

Modelling Cracks and Dislocations with the Extended Finite Element Method

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Mechanical Engineering



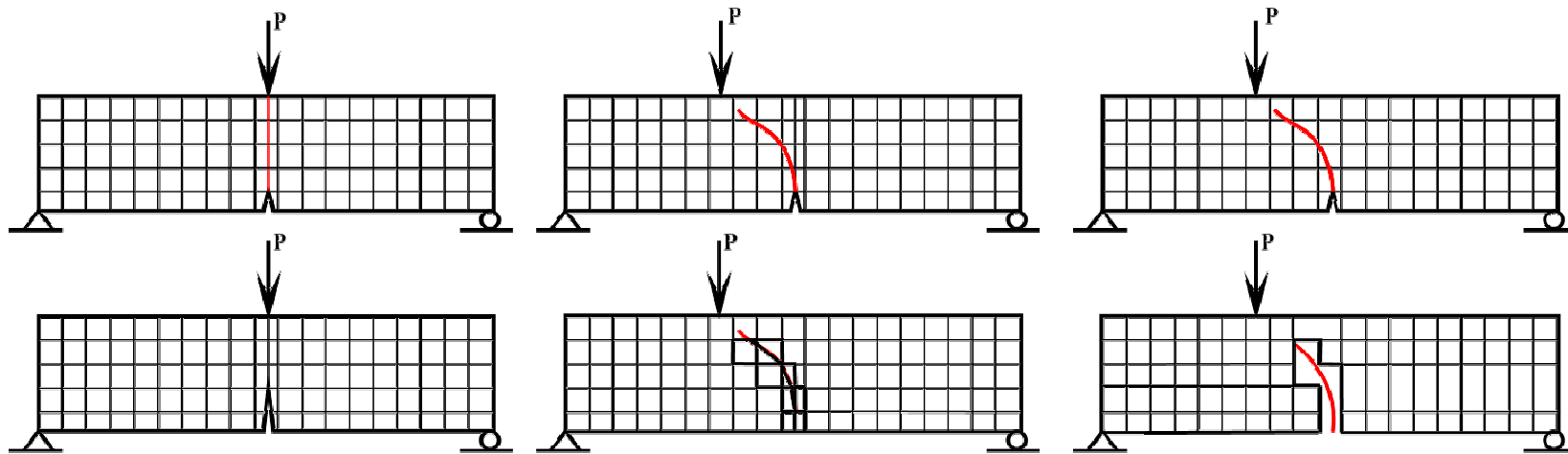
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- Challenges to modelling discontinuities with FEM
- Extended Finite Element Method (XFEM)
- Modelling Cracks
- Some improvements to the XFEM
 - Efficient Numerical Integration
 - Discontinuous Galerkin
- Modelling Dislocations
 - Peach-Koehler force
 - 2D and 3D
 - Thin Shells



- How do we model a crack with the FEM?



$$\mathbf{u}(\mathbf{x}) = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I = \mathbf{u}^C(\mathbf{x})$$

- FEM approximation is continuous, so crack faces must align with element edges
- Remeshing for crack propagation.
 - expensive and complicated in 3D
- Element deletion (crack band model)
 - Mesh dependent results
 - Difficult to achieve consistent fracture energy



- Element deletion is popular in industry because it is very simple
- But, mesh dependent results

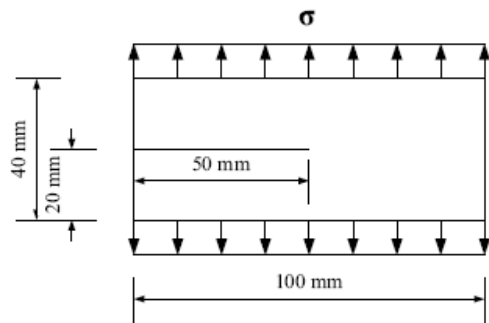
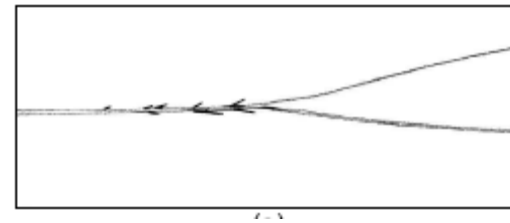


Fig. 3. Setup of a dynamic crack branching problem.

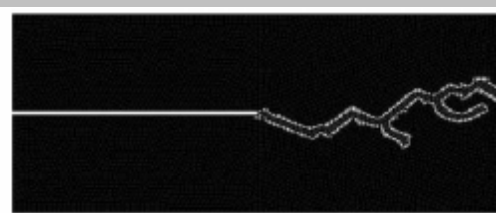


Ramulu M, Kobayashi AS (1985) Int. J. Fracture

Element Deletion (crack band model)

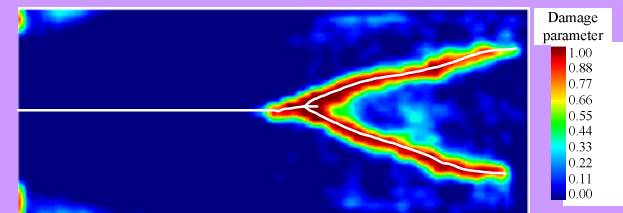


(structured mesh)



(unstructured mesh)

XFEM



(structured mesh)

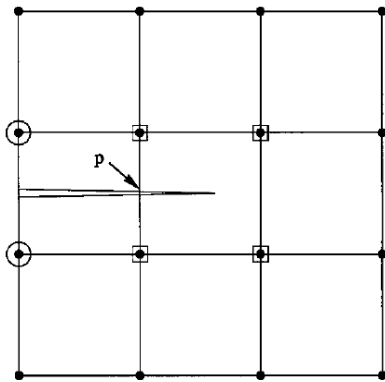


- Challenges to modelling discontinuities with FEM
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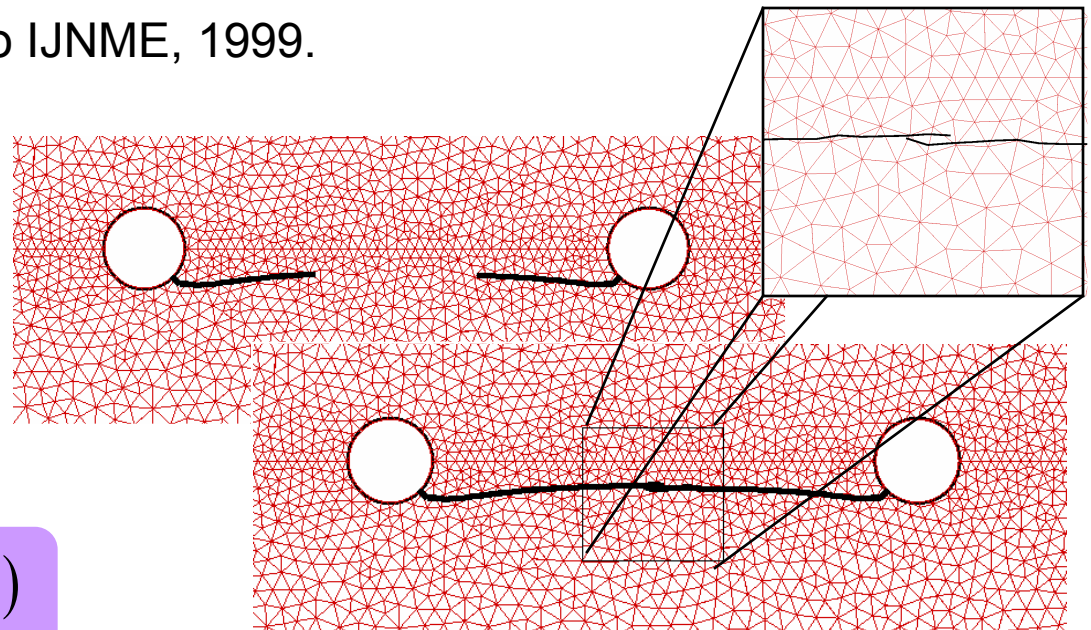


Extended Finite Element Method

- How do we model a crack with the XFEM.
 - Moës, Dolbow, Belytschko IJNME, 1999.



$$\mathbf{u}(\mathbf{x}) = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I + \mathbf{u}^D(\mathbf{x})$$



- XFEM approximation is discontinuous, so crack are arbitrarily located in the elements.
- **No Remeshing** for crack propagation.



$$\mathbf{u} = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I + \underbrace{\sum_{J \in S} N_J(\mathbf{x}) \varphi(\mathbf{x}) \mathbf{a}_J}_{\text{enrichment}}$$

$$\sum_{\forall J} N_J(\mathbf{x}) = 1, \forall \mathbf{x} \in \Omega_S$$

- $\varphi(\mathbf{x})$ is called an enrichment function
- $\varphi(\mathbf{x})$ can be reproduce only exactly in Ω_S .
- Local enrichment



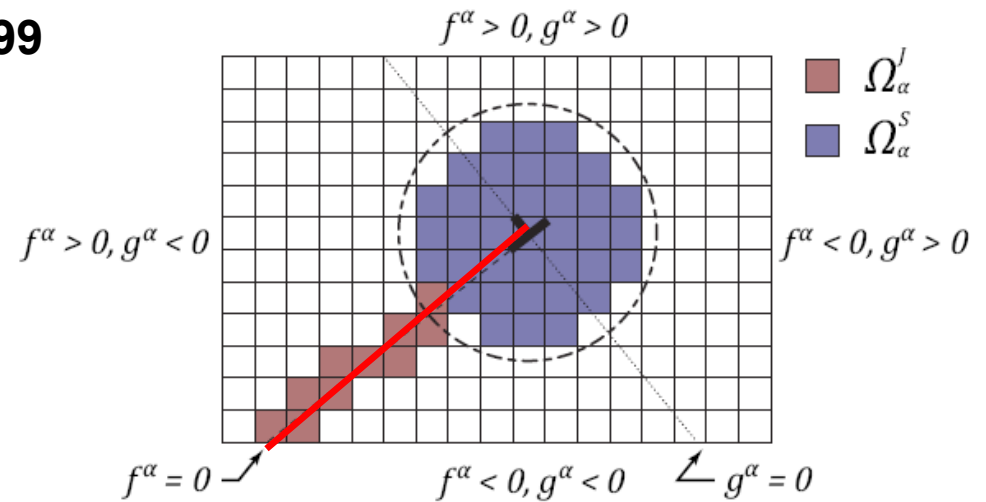
Moës, Dolbow, Belytschko IJNME 1999

Liu, Karihaloo, IJNME 2004

$I \in \{all\ nodes\}$

$J \in \{all\ step\ enriched\ nodes\}$

$K \in \{all\ branch\ enriched\ nodes\}$



$$\mathbf{u}(\mathbf{x}) = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I + \sum_{J \in S^H} N_J(\mathbf{x}) H(-f(\mathbf{x})g(\mathbf{x})) \mathbf{a}_J + K_I \sum_{L \in S^\infty} N_L(\mathbf{x}) \mathbf{u}^{K_I}(\mathbf{x})$$

$$H(z) = \begin{cases} +1, & z \geq 0 \\ 0, & z < 0 \end{cases}$$

$\mathbf{u}^{K_I}(\mathbf{x}) =$ **Mode I asymptotic solution**

$K_I =$ **Mode I SIF**

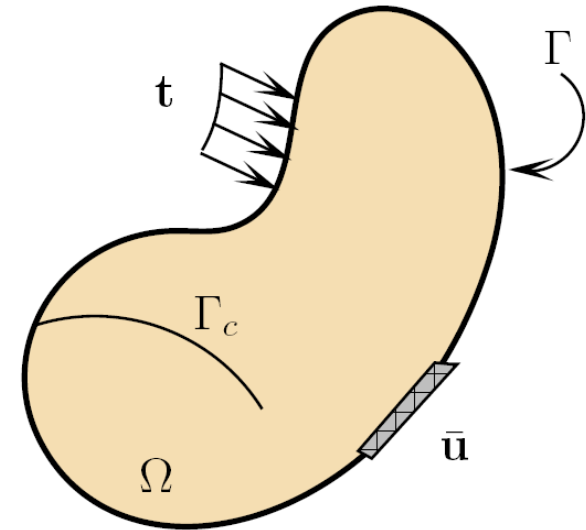


Find $\mathbf{u} \in U^0$, such that

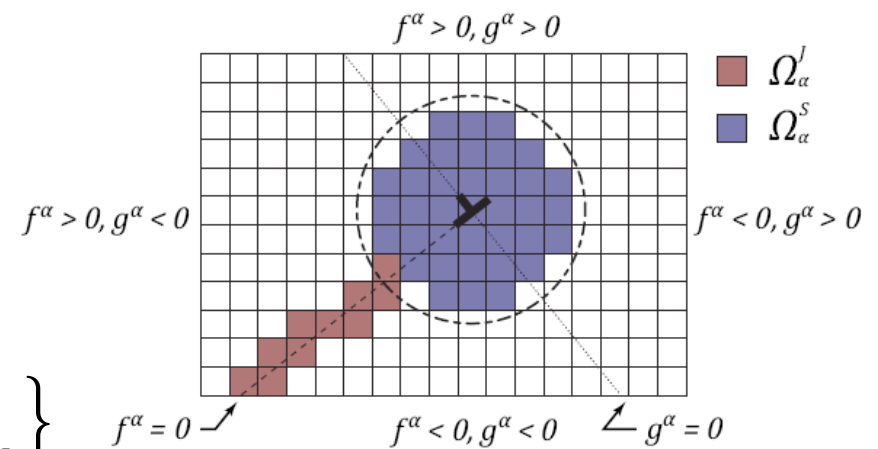
$$\int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\mathbf{u})) : \boldsymbol{\varepsilon}(\mathbf{v}) d\Omega - \int_{\Gamma_t} \mathbf{t} \cdot \mathbf{v} d\Gamma = 0, \forall \mathbf{v} \in U$$

$$\mathbf{u}(\mathbf{x}) = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I$$

$$+ \sum_{J \in S^H} N_J(\mathbf{x}) H(-f(\mathbf{x})g(\mathbf{x})) \mathbf{a}_J + K_I \sum_{L \in S^\infty} N_L(\mathbf{x}) \mathbf{u}^{K_I}(\mathbf{x})$$



$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{ua} & \mathbf{K}_{ub} \\ \mathbf{K}_{ua}^T & \mathbf{K}_{aa} & \mathbf{K}_{ab} \\ \mathbf{K}_{ub}^T & \mathbf{K}_{ab}^T & \mathbf{K}_{bb} \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \mathbf{q} \\ K_I \end{bmatrix} = \begin{bmatrix} \mathbf{f}_d^{ext} \\ \mathbf{f}_q^{ext} \\ \mathbf{f}_K^{ext} \end{bmatrix}$$



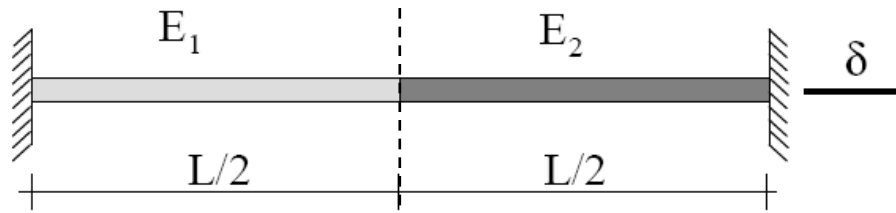
$$\mathbf{d}^T = \{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N\} \quad \mathbf{q}^T = \{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{n_H}\}$$



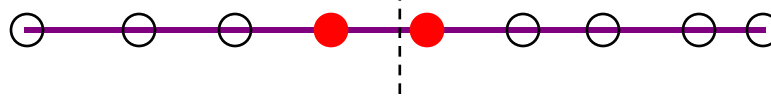
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Blending in XFEM



mesh:

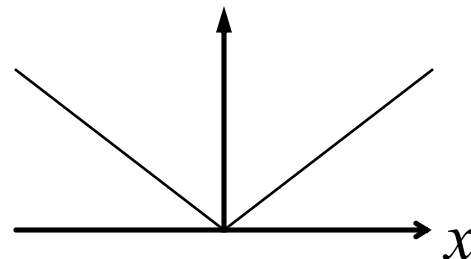


approx:

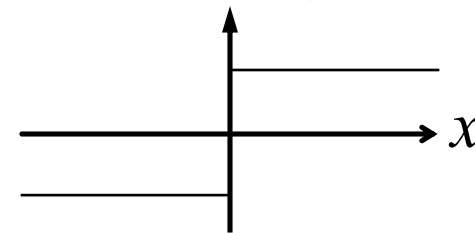
$$u(x) = \sum_{\forall I} N_I(x) u_I + \sum_{J=1}^2 \bar{N}_J(x) \varphi(x) a_J$$

enrichment:

$$\varphi(x) = abs(x)$$



$$\varphi_{,x}(x) = \begin{cases} -1 \\ 1 \end{cases}$$



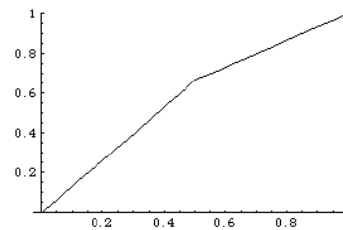


Blending in XFEM

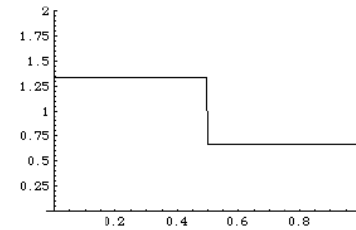


1 element

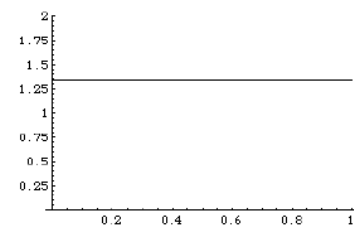
Displacement



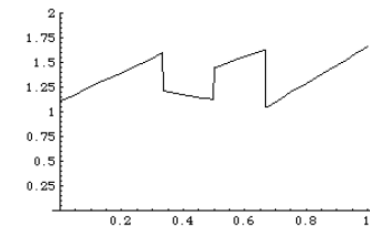
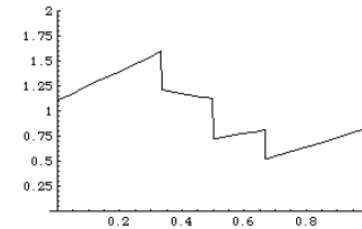
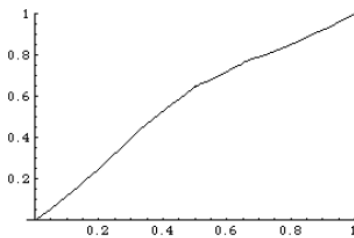
Strain



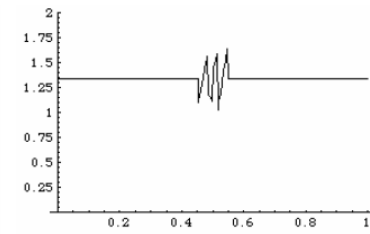
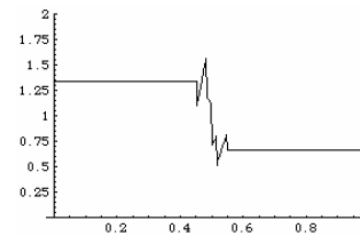
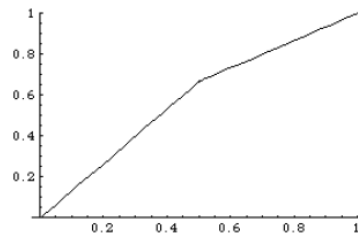
Stress



3 elements



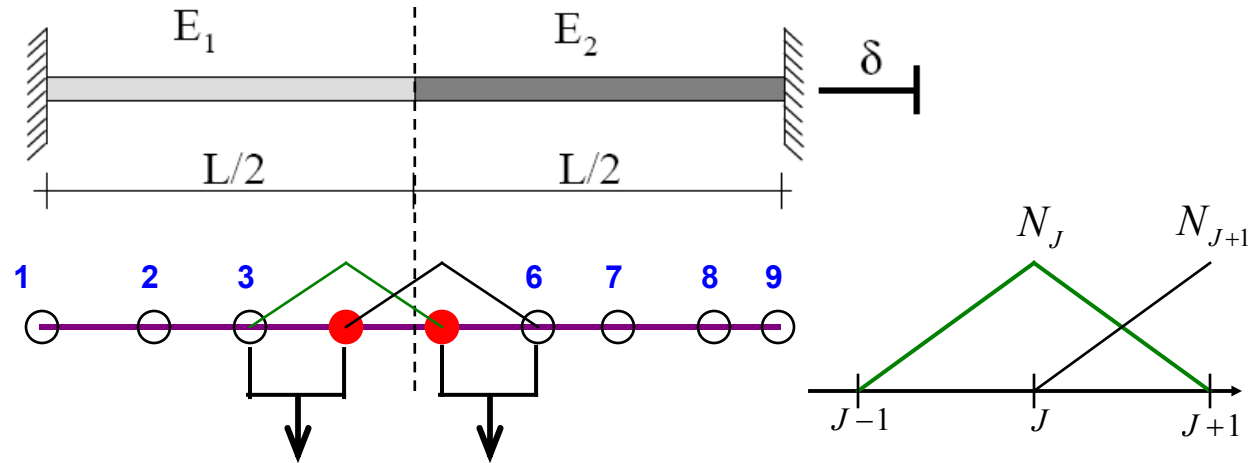
31 elements





Blending in XFEM

mesh:



Blending elements $\longrightarrow \sum_{J \in S} \bar{N}_J(x) \neq 1$

Global:

$$u(x) = \sum_{\forall I} N_I(x) u_I + \sum_{J=1}^2 \bar{N}_J(x) abs(x) a_J$$

Element 3:

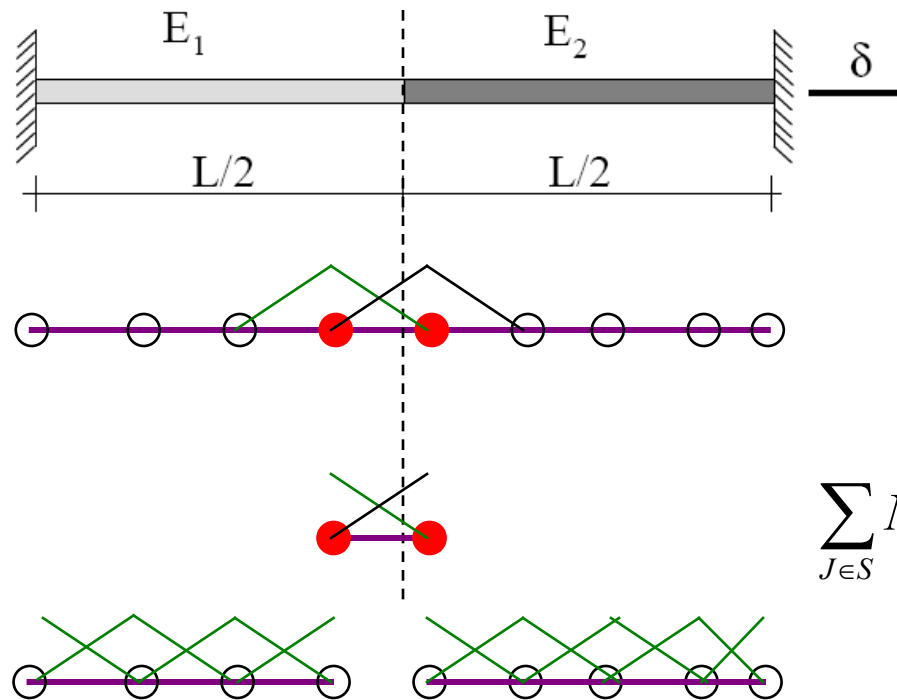
$$\frac{du(x)}{dx} = \sum_{I=3}^4 \frac{dN_I(x)}{dx} u_I^e + \frac{d\bar{N}_1(x)}{dx} abs(x) a_1 + \bar{N}_1(x) H(x) a_1$$

Cannot reproduce a constant strain



- Domain decomposition

mesh:

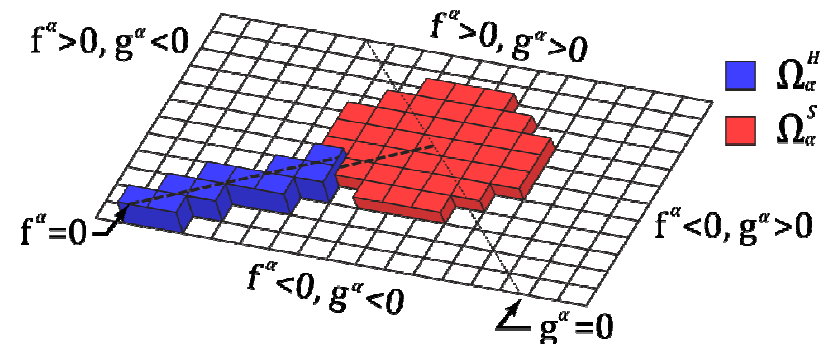
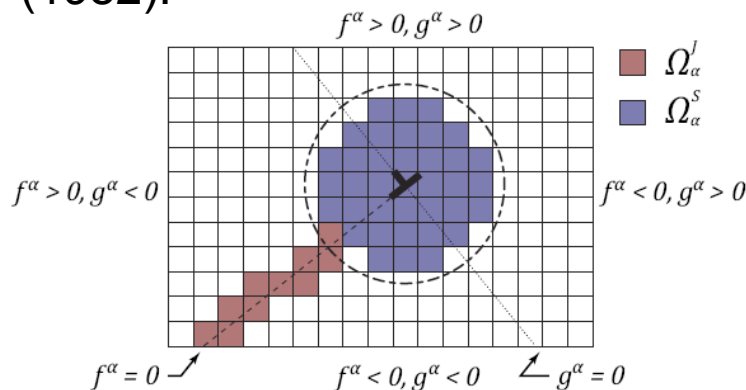
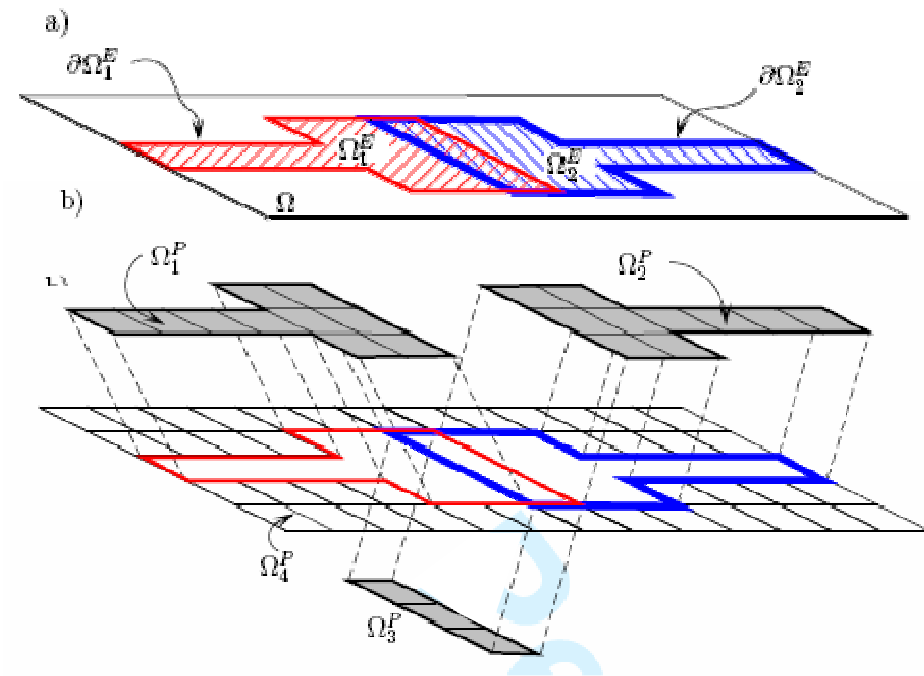


$$\sum_{J \in \mathcal{S}} N_J(x) = 1$$



A Discontinuous Galerkin (DG) XFEM

- Decompose the domain into n_p non-overlapping subdomains (patches).
- Enrichments are applied over a full patch. So enrichment is local and PU property is always satisfied.
- Continuity between patches is enforced with an Internal Penalty method: Wheeler (1978) & Arnold (1982).





$$\delta\Pi = \sum_{\beta=1}^{n_P} \left[\int_{\Omega_{\beta}^P} \boldsymbol{\varepsilon}(\mathbf{v}^{\beta}) \cdot \boldsymbol{\sigma}(\mathbf{u}^{\beta}) d\Omega \right] - \delta W^{ext}$$

$$+ \sum_{\beta=1}^{n_P} \sum_{\theta>\beta}^{n_P} \left[\underbrace{- \int_{\partial\Omega_{\beta\theta}} \llbracket \mathbf{v}^{\beta\theta} \rrbracket \langle \mathbf{t}^{\beta\theta} \rangle d\Gamma}_{\text{consistency}} - \underbrace{\int_{\partial\Omega_{\beta\theta}} \langle \mathbf{t}^{\beta\theta} \rangle \llbracket \mathbf{u}^{\beta\theta} \rrbracket d\Gamma}_{\text{symmetry}} + \underbrace{\frac{\alpha}{A} \int_{\partial\Omega_{\beta\theta}} \llbracket \mathbf{v}^{\beta\theta} \rrbracket \llbracket \mathbf{u}^{\beta\theta} \rrbracket d\Gamma}_{\text{stability}} \right]$$

Ω_{β}^P : domain of patch β

\mathbf{u}^{β} : displacement of patch β

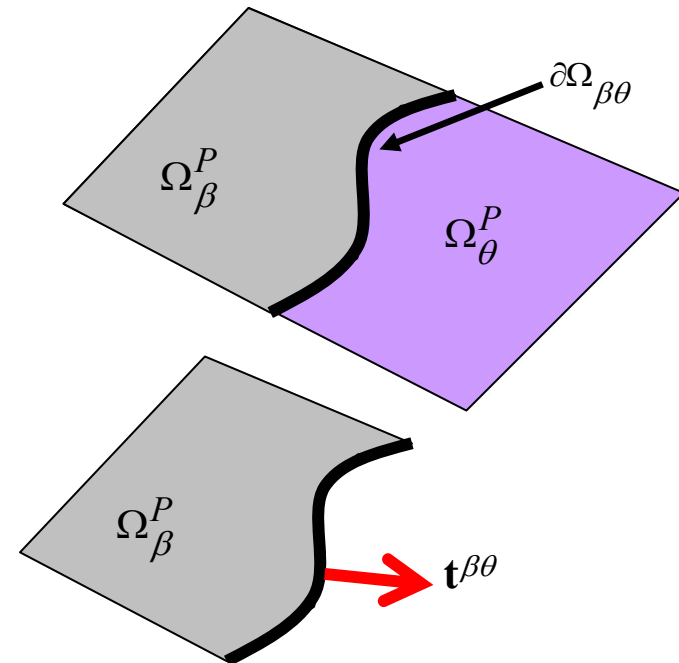
n_P : number of patches

$\partial\Omega_{\beta\theta}$: boundary of patch β and θ

$\mathbf{t}^{\beta\theta}$: traction acting on patch β on $\partial\Omega_{\beta\theta}$

$$\llbracket \mathbf{u}^{\beta\theta} \rrbracket = \frac{1}{2} (\mathbf{u}^{\beta} - \mathbf{u}^{\theta})$$

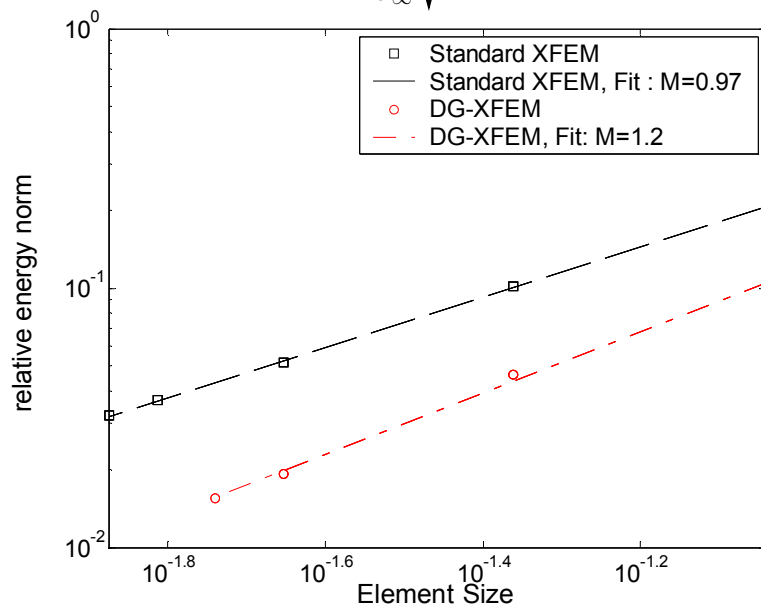
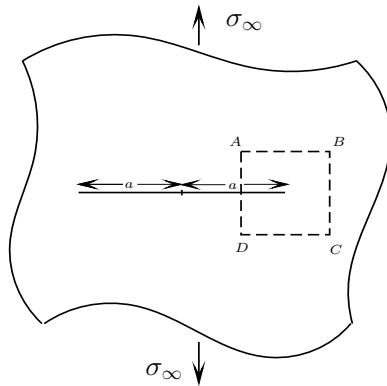
$$\langle \mathbf{t}^{\beta\theta} \rangle = \frac{1}{2} (\mathbf{t}^{\beta} + \mathbf{t}^{\theta})$$



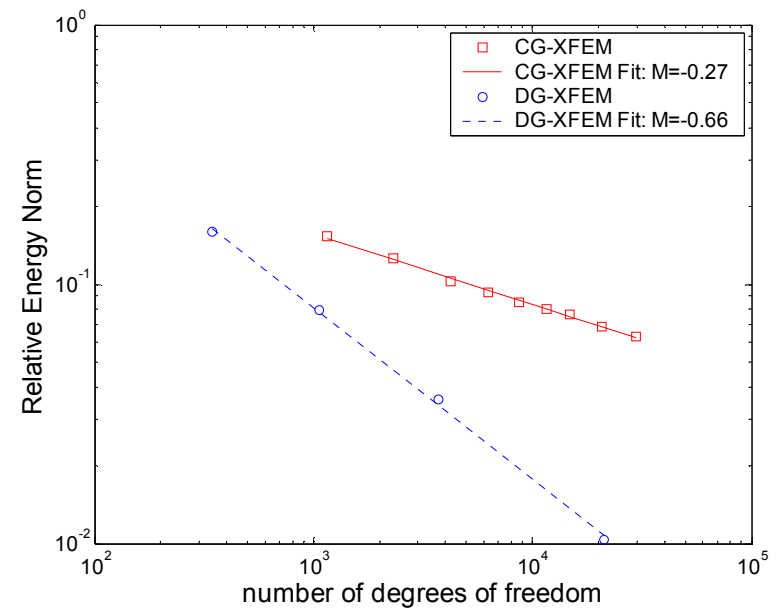
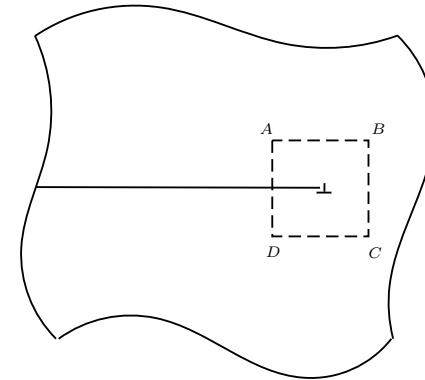


DG-XFEM vs XFEM

Elastic Crack



Edge dislocation





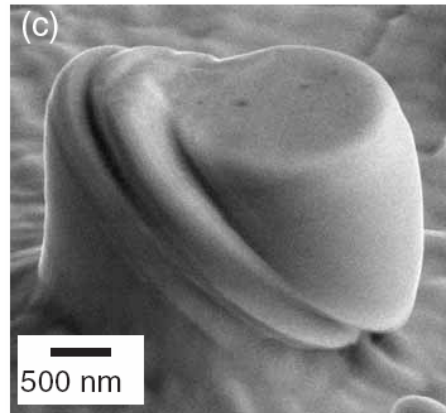
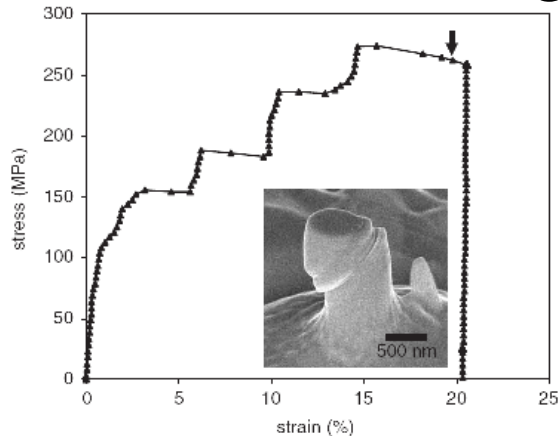
- XFEM for modelling Cracks in continua
- Improved numerical integration of singular enrichments
- Improved accuracy and convergence with discontinuous Galerkin scheme



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- Plasticity in metals is the result of complex processes involving dislocations



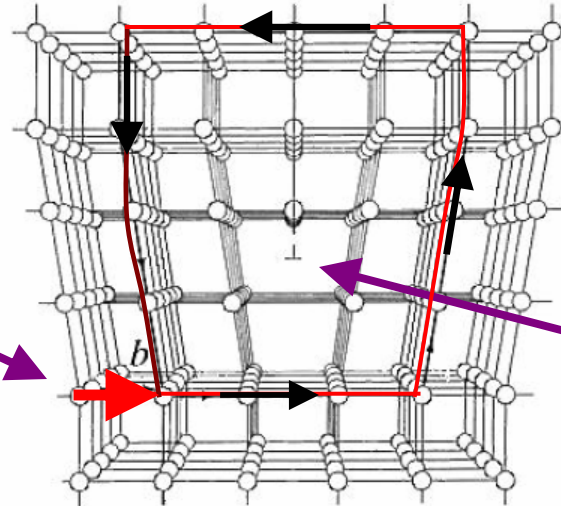
Submicron Au Columns:
Volkert, Phil Mag. 2006

- In MEMS devices material interfaces act as sources for dislocation nucleation.
- Dislocations degrade the electronic properties of the device.



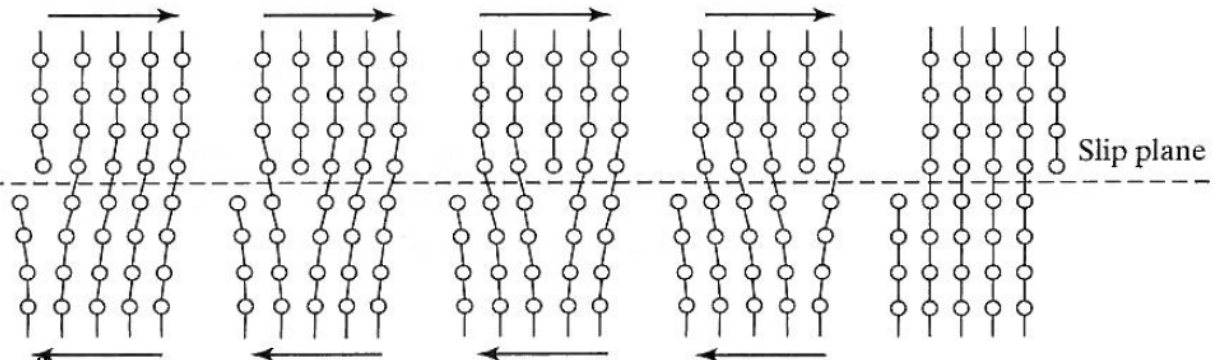
Dislocations

Burgers Vector, b



Core

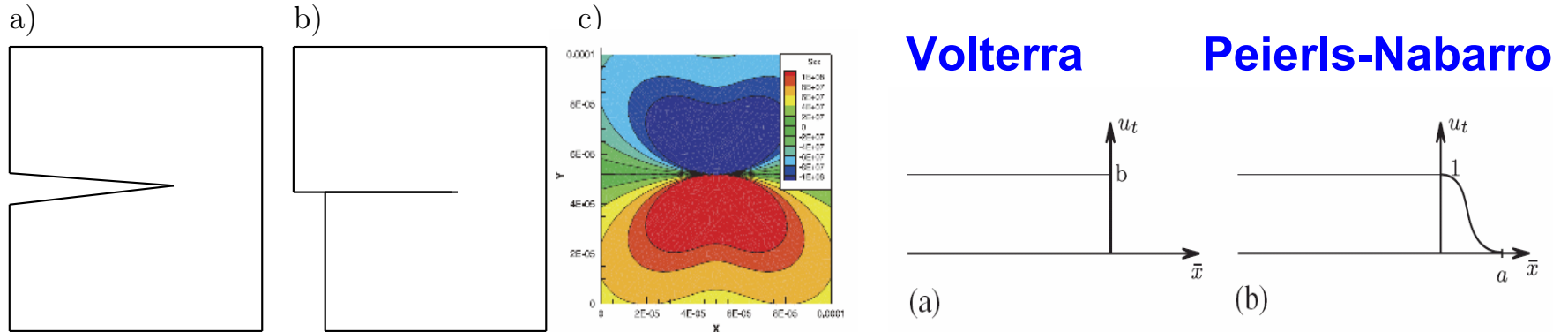
Glide plane



Slip plane



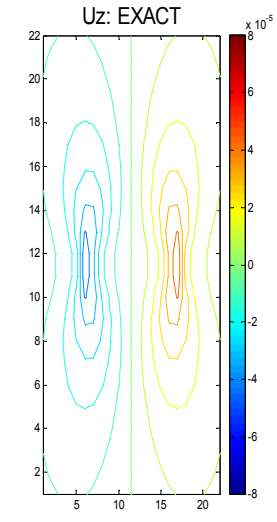
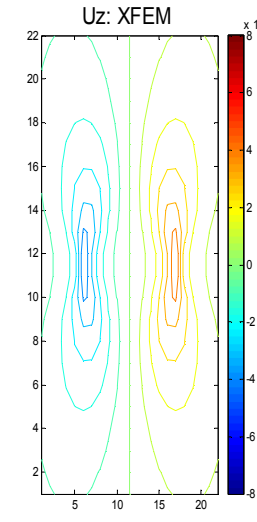
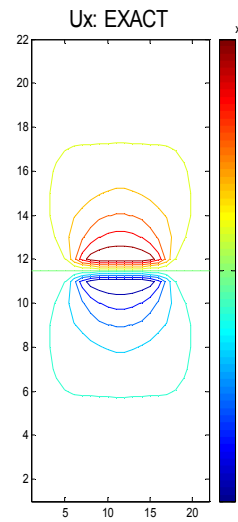
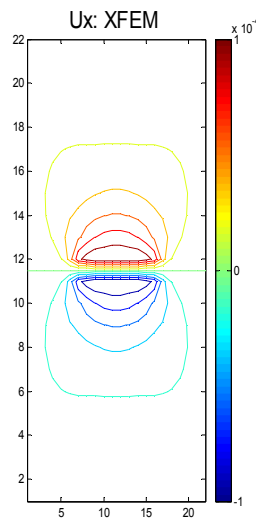
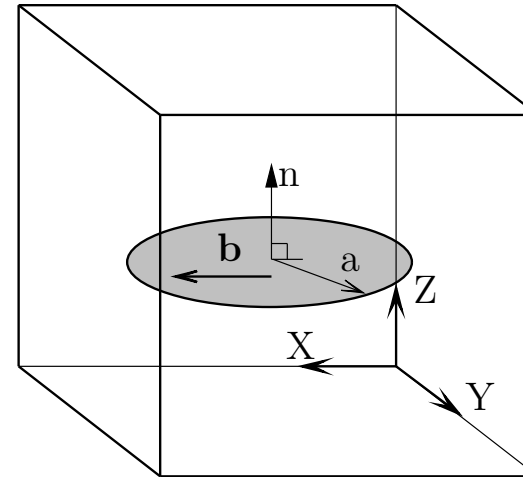
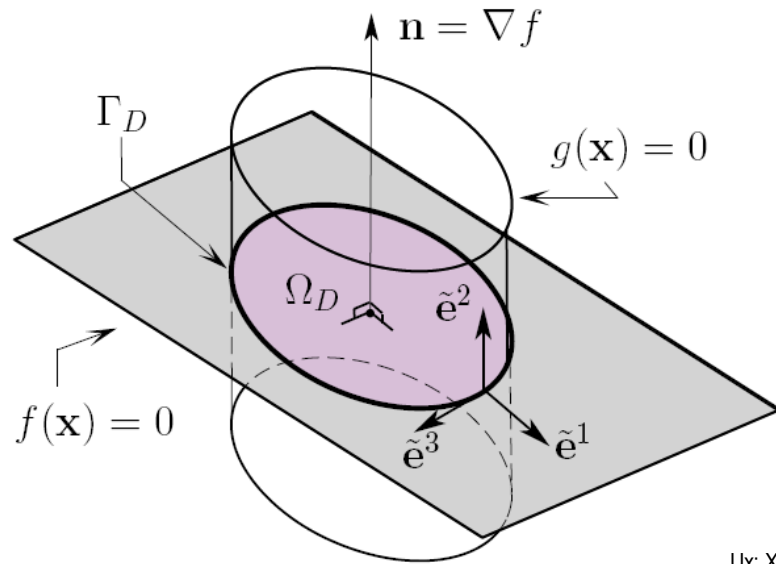
Continuum Model: A New-Old Focus



- (Volterra 1907, Eshelby 1953) the strain field due to a dislocation is completely characterized by the definition of the slip profile along the glide plane.
- The modelling of dislocations can be accomplished by solving the equilibrium equations subject to displacement boundary conditions on internal surfaces.
- Adopt an eXtended Finite Element Method (XFEM) to introduce discontinuities into the finite element approximation space.



Dislocations in 3D





1. Determine static state of stress given number and location of dislocations
2. Calculate driving force on each dislocation (Peach-Koehler force)
3. Update Dislocation positions using a phenomenological law of motion.

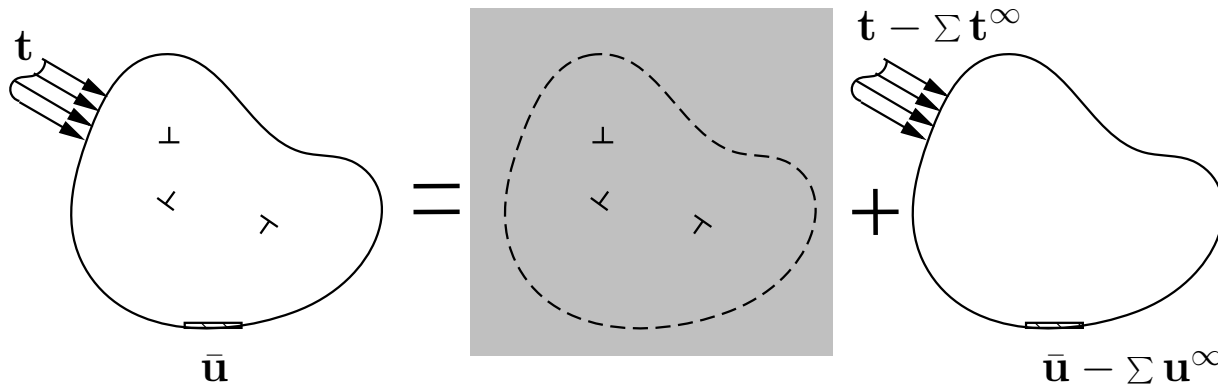
$$\mathbf{F}_{\alpha}^{PK} = \mathbf{M}\ddot{\mathbf{x}}_{\alpha c} + \mathbf{B}\dot{\mathbf{x}}_{\alpha c}$$

Where M = virtual mass, B = lattice drag

4. Apply empirical rules (nucleation, annihilation, etc)
5. Goto 1

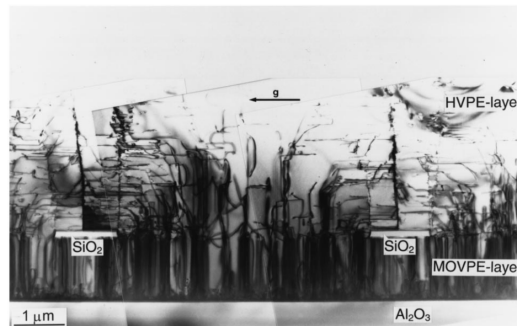


■ Superposition (van der Giessen and Needleman 1995)

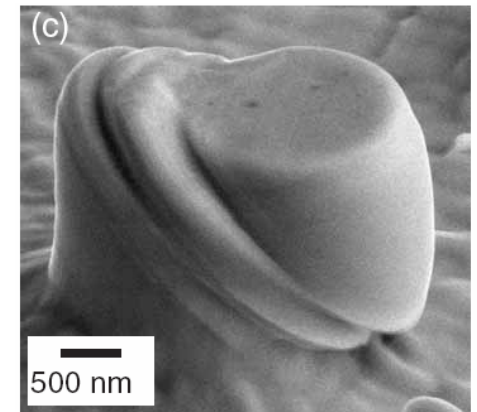


$$\boldsymbol{\sigma}(\mathbf{x}) = \sum_{\alpha=1,n} \boldsymbol{\sigma}_\alpha^\infty(\mathbf{x}) + \boldsymbol{\sigma}^I(\mathbf{x})$$

- Linear
- Isotropic materials
- Single material systems
- Expensive. $O(n^2)$.



Sakai, et al. a APL 1997



Volkert, et al. 2006

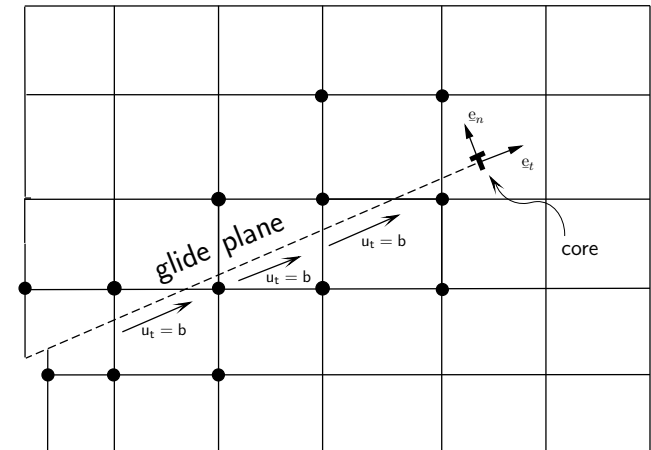


1. Tangential Step Enrichment (Gracie et al IJNME 2007)

$$\mathbf{u}(\mathbf{x}) = \sum_I N_I(\mathbf{x}) \mathbf{u}_I + \mathbf{b} H(f(x)) H(-g(x)) \sum_{J \in S_D} N_J(\mathbf{x})$$

$$H(z) = \begin{cases} 1/2 & \text{if } z > 0 \\ -1/2 & \text{if } z < 0 \end{cases}$$

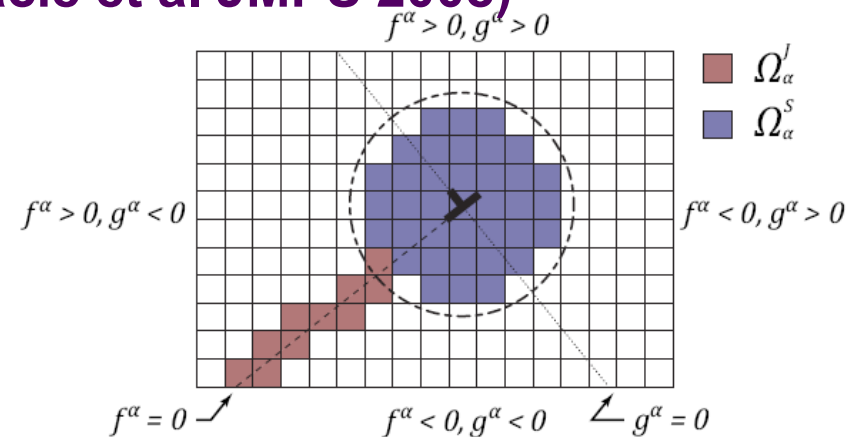
$$f(\mathbf{x}) = \alpha_0 + \alpha_i x_i$$



\mathbf{b} is a known quantity, so no additional degrees of freedom

2. Hybrid (Core+Step) Enrichment (Gracie et al JMPS 2008)

$$\begin{aligned} \mathbf{u}(\mathbf{x}) &= \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I \\ &+ \mathbf{b} \sum_{J \in S^H} N_J(\mathbf{x}) H(f(\mathbf{x})) H(-g(\mathbf{x})) \\ &+ b \sum_{K \in S^\infty} N_K(\mathbf{x}) \mathbf{u}^\infty(\mathbf{x}) \end{aligned}$$





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1. Peach-Koehler formula: Peach and Koehler (1950)

$$\mathbf{F}_l^{PK}(\mathbf{x}_\alpha^C) = \left. \frac{\partial U}{\partial \mathbf{x}_\alpha^C} \right|_{\mathbf{x}_\alpha^c} = \boldsymbol{\xi}_\alpha \times \left(\left[\boldsymbol{\sigma}(\mathbf{x}_\alpha^C) - \boldsymbol{\sigma}_\alpha^D(\mathbf{x}_\alpha^C) \right] \cdot \mathbf{b}_\alpha \right)$$

$\boldsymbol{\sigma}_\alpha^D$ = stress due to dislocation α \mathbf{b} = Burgers vector

$\boldsymbol{\xi}$ = Local tangent to dislocation line

- in superposition methods $\boldsymbol{\sigma}$ is a sum over all dislocations

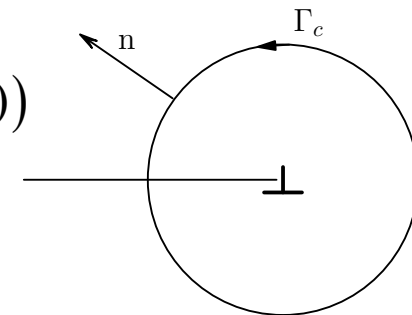
2. J-integral: Eshelby (1951), Rice (1968)

- when the approximation is:

$$\mathbf{u}(\mathbf{x}) = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I + \mathbf{b} \sum_{J \in S^H} N_J(\mathbf{x}) H(f(\mathbf{x})) H(g(\mathbf{x}))$$

we can use the J-integral

$$\mathbf{F}_l^{PK}(\mathbf{x}_\alpha^C) = J_l = - \int_{\Gamma_c} \left[\frac{1}{2} \sigma_{ij} \varepsilon_{ij} \delta_{kl} - \sigma_{ik} u_{i,l} \right] n_k d\Gamma$$



Belytschko, Gracie IJP (2007)



3. Modified Peach-Koehler formula: Gracie et al. JMPS (2008)

- A significant advantage with using the approximation is:

$$\mathbf{u}(\mathbf{x}) = \sum_{\forall I} N_I(\mathbf{x}) \mathbf{u}_I + \mathbf{b} \sum_{J \in S^H} N_J(\mathbf{x}) H(f(\mathbf{x})) H(g(\mathbf{x})) + b \sum_{K \in S^\infty} N_K(\mathbf{x}) \mathbf{u}^\infty(\mathbf{x})$$

Is that a modified Peach-Koehler formula can be used

$$\mathbf{F}_l^{PK}(\mathbf{x}_\alpha^C) = \boldsymbol{\xi}_\alpha \times \left(\left[\boldsymbol{\sigma}^{XFEM}(\mathbf{x}_\alpha^C) - \boldsymbol{\sigma}_\alpha^D(\mathbf{x}_\alpha^C) \right] \cdot \mathbf{b}_\alpha \right)$$

\mathbf{b} = Burgers vector

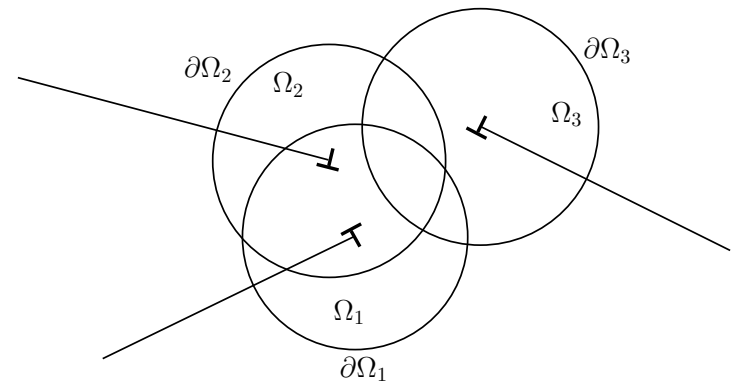
$\boldsymbol{\xi}$ = Local tangent to dislocation line

$\boldsymbol{\sigma}^{XFEM}$ = Stress from XFEM approximation

$\boldsymbol{\sigma}_\alpha^D$ = stress due to dislocation α

- in XFEM $\boldsymbol{\sigma}^{XFEM}$ is a sum over a subset of all dislocations
- more efficient than superposition of all dislocations

Gracie, Oswald, Belytschko JMPS (2008)

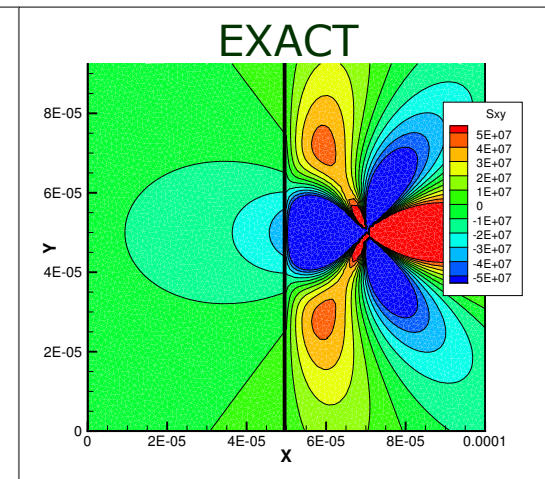
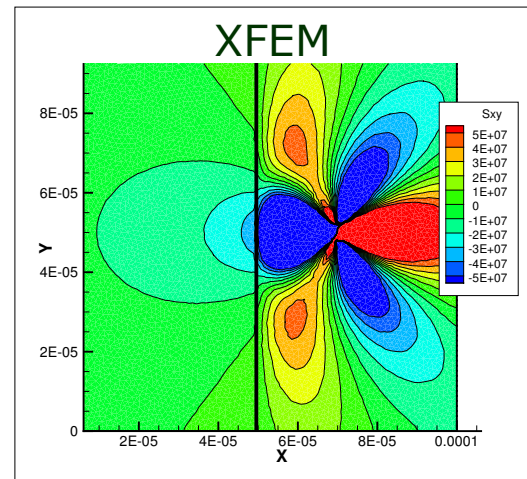
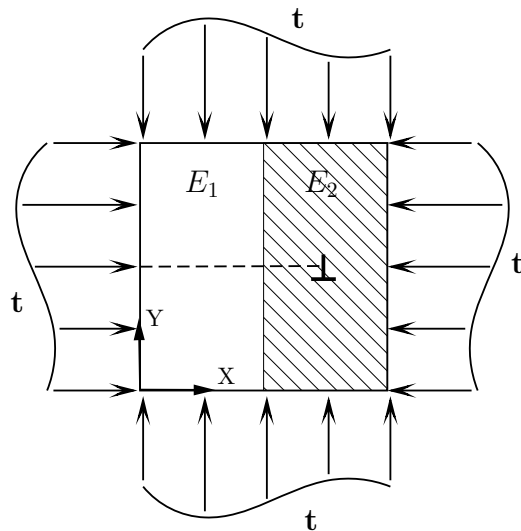
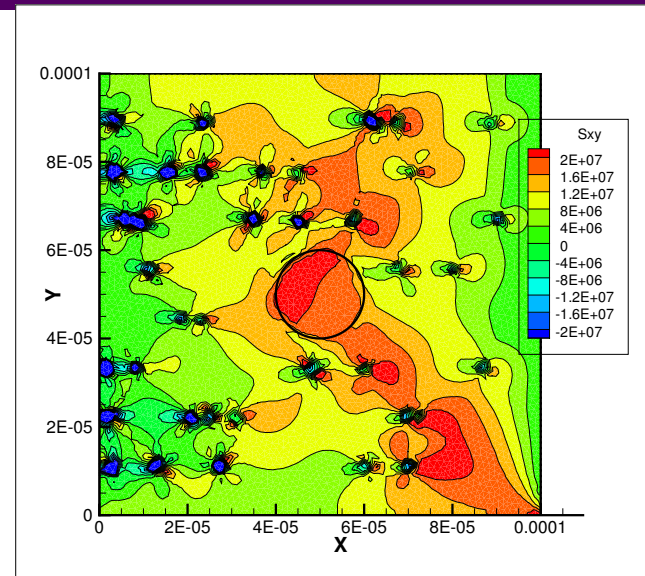
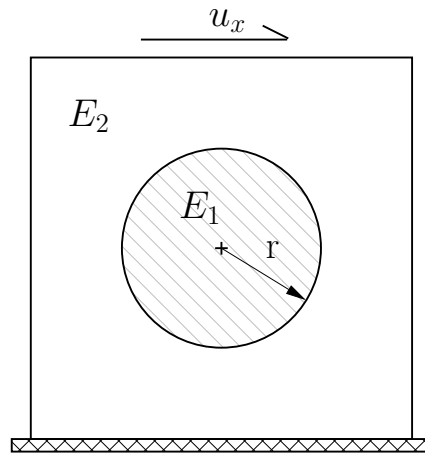




- Challenges to modelling discontinuities with FEM
- Extended Finite Element Method (XFEM):
Modelling Cracks
- Some improvements to the XFEM
 - Efficient Numerical Integration
 - Discontinuous Galerkin
- **Modelling Dislocations**
 - Approximations
 - Peach-Koehler force
 - **2D and 3D**
 - Thin Shells



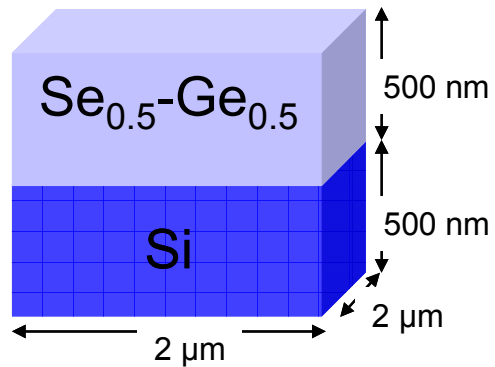
Application to interface problems



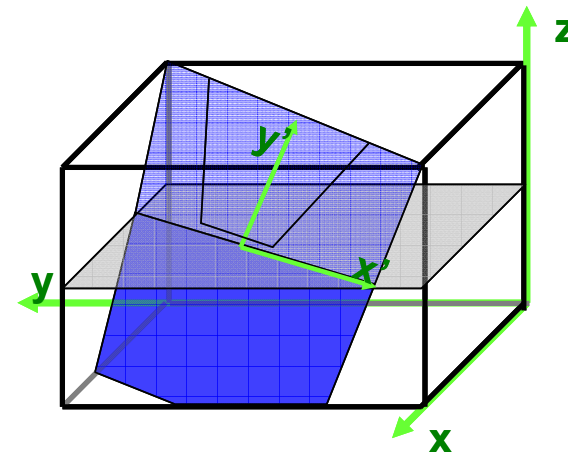
Belytschko & Gracie IJP (2007)



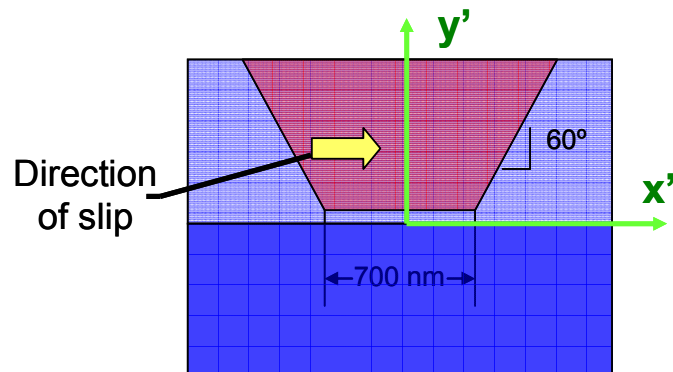
Misfit dislocations in layered anisotropic materials



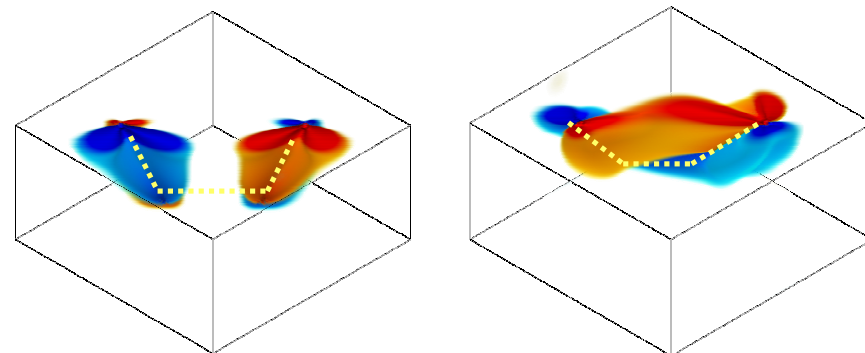
Si/SiGe layered system – lattice mismatch leads to misfit dislocations



Schematic of dislocation on (111) glide plane in layered system



Cross section of (111) glide plane showing slip across the shaded region



Stress contours (left) σ_{xy} , (right) σ_{xx} , resulting from misfit dislocation and threading segments

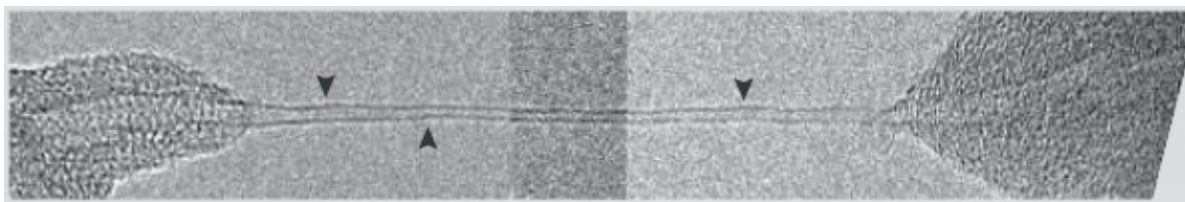
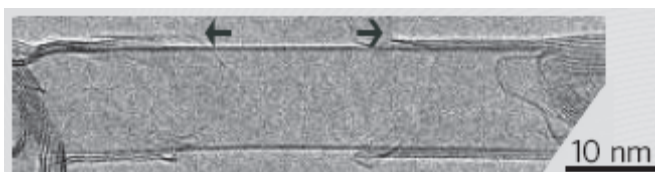


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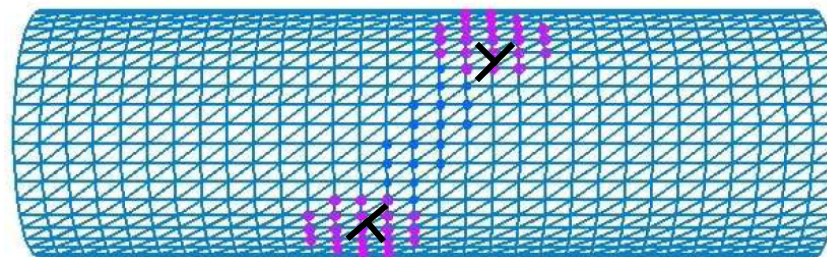
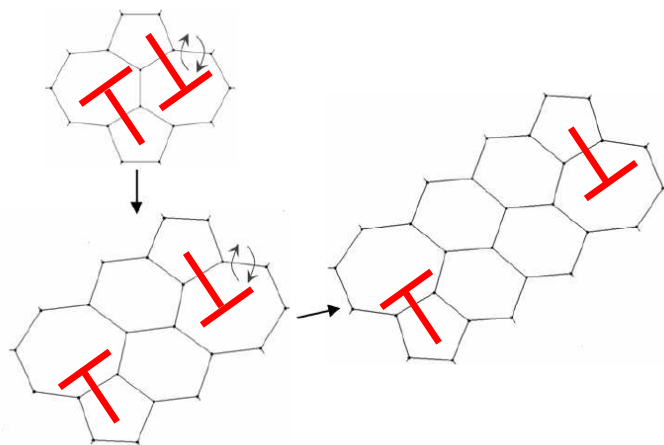


Plasticity in Carbon Nanotubes

- Plasticity in carbon nanotubes at high temperatures (Huang, Nature 2006)



- Dislocations are mechanism for plasticity (Yakobson Group 2006, 2007)

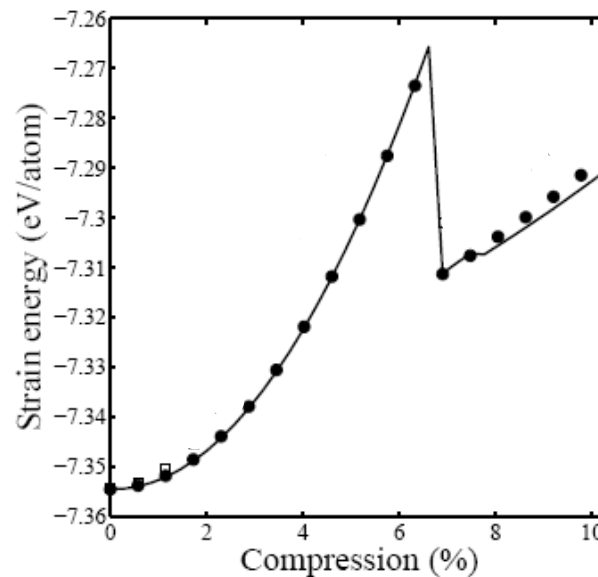




- Buckling of perfect nanotubes: **Arroyo (2002) thesis**
 - Kirchhoff-Love thin shell versus atomistics
- Atomistics are expensive, restricted to short tubes of small diameter



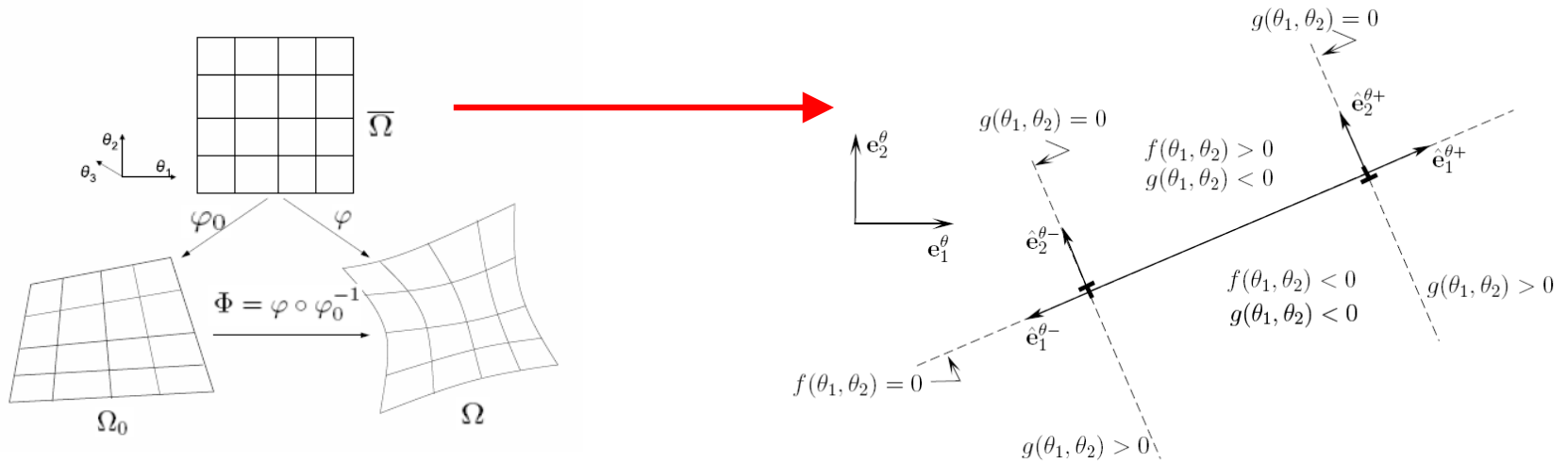
(a)



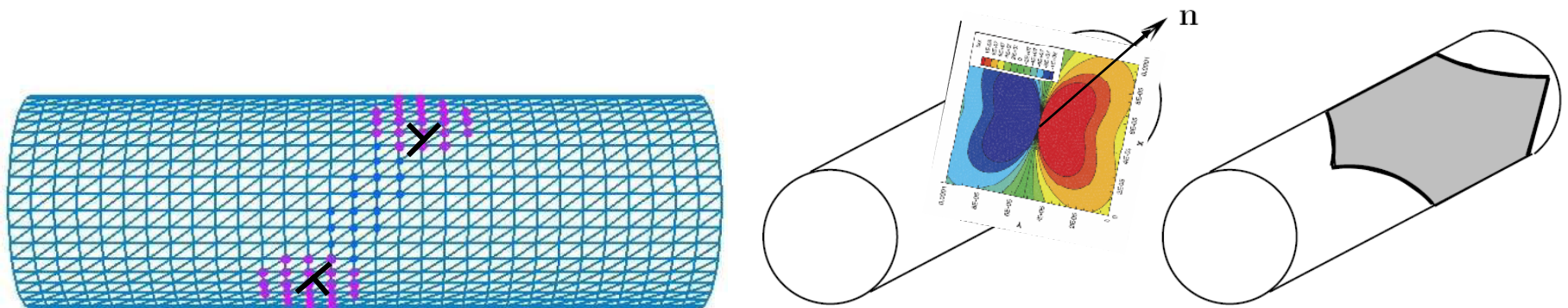
(b)



XFEM dislocations model for shells



$$\mathbf{u}^D(\theta_1, \theta_2) = \sum_{J \in S^H} N_J(\theta_1, \theta_2) \Psi^H(\theta_1, \theta_2) + \sum_{K \in S^H} N_K(\theta_1, \theta_2) \Psi^\infty(\theta_1, \theta_2)$$

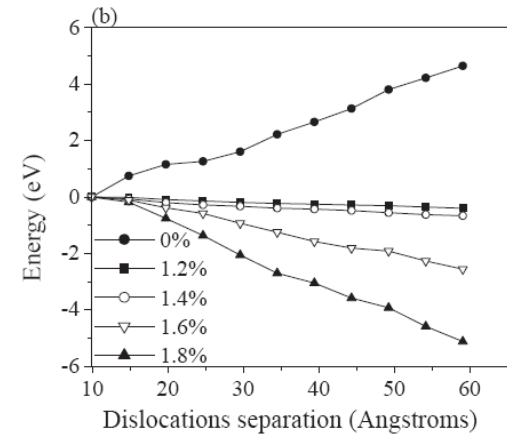
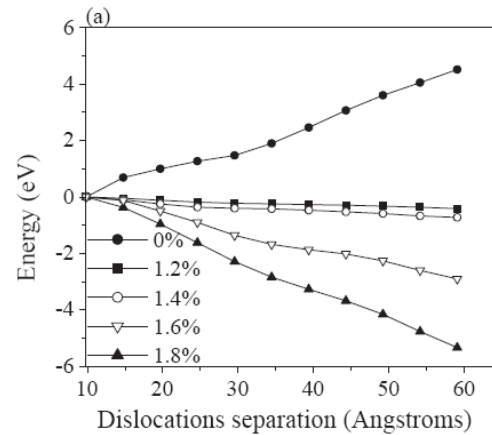




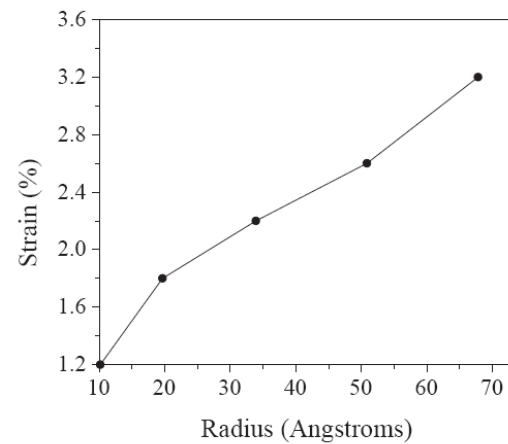
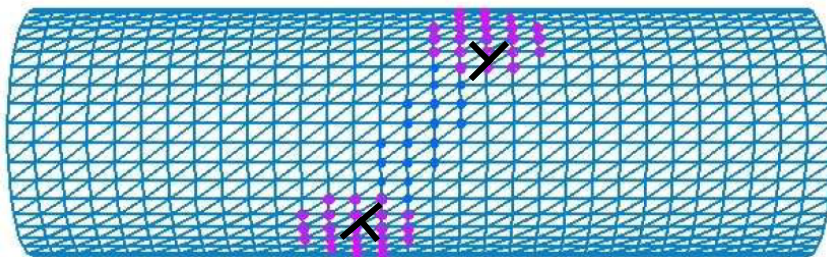
Carbon nanotube with dislocation pair

■ [15,15] CNT

D=10 Å
L=249.6 Å
E = 730 GPa
 $\nu = 0.4$
b = 2.46 Å
765 nodes
6120 atoms



■ [15,15] CNT to [100,100] CNT





- Methods for modelling discontinuities in continua
 - Cracks and Dislocations
- Improved integration of singular enrichments
- Improved accuracy and convergence with discontinuous Galerkin scheme
- Applications to dislocations in 2D, 3D and shells
- Methods for computing of the Peach-Koehler force



■ Collaborators

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- Dr. R. Khare: *Department of Mechanical Engineering, Northwestern University*
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- 1. Gracie**, Oswald, and Belytschko, *On a new extended finite element method for dislocations: core enrichments*. Journal of Mechanics and Physics of Solids, 56:200-214, 2008.
- 2. Gracie**, Wang, and Belytschko, *Blending in the eXtended Finite Element Method by Discontinuous Galerkin and Assumed Strain Methods*. International Journal for Numerical Methods in Engineering (accepted 2007)
- 3. Gracie**, Ventura, and Belytschko. *A new fast*