Bridging Singularities and Nonlinearities Across Scales

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C. Armando Duarte Dept. of Civil and Environmental Engineering Computational Science and Engineering

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illinois.edu



The US Air Force has expended six decades and untold resources in attempts to field a reusable hypersonic vehicle*

Scientific challenge:

"An inability to computationally capture the <u>material</u> evolution and degradation within a <u>structural component</u>"



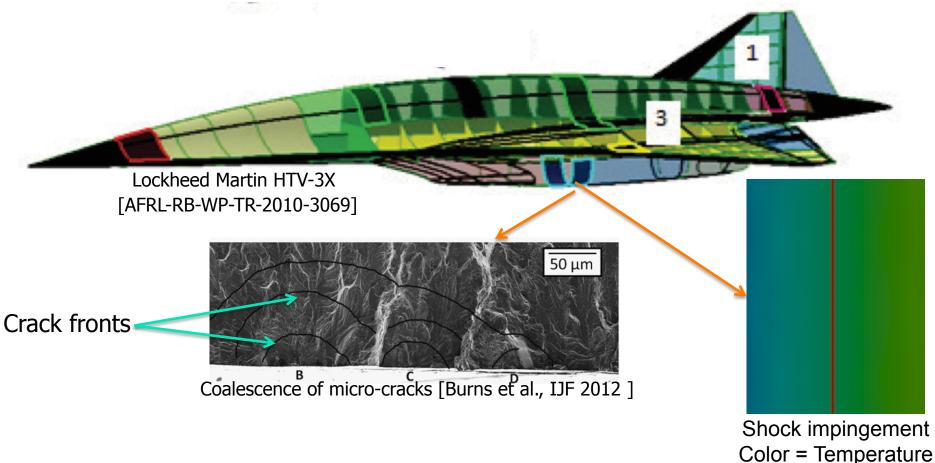
X-15 (1959)

X-51a (2010)

*[T. G. Eason et al., 2013]



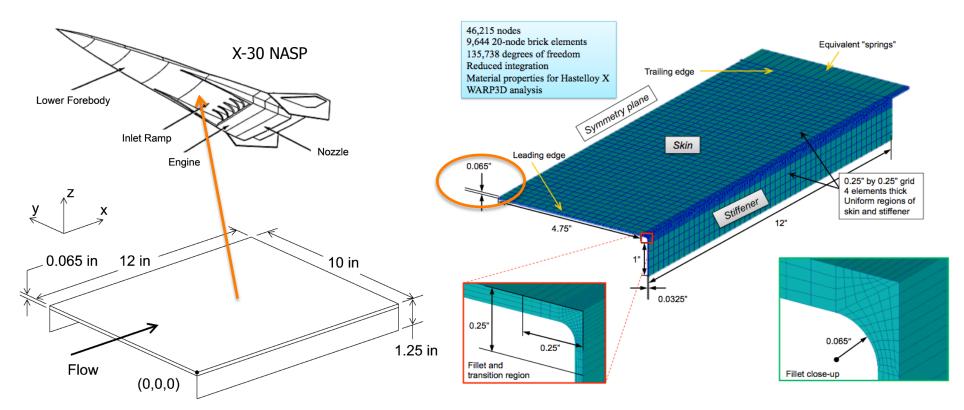
• The analysis of hypersonic aircrafts involves multiple spatial and temporal scales: From airframe scale to material microscale, loading scale, etc





Motivation: Multiscale Structural Analysis

 Thermo, mechanical and acoustic loads lead to highly localized non-linear 3-D stress fields: Finite element models with fine meshes are required



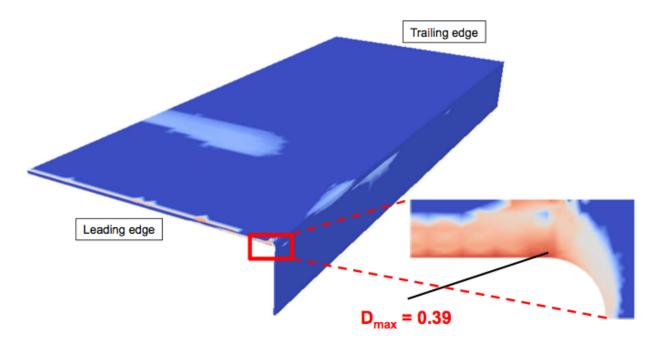
Representative hypersonic skin panel [Sobotka et al., 2013]

3-D FEM: Large aspect ratio of elements may lead to numerical instabilities during analysis [Sobotka et al., 2013]



Motivation: Multiscale Structural Analysis

- Highly localized non-linear 3-D effects
- Most of the structure remains linear elastic
- Q: How to efficiently capture these localized non-linear 3-D effects?
- Q: How to avoid numerical stability issues caused by aspect ratio of elements?
- Strategy: A Generalized FEM for multiscale structural analysis





- Motivation
- Generalized finite element methods: Basic ideas
- Bridging scales with GFEM:
 - Global-local enrichments for localized non-linearities
 - Global-local enrichment for heterogeneous materials and parallelization of fine-scale computations
- Conclusions and outlook



Early works on Generalized FEMs

- Babuska, Caloz and Osborn, 1994 (Special FEM).
- Duarte and Oden, 1995 (Hp Clouds).
- Babuska and Melenk, 1995 (PUFEM).
- Oden, Duarte and Zienkiewicz, 1996 (Hp Clouds/GFEM).
- Duarte, Babuska and Oden, 1998 (GFEM).
- Belytschko et al., 1999 (Extended FEM).
- Strouboulis, Babuska and Copps, 2000 (GFEM).
- Basic idea:
 - Use a partition of unity to build Finite Element shape functions
- Review paper

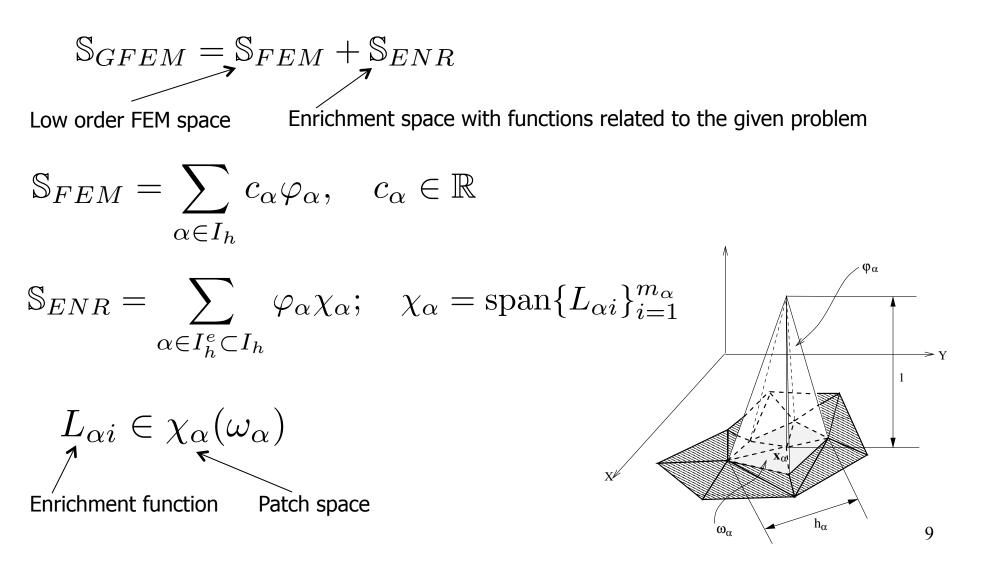
Belytschko T., Gracie R. and Ventura G. A review of extended/generalized finite element methods for material modeling, *Mod. Simul. Matl. Sci. Eng.*, 2009

"The XFEM and GFEM are basically <u>identical</u> methods: the name generalized finite element method was adopted by the Texas school in 1995–1996 and the name extended finite element method was coined by the Northwestern school in 1999."



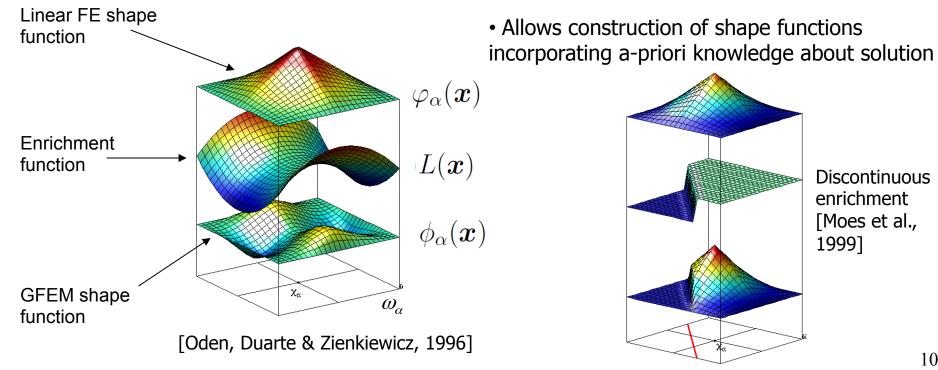
Generalized Finite Element Method

• GFEM is a Galerkin method with special test/trial space given by



Generalized Finite Element Method

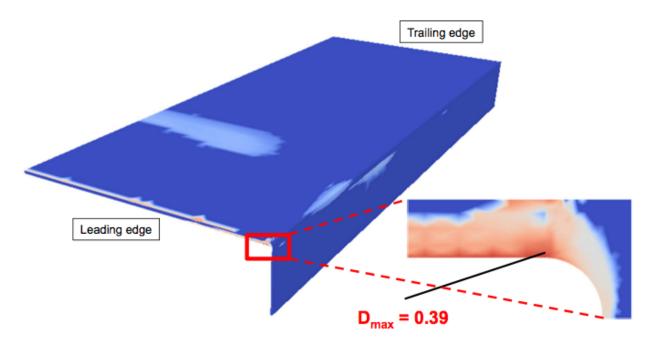
$$S_{ENR} = \sum_{\alpha \in I_h^e \subset I_h} \varphi_\alpha \chi_\alpha; \quad \chi_\alpha = \operatorname{span}\{L_{\alpha i}\}_{i=1}^{m_\alpha}$$
$$\phi_{\alpha i}(x) = \varphi_\alpha(x) L_{\alpha i}(x) \qquad \sum_{\alpha} \varphi_\alpha(x) = 1$$





Multiscale Structural Analysis

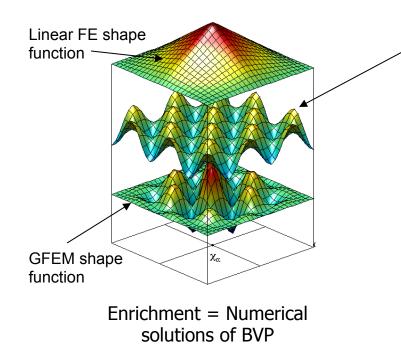
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Bridging Scales with Global-Local Enrichment Functions*

Enrichment functions computed from solution of local boundary value problems: <u>Global-Local enrichment functions</u>

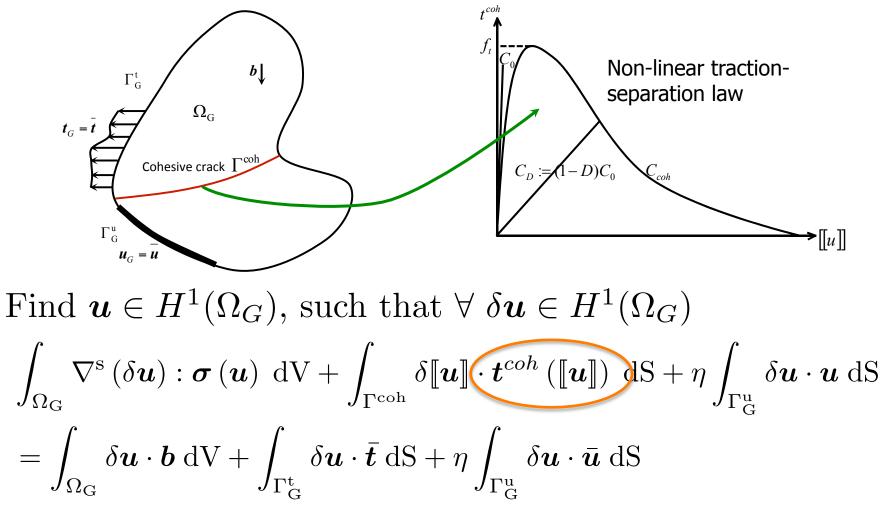


- Idea: Use available numerical solution at a simulation step to build shape functions for next step (quasi-static, transient, non-linear, etc.)
- Enrichment functions are produced numerically on-the-fly through a global-local analysis
- Use a *coarse* mesh enriched with Global-Local (GL) functions
- GFEM^{gl} = GFEM with global-local enrichments

*[Duarte et al. 2005, 2007, 2008, 2010, 2011, 2014]



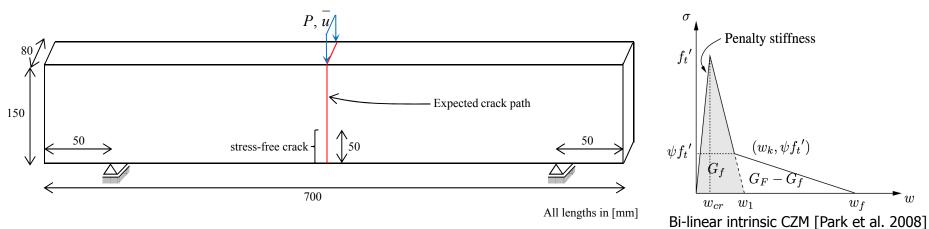
• Model Problem: Simulation of propagating cracks using cohesive fracture models



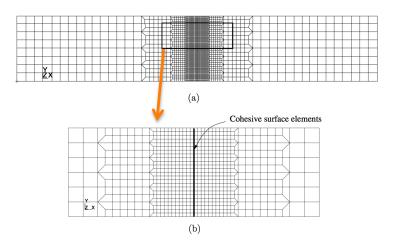
*[with Jongheon Kim]



• Three-Point Bending Beam



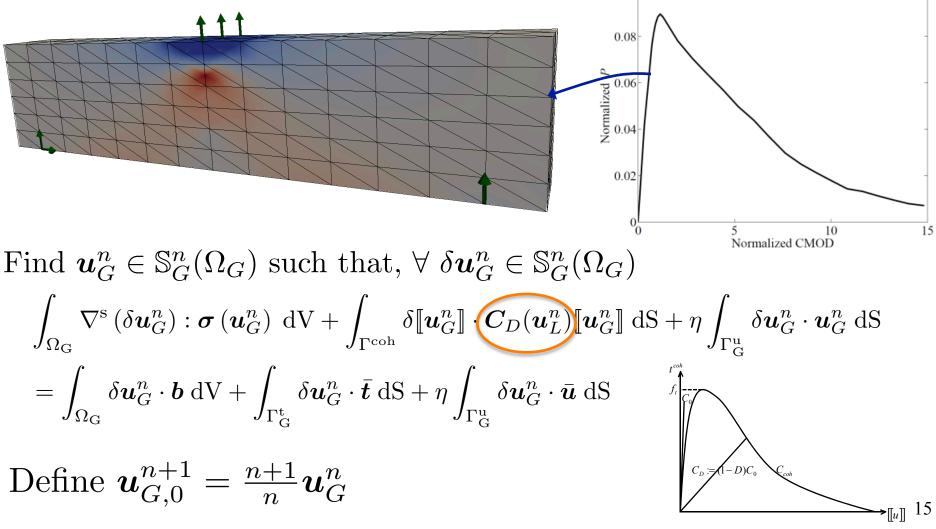
• Typical FEM discretization [Park et al. 2008]



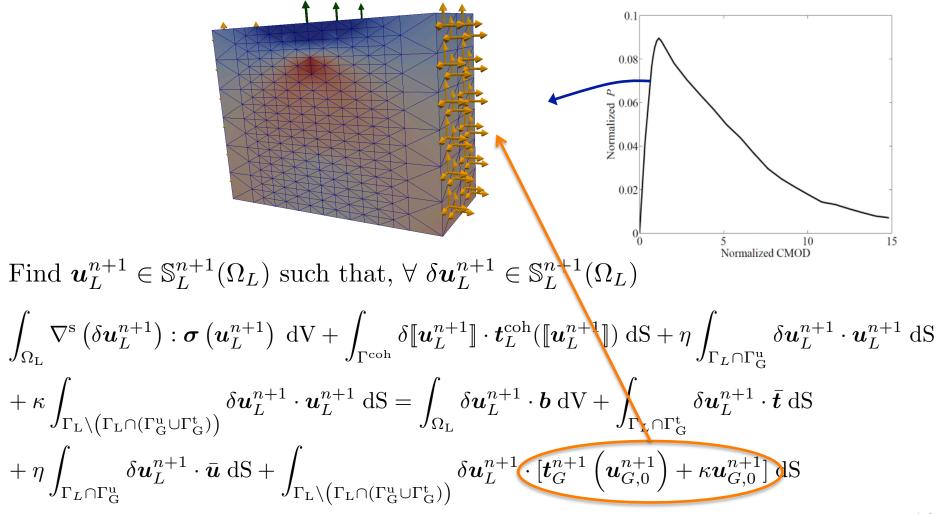
Goals:

- Solve problem on a coarse global mesh.
- Non-linear iterations at fine scales <u>only</u>.

Let $\boldsymbol{u}_G^n \in \mathbb{S}_G^n(\Omega)$ and $\boldsymbol{u}_L^n \in \mathbb{S}_L^n(\Omega)$, GFEM solutions of global and local problems at load step n

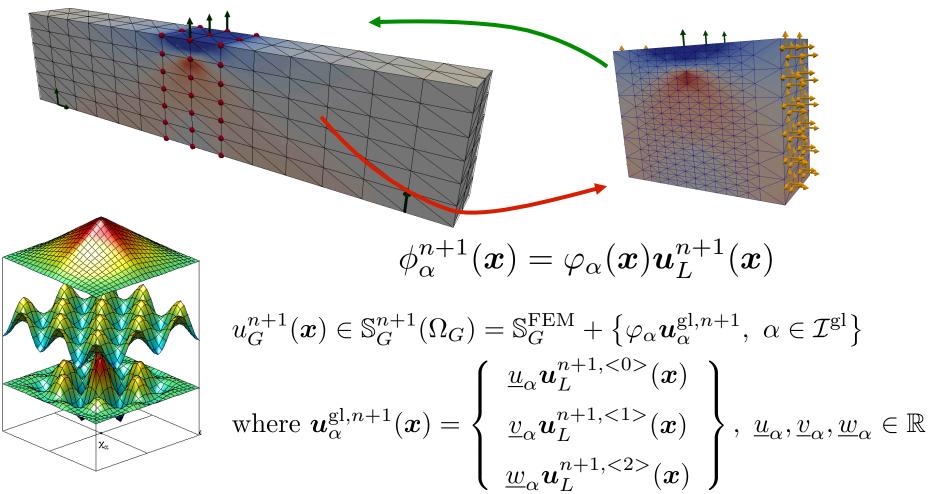


Solve following non-linear *local* problem at load step n+1 using, e.g., *hp-*GFEM



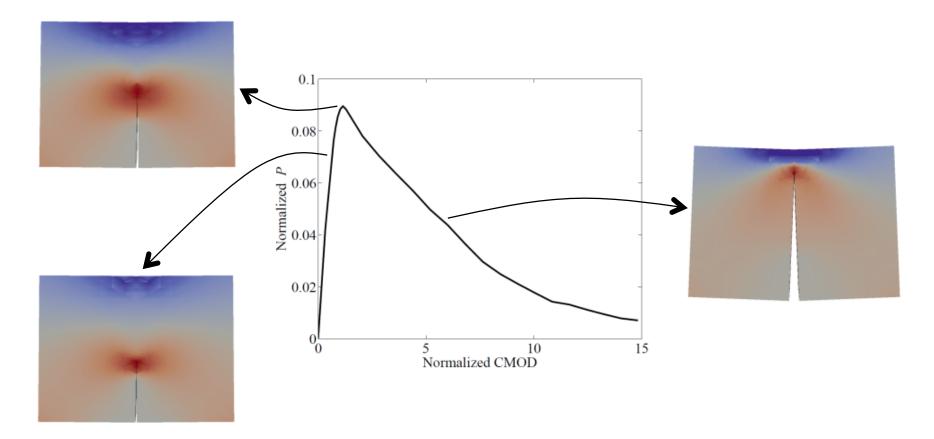
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• **Defining Step:** Global space is enriched with non-linear local solution



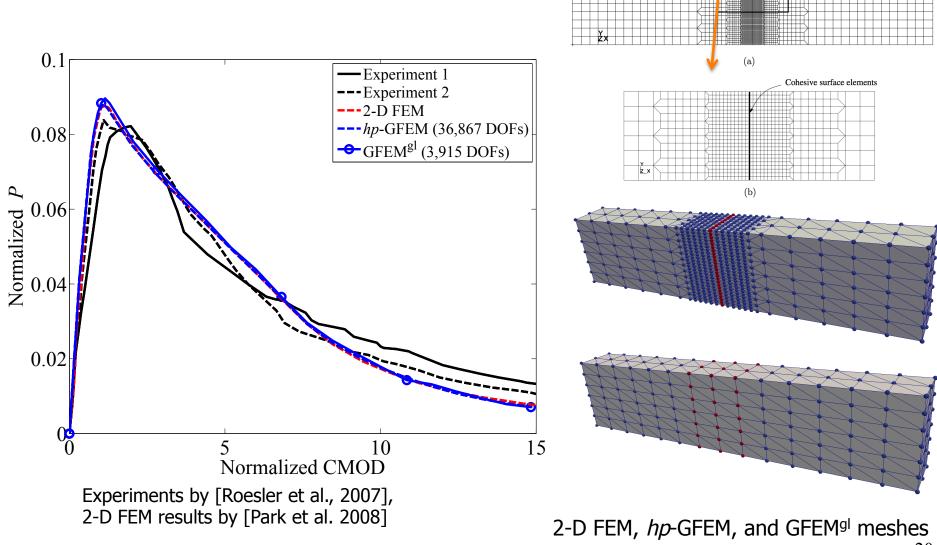
• Discretization spaces updated on-the-fly with global-local enrichment functions





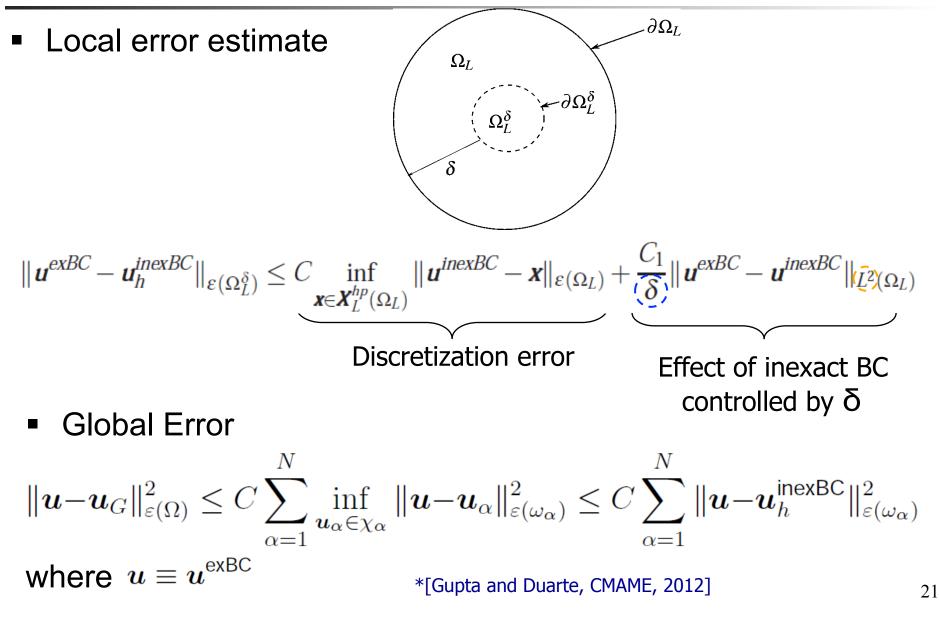
• On-the-fly updating of global-local enrichment functions during the non-linear iterative solution process







A-Priori Error Estimate*



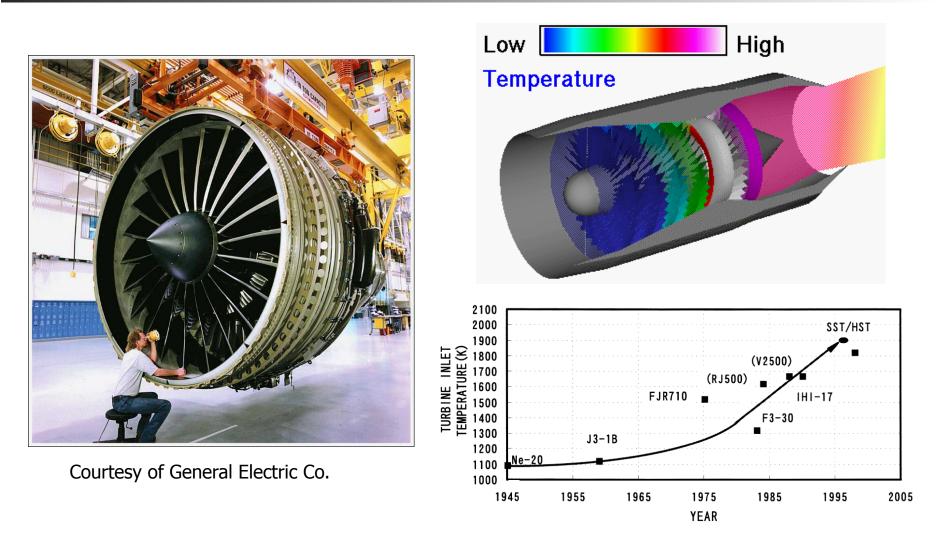


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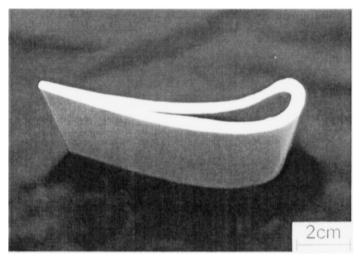
From Micro to Macro Scales



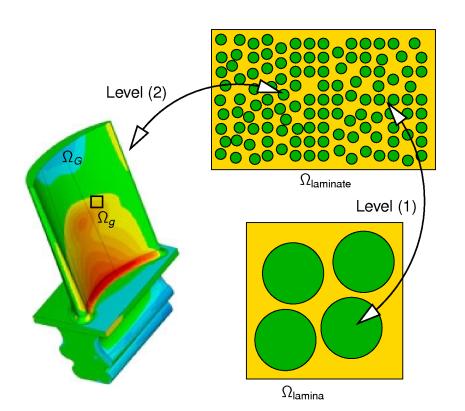
• The performance of a turbine increases with its operational temperature



• High operational temperatures require new materials like Ceramic Matrix Composites (CMC)



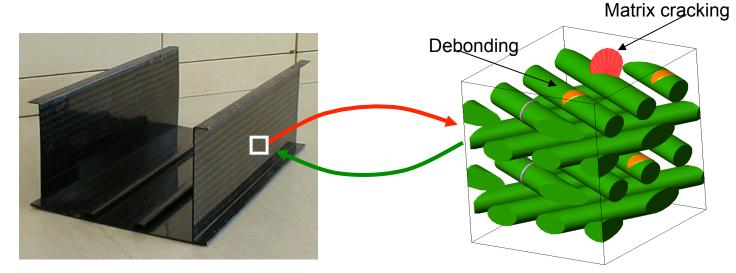
Turbine component made of CMC



Structural performance depends strongly on micro-scale details



- Failure of Heterogeneous Materials
 - Damage characterization in composite materials involves complex multi-scale phenomena



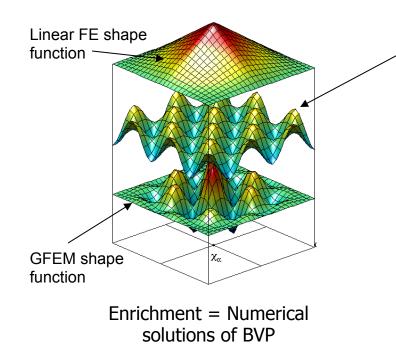
Damage in composite materials

- Homogenization approaches can not be used near singularities:
 - Can not predict local stress state since it converges in L_2 norm
 - Failure depends on local quantities as opposed to averaged [A. Needleman]



Bridging Material and Structural Scales with Global-Local Enrichment Functions

Enrichment functions computed from solution of local boundary value problems: <u>Global-Local enrichment functions</u>



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Global-Local Enrichments for Heat Equation*

$$\rho c \frac{\partial u}{\partial t} = \nabla (\kappa(\boldsymbol{x}) \nabla u) + Q(\boldsymbol{x}, t) \quad \text{in} \quad \Omega$$

where $u(\boldsymbol{x}, t)$ is the temperature field, ρc is the volumetric heat capacity and $Q(\boldsymbol{x}, t)$ is the internal heat source. $\kappa(\boldsymbol{x})$ may be oscillatory.

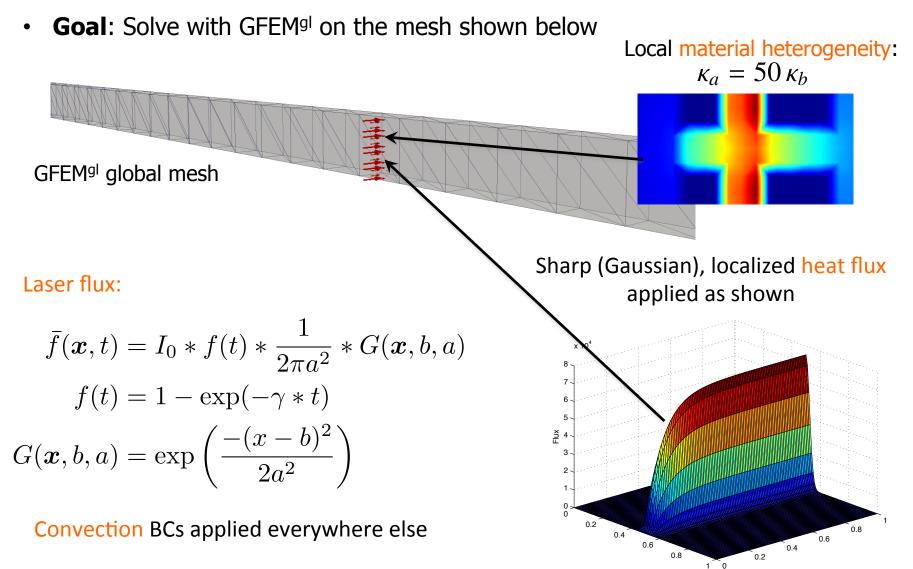
$$-\kappa \frac{\partial u}{\partial n} = \eta \left(\bar{u} - u \right) \quad \text{on} \quad \Gamma_c$$
$$-\kappa \frac{\partial u}{\partial n} = \bar{f} \quad \text{on} \quad \Gamma_f$$

$$u(\boldsymbol{x},0) = u^0(\boldsymbol{x})$$
 at t^0

where $u^0(\boldsymbol{x})$ is the prescribed temperature field at time $t = t^0$

*[O'Hara et al., CMAME, 2011; Plews and Duarte, 2014]

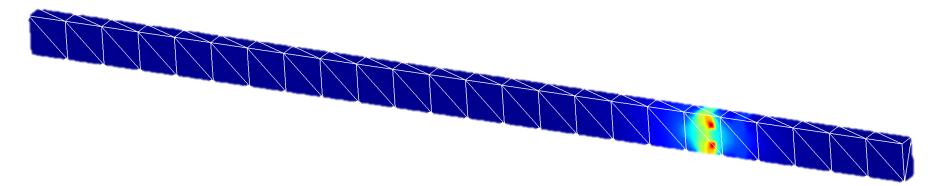
Bridging Material and Structural Scales with Global-Local Enrichment Functions



Location



Let $u_G^n(\boldsymbol{x}) \in \mathbb{S}_G^{GFEM,n}(\Omega)$ be the GFEM solution at time $t = t^n = n\Delta t$

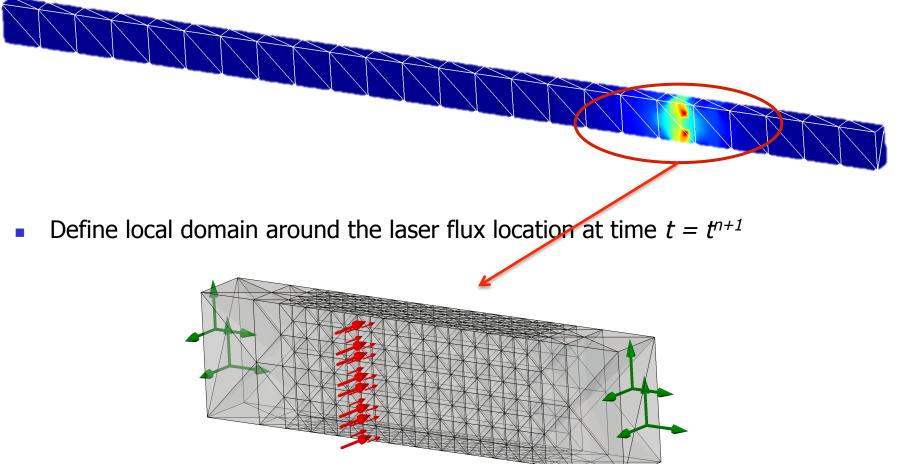


Find $u_G^n \in \mathbb{S}_G^{\text{GFEM},n}(\Omega_G)$ such that, $\forall w_G^n \in \mathbb{S}_G^{\text{GFEM},n}(\Omega_G)$

$$\frac{\rho c}{\Delta t} \int_{\Omega} w_{G}^{n} u_{G}^{n} d\Omega + \int_{\Omega} \left(\nabla w_{G}^{n} \right)^{T} \kappa \nabla u_{G}^{n} d\Omega + \eta \int_{\Gamma_{c}} w_{G}^{n} u_{G}^{n} d\Gamma = \frac{\rho c}{\Delta t} \int_{\Omega} w_{G}^{n} u_{G}^{n-1} d\Omega + \int_{\Gamma_{f}} \bar{f}^{n} w_{G}^{n} d\Gamma + \eta \int_{\Gamma_{c}} \bar{u}^{n} w_{G}^{n} d\Gamma + \int_{\Omega} Q^{n} w_{G}^{n} d\Omega$$

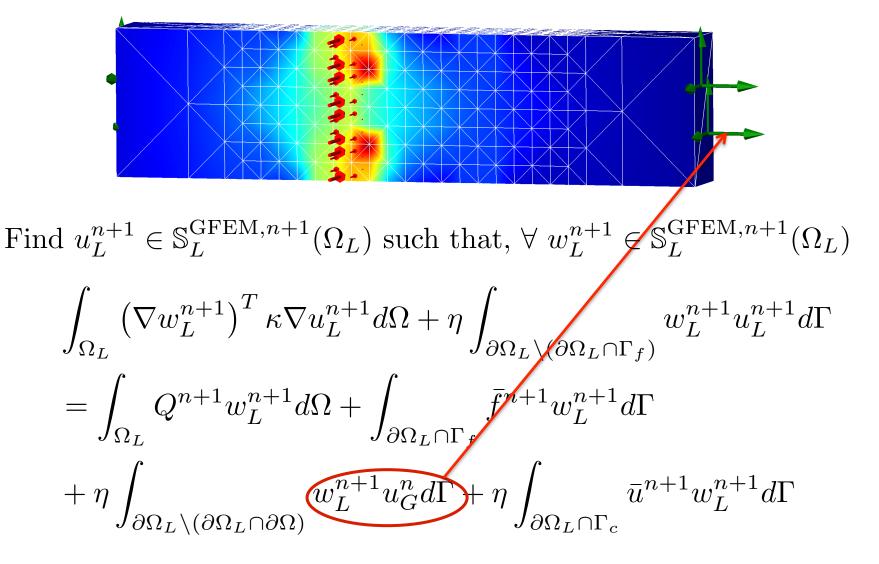


Let $u_G^n(\boldsymbol{x}) \in \mathbb{S}_G^{GFEM,n}(\Omega)$ be the GFEM solution at time $t = t^n = n\Delta t$

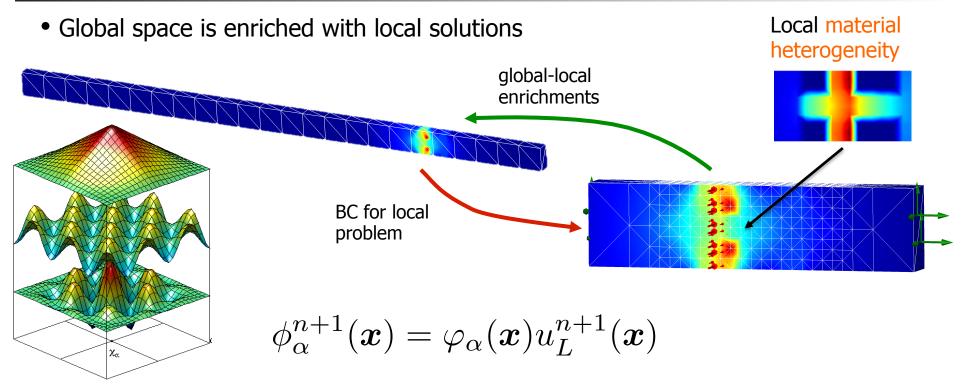




• Solve following *local problem* at time $t = t^{n+1}$ using, e.g., *hp*-GFEM







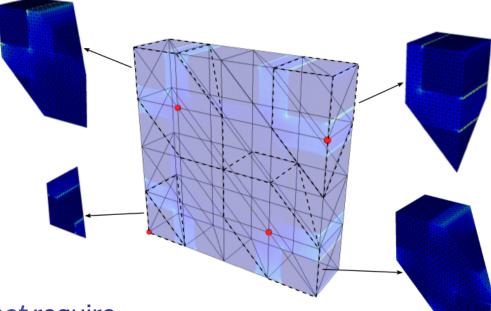
Find
$$u_G^{n+1}(\boldsymbol{x}) \in \mathbb{S}_G^{\text{GFEM},n+1}(\Omega) = \mathbb{S}_G^{\text{FEM}} + \left\{ \varphi_{\alpha} u_{\alpha}^{\text{gl},n+1}, \ \alpha \in \mathcal{I}^{\text{gl}} \right\}$$

where $u_{\alpha}^{\text{gl},n+1}(\boldsymbol{x}) = \underline{u}_{\alpha} u_L^{n+1}(\boldsymbol{x}) \in \chi_{\alpha}^{n+1}, \ \underline{u}_{\alpha} \in \mathbb{R}$

• Discretization spaces updated on-the-fly with global-local enrichment functions



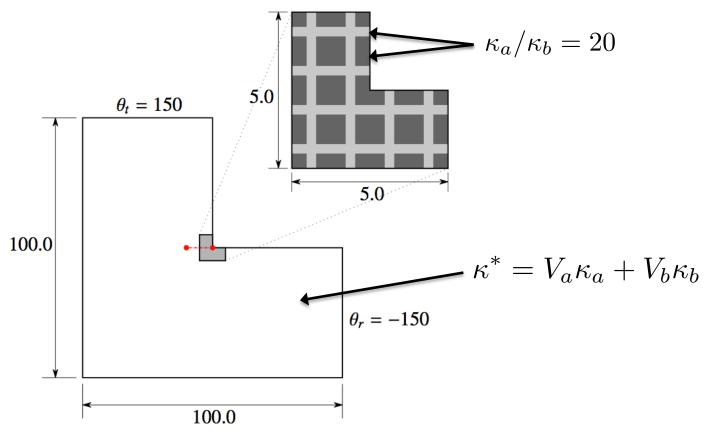
- Subdivide local problem into 'sub-local' domains
 - Each global patch/cloud (node support) = One sub-local domain



- GFEM^{gl} does not require
 - Communication among sub-local problems
 - Continuity across sub-local boundaries
- Analyze fine scale efficiently in parallel [Kim et al. 2010]

Example: Steady-State Heat Transfer on L-Shaped Domain*

Heat flux singularity and material heterogeneity at reentrant corner



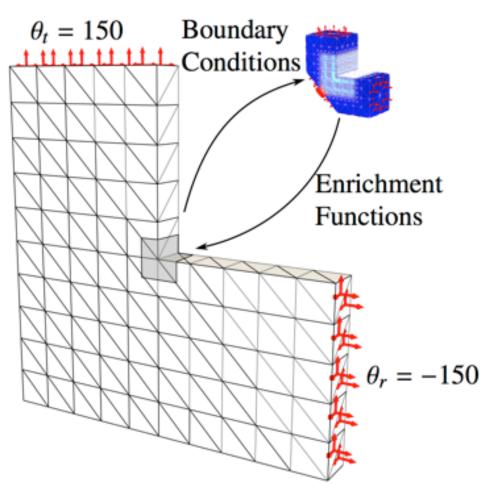
- Homogenization not valid at corner
- Adopt GFEM^{gl} to capture interaction between material and global scales



Steady-State Heat Transfer on L-Shaped Domain

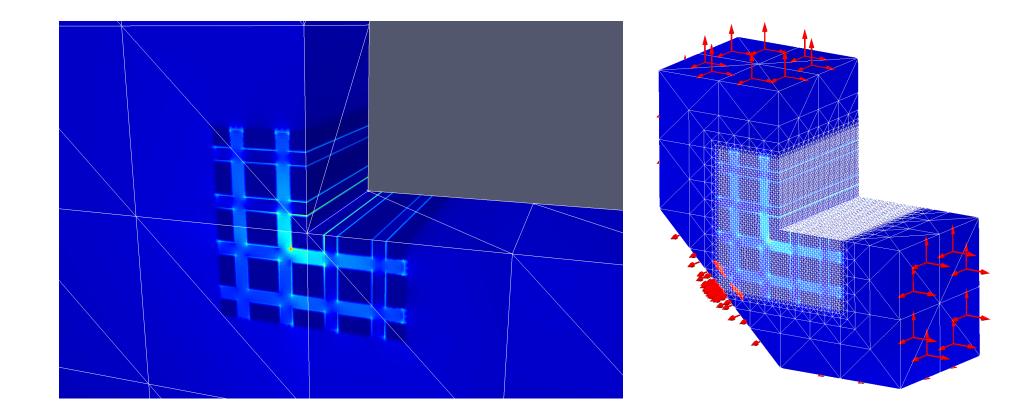
GFEM^{gl} discretizations

- Coarse global mesh
- Refine heavily in sub-*local* problems
- Solve sub-local problems in parallel
- Global-local enrichments in neighborhood of corner only, polynomial enrichment elsewhere



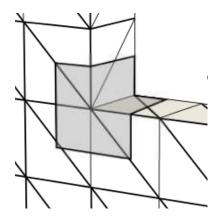


• GFEM^{gl} discretizations: Fine-scale mesh is *non-conforming* with global mesh

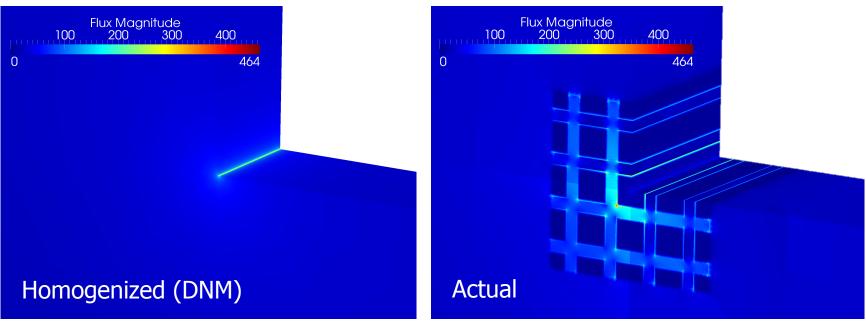




 GFEM^{gl} resolves localized gradients and singularities on a coarse global mesh

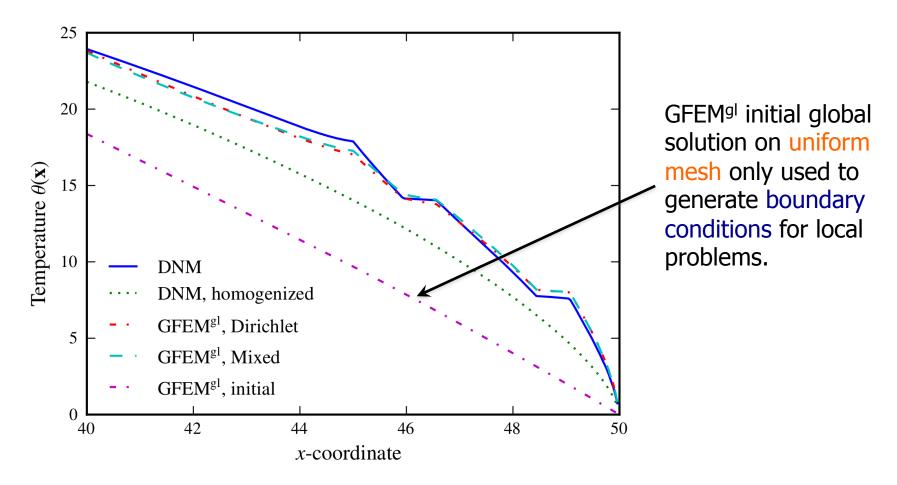


Heat flux at re-entrant corner



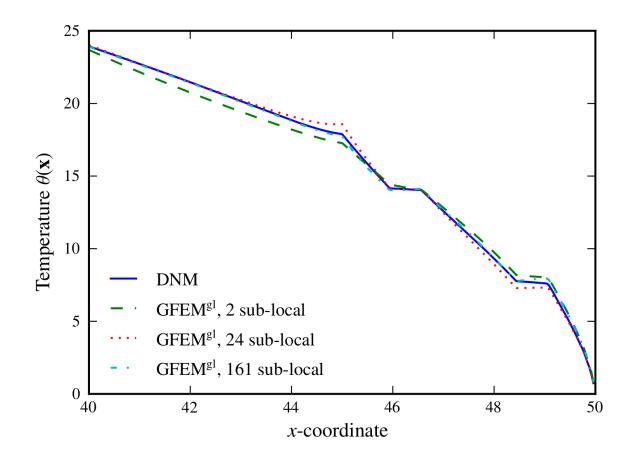


 Solution in neighborhood of reentrant corner: GFEM^{gl} with two sub-local problems





Pointwise convergence of GFEM^{gl} solution in neighborhood of reentrant corner





Computational cost and parallelism

| Method | Sub-local prob. | Global dofs | Energy ($\times 10^6$) | % difference | Sol. time (s) |
|--------------------|-----------------|-------------|--------------------------|--------------|---------------|
| DNM (parallel) | _ | 1,676,652 | 3.376 | _ | 177.4 |
| GFEM ^{gl} | 24 | 880 | 3.377 | 0.05% | 281.6 |
| | 161 | 1.789 | 3.377 | 0.03% | 60.8 |
| | 864 | 4,440 | 3.375 | 0.01% | 30.2 |

- Global mesh refined to generate more sub-local problems
- Identical mesh size maintained in sub-local problems and DNM
- Server: 24 cores, 2 Intel Xeon E5-2697 v2 2.70GHz processors
- Pardiso parallel sparse solver adopted
- Solution time includes assembly, factorization and solve
- Efficiency and accuracy increase with number of sub-local problems



Computational cost and parallelism

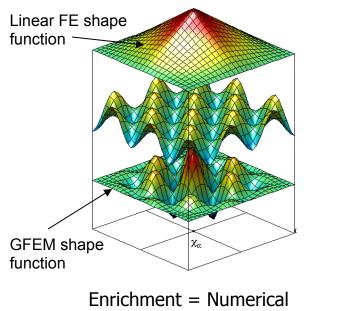
| Method | Sub-local prob. | Factorize/solve (s) | Speedup | Efficiency |
|-------------------------------|-----------------|---------------------|---------|------------|
| DNM (serial) | _ | 1373.1 | - | — |
| DNM (parallel) | _ | 145.8 | 9.42 | 0.393 |
| GFEM ^{gl} (parallel) | 24 | 253.0 | 5.43 | 0.226 |
| | 161 | 42.0 | 32.66 | 1.361 |
| | 864 | 10.3 | 133.01 | 5.542 |

- Speedup and efficiency computed w.r.t. DNM serial solution
- Efficiency over 100% relative to DNM with nearly identical accuracy
- Pardiso parallel sparse solver adopted
- Efficiency and accuracy increase with number of sub-local problems



GFEM^{gl}: Discretization Method at Fine Scale

 Enrichment functions can be computed with almost any available discretization method: GFEM, FEM, BEM, Meshfree, Peridynamics, etc.



solutions of BVP

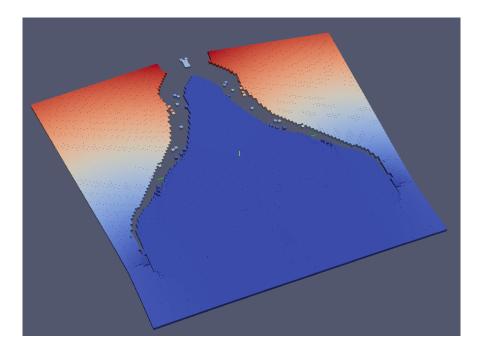
- Simulation of impact and fragmentation using Peridynamics [Sa Wu and Marc A. Schweitzer, Bonn University]*
- Initial conditions for Peridynamics from GFEM sol.
- Use Peridynamics enrichments only where it is needed

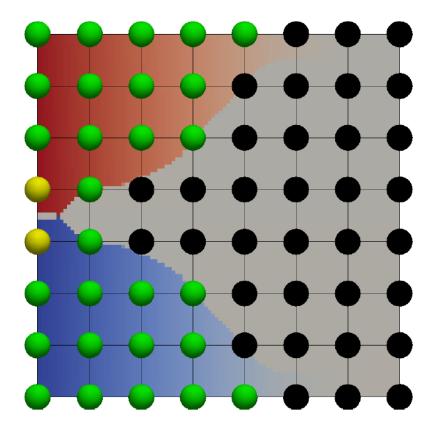
* http://schweitzer.ins.uni-bonn.de/people/wu.html



GFEM^{gl}: Discretization Method at Fine Scale

 Peridynamics solution (left) used as enrichment at macro-scale GFEM mesh (right) *





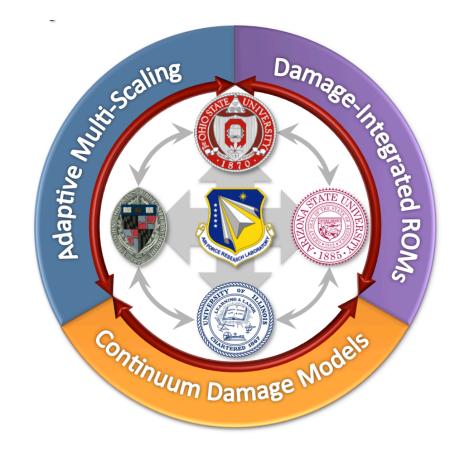
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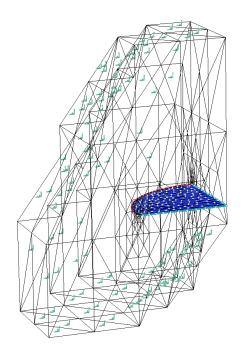


- Generalized FEMs offer significant **flexibility** and attractive features
- It enables the solution of problems that are difficult or not practical with the FEM:
 - Multiscale problems:
 - Fine-scale computations are naturally parallelizable
 - Can adopt different discretization methods at each scale without difficulty or introduction of additional fields (LM, mortar, etc.)
 - Coalescence of 3-D fractures: Hydraulic fracturing of oil and gas reservoirs
- Transition to Labs and Industries: Non-intrusive integration with existing FEA software



• AFRL-University Collaborative Center in Structural Sciences (C²S²)





Questions?

caduarte@illinois.edu

http://gfem.cee.illinois.edu/

