Bridging Scales with a Generalized Finite Element method

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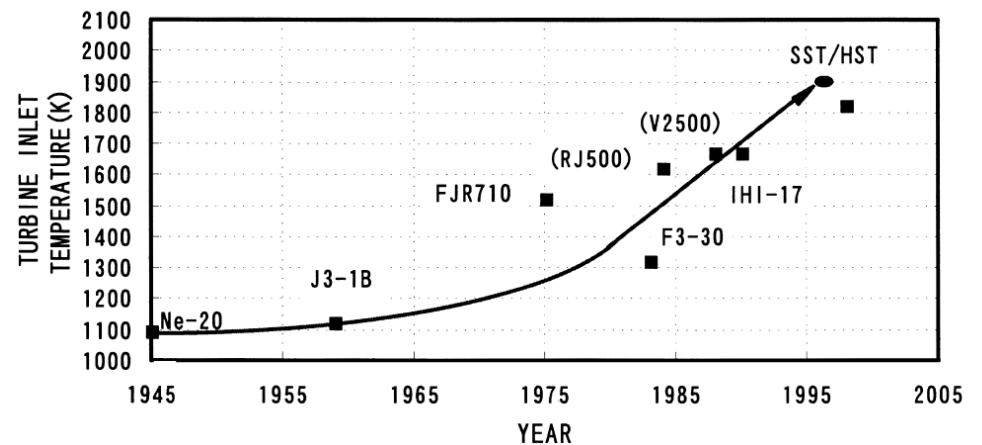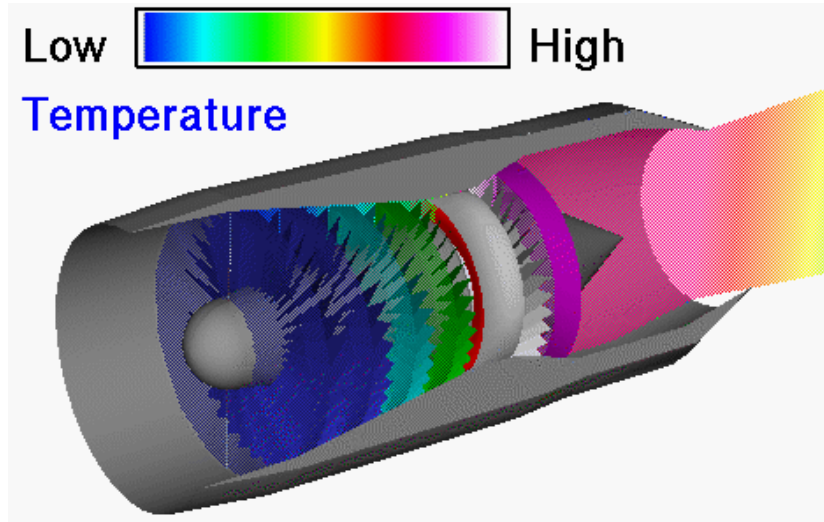University of Illinois at Urbana-Champaign, Urbana, IL

1

Motivation: From Micro to Macro

Courtesy of General Electric Co.
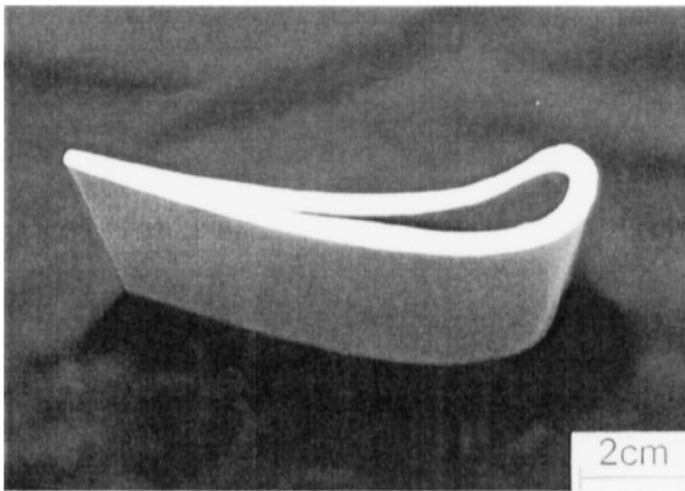

- The performance of a turbine increases with its operational temperature
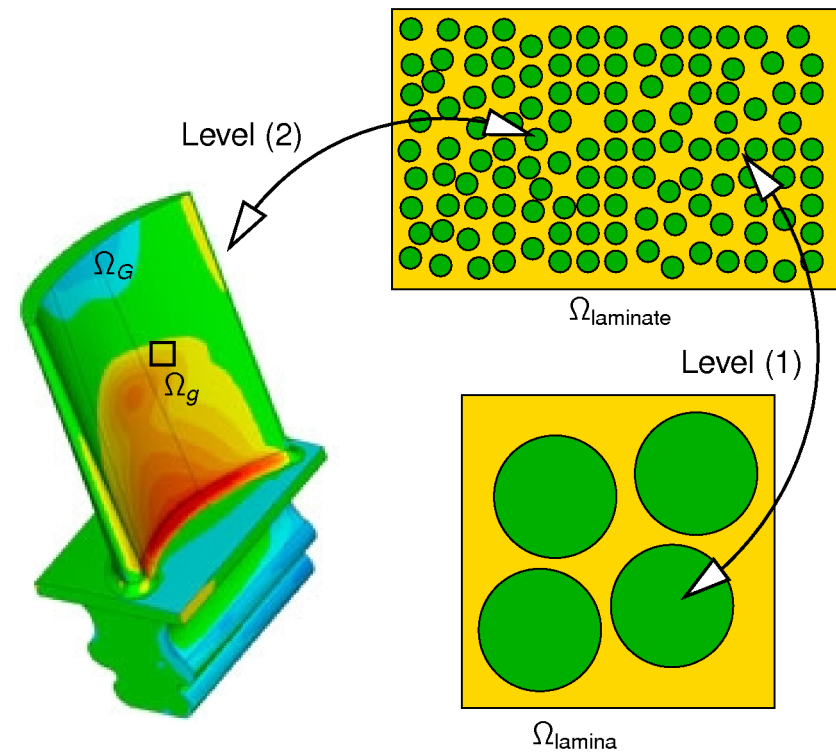
- High operational temperatures require new materials like Ceramic Matrix Composites (CMC)

Turbine component made of CMC

Level (2)

Ω_G

Ω_g

$\Omega_{laminate}$
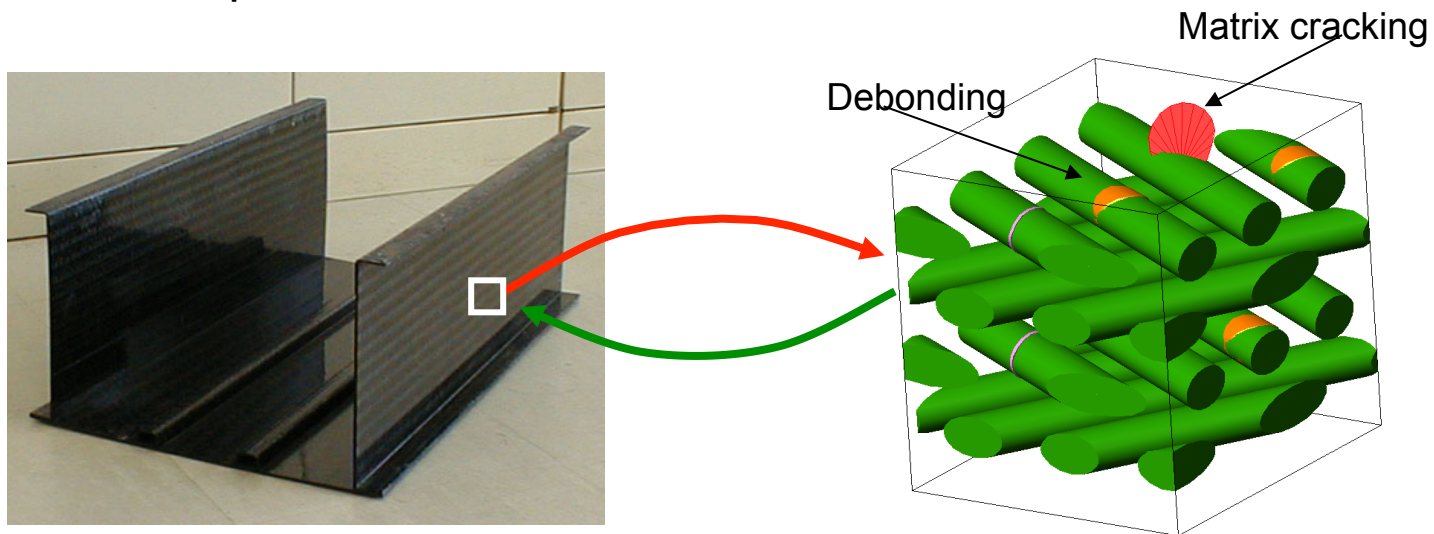
Level (1)

Ω_{lamina}

Structural performance depends strongly on micro-scale details

Motivation: From Micro to Macro

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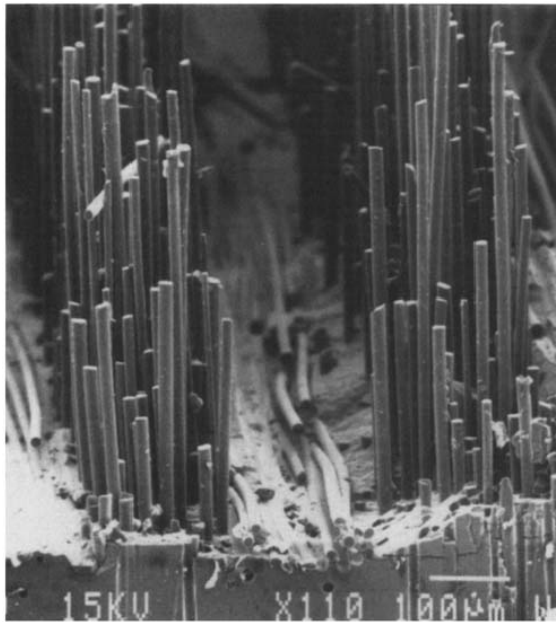

Damage in composite materials

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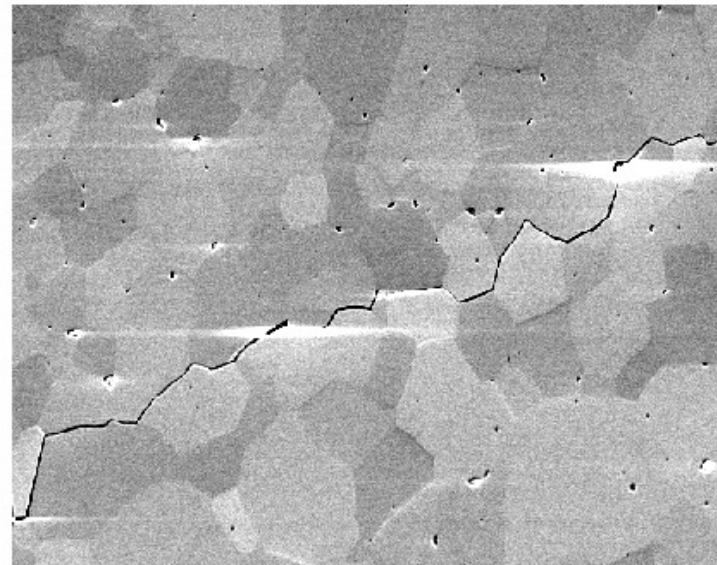 - Failure depends on local quantities as opposed to averaged [A. Needleman]

Multi-Scale Problems: Computational Challenges

- Discretization of fine-scale features like fibers and polycrystalline grains
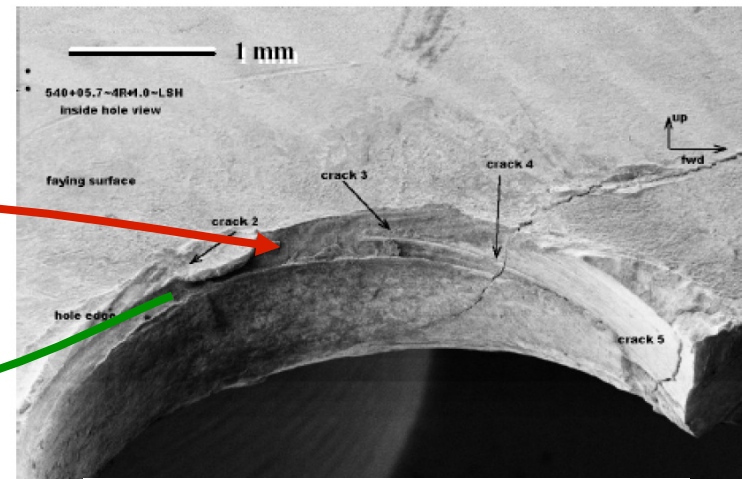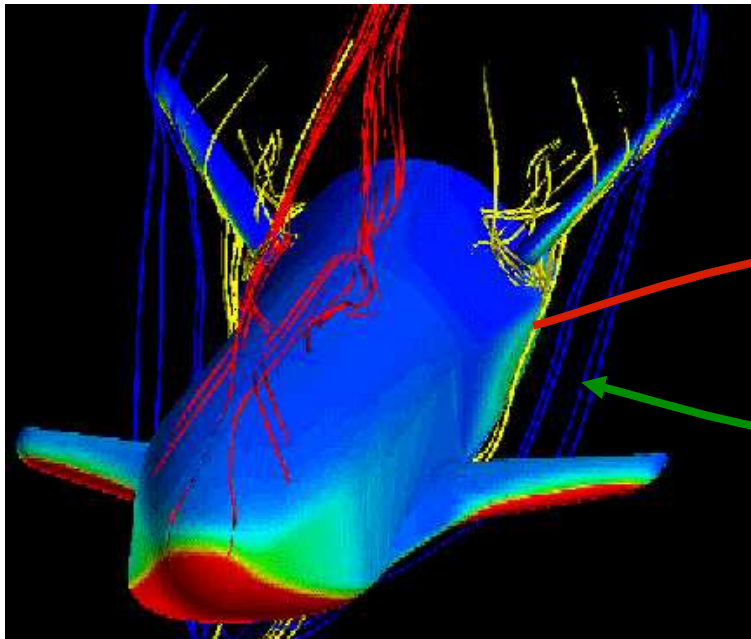

Fracture Surface of CMC

[Saether & Ta'asan, 2004]

Inter-granular Fracture

- Advances in existing computational methods are needed
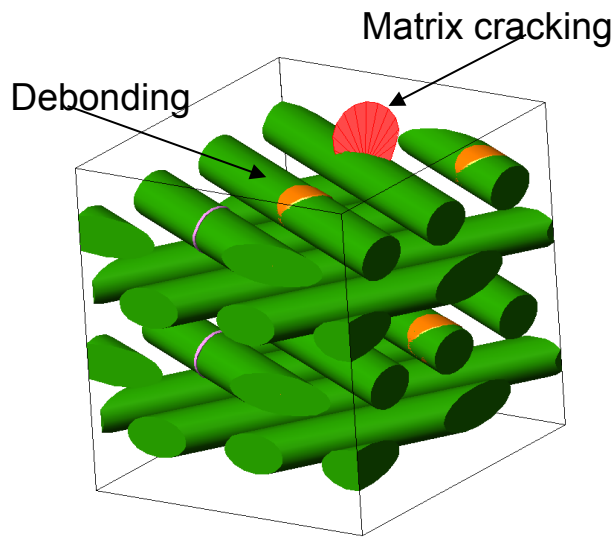- Increasing computational power alone is not enough

Multiple cracks around a rivet hole

[Sandia National Lab, 2005]

Multi-scale Problems

Matrix cracking

Debonding

Damage in composite materials

1 mm

540+05.7~4R+1.0~LSH
inside hole view

faying surface

crack 2

crack 3

crack 4

up
fwd

hole edge

crack 5

Multiple cracks around a rivet hole

[Sandia National Lab, 2005]

250 mm

125 μm

Thermal loads on
hypersonic aircrafts
(dimensions not to scale)

- Predictive simulations require modeling of phenomena spanning several spatial and temporal scales
- Advances in existing computational methods are needed
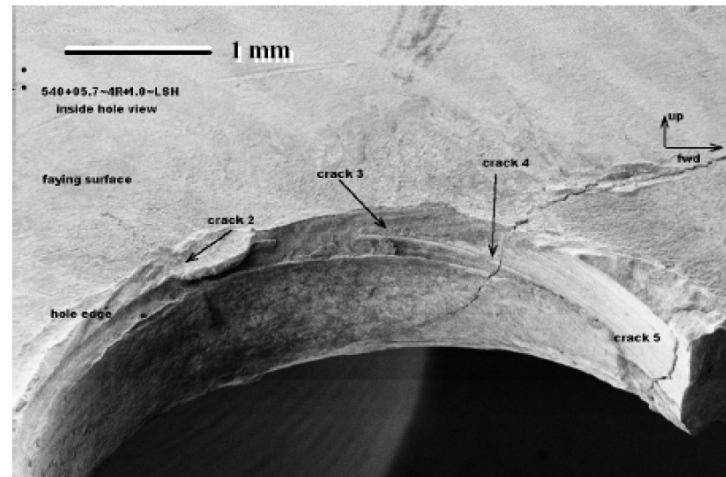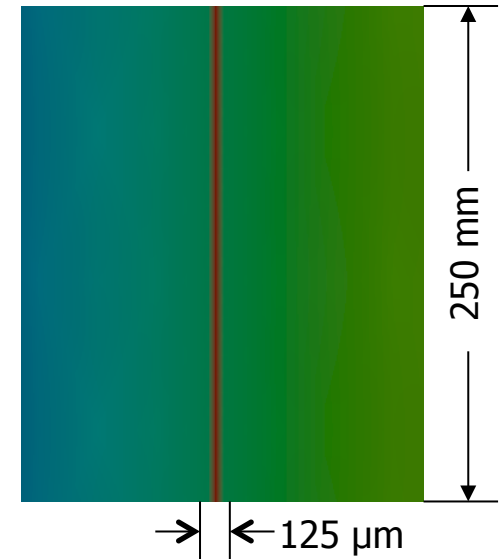- Increasing computational power alone is not enough

Outline

- Generalized finite element methods: Basic ideas

- GFEM for polycrystals and fibers

- Bridging scales with the GFEM:

  – Global-local enrichments

- Applications and mathematical analysis

- Transition: Non-intrusive implementation in Abaqus

- Assessment and closing remarks

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

- Recent review papers

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

  Fries, T.-P. and Belytschko, T. The generalized/extended finite element method: An
  overview of the method and its applications, *Int. J. Num. Meth. Eng.,* 2010.
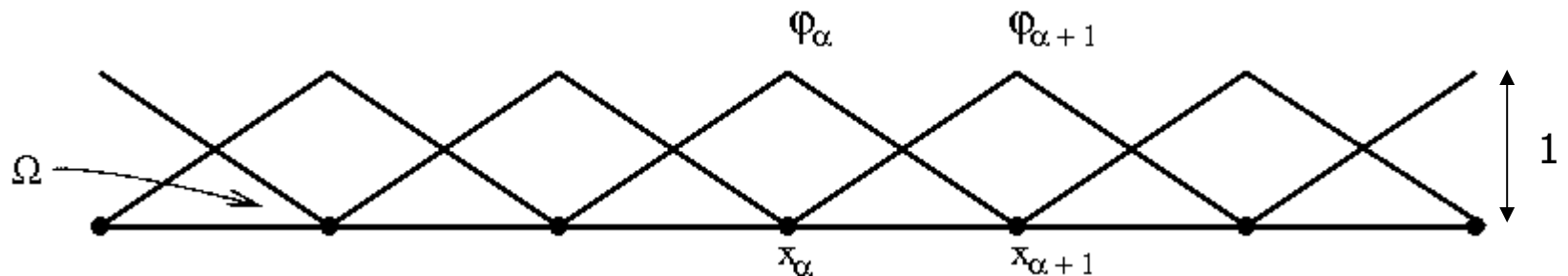
Generalized Finite Element Method

GFEM can be interpreted as a FEM with shape functions built using the concept of a partition of unity

Partition of Unity (PoU)

$$\sum_\alpha \varphi_\alpha(x) = 1 \qquad \forall \ x \in \Omega$$

- φ_α = Linear FEM shape function

Generalized Finite Element Method

- GFEM shape function = FE shape function * enrichment function

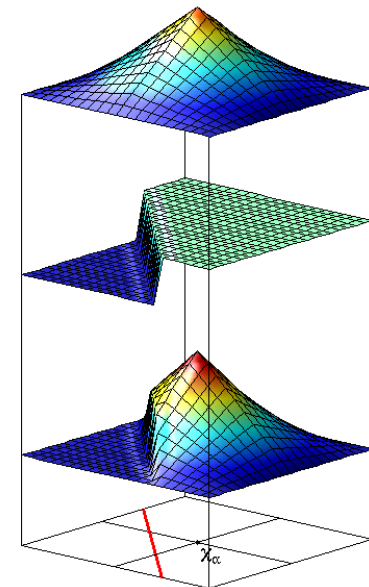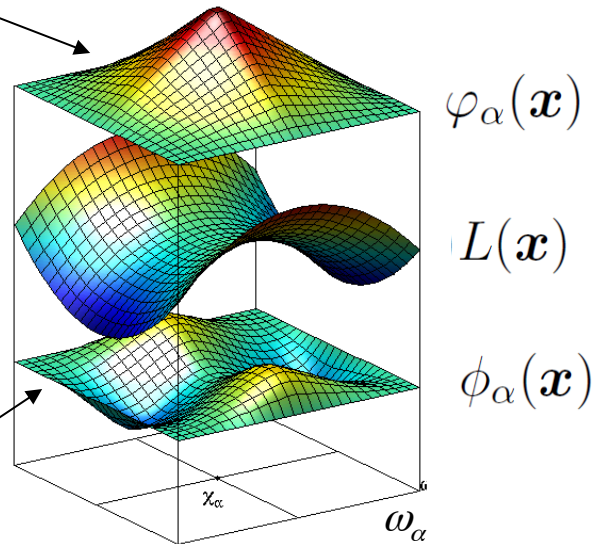$$\phi_\alpha(\boldsymbol{x}) = \varphi_\alpha(\boldsymbol{x}) L(\boldsymbol{x})$$

• Allows construction of shape functions incorporating a-priori knowledge about solution

Linear FE shape function

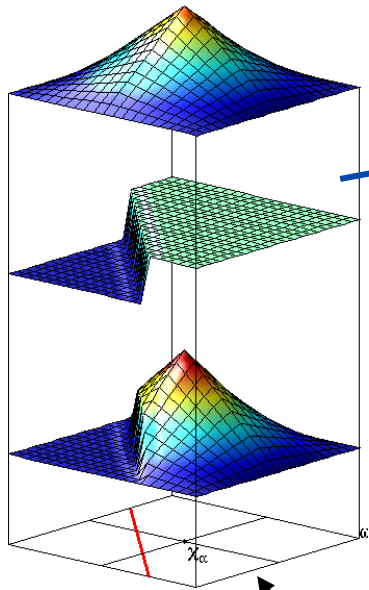Enrichment function

GFEM shape function

$\varphi_\alpha(\boldsymbol{x})$

$L(\boldsymbol{x})$

$\phi_\alpha(\boldsymbol{x})$

χ_α

ω_α

Discontinuous enrichment [Moes et al.]

χ_α

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GFEM Approximation for 3-D Cracks

$$X^{hp}(\Omega) = \left\{ u = \sum_{\alpha=1}^{N} \underbrace{\varphi_\alpha(x)}_{\text{PoU}} \left[\underbrace{\hat{u}_\alpha(x)}_{\text{polynomial}} + \underbrace{\mathcal{H}\tilde{u}_\alpha(x)}_{\text{discontinuous}} + \underbrace{\breve{u}_\alpha(x)}_{\text{singular}} \right] \right\}$$
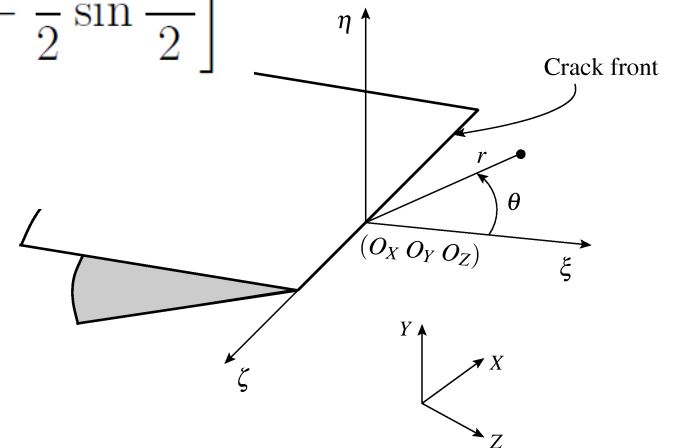
$$\breve{L}_{\alpha 1}^{\xi}(r,\theta) = \sqrt{r}\left[\left(\kappa - \frac{1}{2}\right)\cos\frac{\theta}{2} - \frac{1}{2}\cos\frac{3\theta}{2}\right]$$

$$\breve{L}_{\alpha 1}^{\eta}(r,\theta) = \sqrt{r}\left[\left(\kappa + \frac{1}{2}\right)\sin\frac{\theta}{2} - \frac{1}{2}\sin\frac{3\theta}{2}\right]$$

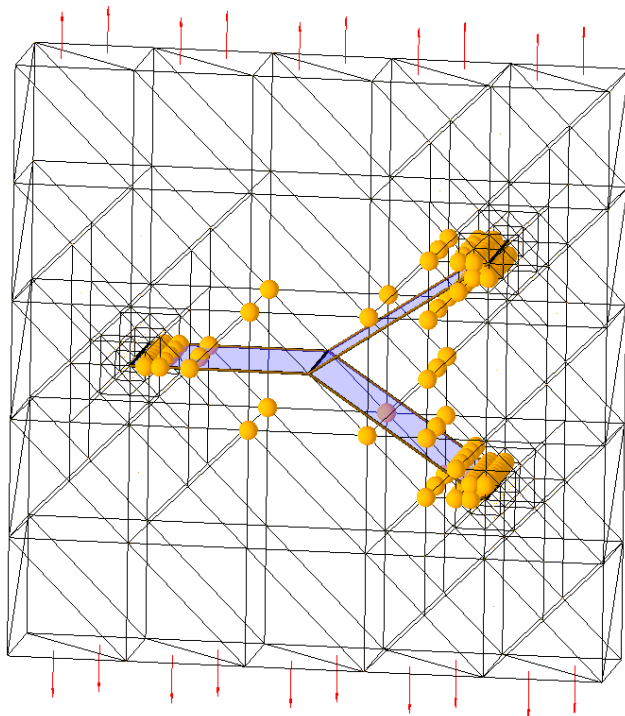$$\breve{L}_{\alpha 1}^{\zeta}(r,\theta) = \sqrt{r}\sin\frac{\theta}{2}$$

[Duarte and Oden 1996]

cloud or patch α
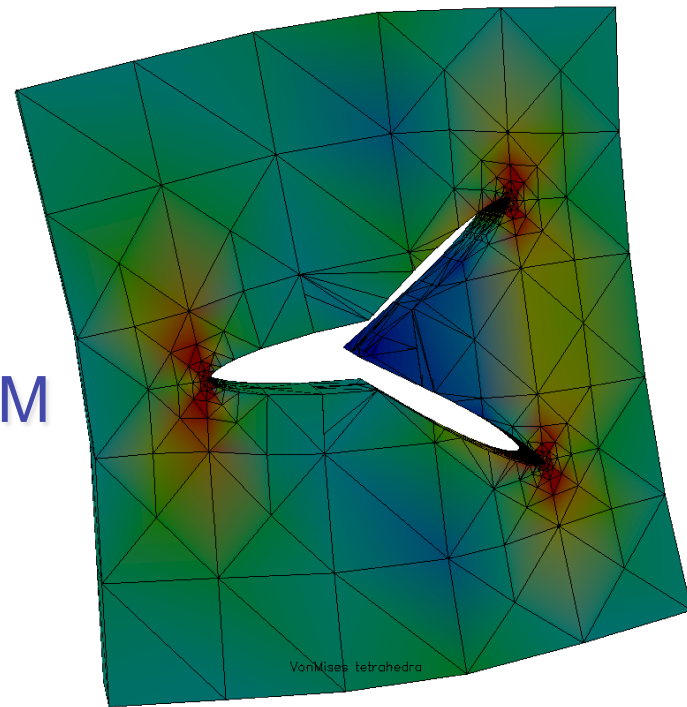
Crack front

$(O_X\, O_Y\, O_Z)$

Modeling Cracks with hp-GFEM

- Discontinuities modeled via enrichment functions, *not* the FEM mesh
- Mesh refinement *still required* for acceptable accuracy

hp-GFEM

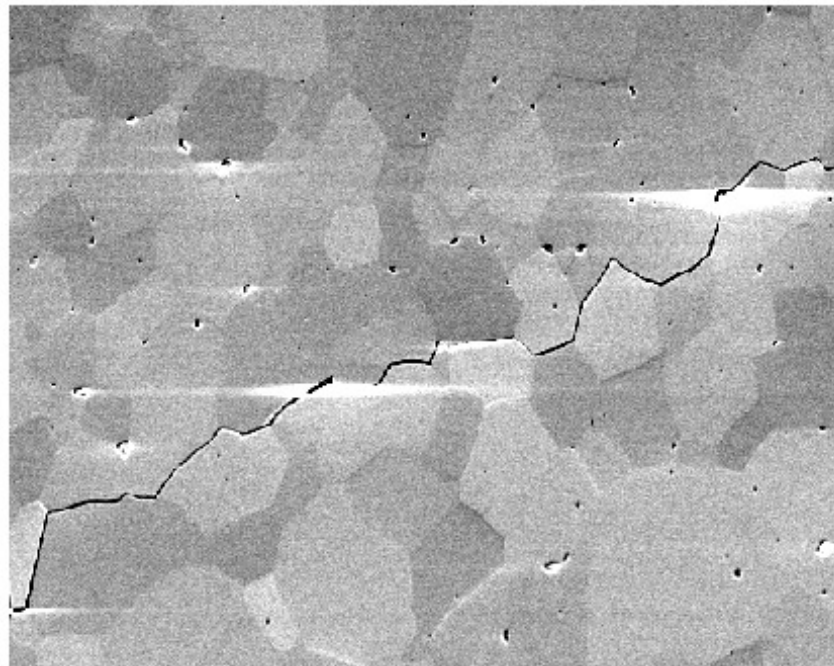● = Nodes with discontinuous enrichments

[Duarte, Reno and Simone, Int. J. Num. Meth. Eng., 2007]

Von Mises stress

Discretization of Micro Scales: GFEM for Polycrystals
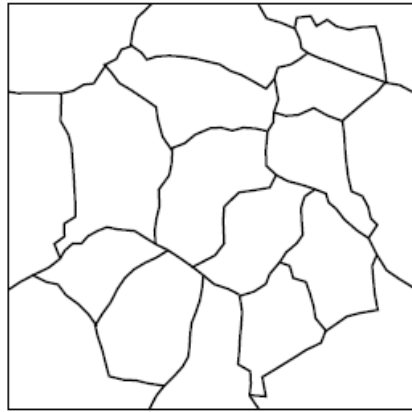
- **Goals:**

  - Modeling inter-granular crack propagation
  - What is the role of grain boundary parameters on the path of a crack ?
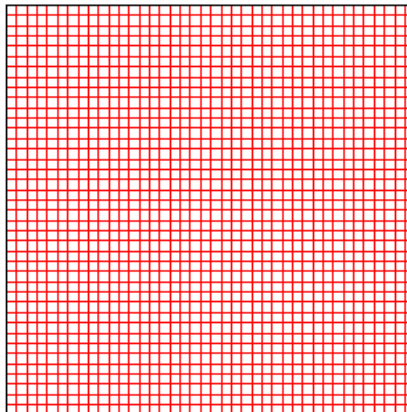

[Saether & Ta'asan, 2004]

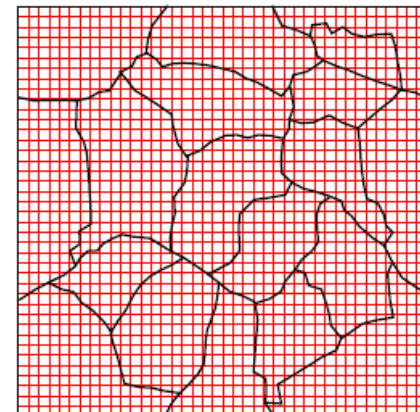# GFEM for Polycrystals*

| polycrystal topology | + | background mesh | = | GFEM for polycrystals |

- Grain boundaries cut elements
- Grain junctions within elements
- Any constitutive relation at grains
- Any traction-separation law at grain boundaries

(*) Simone, Duarte & Van der Giessen, IJNME 2006

• Grains interact through cohesive laws

$\mathcal{G}_1$ $\mathcal{G}_3$ $\mathcal{G}_2$
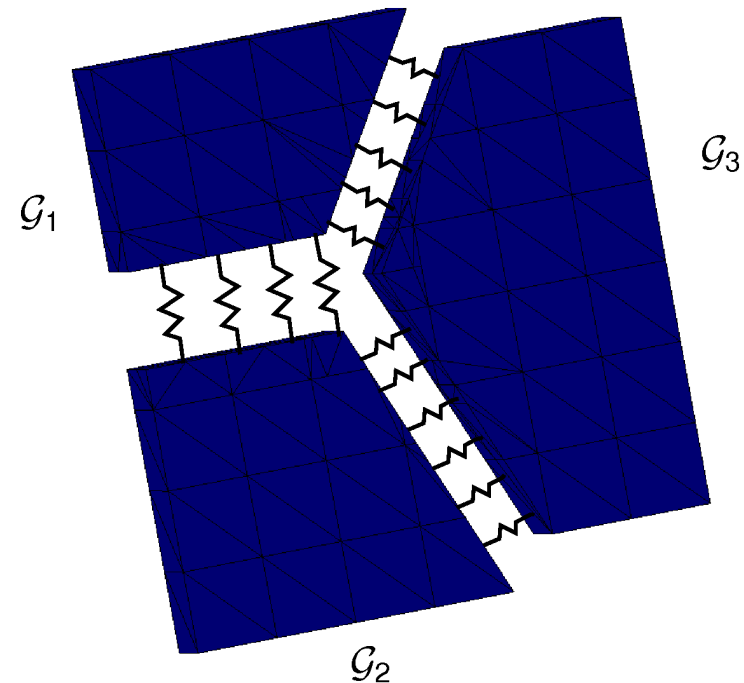
• Displacement decomposition

$$\boldsymbol{u} = \hat{\boldsymbol{u}} + \sum_{i=1}^{N_\mathcal{G}} \mathcal{H}_i \tilde{\boldsymbol{u}}_i \quad \text{with} \quad \mathcal{H}_i(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \mathcal{G}_i \\ 0 & \text{otherwise} \end{cases}$$

- Grain boundaries cut elements; Grain junctions within elements

- Mesh refinement still required for acceptable accuracy
    - split cut elements...as if there were no discontinuities: Preserve aspect ratio
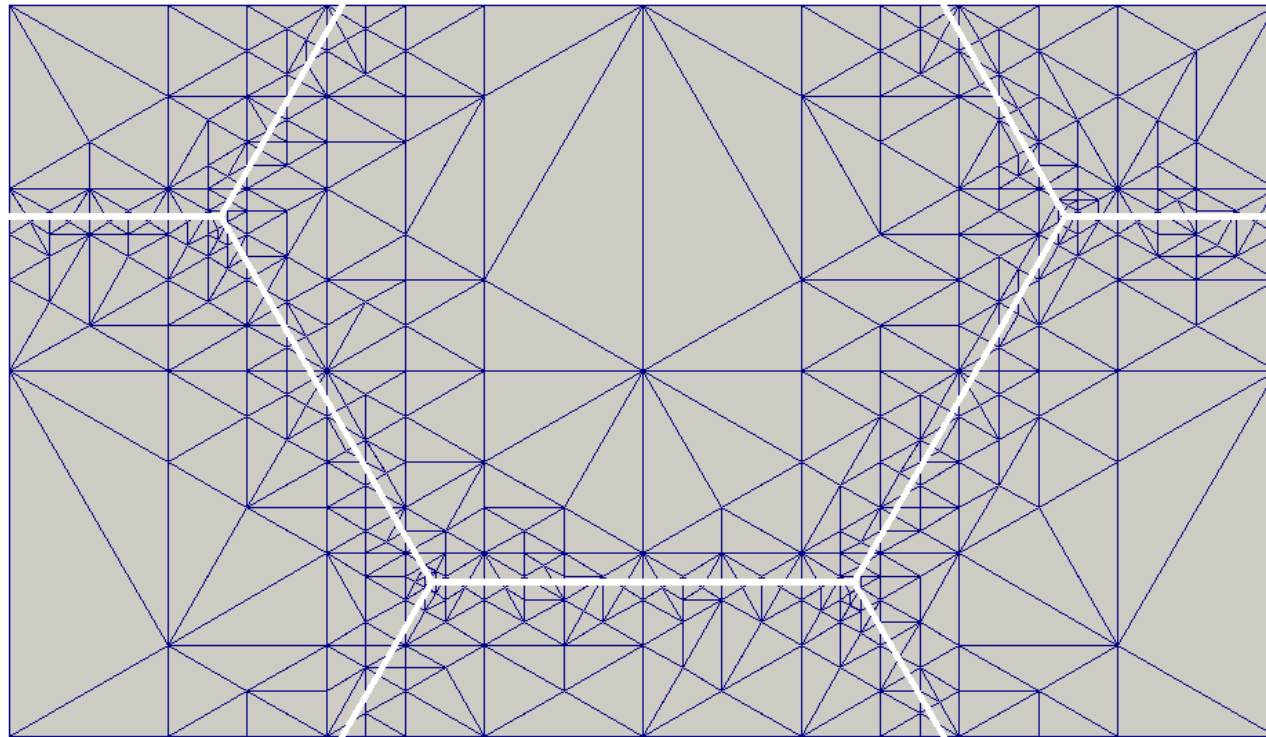
GFEM for Polycrystals

- Effect of grain boundary parameters on crack path (*)

$K_{lc} = 1.7$ MPa$\sqrt{m}$, $\sigma_{max} = 0.6$ GPa

$K_{lc} = 4.0$ MPa$\sqrt{m}$, $\sigma_{max} = 0.6$ GPa
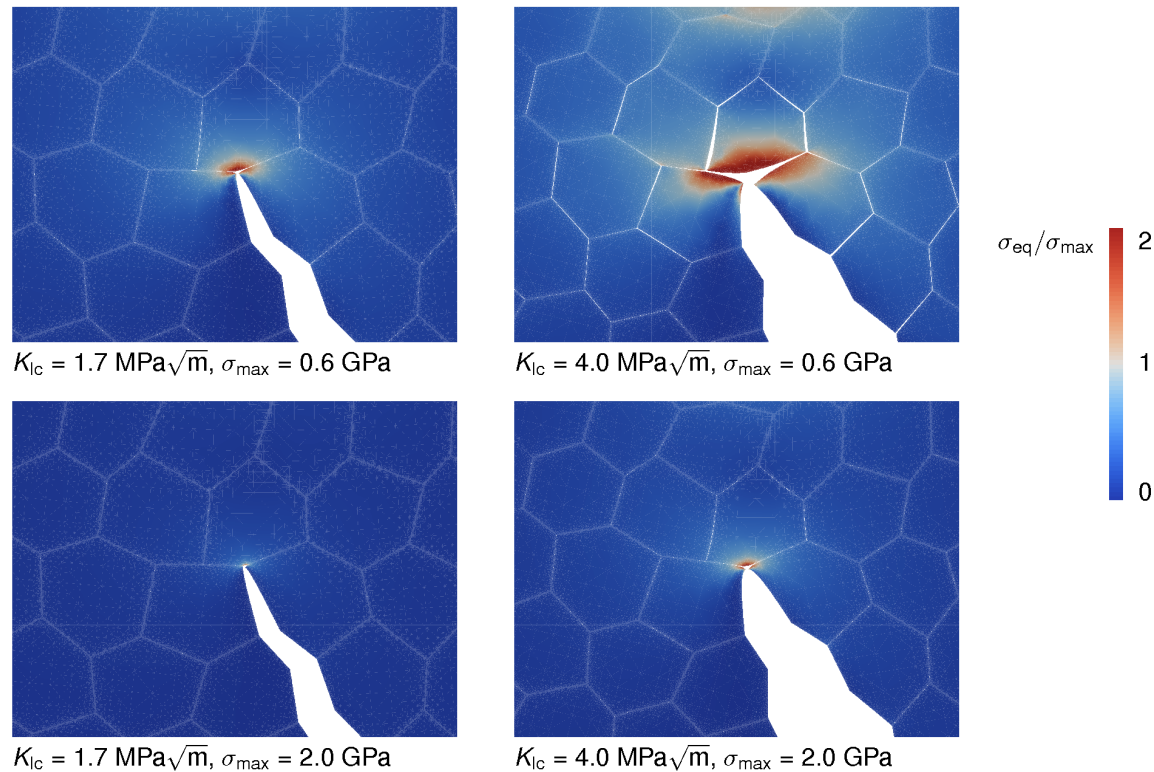
σ_{eq}/σ_{max}

$K_{lc} = 1.7$ MPa$\sqrt{m}$, $\sigma_{max} = 2.0$ GPa
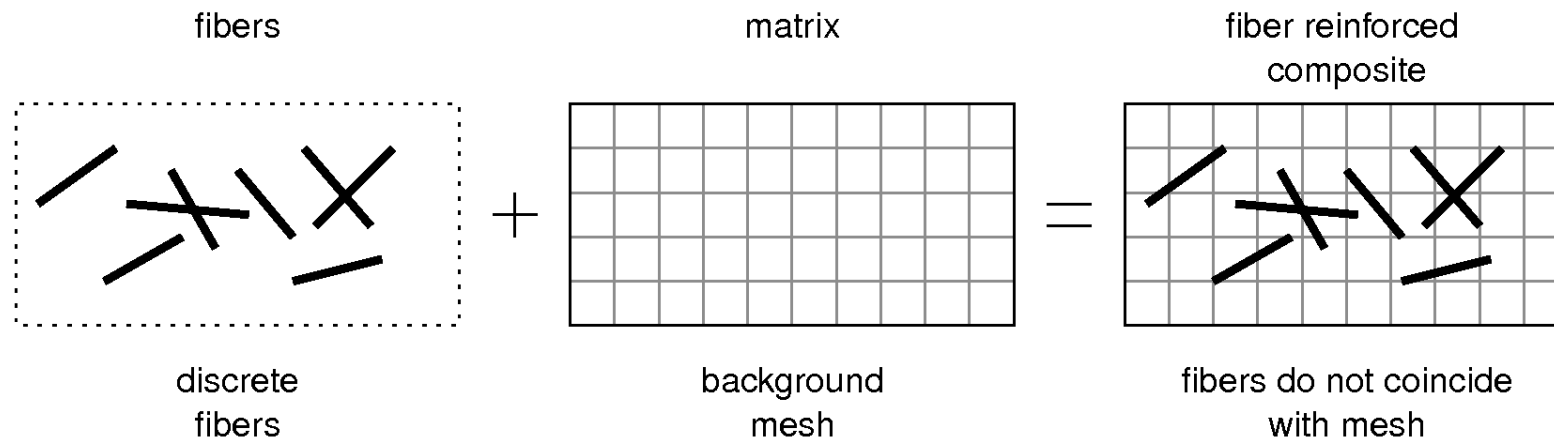
$K_{lc} = 4.0$ MPa$\sqrt{m}$, $\sigma_{max} = 2.0$ GPa

- Crack path is insensitive to variations of grain boundary parameters

(*) Shabir, Van der Giessen, Duarte and Simone, MSMSE, 2011

- Enrichment functions are used to represent fiber-matrix material-interfaces
- Fibers do not have to coincide with FE mesh

(*) Radtke, Simone and Sluys, IJNME, 2010

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Bridging Scales with Global-Local Enrichment Functions

- How to account for interactions among scales?
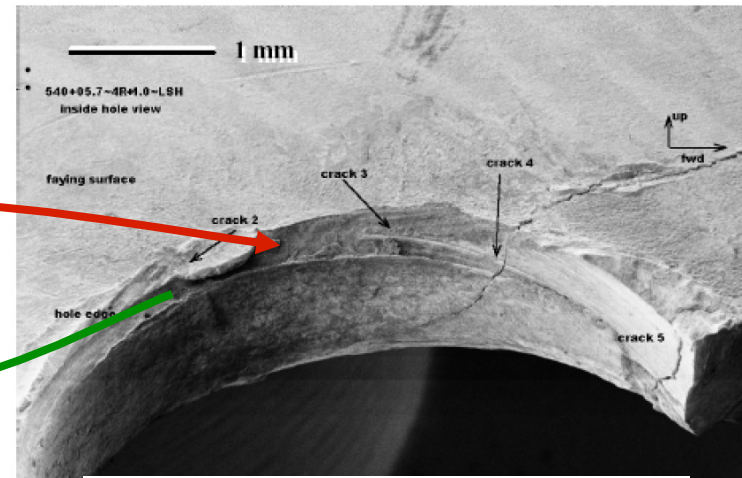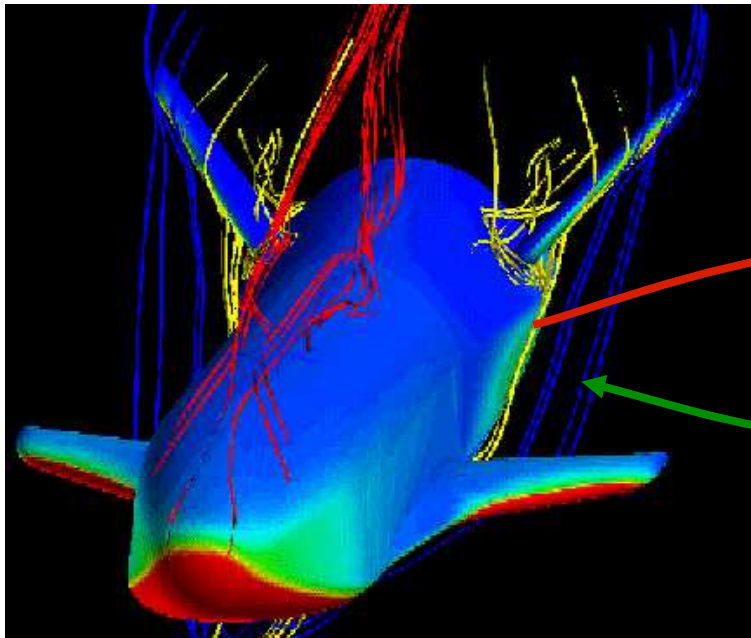
Multiple cracks around a rivet hole

[Sandia National Lab, 2005]

Goal:

- Capture fine scale effects on *coarse* meshes at the global (structural) scale

Bridging Scales with Global-Local Enrichment Functions *
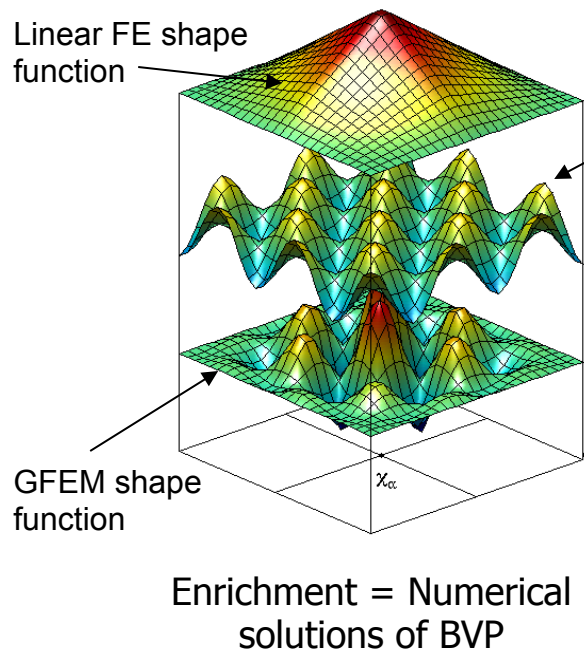
■ Enrichment functions computed from solution of local boundary value problems: <u>Global-Local enrichment functions</u>

Linear FE shape function

GFEM shape function

χ_α

Enrichment = Numerical solutions of BVP

■ **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 (G-L) functions

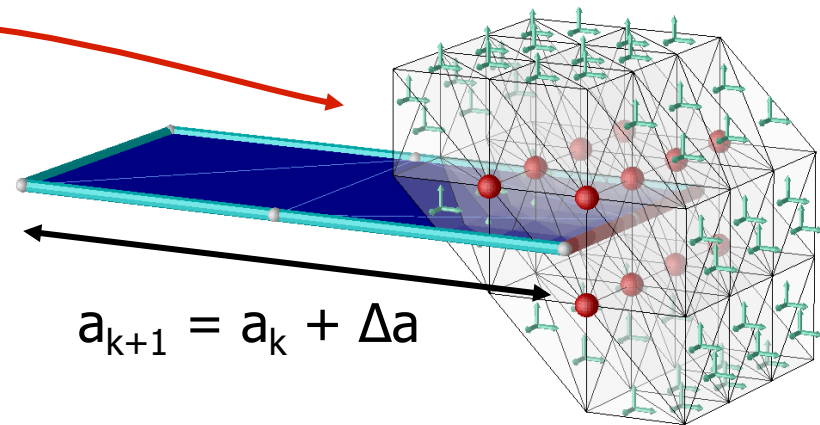***** Duarte et al. 2005, 2007, 2008, 2010, 2011

Global-Local Enrichments for 3-D Fractures

- u_G^k solution of global problem at crack step k
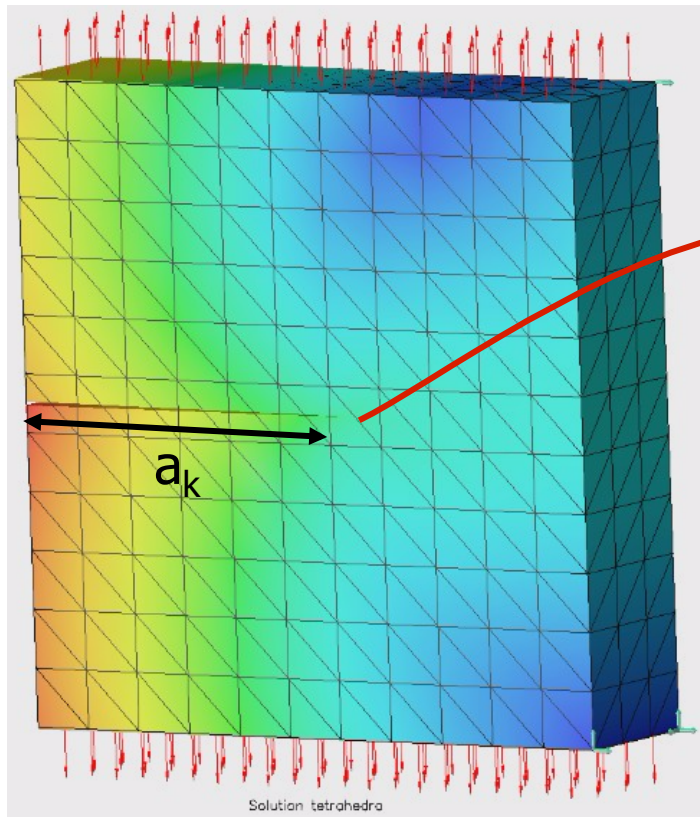
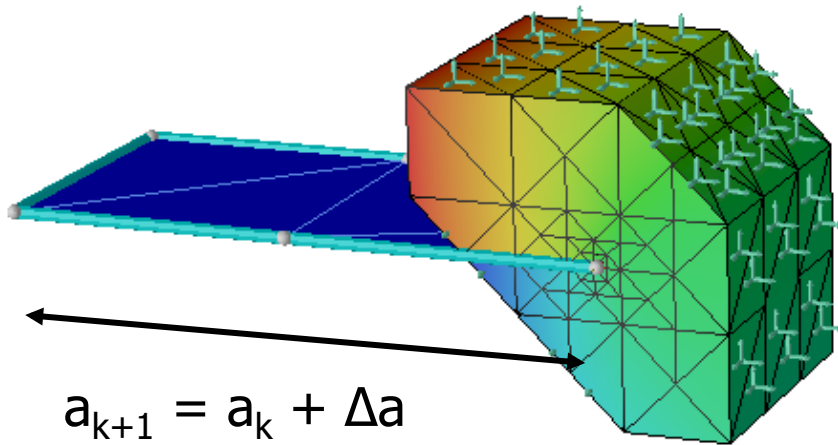- Define local domain containing crack front at step k+1

$$a_{k+1} = a_k + \Delta a$$

Local problem with crack size a_{k+1}

$u_G^k \in X_G^k(\Omega)$ = solution of global problem with crack size a_k

Global-Local Enrichments for 3-D Fractures

- Solve local problem at step k using *hp*-GFEM

Boundary conditions for local problems provided by global solution:

$$u_L^k = u_G^k \quad \text{on} \quad \partial\Omega_L^k \setminus (\partial\Omega_L^k \cap \partial\Omega)$$

$a_{k+1} = a_k + \Delta a$

$$X_L^k(\Omega_L^k) = \textit{hp-GFEM space}$$
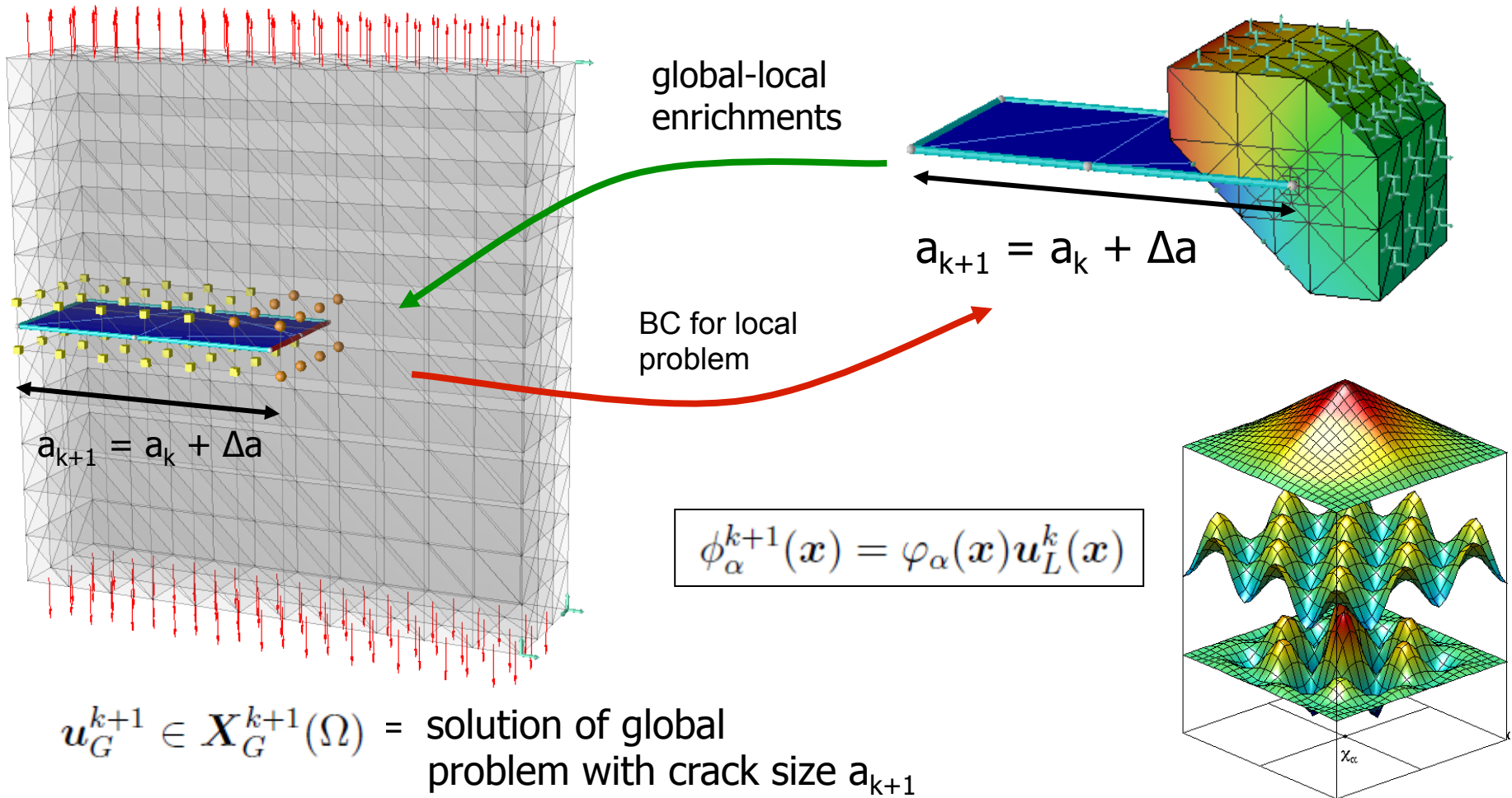
Find $u_L^k \in X_L^k(\Omega_L^k) \subset H^1(\Omega_L^k)$ such that $\forall\, v_L^k \in X_L^k(\Omega_L^k)$

$$\int_{\Omega_L^k} \boldsymbol{\sigma}(u_L^k) : \boldsymbol{\varepsilon}(v_L^k)\,d\boldsymbol{x} + \kappa \int_{\partial\Omega_L^k \setminus (\partial\Omega_L^k \cap \partial\Omega)} u_L^k \cdot v_L^k\,ds$$

$$= \int_{\partial\Omega_L^k \cap \partial\Omega^\sigma} \bar{t} \cdot v_L^k\,ds + \kappa \int_{\partial\Omega_L^k \setminus (\partial\Omega_L^k \cap \partial\Omega)} u_G^k \cdot v_L^k\,ds$$

Global-Local Enrichments for 3-D Fractures

- **Defining Step**: Global space is enriched with local solutions

global-local
enrichments

$$a_{k+1} = a_k + \Delta a$$

BC for local
problem

$$a_{k+1} = a_k + \Delta a$$

$$\phi_\alpha^{k+1}(x) = \varphi_\alpha(x) u_L^k(x)$$

$u_G^{k+1} \in X_G^{k+1}(\Omega) =$ solution of global
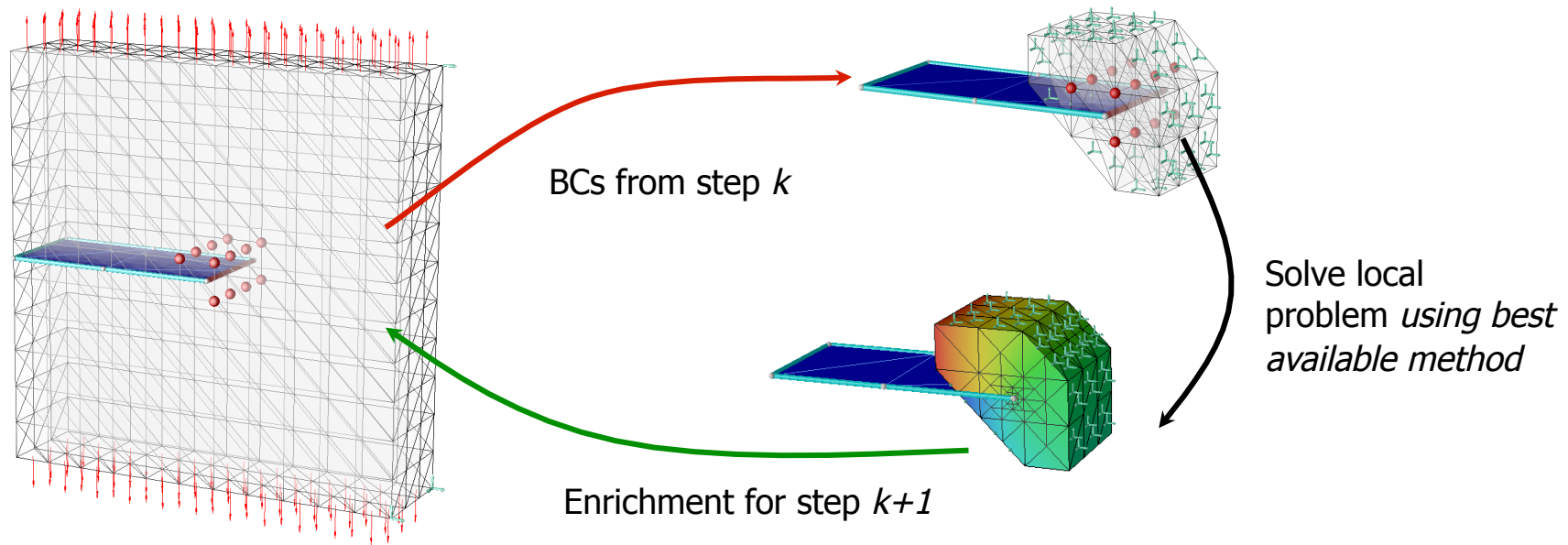problem with crack size a_{k+1}

- Procedure may be repeated: Update local BCs and enrichment functions

Global-Local Enrichments for Crack Growth

- **Summary:** Use solution of global problem at simulation k to build enrichment functions for step $k+1$

BCs from step k

Solve local problem *using best available method*

Enrichment for step $k+1$

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

$$X_G^{k+1}(\Omega_G) = \left\{ u = \underbrace{\sum_{\alpha=1}^{N} \varphi_\alpha(x)\hat{u}_\alpha(x)}_{\text{coarse-scale approx.}} + \underbrace{\sum_{\beta\in\mathcal{I}_{gl}^k} \varphi_\beta(x)u_\beta^{gl(k)}(x)}_{\text{fine-scale approx.}} \right\} \qquad u_\beta^{gl(k)} = \text{G-L enrichment}$$
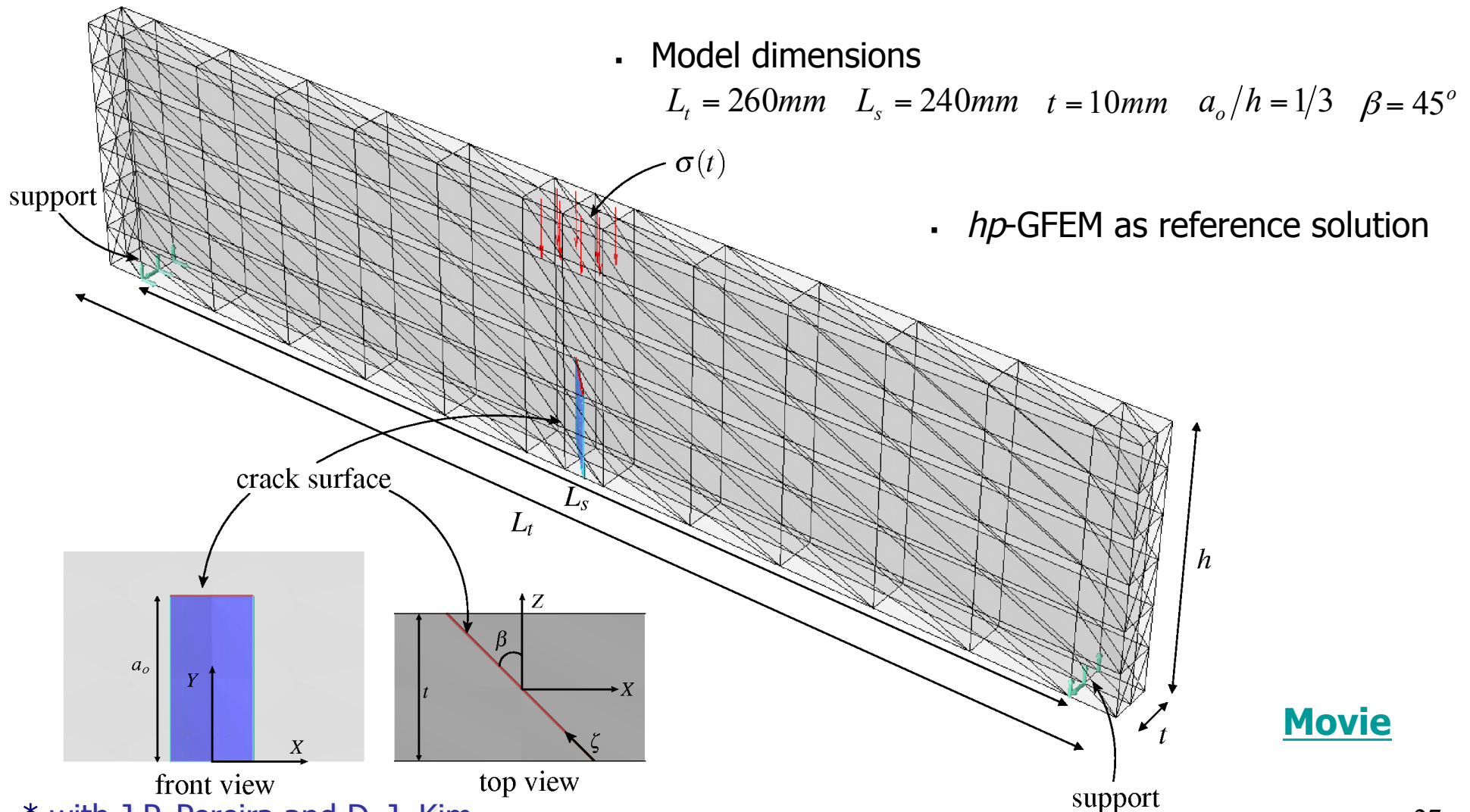
Edge-Notched Beam with Slanted Crack *

- **Fatigue Crack Growth: hp-GFEM and GFEM^{gl} solutions**

- Model dimensions

$$L_t = 260mm \quad L_s = 240mm \quad t = 10mm \quad a_o/h = 1/3 \quad \beta = 45^o$$

$\sigma(t)$

- hp-GFEM as reference solution

support

crack surface

L_s

L_t

h

a_o

Y

X

front view

Z
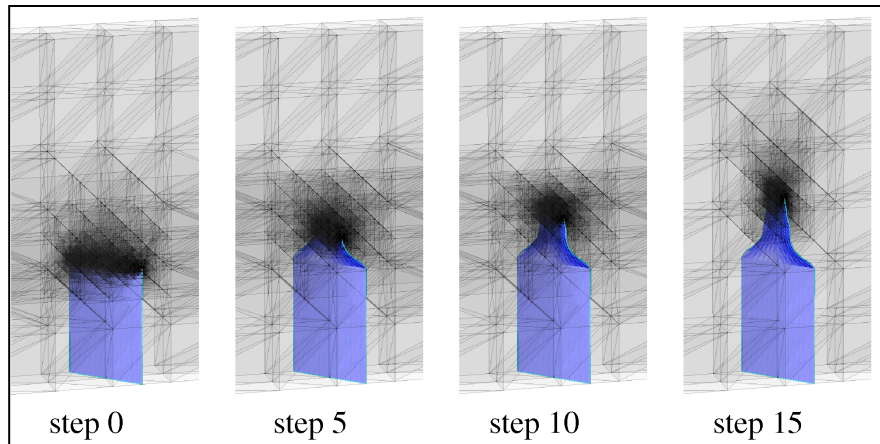
β

t
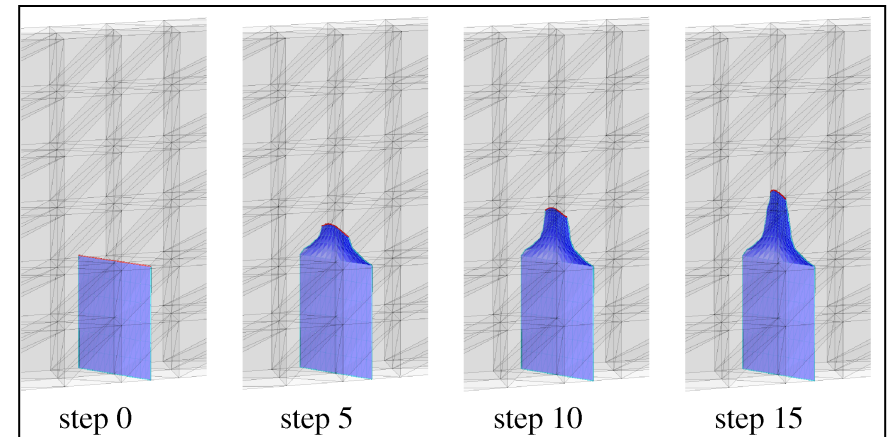
X

ζ

top view

t

support

Movie

* with J.P. Pereira and D.-J. Kim

Edge-Notched Beam with Slanted Crack
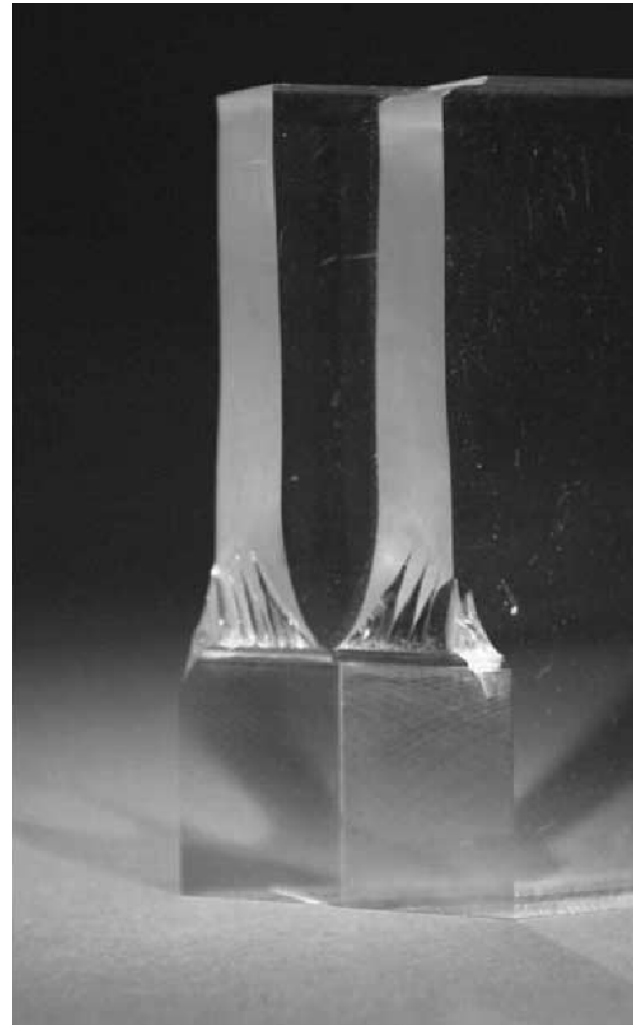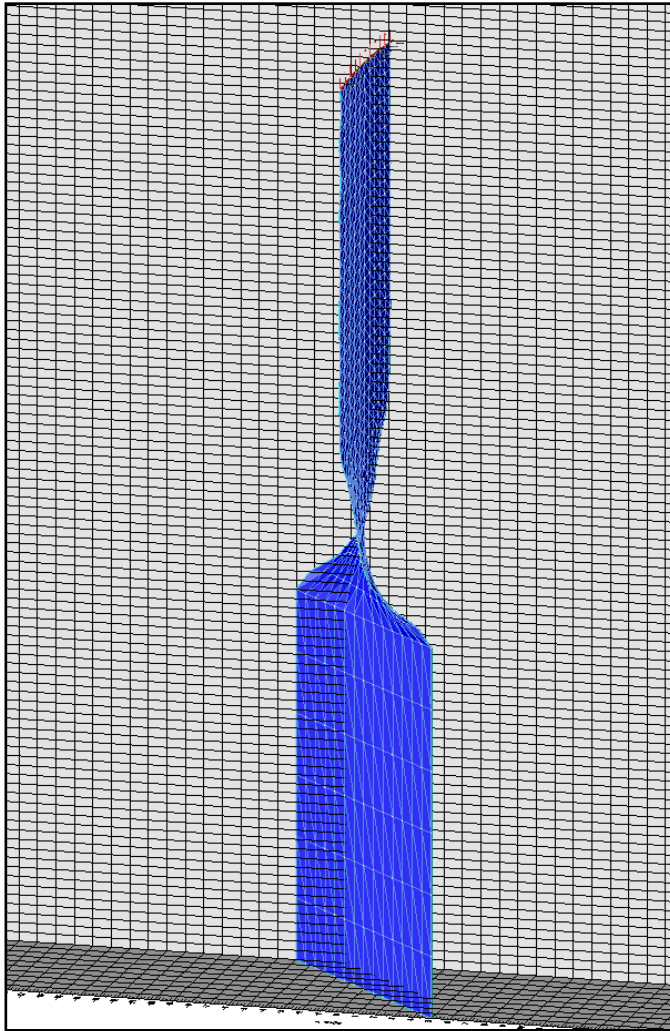

Available Methods – *hp*-GFEM/FEM

Two-Scale Generalized FEM – GFEM[gl]

- Mesh with elements that are orders of magnitude larger than in a FEM mesh
- Fully compatible with FEM
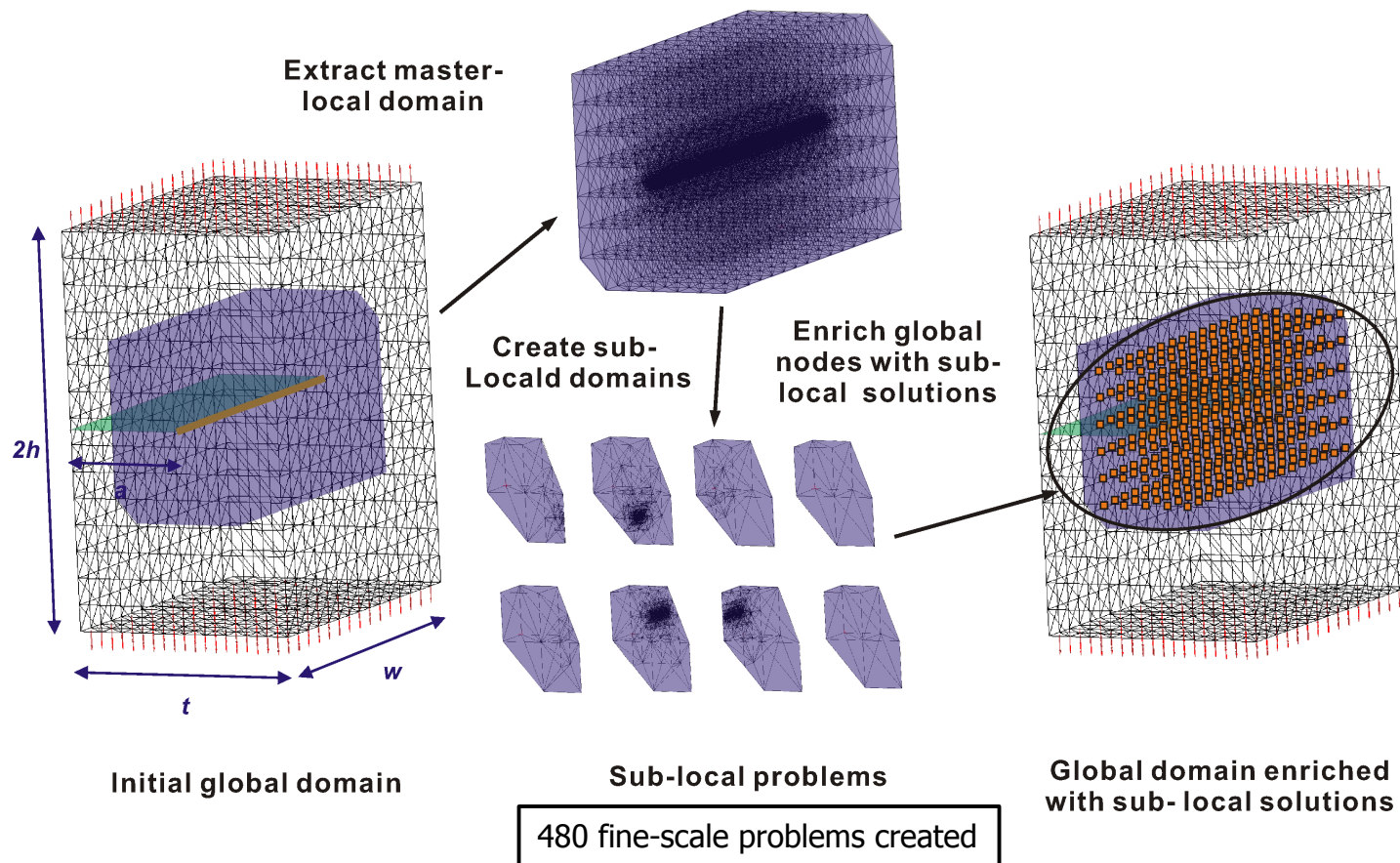- Single field formulation: Does not introduce stability (LBB) issues

[Buchholz et al., 2004]

Parallel Computation of Enrichment Functions *

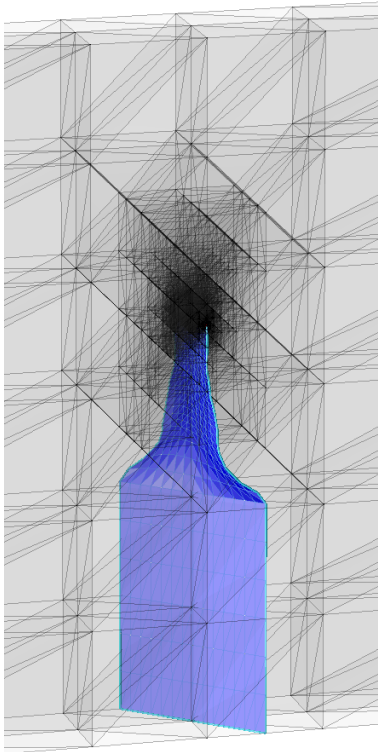- A large number of small fine-scale problems can be created instead of a single one
- *No communication is involved in their parallel solution*

Extract master-local domain

Create sub-Locald domains

Enrich global nodes with sub-local solutions

2h

w

t

Initial global domain

Sub-local problems

480 fine-scale problems created

Global domain enriched with sub- local solutions
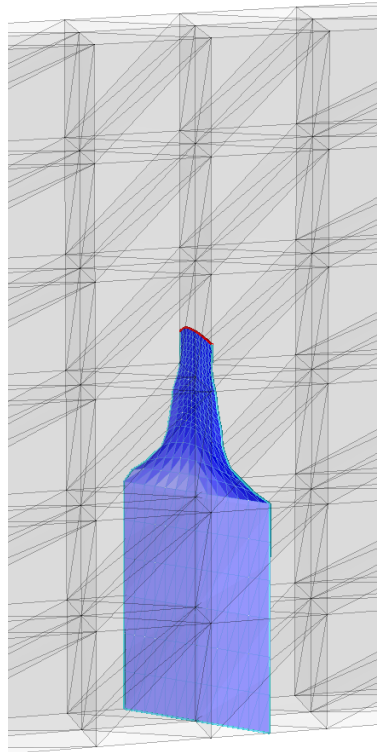
*with D.-J. Kim and N. Sohb
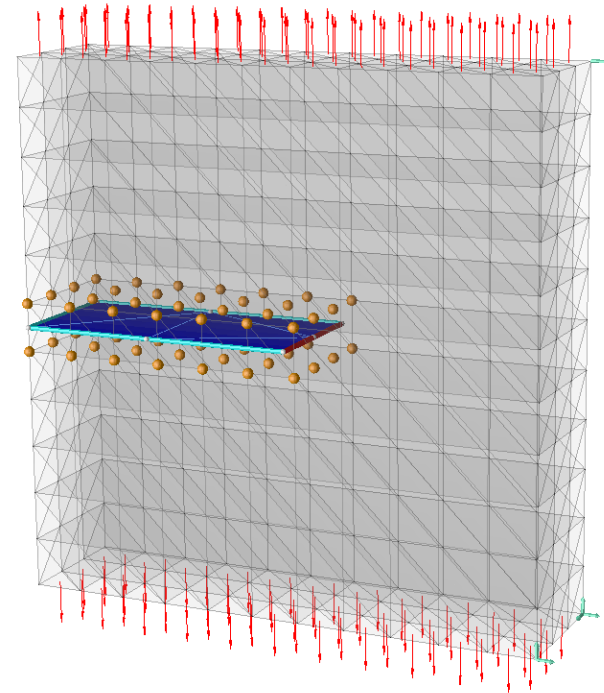
Mathematical Analysis *

hp-GFEM/FEM   GFEM^{gl}

GFEM^{gl}: Error controlled through
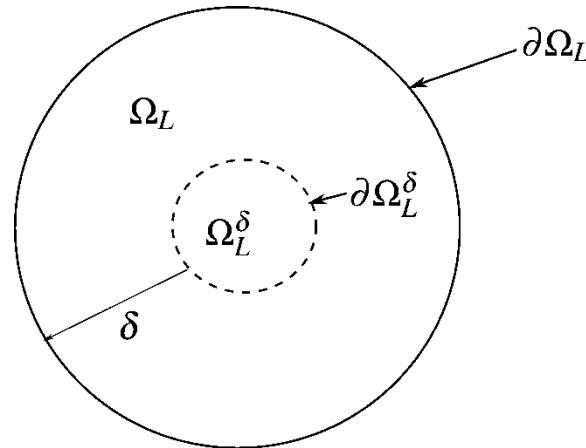   global-local enrichments

Questions:

- What are the effects of inexact BCs at fine-scale problems?
- How to control them?

*with Varun Gupta

A-Priori Error Estimate

- Local error estimate

$$\|\boldsymbol{u}^{exBC} - \boldsymbol{u}_h^{inexBC}\|_{\varepsilon(\Omega_L^\delta)} \leq C \underbrace{\inf_{\boldsymbol{x} \in \boldsymbol{X}_L^{hp}(\Omega_L)} \|\boldsymbol{u}^{inexBC} - \boldsymbol{x}\|_{\varepsilon(\Omega_L)}}_{\text{Discretization error}} + \underbrace{\frac{C_1}{\delta} \|\boldsymbol{u}^{exBC} - \boldsymbol{u}^{inexBC}\|_{L^2(\Omega_L)}}_{\text{Effect of inexact BC}}$$

- Global Error [Babuska and Melenk, 1996]

$$\|\boldsymbol{u} - \boldsymbol{u}_G\|_{\varepsilon(\Omega)}^2 \leq C \sum_{\alpha=1}^{N} \inf_{\boldsymbol{u}_\alpha \in \chi_\alpha} \|\boldsymbol{u} - \boldsymbol{u}_\alpha\|_{\varepsilon(\omega_\alpha)}^2 \leq C \sum_{\alpha=1}^{N} \|\boldsymbol{u} - \boldsymbol{u}_h^{inexBC}\|_{\varepsilon(\omega_\alpha)}^2$$

where $\boldsymbol{u} \equiv \boldsymbol{u}^{exBC}$

Strategy I: Multiple Global-Local Iterations

BCs from step t

Solve local problem
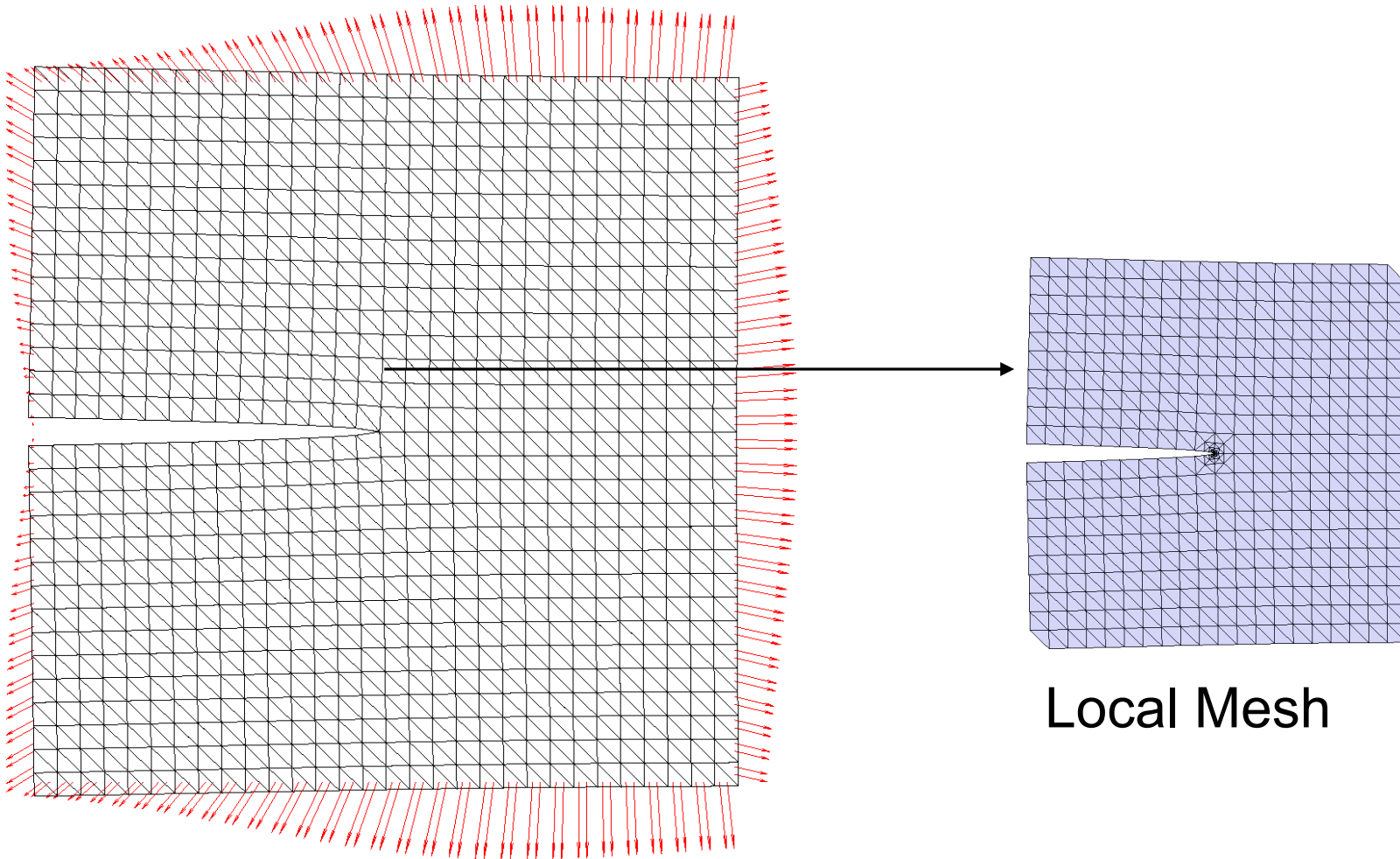
Enrichment for step $t+1$
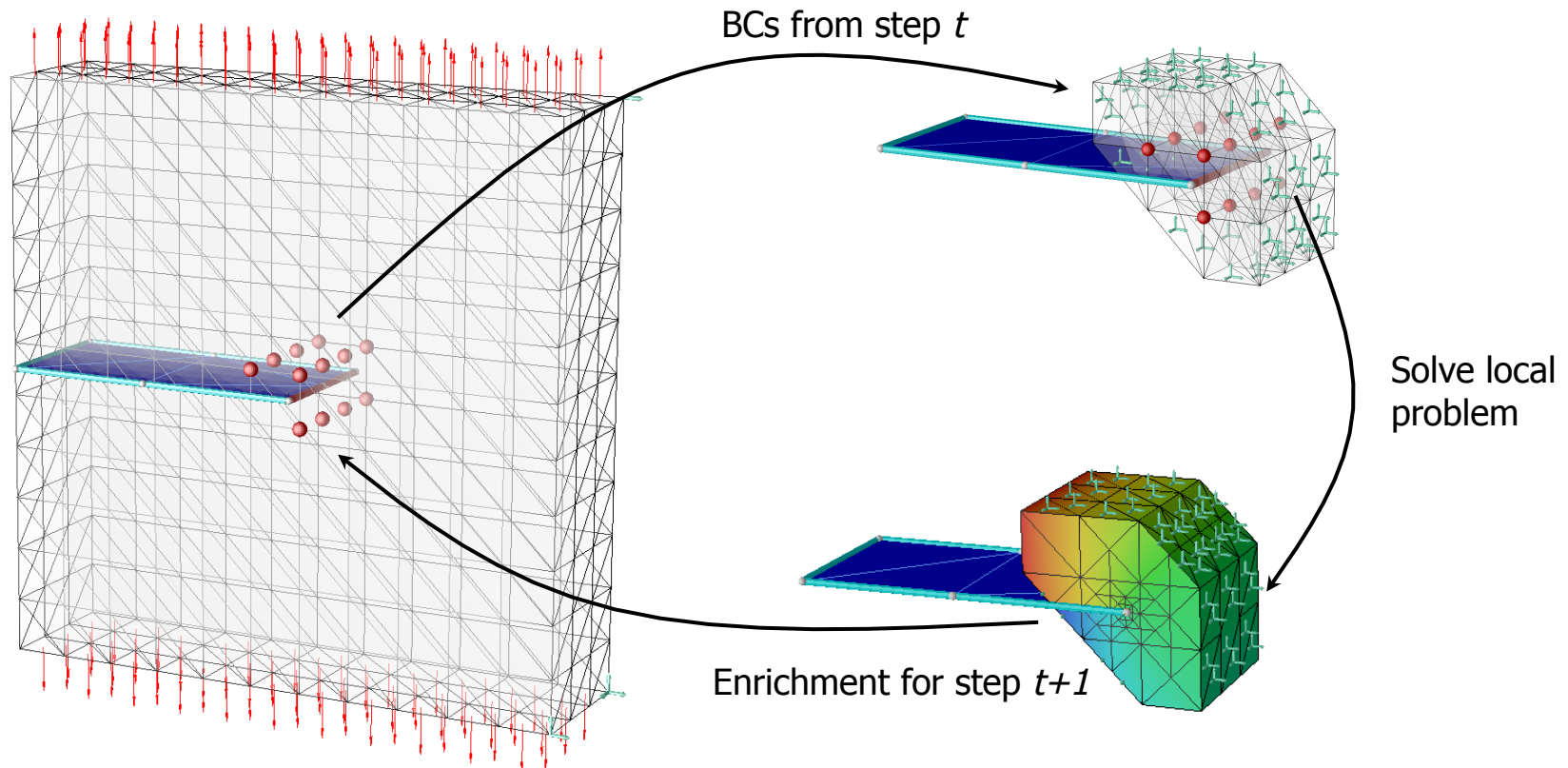
- Repeat Global-local-Global cycle before advancing crack

Strategy I: Multiple Global-Local Iterations

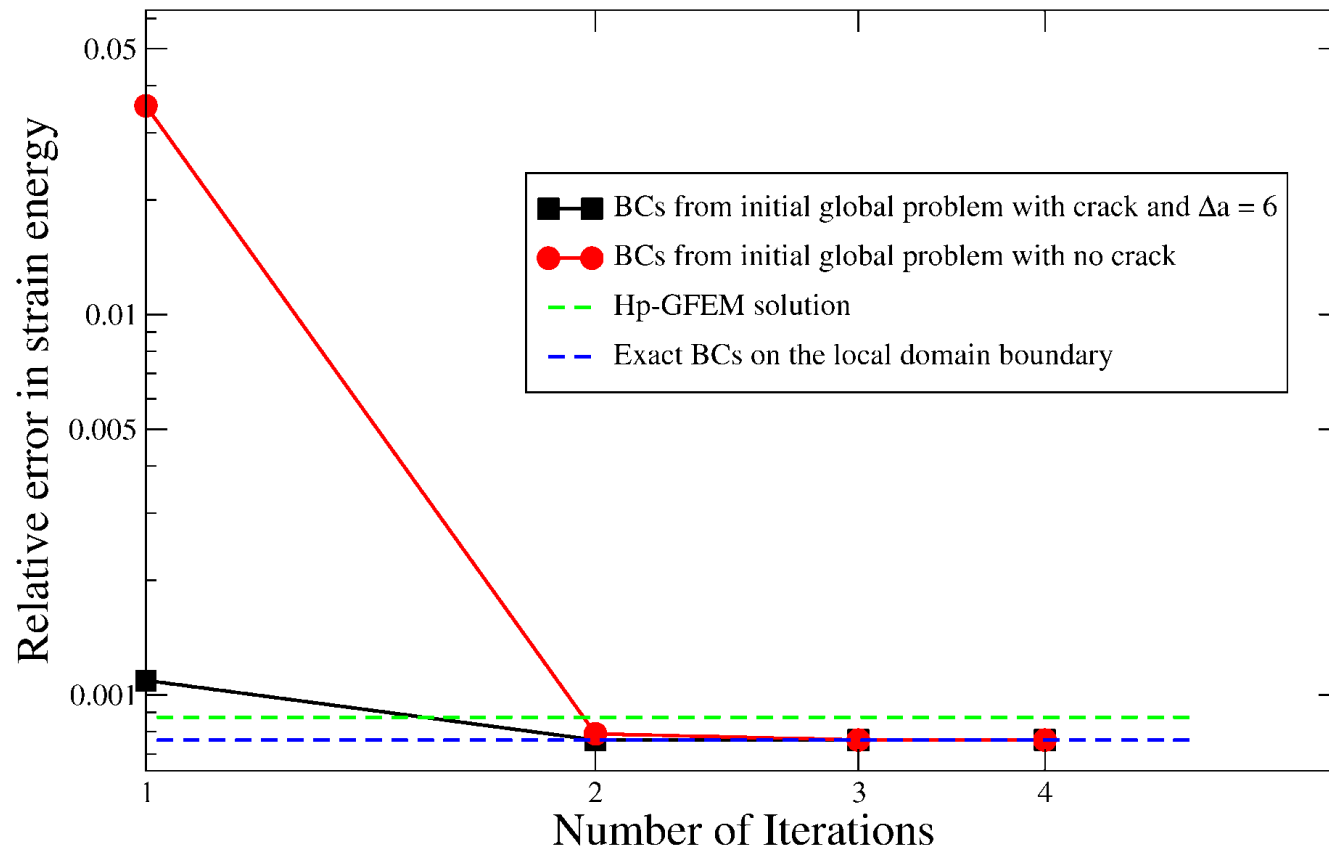- 30" x 30" x 1" edge-crack panel loaded with Mode I tractions

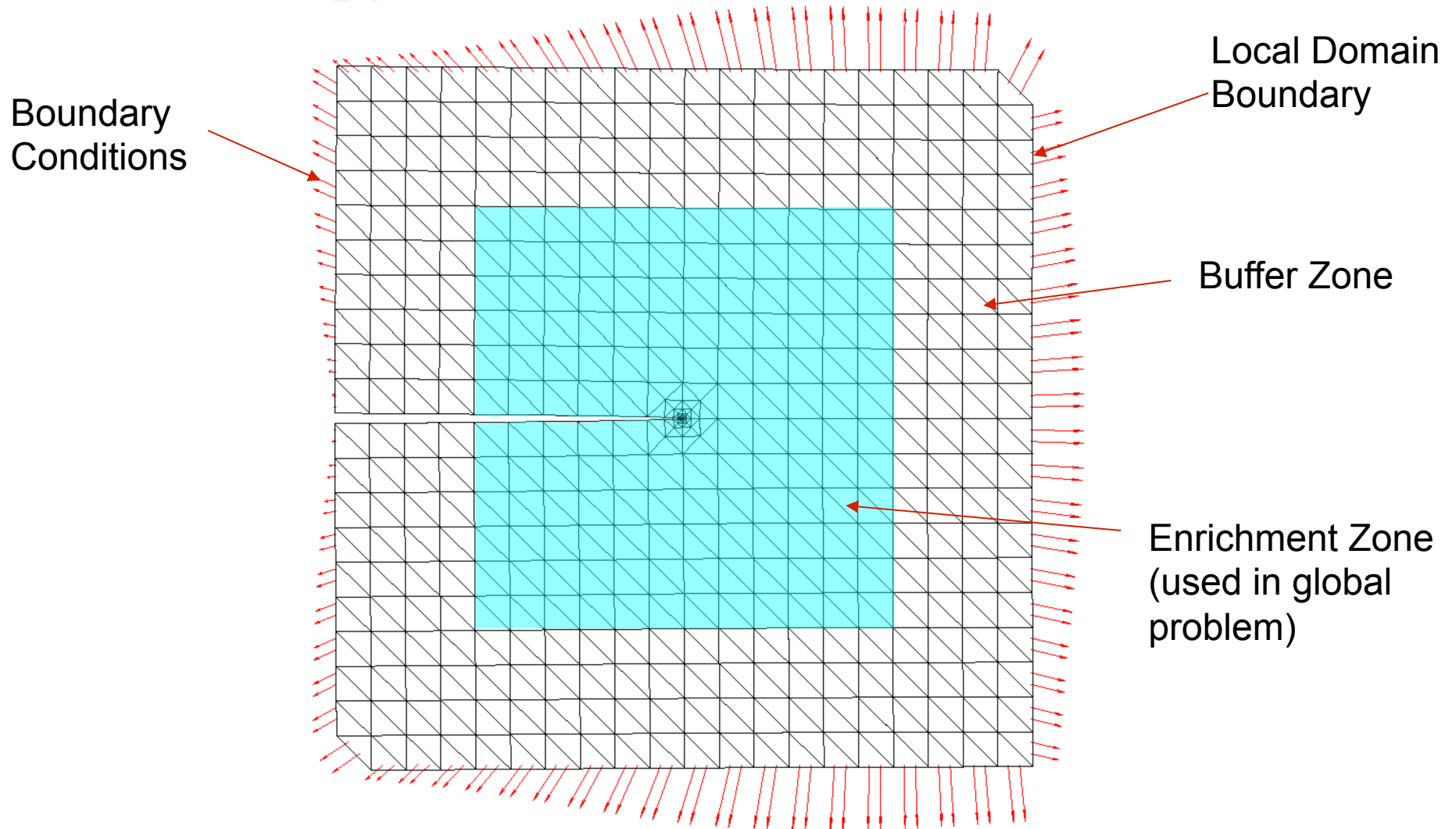Local Mesh

Strategy I: Multiple Global-Local Iterations

Relative Error in Strain Energy

- GFEM^{gl} can deliver same accuracy as hp-GFEM (DNS)

Strategy II: Buffer Zone in Local Domain

Boundary Conditions

Local Domain Boundary

Buffer Zone

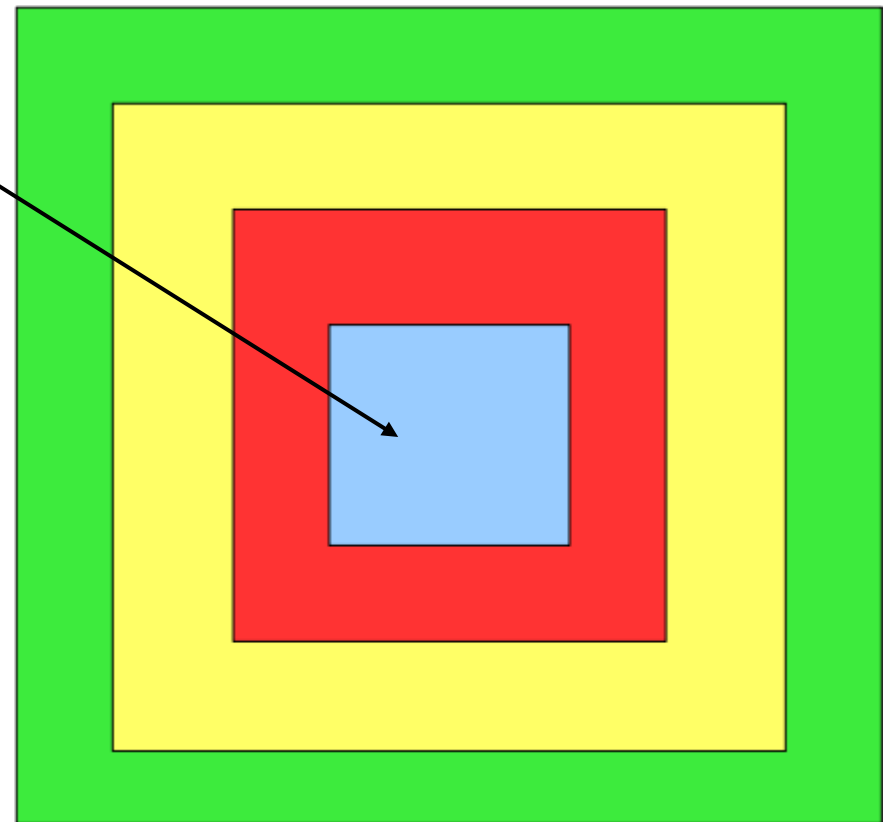Enrichment Zone (used in global problem)

Strategy II: Buffer Zone in Local Domain

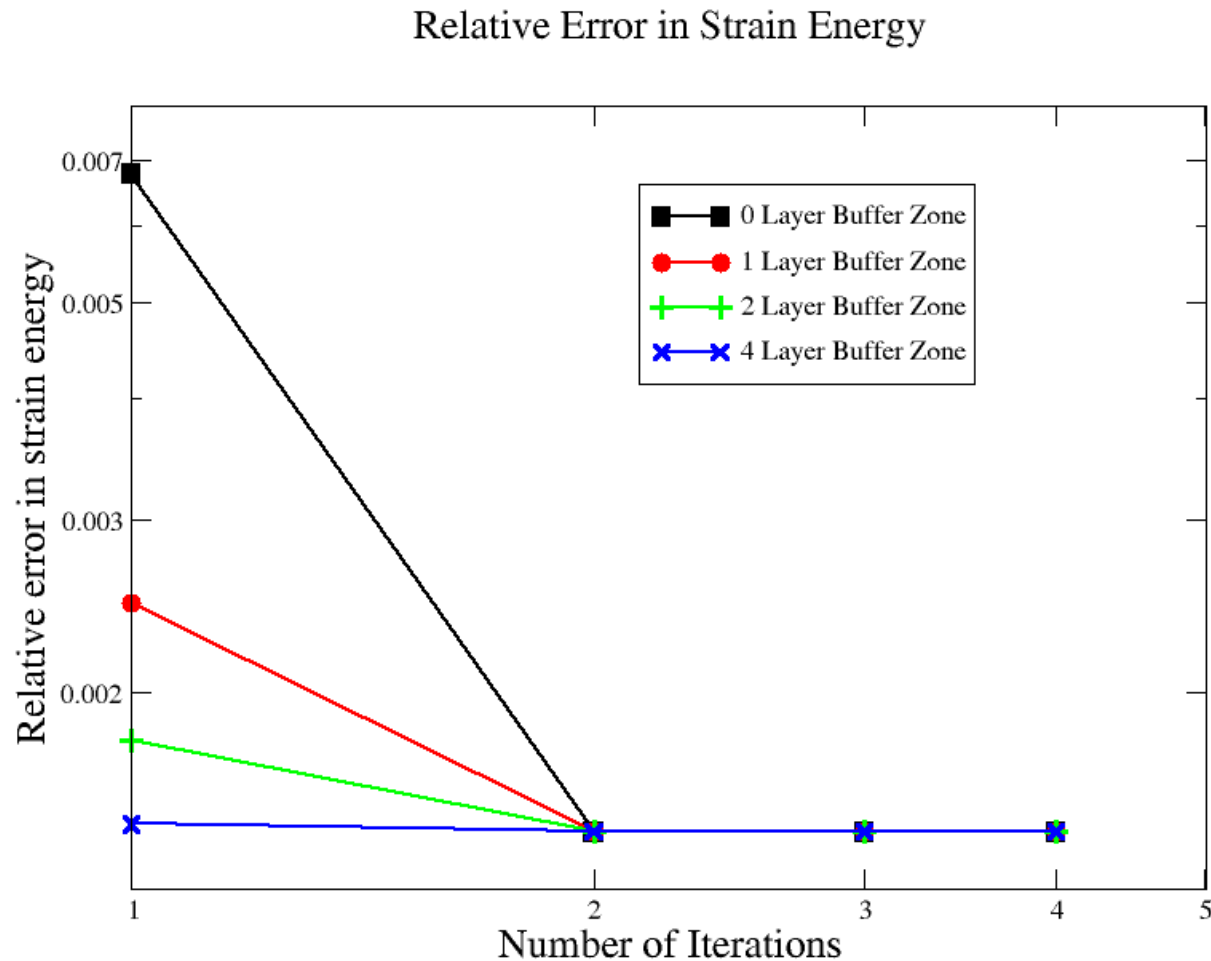- Buffer Zone Sizes Considered

  - Enrichment Zone: 4" X 4" blue square region

  - Buffer zone (in terms of number of layers of elements):

    - Red - 1 layer

    - Yellow - 2 layers

    - Green - 4 layers

Not to scale

Strategy II: Buffer Zone in Local Domain

Relative Error in Strain Energy

- BCs from global problem *without* a crack

Outline

- Generalized finite element methods: Basic ideas

- Bridging scales with the GFEM:

  – Global-local enrichments

- Applications and mathematical analysis

- **Transition: Non-intrusive implementation in Abaqus**

- **Extension to nonlinear problems**

- **Closing remarks**

Computation of Solution at a Crack Step

$$u_G = \underbrace{\tilde{u}^0}_{\text{coarse scale (polynomial)}} + \underbrace{u^{gl}}_{\text{fine scale (G-L)}} = [N^0 \, N^{gl}] \begin{bmatrix} \underline{\tilde{u}}^0 \\ \underline{u}^{gl} \end{bmatrix}$$

$\underline{\tilde{u}}^0 = $ DOFs associate with coarse scale discretization

$\underline{u}^{gl} = $ DOFs associate with G-L (hierarchical) enrichments

$$\dim(\underline{u}^{gl}) << \dim(\underline{\tilde{u}}^0)$$

This leads to

$$\begin{bmatrix} K^0 & K^{0,gl} \\ K^{gl,0} & K^{gl} \end{bmatrix} \begin{bmatrix} \underline{\tilde{u}}^0 \\ \underline{u}^{gl} \end{bmatrix} = \begin{bmatrix} F^0 \\ F^{gl} \end{bmatrix}$$

Computed by FEM code

Solve using, e.g., static condensation of $\underline{u}^{gl}$

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Computation of Solution at a Crack Step

From the first equation

$$\tilde{\underline{u}}^0 = (K^0)^{-1}F^0 - (K^0)^{-1}K^{0,\text{gl}}\,\underline{u}^{\text{gl}}$$
$$= \underline{u}^0 - S^{0,\text{gl}}\,\underline{u}^{\text{gl}}$$

Where

$$S^{0,\text{gl}} := (K^0)^{-1}K^{0,\text{gl}}$$

$$K^0 \quad \underbrace{S^{0,\text{gl}}}_{\text{pseudo coarse scale solutions}} \quad = \quad \underbrace{K^{0,\text{gl}}}_{\text{pseudo coarse scale loads}}$$

$S^{0,\text{gl}}$ = Pseudo coarse scale solutions computed through forward and backward substitutions on K^0

(by FEM code)

From the second equation and the above

$$K^{gl} \underline{u}^{gl} = F^{gl} - K^{gl,0} \left[\underline{u}^0 - S^{0,gl} \underline{u}^{gl} \right]$$

Thus

$$\underbrace{\left[K^{gl} - K^{gl,0} S^{0,gl} \right]}_{\widehat{K}^{gl}} \underline{u}^{gl} = \underbrace{F^{gl} - K^{gl,0} \underline{u}^0}_{\widehat{F}^{gl}}$$

$$\widehat{K}^{gl} \underline{u}^{gl} = \widehat{F}^{gl}$$

$$\tilde{\underline{u}}^0 = \underline{u}^0 - S^{0,gl} \underline{u}^{gl}$$

$$u_E = \tilde{\underline{u}}^0 + \underline{u}^{gl} = \left[N^0 N^{gl} \right] \begin{bmatrix} \tilde{\underline{u}}^0 \\ \underline{u}^{gl} \end{bmatrix}$$

Computation of u_G involves forward- and back-substitutions on K^0

Non-Intrusive Implementation in Existing FEM Codes

- Different solvers can be used to solve coarse and fine-scale problems

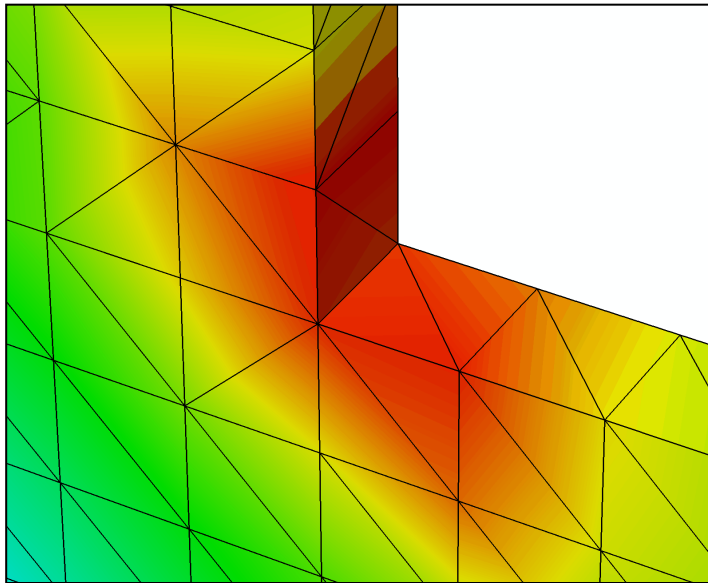**GFEM Code**

FEM Code

Global solution
BC for local prob.

Local solution
Global-local enrichment

Pseudo loads

Initial global solution
Uncracked domain

Pseudo solutions

Enriched global solution
Compute quantities of interest
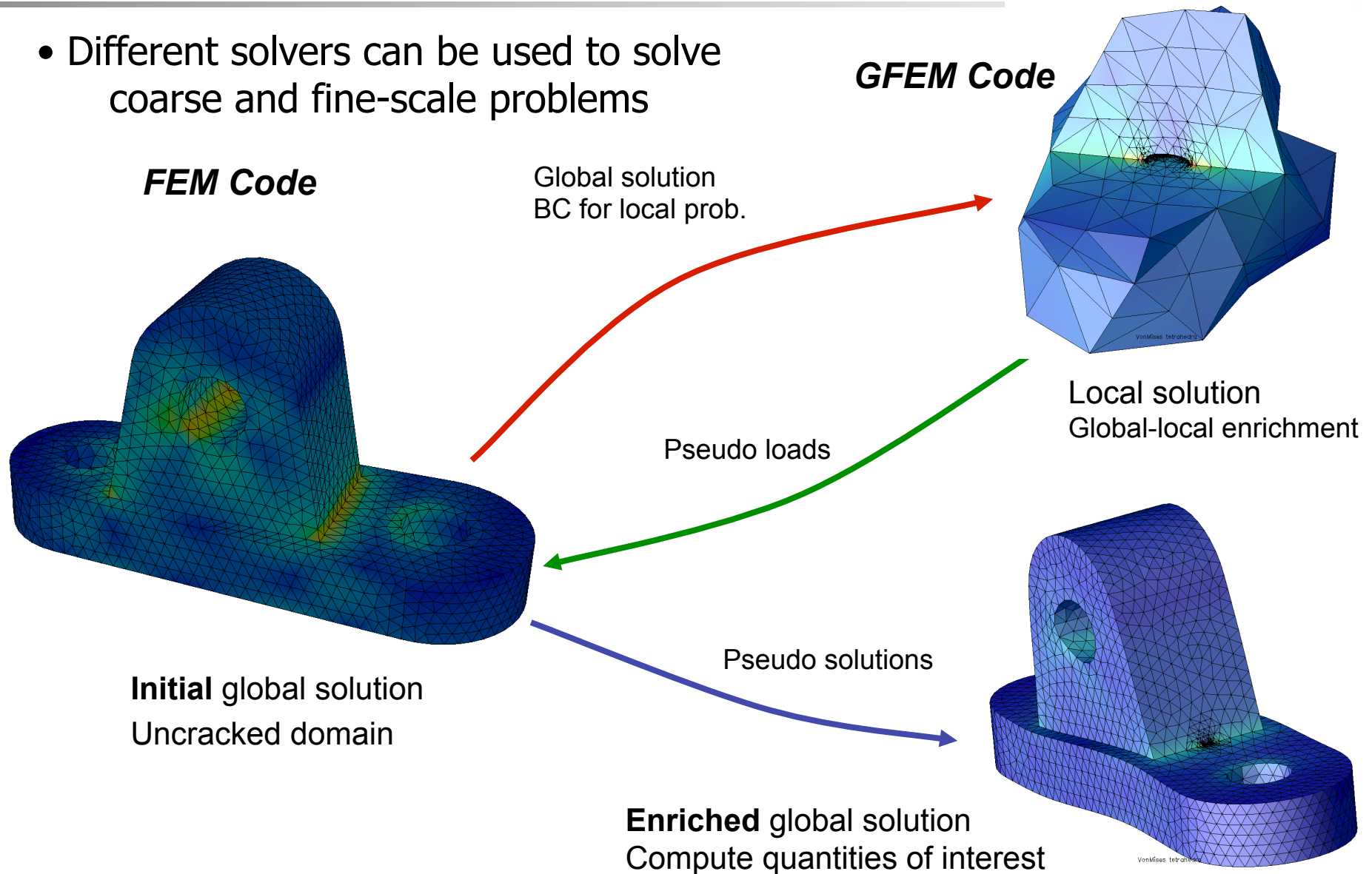
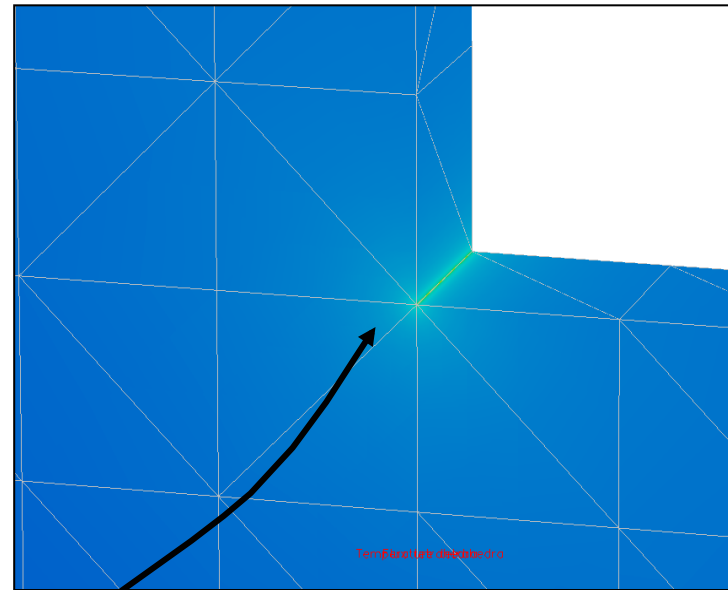- **Singularities in thermal fields**

Coarse-Scale Abaqus Solution
at critical region

Abaqus + GFEM Solution

$$e^r_{U,IG} = 11.9\%$$
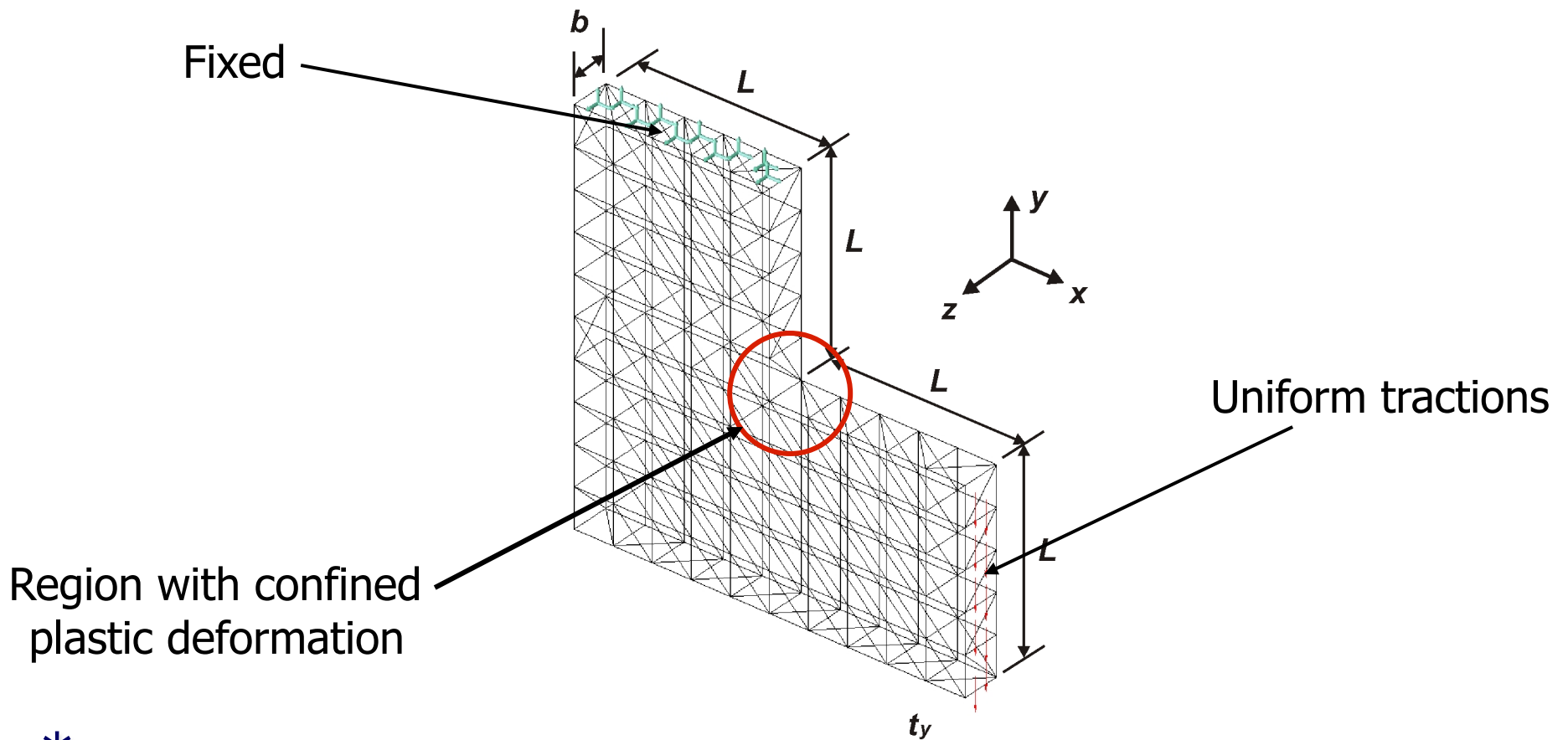
$$e^r_{U,EG} = 0.63\%$$

- Able to effectively capture sharp flux singularity adding only 16 global-local degrees of freedom to Abaqus model

*with J. Plews, Piyush Gupta and T. Eason

Enrichment Functions for Confined Plasticity Problems *

- **J_2 plasticity with isotropic hardening**

Fixed

Region with confined
 plasticity deformation

Uniform tractions
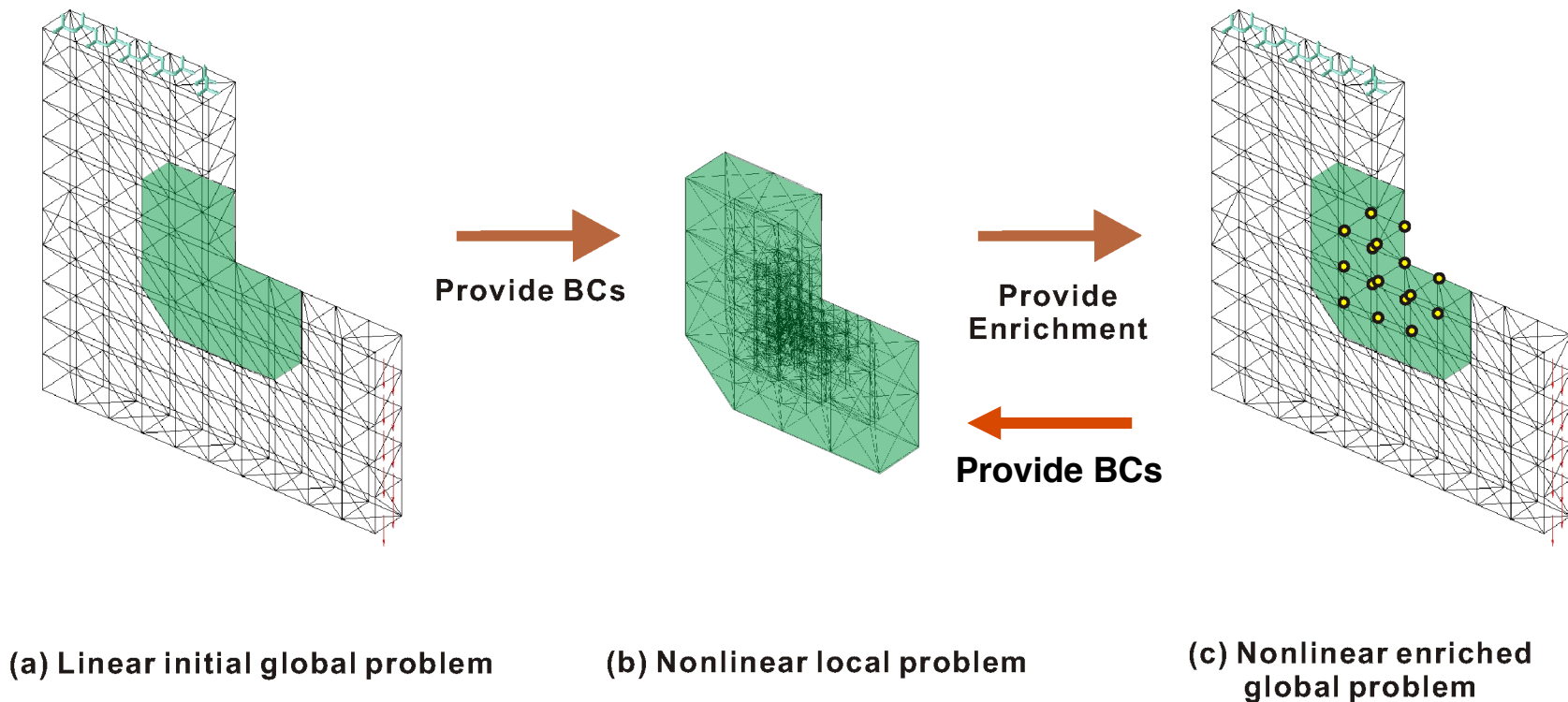
b

L

L

L

L

t_y

y

x

z

*with D.-J. Kim and S. Proenca

Enrichment Functions for Confined Plasticity Problems

- **Key Idea:**
  - Use nonlinear local solution as enrichment for global problem solved on a *coarse mesh*
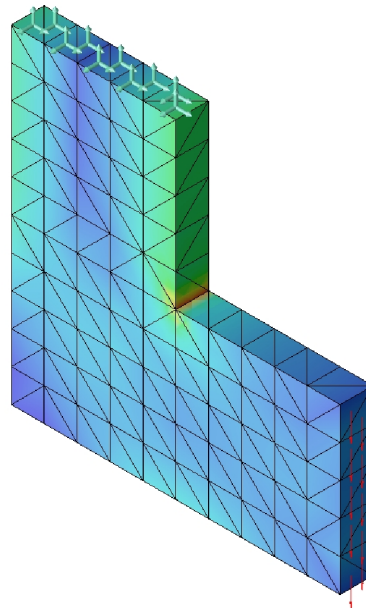

Provide BCs

Provide Enrichment

Provide BCs

(a) Linear initial global problem

(b) Nonlinear local problem

(c) Nonlinear enriched global problem

  - G-L enrichments can be updated during iterative solution of nonlinear global problem
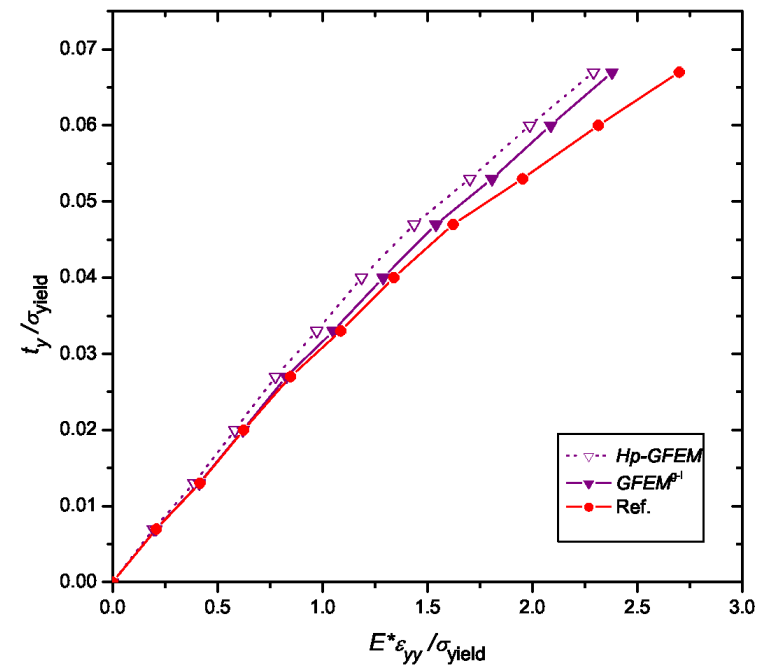
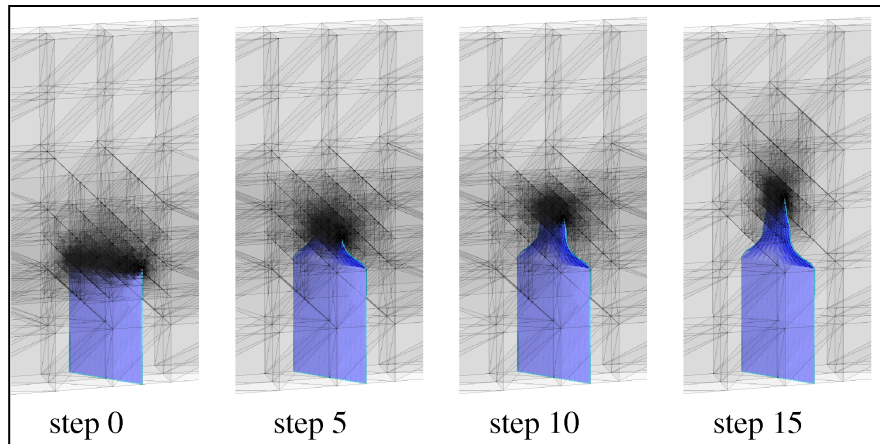# Enrichment Functions for Confined Plasticity Problems
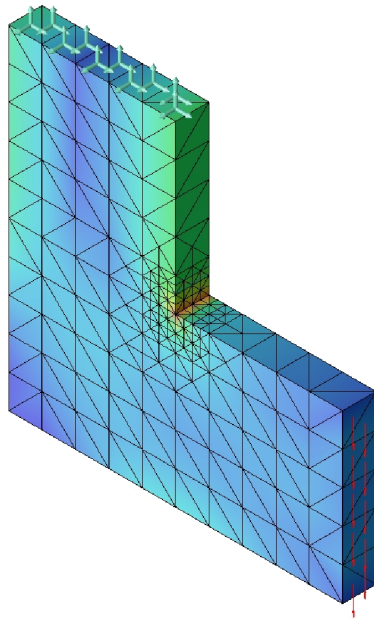
(a) *Hp-GFEM*

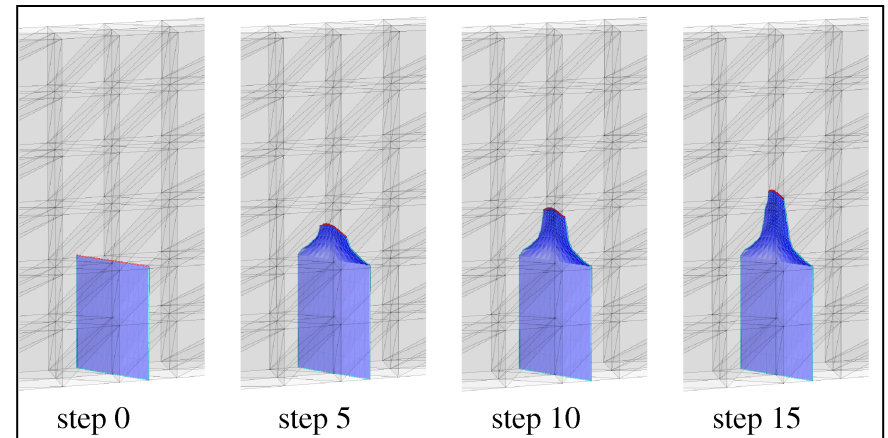(b) *GFEM* [g-l]

Von Mises stress distribution at final load step

Load-displacement curves for *hp*-GFEM and GFEM[gl]

Concluding Remarks

Available methods require AMR
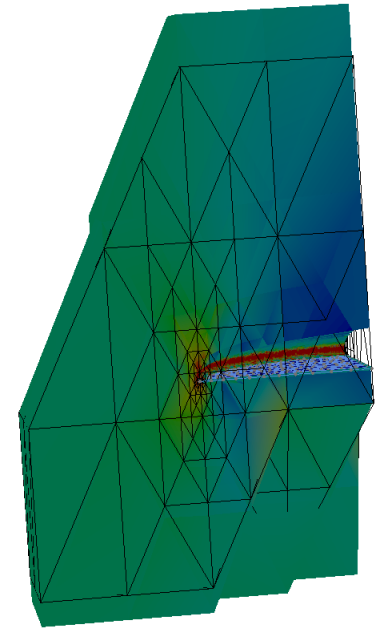

Multiscale Generalized FEM

- **F**AST: Coarse-scale model of much reduced dimension than FEM; Fine-Scale computations are intrinsically parallelizable; recycle coarse scale solution

- **A**CCURATE: Can deliver same accuracy as adaptive mesh refinement (AMR) on meshes with elements that are orders of magnitude larger than in the FEM

- **S**TABLE: Uses single-field variational principles

- **T**RANSITION: Fully compatible with FEM
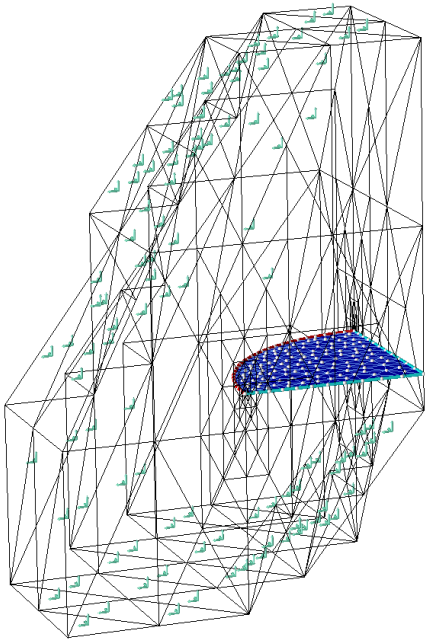
Questions?

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

Support: