{\Omega_0^e} \nabla_0 \cdot \mathbf{P}^T \cdot \boldsymbol{\delta \varphi} d\Omega = 0$$



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• Weak formulation obtained by integration by parts on each element Ω^{e}



$$\sum_{e} \int_{\Omega_{0}^{e}} \nabla_{0} \cdot \mathbf{P}^{T} \cdot \delta \boldsymbol{\varphi} d\Omega = 0$$
$$\sum_{e} \int_{\Omega_{0}^{e}} -\mathbf{P} \cdot \nabla_{0} \delta \boldsymbol{\varphi} d\Omega + \sum_{e} \int_{\partial \Omega_{0}^{e}} \delta \boldsymbol{\varphi} \cdot \mathbf{P} \cdot \mathbf{N} d\partial \Omega = 0$$

- Discontinuous Galerkin (DG) methods (2)
 - Formulation in terms of the first Piola-Kirchhoff stress tensor P

$$\nabla_0 \cdot \mathbf{P}^T = 0 \text{ in } \Omega_0 \qquad \& \qquad \begin{cases} \mathbf{P} \cdot \mathbf{N} = \overline{\mathbf{T}} \text{ on } \partial_N \Omega_0 \\ \mathbf{\varphi} = \overline{\mathbf{\varphi}} \text{ on } \partial_D \Omega_0 \end{cases}$$

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• Discontinuous Galerkin (DG) methods (3)

 $\int_{\Omega_0} \mathbf{P} : \nabla_0 \delta \boldsymbol{\varphi} d\Omega + \int_{\partial_1 \Omega_0} [\![\delta \boldsymbol{\varphi} \cdot \mathbf{P}]\!] \cdot \mathbf{N}^- d\partial \Omega = \int_{\partial_N \Omega_0} \overline{\mathbf{T}} \cdot \delta \boldsymbol{\varphi} d\partial \Omega$



Discontinuous Galerkin (DG) methods (3) ۲

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Introduction of a consistent numerical flux

 $\int_{\Omega_{0}} \mathbf{P} : \nabla_{0} \delta \boldsymbol{\varphi} d\Omega + \int_{\partial_{1} \Omega_{0}} [\![\delta \boldsymbol{\varphi}]\!] \cdot \langle \mathbf{P} \rangle \cdot \mathbf{N}^{-} d\partial \Omega = \int_{\partial_{N} \Omega_{0}} \overline{\mathbf{T}} \cdot \delta \boldsymbol{\varphi} d\partial \Omega$



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• Weak enforcement of the compatibility & symmetrization

$$\int_{\Omega_0} \mathbf{P} : \nabla_0 \delta \varphi d\Omega + \int_{\partial_1 \Omega_0} [\![\delta \varphi]\!] \cdot \langle \mathbf{P} \rangle \cdot N^- d\partial \Omega + \int_{\partial_1 \Omega_0} [\![\varphi]\!] \cdot \langle \mathbf{C}^{\mathrm{el}} : \nabla_0 \delta \varphi \rangle \cdot N^- d\partial \Omega$$

$$= \int_{\partial_N \Omega_0} \overline{\mathbf{T}} \cdot \delta \varphi d\partial \Omega$$

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• Weak enforcement of the compatibility & symmetrization

$$\begin{split} &\int_{\Omega_0} \mathbf{P} : \nabla_0 \delta \varphi d\Omega + \int_{\partial_1 \Omega_0} [\![\delta \varphi]\!] \cdot \langle \mathbf{P} \rangle \cdot N^- d\partial \Omega + \int_{\partial_1 \Omega_0} [\![\varphi]\!] \cdot \langle C^{\mathrm{el}} : \nabla_0 \delta \varphi \rangle \cdot N^- d\partial \Omega \\ &= \int_{\partial_N \Omega_0} \overline{T} \cdot \delta \varphi d\partial \Omega \end{split}$$

• Stabilization controlled by a parameter β_s for all mesh sizes h^s

$$\int_{\Omega_0} \mathbf{P} : \nabla_0 \delta \boldsymbol{\varphi} d\Omega + \int_{\partial_1 \Omega_0} [\![\delta \boldsymbol{\varphi}]\!] \cdot \langle \mathbf{P} \rangle \cdot N^- d\partial \Omega + \int_{\partial_1 \Omega_0} [\![\boldsymbol{\varphi}]\!] \cdot \langle \boldsymbol{C}^{\mathrm{el}} : \nabla_0 \delta \boldsymbol{\varphi} \rangle \cdot N^- d\partial \Omega$$

$$+ \int_{\partial_{\mathrm{I}}\Omega_{0}} \llbracket \varphi \rrbracket \otimes N^{-} : \langle \frac{\beta_{s} C^{\mathrm{el}}}{h^{s}} \rangle : \llbracket \delta \varphi \rrbracket \otimes N^{-} d\partial \Omega = \int_{\partial_{N}\Omega_{0}} \overline{T} \cdot \delta \varphi d\partial \Omega$$

[Noels & Radovitzky, IJNME 2006]



- Hybrid Discontinuous Galerkin/Extrinsic Cohesive Law method
 - Final DG formulation

$$\int_{\Omega_0} \mathbf{P} : \nabla_0 \delta \boldsymbol{\varphi} d\Omega + \int_{\partial_1 \Omega_0} [\![\delta \boldsymbol{\varphi}]\!] \cdot \langle \mathbf{P} \rangle \cdot N^- d\partial \Omega + \int_{\partial_1 \Omega_0} [\![\boldsymbol{\varphi}]\!] \cdot \langle \boldsymbol{C}^{\mathrm{el}} : \nabla_0 \delta \boldsymbol{\varphi} \rangle \cdot N^- d\partial \Omega \\ + \int_{\partial_1 \Omega_0} [\![\boldsymbol{\varphi}]\!] \otimes N^- : \langle \frac{\beta_s \boldsymbol{C}^{\mathrm{el}}}{h^s} \rangle : [\![\delta \boldsymbol{\varphi}]\!] \otimes N^- d\partial \Omega = \int_{\partial_N \Omega_0} \overline{\boldsymbol{T}} \cdot \delta \boldsymbol{\varphi} d\partial \Omega$$

• Interface terms integrated on an interface element





- Hybrid Discontinuous Galerkin/Extrinsic Cohesive Law method
 - Final DG formulation

 $\int_{\Omega_0} \mathbf{P} : \nabla_0 \delta \boldsymbol{\varphi} d\Omega + \int_{\partial_1 \Omega_0} [\![\delta \boldsymbol{\varphi}]\!] \cdot \langle \mathbf{P} \rangle \cdot N^- d\partial \Omega + \int_{\partial_1 \Omega_0} [\![\boldsymbol{\varphi}]\!] \cdot \langle \boldsymbol{C}^{\mathrm{el}} : \nabla_0 \delta \boldsymbol{\varphi} \rangle \cdot N^- d\partial \Omega \\ + \int_{\partial_1 \Omega_0} [\![\boldsymbol{\varphi}]\!] \otimes N^- : \langle \frac{\beta_s \boldsymbol{C}^{\mathrm{el}}}{h^s} \rangle : [\![\delta \boldsymbol{\varphi}]\!] \otimes N^- d\partial \Omega = \int_{\partial_N \Omega_0} \overline{\boldsymbol{T}} \cdot \delta \boldsymbol{\varphi} d\partial \Omega$

- Interface terms integrated on an interface element
- Taking advantage of the interface elements
 - Check is fracture criterion is reached (α : 0->1)
 - If so, use the extrinsic cohesive law

$$\int_{\Omega_0} \mathbf{P} \cdot \nabla_0 \delta \boldsymbol{\varphi} d\Omega + \alpha \int_{\partial_I \Omega} [\![\delta \boldsymbol{\varphi}]\!] \cdot \bar{\boldsymbol{t}} \cdot \boldsymbol{n}^- d\partial \Omega +$$

$$(1 - \alpha) \int_{\partial_{I}\Omega_{0}} [\![\delta\varphi]\!] \cdot \langle \mathbf{P} \rangle \cdot N^{-} d\partial\Omega + (1 - \alpha) \int_{\partial_{I}\Omega_{0}} [\![\varphi]\!] \cdot \langle \mathbf{C}^{\mathrm{el}} : \nabla_{\mathbf{0}}\delta\varphi \rangle \cdot N^{-} d\partial\Omega + (1 - \alpha) \int_{\partial_{I}\Omega_{0}} [\![\varphi]\!] \otimes N^{-} : \langle \frac{\beta_{s}\mathbf{C}^{\mathrm{el}}}{h^{s}} \rangle : [\![\delta\varphi]\!] \otimes N^{-} d\partial\Omega = \int_{\partial_{N}\Omega_{0}} \overline{\mathbf{T}} \cdot \delta\varphi d\partial\Omega$$





- Efficient // implementation
 - Based on the ghost-faces method
 - Initial mesh





- Efficient // implementation (2)
 - Based on the ghost-faces method
 - Partitioned mesh (METIS)
 - Internal forces can be computed
 - At bulk elements
 - At interface elements in the partitions









- Efficient // implementation (2)
 - Based on the ghost-faces method
 - Partitioned mesh (METIS)
 - Internal forces can be computed
 - At bulk elements
 - At interface elements in the partitions
 - Interface elements at processors boundaries?









- Efficient // implementation (3)
 - Based on the ghost-faces method

- Create ghost elements
 - Internal forces can be computed at processors boundaries interfaces
 - If deformation of ghost
 elements is correct





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- Efficient // implementation (4)
 - Based on the ghost-faces method



- Update positions of ghost elements nodes
 - Only exchange



- **Composite materials**
 - UD carbon-fiber (60%) reinforced epoxy
 - Elasto-plastic matrix
 - Transverse anisotropic fibers •
 - Interface failure: •
 - $\sigma_{c} = 45 \text{ MPa}, G_{c} = 100 \text{ J/m}^{2}$
 - Intra-matrix failure:
 - $\sigma_{c} = 83 \text{ MPa}, G_{c} = 78 \text{ J/m}^{2}$ [Sato et al., 1986]



Transverse loading experiments ۲







- Micro-models
 - Study of the cell size effect (3D random cells)





• Consider a transverse loading δu^m on the cells



Simulations



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z x

• Micro-Meso fracture model for intra-laminar failure





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• Micro-Meso fracture model for intra-laminar failure



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• Micro-Meso fracture model for intra-laminar failure



- Micro-Meso fracture model for intra-laminar failure (2)
 - Scale transition after softening onset
 - Should not depend on the RVE size





- Micro-Meso fracture model for intra-laminar failure (2)
 - Scale transition after softening onset
 - Should not depend on the RVE size
 - The displacement δu^m of the RVE needs to be corrected
 - Mesoscopic surface traction directly obtained

 $\delta \bar{t} = \boldsymbol{\sigma} \cdot \boldsymbol{e}_X$

Compute a mesoscopic opening (increment)

 $\delta \boldsymbol{u}^{M} = \delta \boldsymbol{u}^{m} - L_{\text{cell}} \boldsymbol{C}^{\text{el}^{-1}} : \boldsymbol{e}_{X} \otimes \boldsymbol{e}_{X} \cdot \boldsymbol{\delta} \bar{\boldsymbol{t}} - \delta \boldsymbol{u}_{0}^{m}$ which accounts for the change in the structural stiffness *C* due to irreversible processes

$$\delta \boldsymbol{u}_0^m = L_{\text{cell}} \left(\boldsymbol{C}^{-1} - \boldsymbol{C}^{\text{el}^{-1}} \right) : \boldsymbol{e}_X \otimes \boldsymbol{e}_X \cdot \boldsymbol{\delta} \bar{\boldsymbol{t}}$$

[Verhoosel et al., IJNME 2010]



- Micro-Meso fracture model for intra-laminar failure (2)
 - Scale transition after softening onset
 - Should not depend on the RVE size
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 $\delta \bar{t} = \sigma \cdot e_{Y}$

Compute a mesoscopic opening (increment)

 $\delta \boldsymbol{u}^{M} = \delta \boldsymbol{u}^{m} - L_{\text{cell}} \boldsymbol{\mathcal{C}}^{\text{el}^{-1}} : \boldsymbol{e}_{X} \otimes \boldsymbol{e}_{X} \cdot \boldsymbol{\delta} \boldsymbol{\bar{t}} - \delta \boldsymbol{u}_{0}^{m}$ which accounts for the change in the structural stiffness C due to irreversible processes

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[Verhoosel et al., IJNME 2010]

- Corresponds to a meso-scale cohesive law
 - Area converges to the apparent energy release rate of the composite: 122 J/m2
 - To be compared to G_c of epoxy (78 J/m2) •



- Comparison with experiments
 - Loading curve can be compared up to strain softening
 - Similar failure mode







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Conclusions

• Hybrid DG/ECL method

- Efficient parallel computational method
- Can be used to simulate micro failure
- Micro-meso model
 - Meso-scale cohesive law can be extracted from simulations
 - Small cells can provide accurate results
- Perspectives
 - Loading direction effects
 - Computational multiscale failure

