

Discretisation, Multiscale Mechanics Problems & Surgical Simulation

Stéphane Bordas & Pierre Kerfriden
University of Luxembourg and Cardiff University

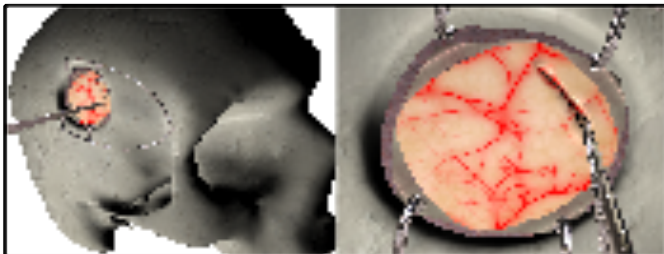


University of Limerick, Ireland
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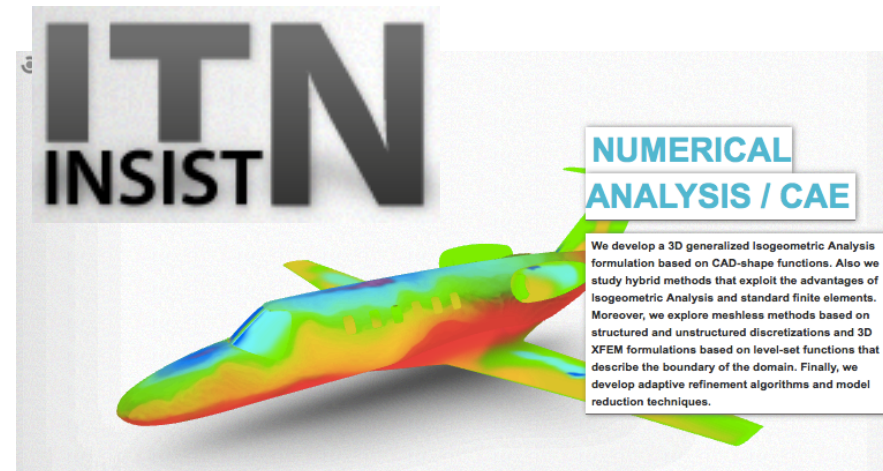




- A small, young, dynamic university
- 3 languages (English, German, French); bilingual and trilingual degrees
- Strong mathematics and Comp. Sc.
- RUES: 3 professors in computational mechanics, 30 collaborators
- Computational sciences priority 1
- Strong local industry
- Strong and supportive national funding
- 7 EU projects in engineering, of which RealTcut: ERC Starting Grant (Bordas)



- A large, established university (1883)
- 95% 3 or 4* at RAE2008 in Civil
- Over 100 EU projects awarded of which ITN: INSIST
- Mechanics Research: 40 researchers, 14 faculty members
- Advanced manufacturing and characterisation





Advisor: Brian Moran
Now vice-provost for
faculty affairs at KAUST

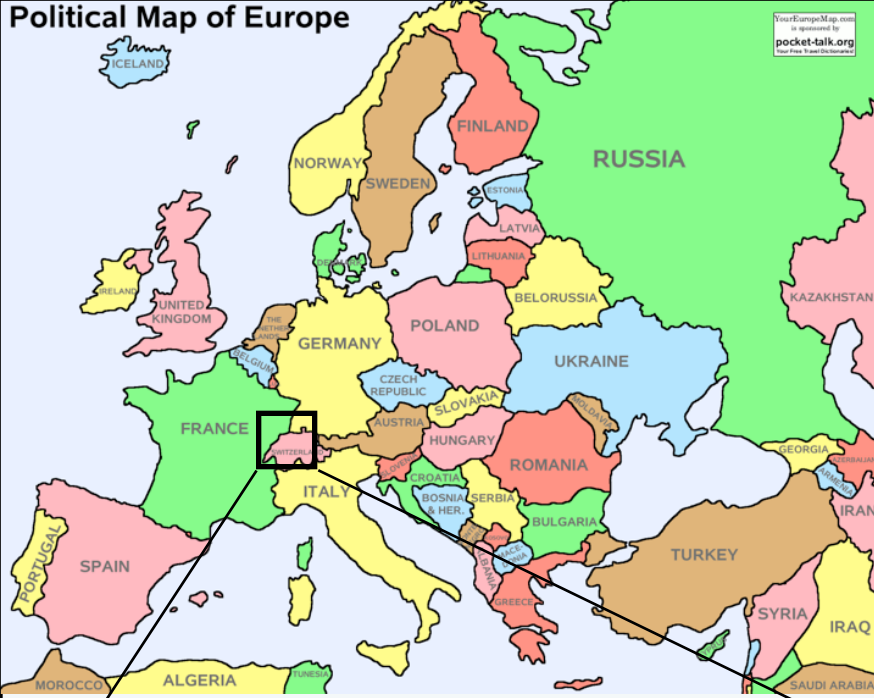


1997-2003

MSc Geotechnical Engineering

PhD. Damage Tolerance of Aerospace Structures (XFEM)
and Biofilm Growth

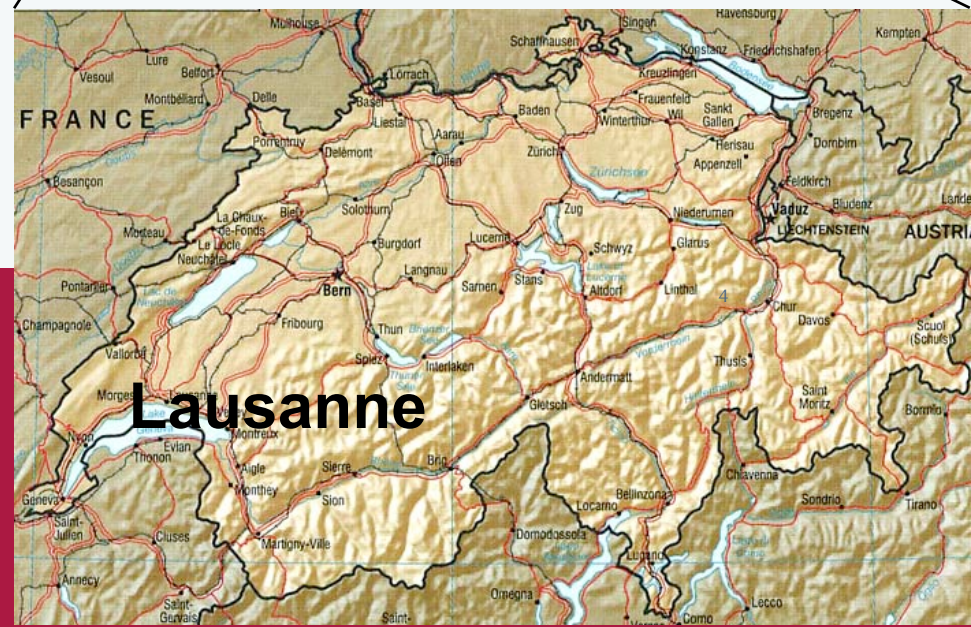
Political Map of Europe



Post-doc 2003-2006 -
Meshless/XFEM Geomechanics



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

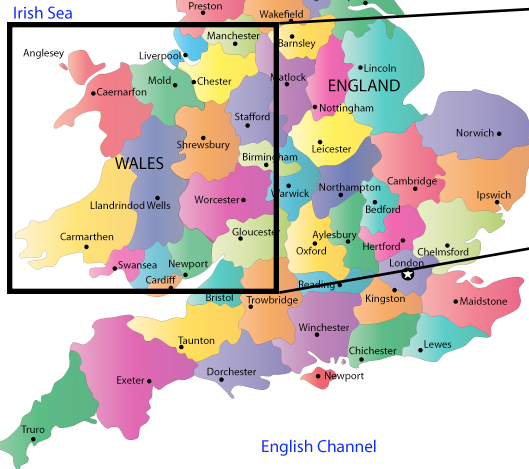
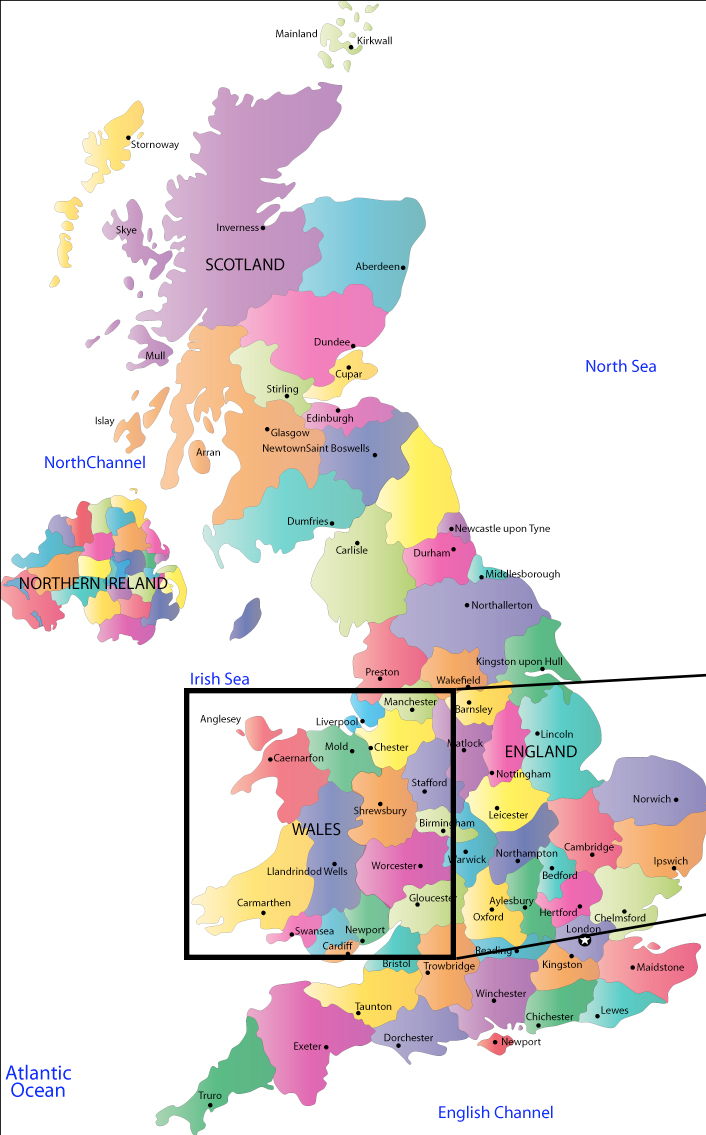




Lecturer in
civil
engineering



UNIVERSITY
of
GLASGOW



CARDIFF
UNIVERSITY

PRIFYSGOL
CAERDYDD

I M A M
Institute of Mechanics
& Advanced Materials







2

4

5

1

6

3



Luxembourg: 2,586.4 km²

Paris region: 12,012 km²



geodynamics, faults, ice



intuitive design of surgical simulators



methods



nano/characterisation, Si



concrete/fibers, cracks



meshfree, diffpack...



FSI, advanced num...



CAD - isogeometry...



antennas, EMS, data



inverse problems damage



geodesy (need to be taught!)



moving boundaries



dynamics, maths



energy



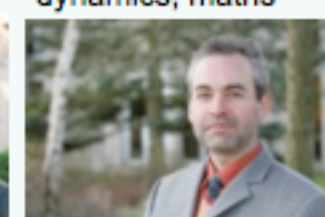
FE, mechanics, fibres, health monitoring, multifield, biomechanics



chemistry, moving fronts, biofilms, concrete



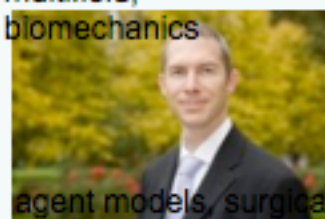
Bauphysik, acoustics isogeometric BEM?



steel, multi-materials, acoustics, multiphysics



hydraulics, biofilms



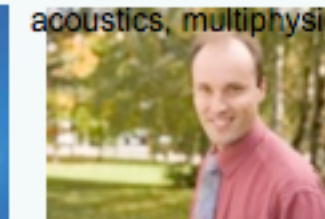
agent models, surgical robots



laser techno



geodynamics, faults, ice geomechanics/meshfree/DEM





Prof. Stéphane Bordas, Director.
Extended FEM/ Meshless



Prof. Feodor Borodich
Theoretical/Nano mechanics, contact, adhesion



Prof. Pwt Evans
Contact mechanics, tribology



Dr. Paul Howson
Transcendental eigenvalue problems



Prof. Bhushan Karihaloo
Advanced materials, theoretical mechanics



Prof. David Kennedy
Eigenvalue problems, advanced numerical methods



Dr. Pierre Kerfriden
Multiscale, model order reduction, fracture



Dr. Siva Kulasegaram
Meshless methods



Prof. Ray Snidle
Contact mechanics, tribology



Dr. Lars Beex
Multiscale methods



Dr. Hanxing Zhu
Theoretical mechanics, cellular materials

The institute

- 6 professors, 6 lecturers/senior lecturers
- 10 post-doc fellows
- 17 PhD students
- ~ £1.0M funding annually



Theoretical & Computational

Tribology & Contact Mechanics

Experiments

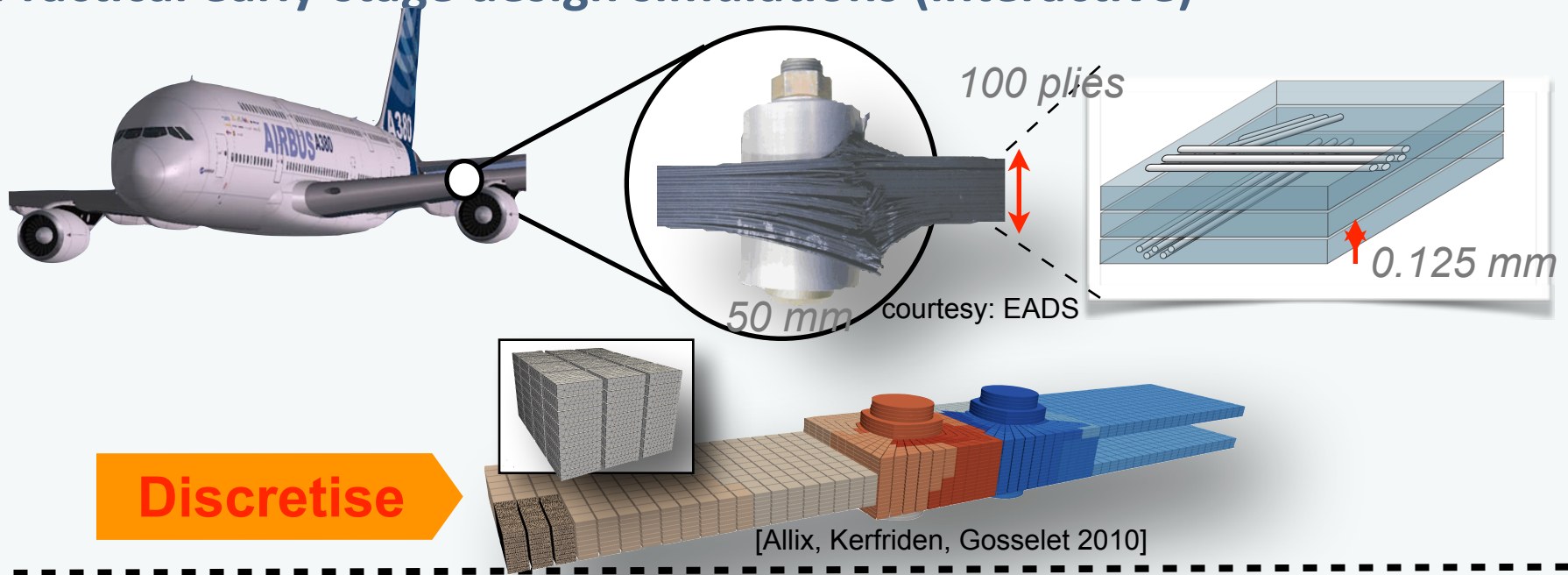
Theory

Computational Mechanics

Motivation: multiscale fracture of engineering structures and materials

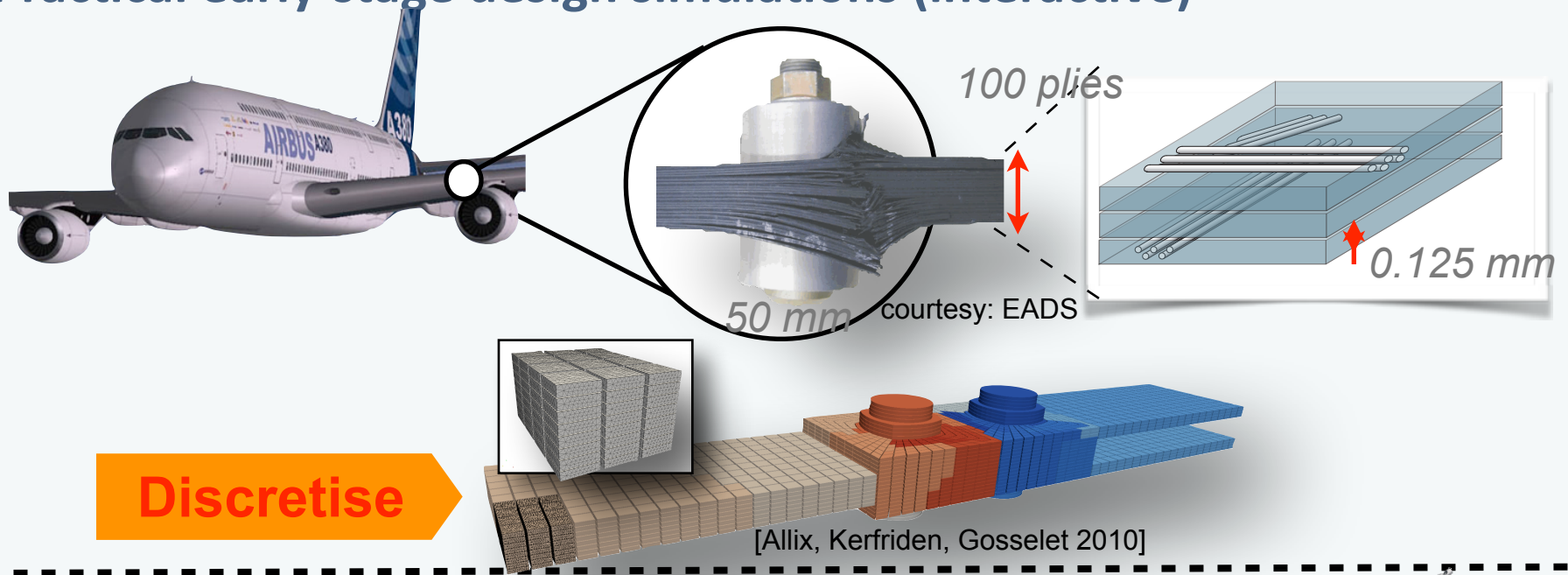
Motivation: multiscale fracture of engineering structures and materials

Practical early-stage design simulations (interactive)

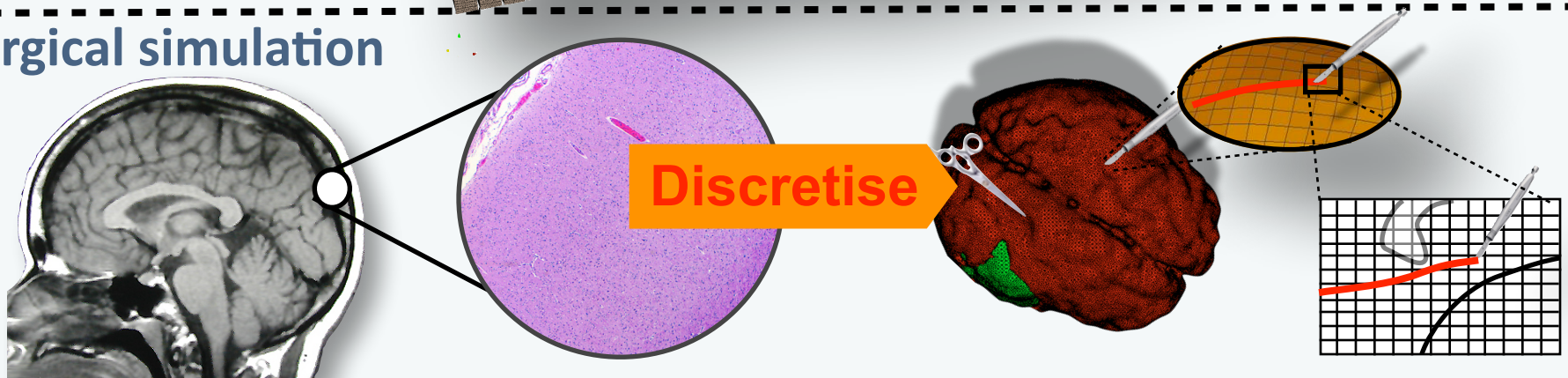


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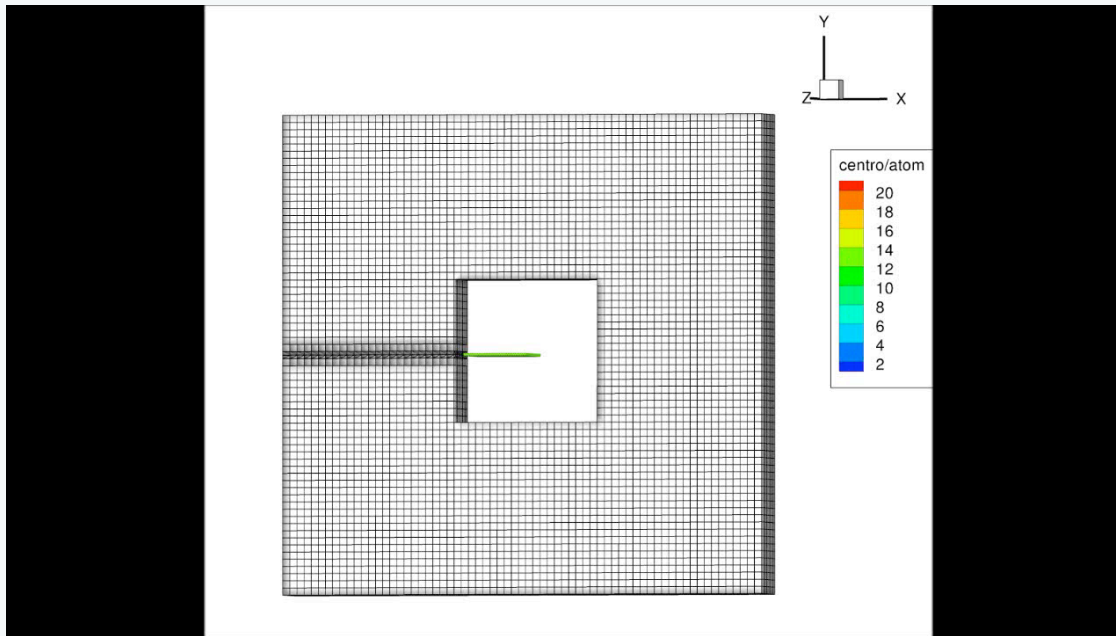
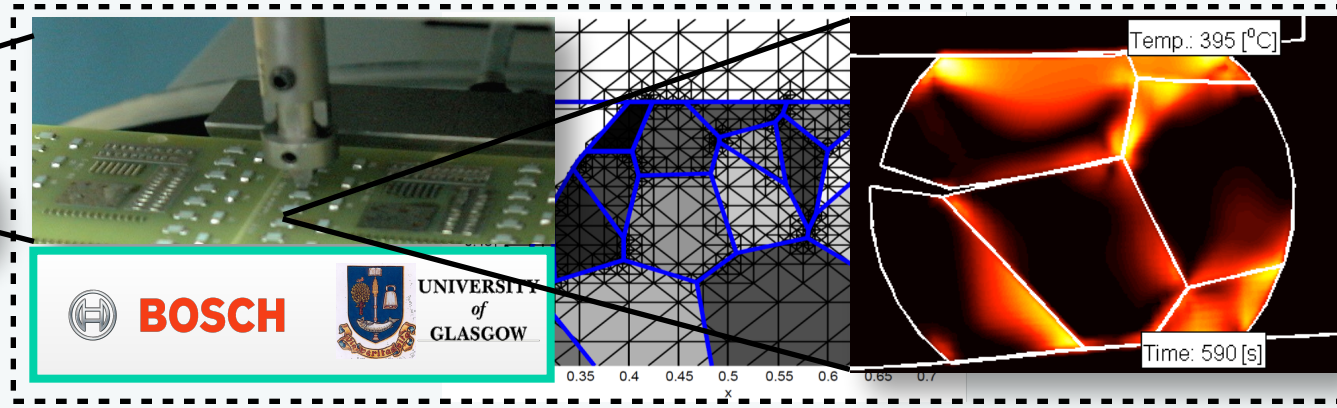
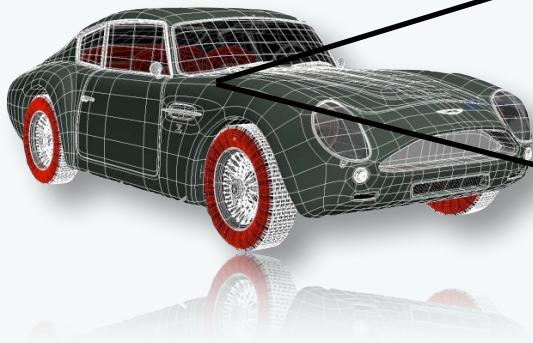
Surgical simulation



- ▶ Reduce the problem size while controlling the error (in QoI) when solving very large (multiscale) mechanics problems

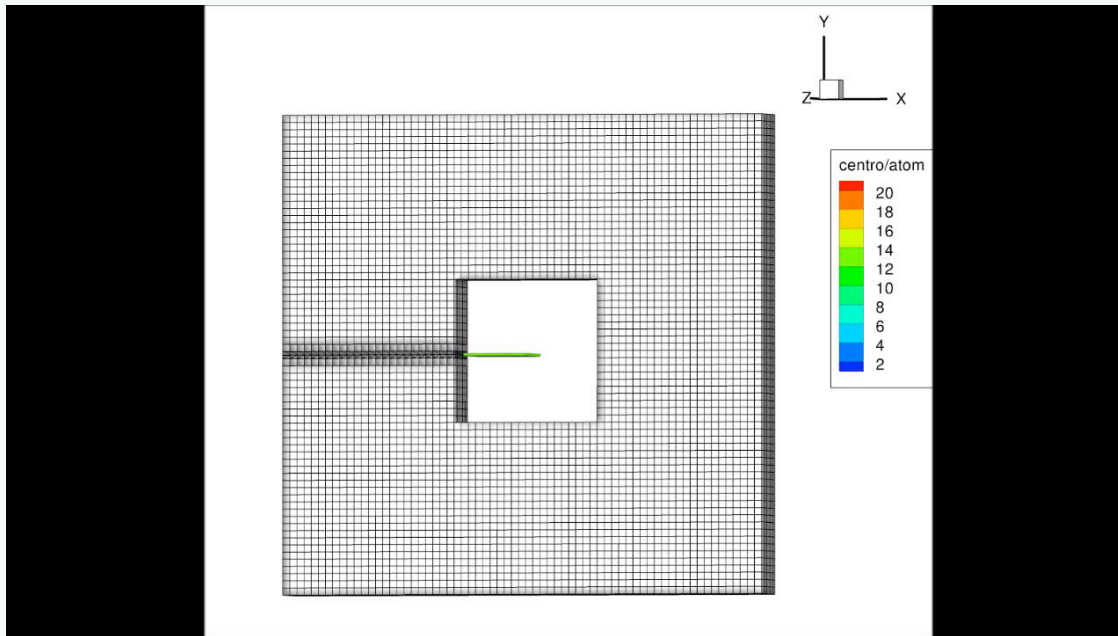
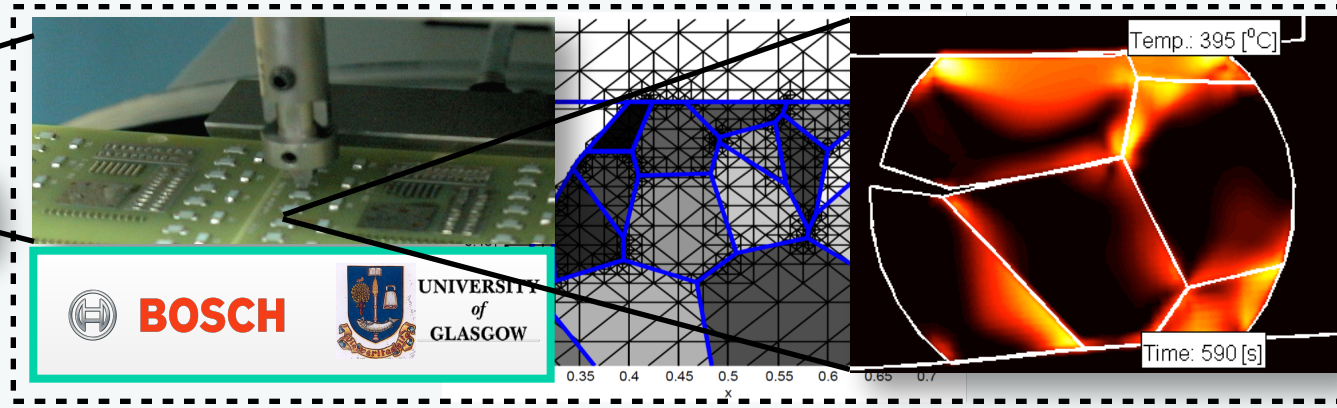
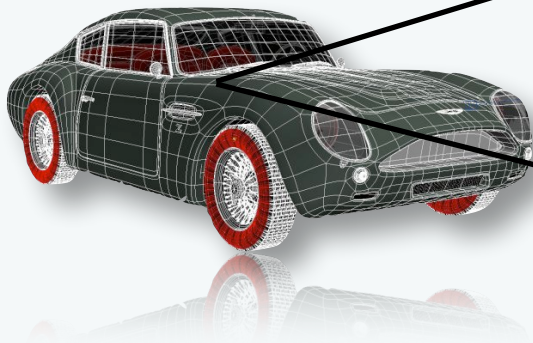
Motivation: multiscale fracture of engineering structures and materials

Solder joint durability (microelectronics), Bosch GmbH



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Discretization

- ➔ partition of unity enrichment
- ✓ (enriched) meshless methods
- ✓ level sets

- ➔ isogeometric analysis
- ➔ implicit boundaries

Model reduction ¹⁵

- ✓ multi-scale & homogenisation
- ✓ algebraic model reduction (using POD)
- ✓ Newton-Krylov, “local/global”, domain decomposition

Error control

- ✓ XFEM: goal-oriented error estimates
 - ▶ used by CENAERO (Morfeo XFEM)
- ✓ meshless methods for fracture
- ✓ error estimation for reduced models

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Part I. Streamlining the CAD-analysis transition

Part II. Some advances in enriched FEM

Part III. Application to H cutting of Si wafers

Part IV. Application to interactive cutting sim.

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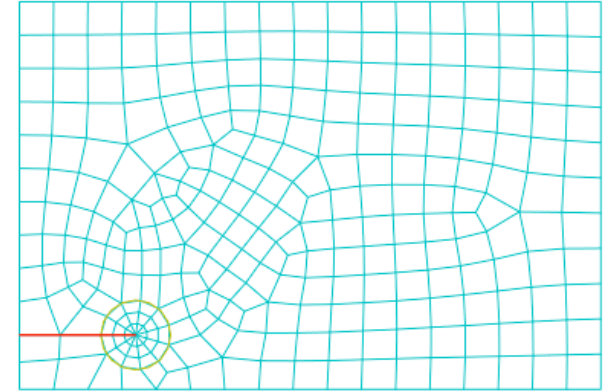
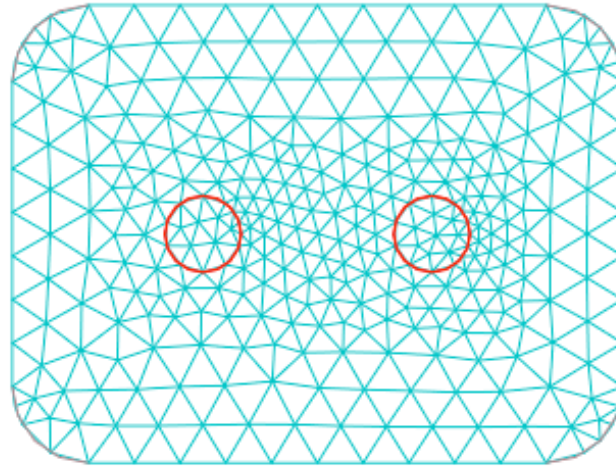
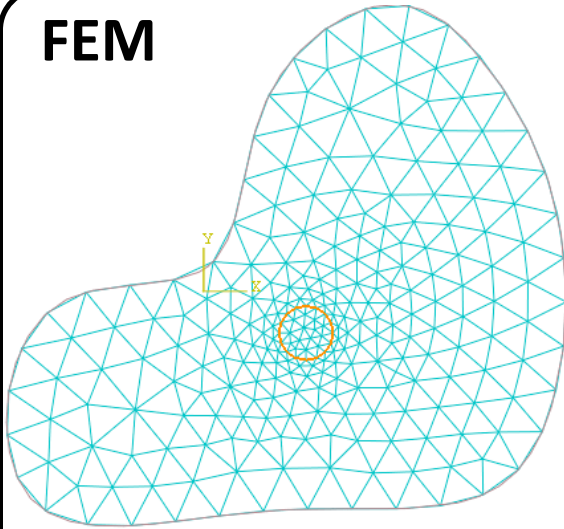
Part I. Streamlining the CAD-analysis transition

Coupling, or decoupling?

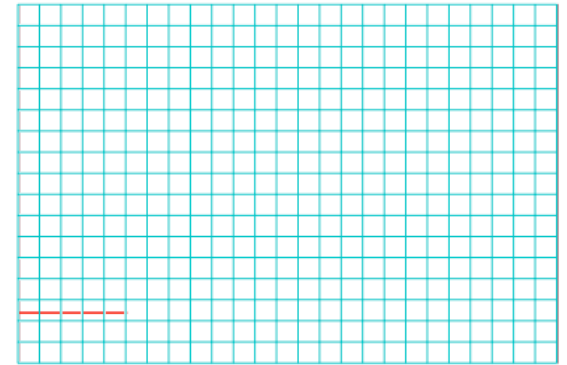
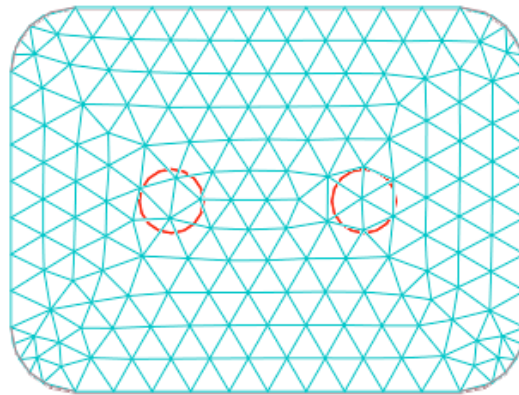
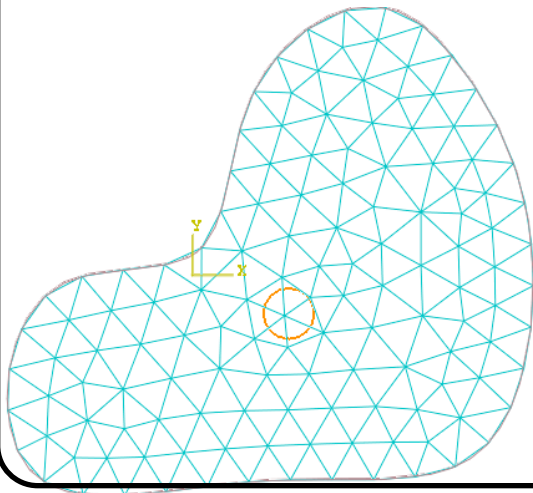
Motivation: free boundary problems - mesh burden



FEM



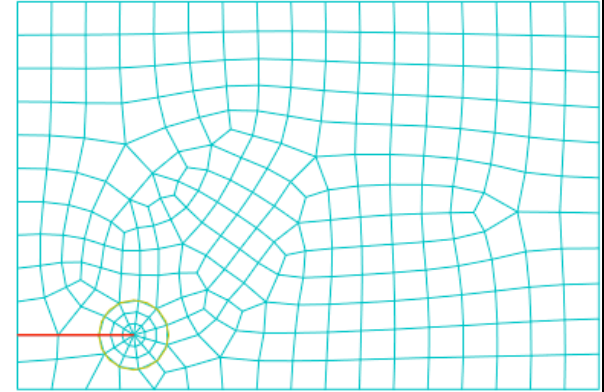
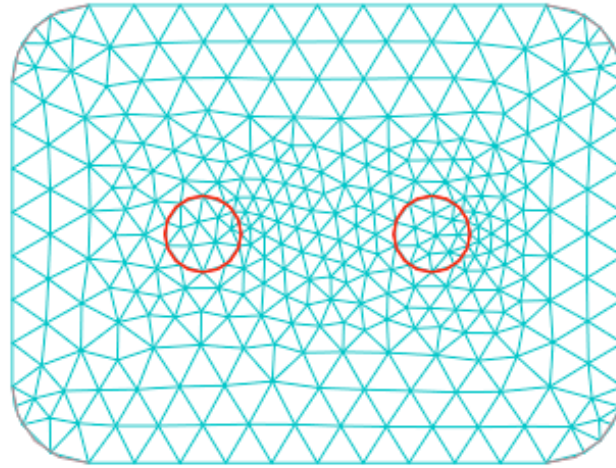
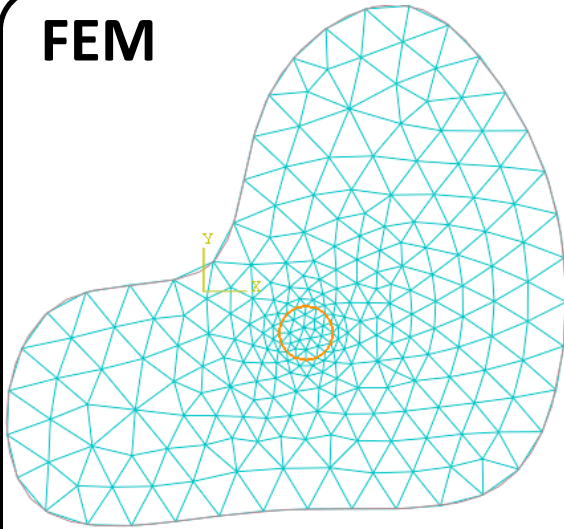
XFEM



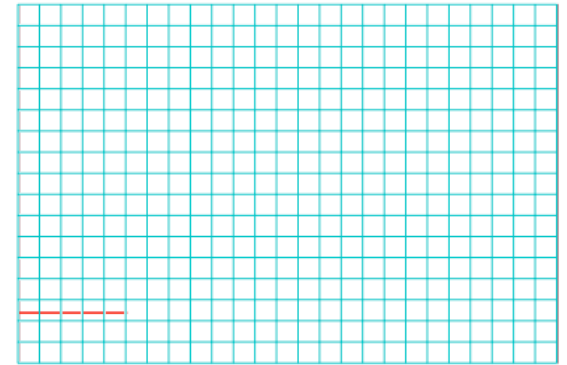
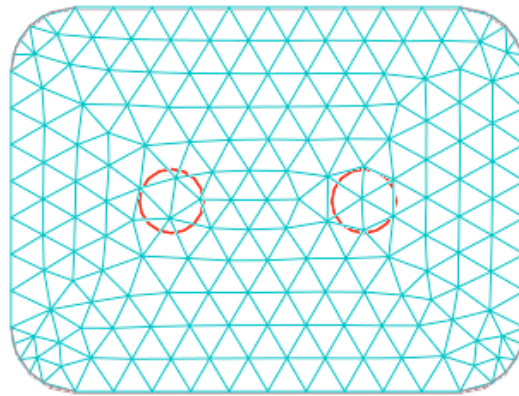
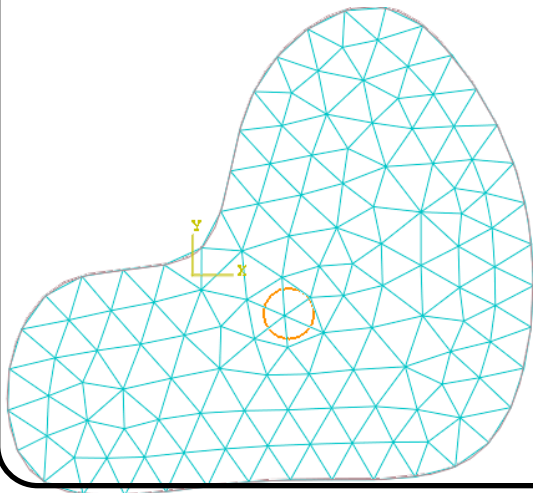
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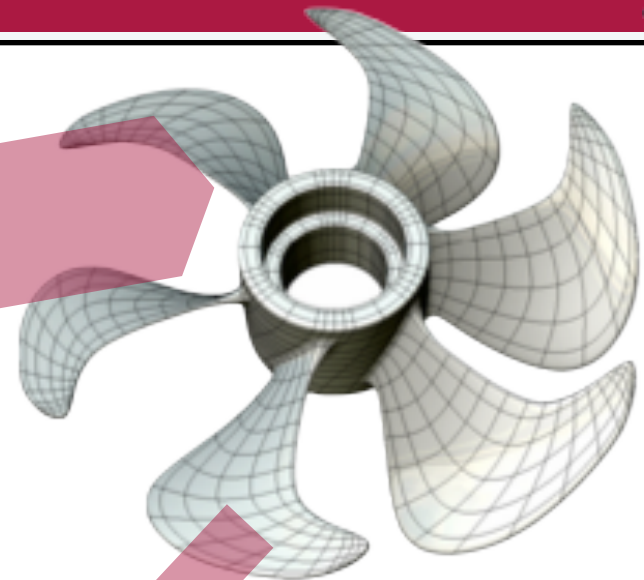
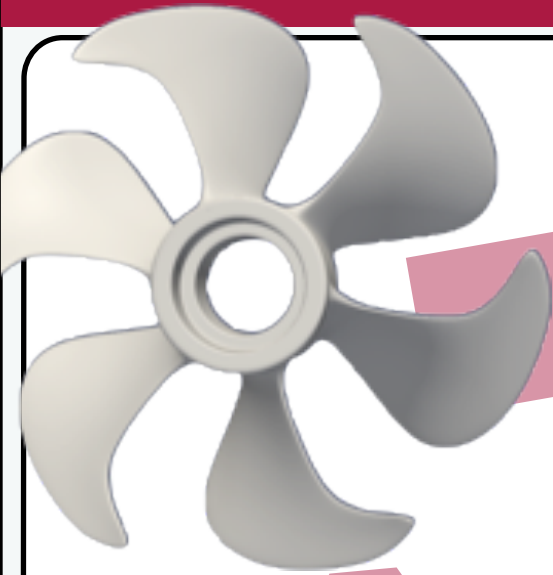


FEM

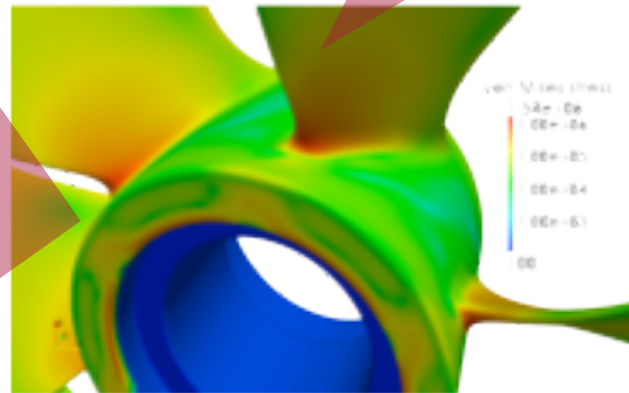
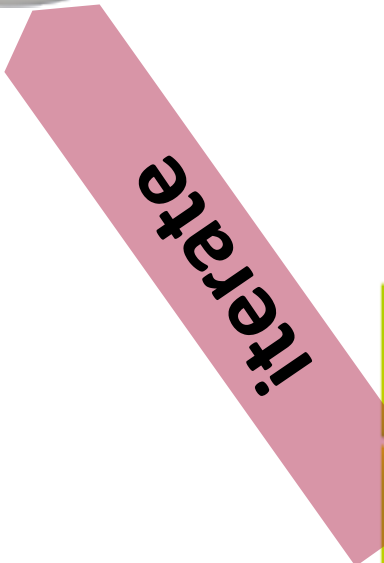


XFEM



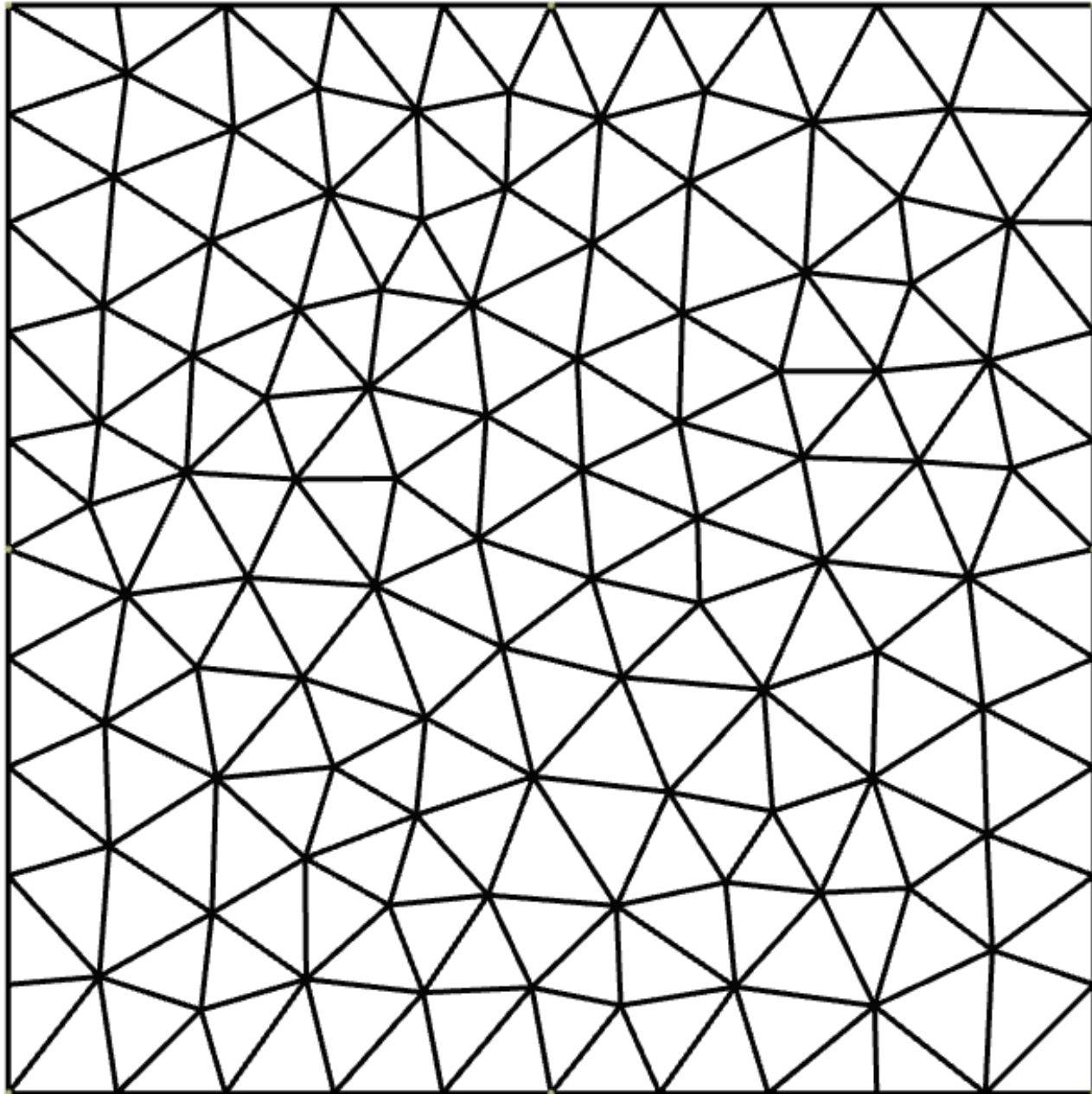


calculate

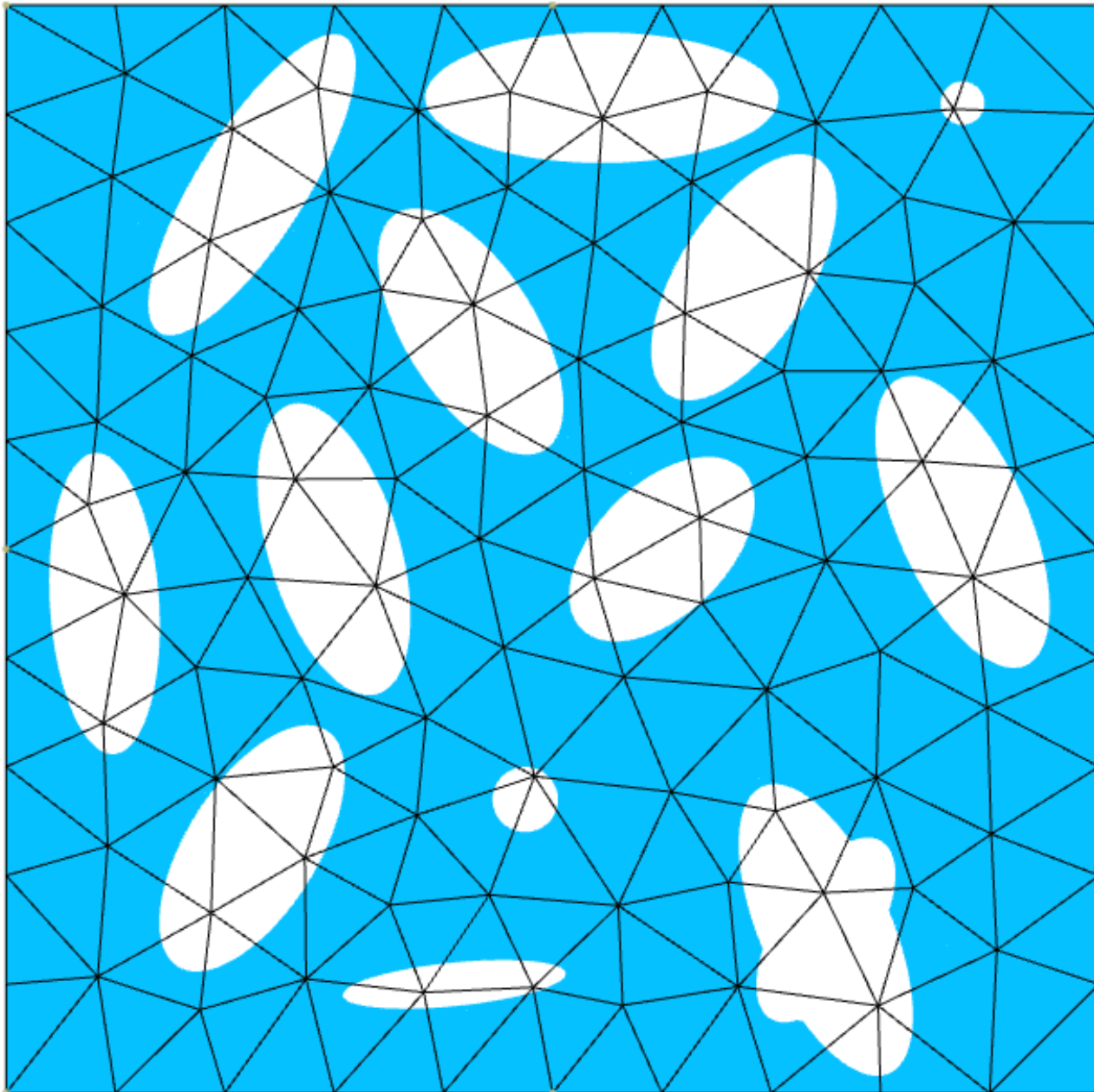


stress distribution

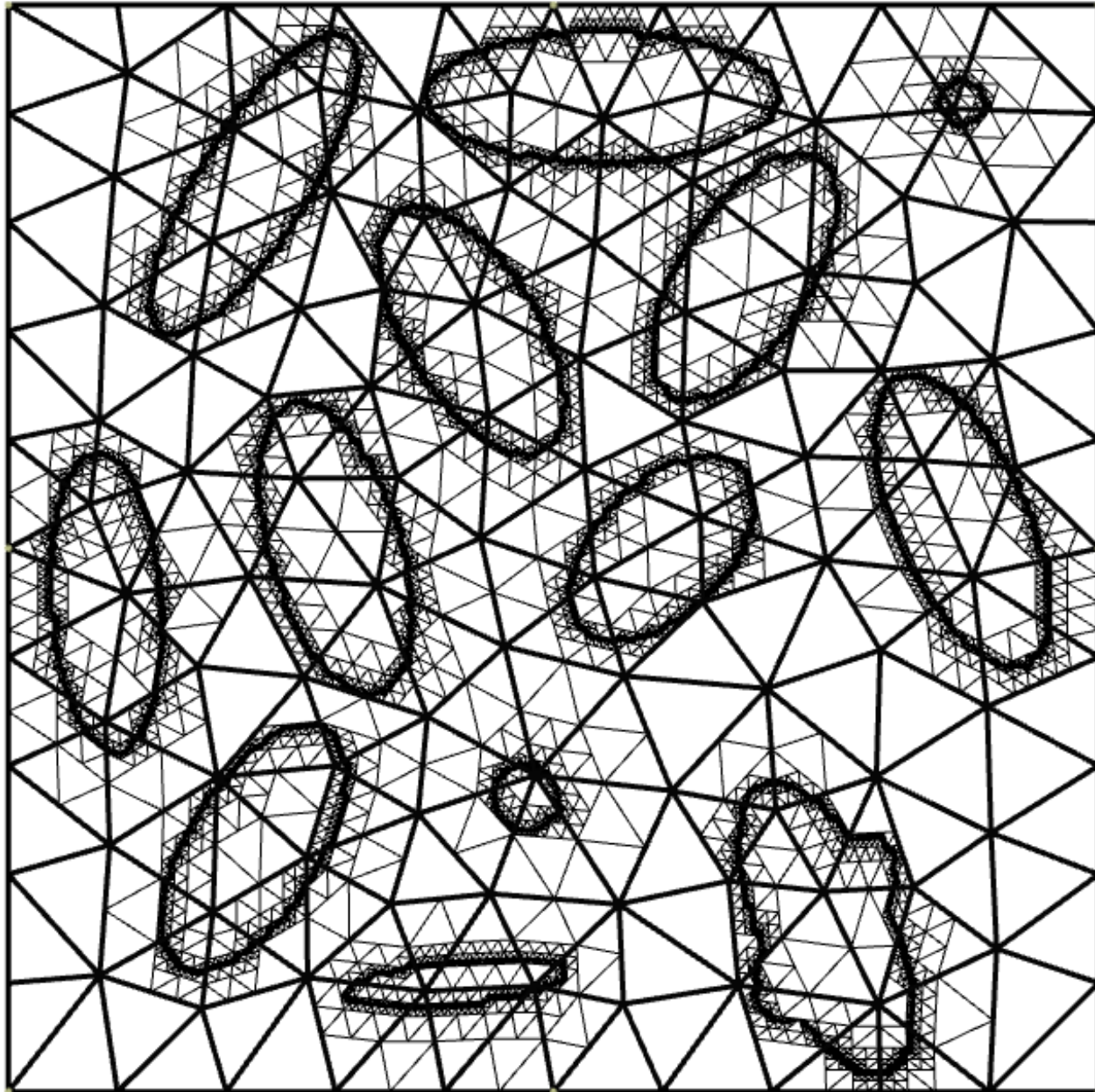
One would like to be able to use such a mesh



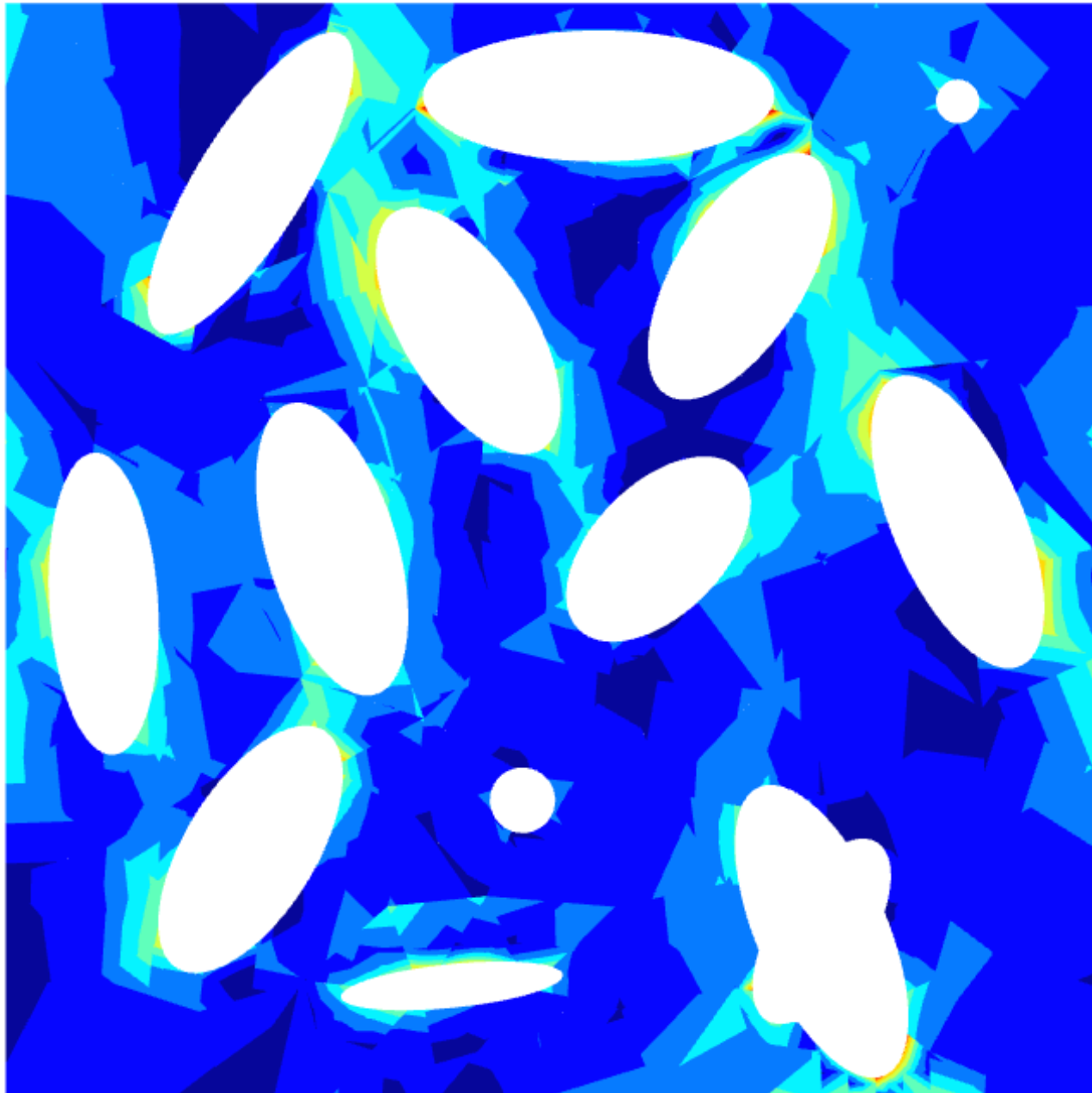
Superimpose the geometry onto an arbitrary background mesh



Compute interactions between the geometry and the mesh

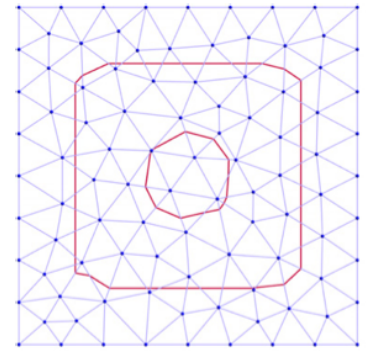


Perform the analysis

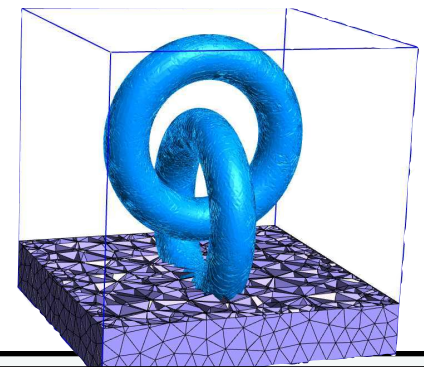
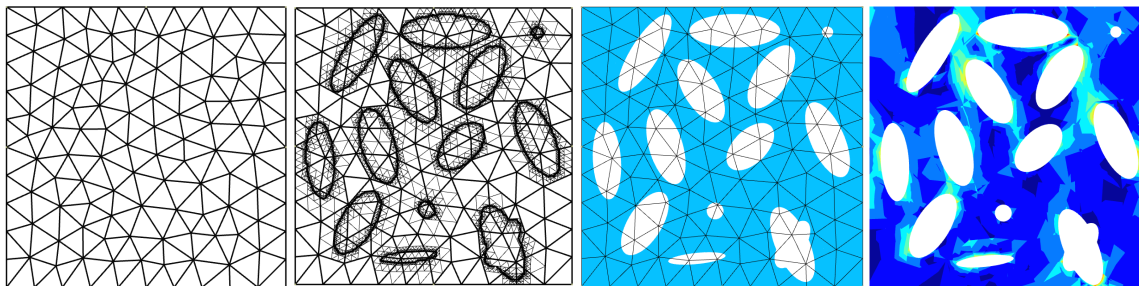


Paradigm 1: Separate field and boundary discretisation

- Immersed boundary method (Mittal, *et al.* 2005)
- Fictitious domain (Glowinski, *et al.* 1994)
- Embedded boundary method (Johansen, *et al.* 1998)
- Virtual boundary method (Saiki, *et al.* 1996)
- Cartesian grid method (Ye, *et al.* 1999, Nadal, 2013)

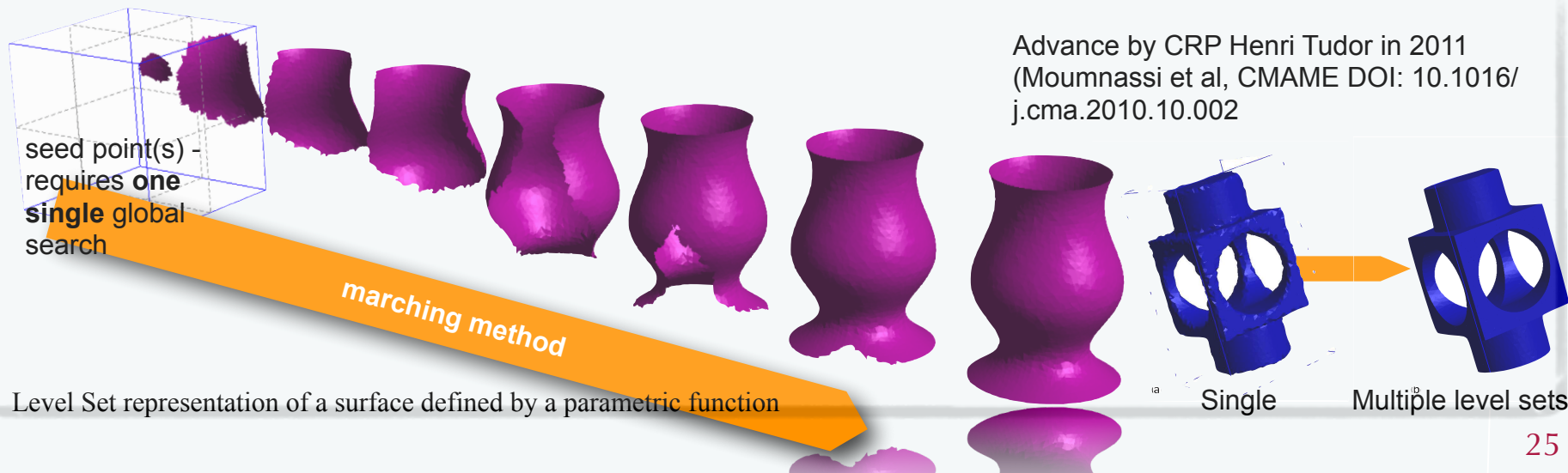
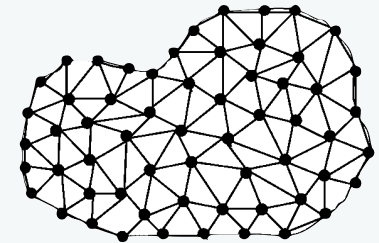
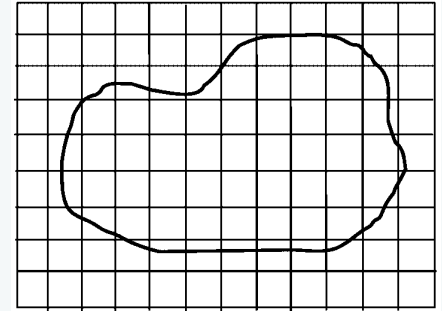


- ✓ Easy adaptive refinement + error estimation (Nadal, 2013)
- ✓ Flexibility of choosing basis functions
- Accuracy for complicated geometries? BCs on implicit surfaces?
- ➔ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi, *et al.* 2011)

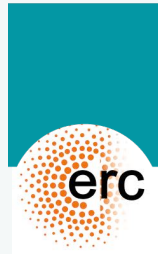


● Objectives

- ▶ insert surfaces in a structured mesh
 - without meshing the surfaces (boundary, cracks, holes, inclusions, etc.)
 - directly from the underlying CAD model
 - model arbitrary solids, including sharp edges and vertices
- ▶ keep as much as possible of the mesh as the CAD model evolves, i.e. reduce mesh dependence of the implicit boundary representation
- ▶ maintain the convergence rates and implementation simplicity of the FEM



ITN
INSIST



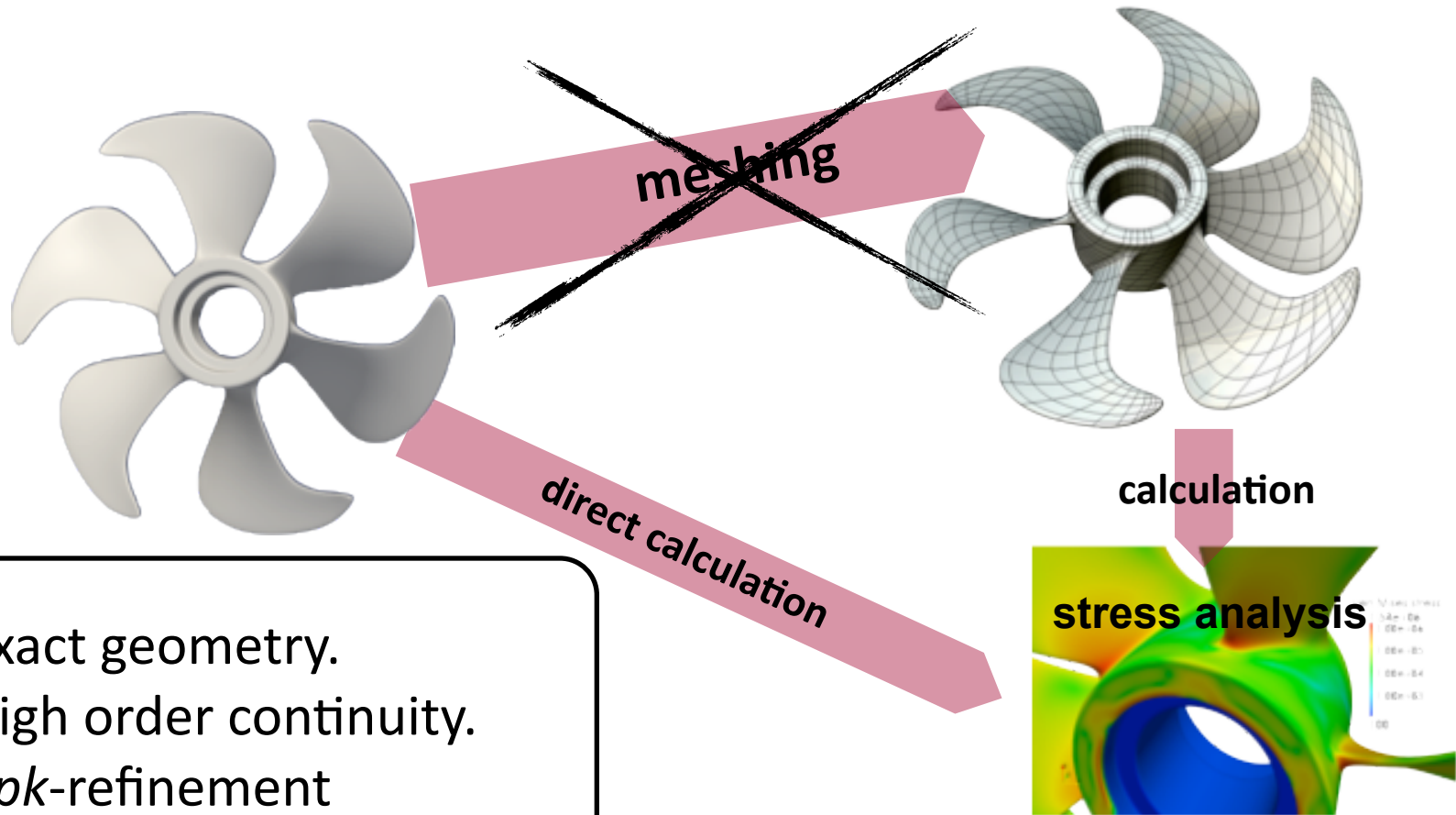
Faculty of Sciences,
Technology
and Communication

Paradigm 2 : IGA

Couple Geometry and Approximation



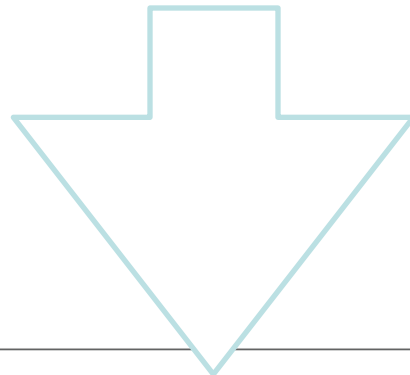
Approximate the unknown fields with the same basis functions (NURBS, T-splines ...) as that used to generate the CAD model



- Exact geometry.
- High order continuity.
- *hpk*-refinement

1. Generate a **volume** discretization using the **surface** geometry only?
2. Realistic solids can in general not be represented by only one volume (patch) and multiple **patches** must be **glued** together to avoid “leaks” (Nitsche, T-splines, PHT-splines, RL/LR-splines)
3. Refinement must be done everywhere in the domain (T, PHT... splines)

3 KEY QUESTIONS FOR IGA



Isogeometric Analysis with BEM

Boundary
representation



Domain
representation

1. IGABEM with NURBS for 2D elastic problems (Simpson, *et al.* CMAME, 2011).
2. IGABEM with T-splines for 3D elastic problems (Scott, *et al.* CMAME, 2012).
3. IGABEM with T-splines for 3D acoustic problems (Simpson, *et al.* 2013 - MAFELAP2013 TH1515).

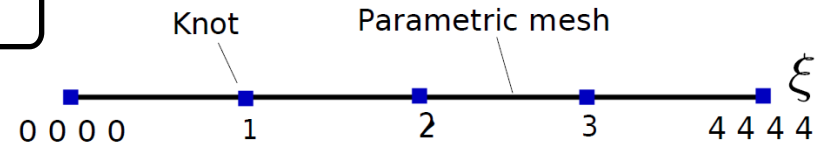
Difficulties in dealing with nonlinear problems and non-homogeneous materials.

Non-uniform rational B-splines

Knot vector

a non-decreasing set of coordinates in the parametric space.

$$\Xi = \{\xi_1, \xi_2, \dots, \xi_{n+p+1}\}$$



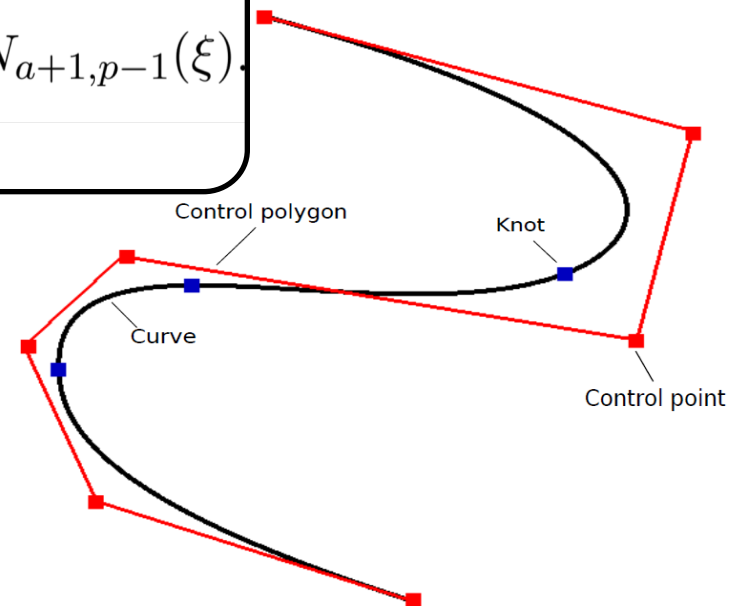
B-spline basis function

$$N_{a,0}(\xi) = \begin{cases} 1, & \text{if } \xi_a \leq \xi < \xi_{a+1} \\ 0, & \text{otherwise.} \end{cases}$$

$$N_{a,p}(\xi) = \frac{\xi - \xi_a}{\xi_{a+p} - \xi_a} N_{a,p-1}(\xi) + \frac{\xi_{a+p+1} - \xi}{\xi_{a+p+1} - \xi_{a+1}} N_{a+1,p-1}(\xi)$$

NURBS basis function

$$R_{a,p}(\xi) = \frac{N_{a,p}(\xi)w_a}{W(\xi)} = \frac{N_{a,p}(\xi)w_a}{\sum_{\hat{a}=1}^n N_{\hat{a},p}w_{\hat{a}}}$$



Properties of NURBS



- Partition of Unity

$$\sum_{i=1}^n R_{i,p}(\xi) = 1$$

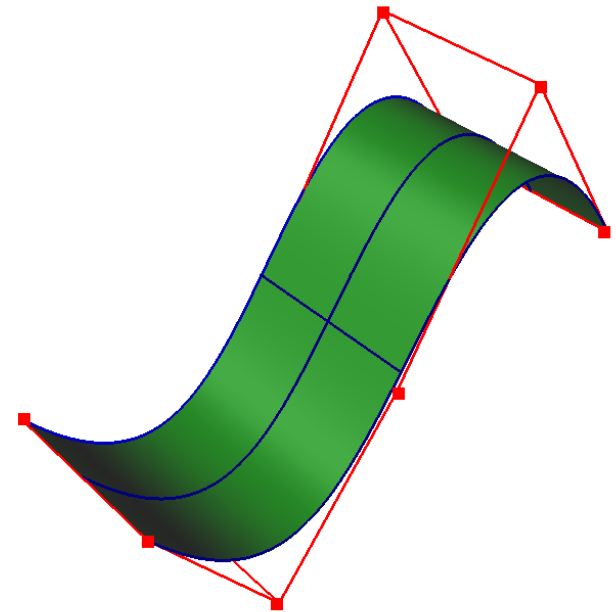
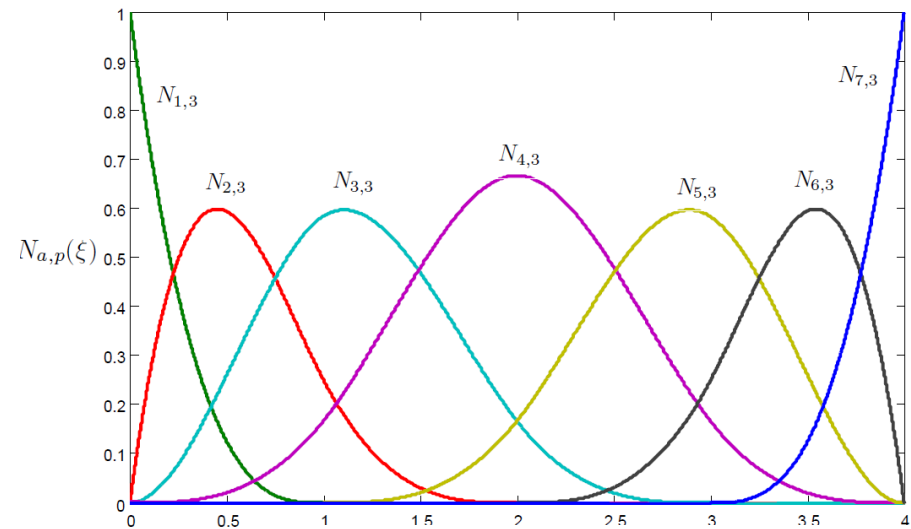
- Non-negative

- $p-1$ continuous derivatives

- Tensor product property

$$S(\xi, \eta) = \sum_{i=1}^n \sum_{j=1}^m R_{i,p}^1(\xi) R_{j,q}^2(\eta) \mathbf{B}_{i,j}$$

$$\sum_{i=1}^n \sum_{j=1}^m R_{i,p}^1(\xi) R_{j,q}^2(\eta) = \left(\sum_{i=1}^n R_{i,p}^1(\xi) \right) \left(\sum_{j=1}^m R_{j,q}^2(\eta) \right)$$



NURBS to T-splines



www.tsplines.com

(NURBS geometry)



www.tsplines.com

(T-splines geometry)

NURBS

- No watertight geometry
- No local refinement scheme

T-splines

- Local knot vector (as Point-based splines)
- Global topology

Y. Bazilevs, V.M. Calo, J.A. Cottrell, J.A. Evans, T.J.R. Hughes, S. Lipton, M.A. Scott, and T.W. Sederberg. Isogeometric analysis using T-splines. CMAME, 199(5-8):229–263, 2010.

IGABEM formulation

Regularised form of boundary integral equation for 2D linear elasticity

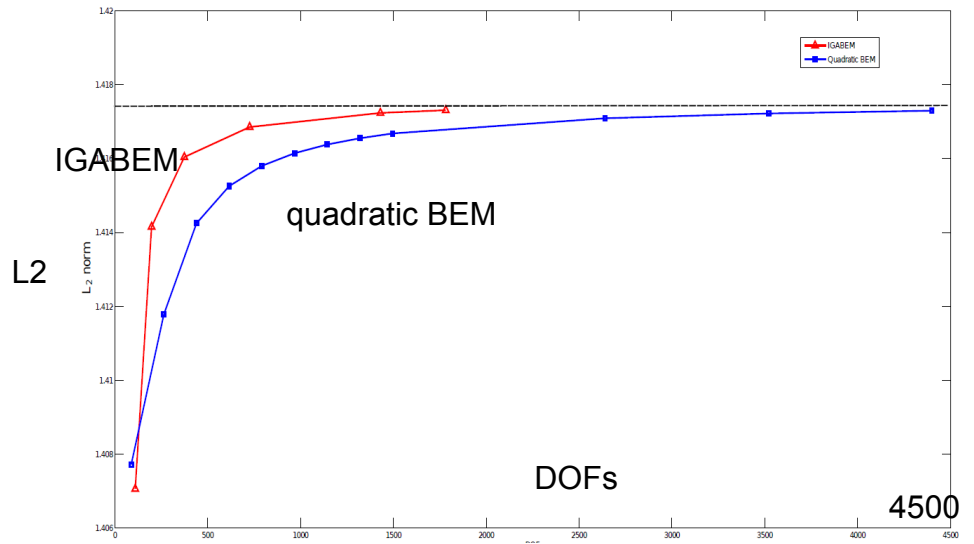
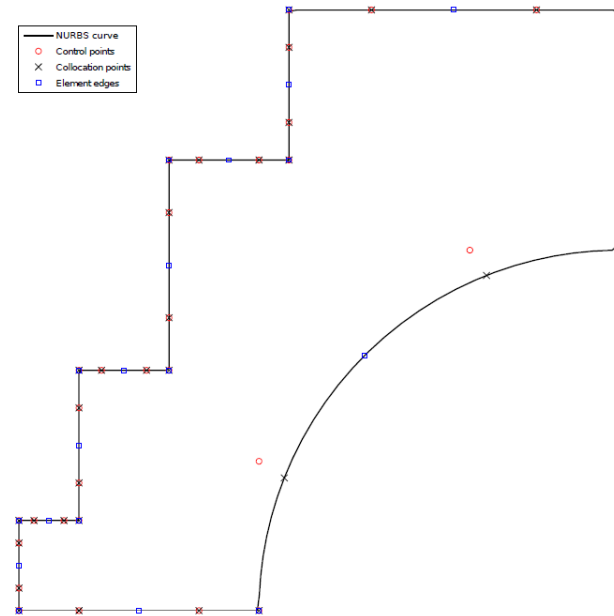
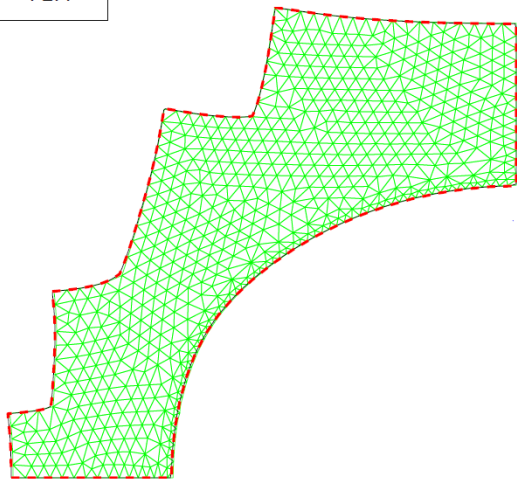
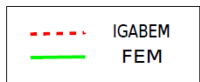
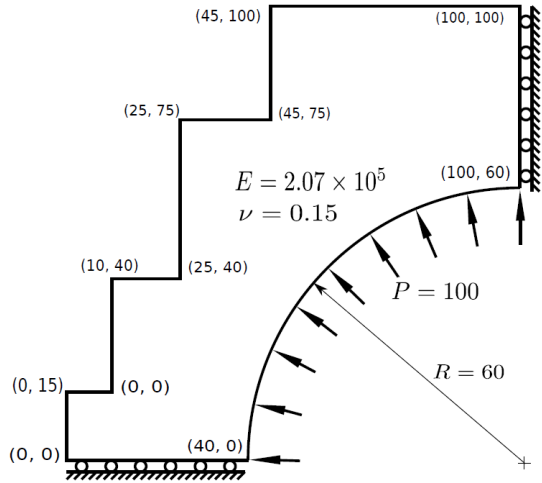
$$\int_{\Gamma} \mathbf{T}(\mathbf{s}, \mathbf{x}) [\mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{s})] d\Gamma(\mathbf{x}) = \int_{\Gamma} \mathbf{U}(\mathbf{s}, \mathbf{x}) \mathbf{t}(\mathbf{x}) d\Gamma(\mathbf{x})$$

where \mathbf{x} and \mathbf{s} are field point and source point respectively, \mathbf{u} and \mathbf{t} are displacement and traction around the boundary, \mathbf{T} and \mathbf{U} are fundamental solutions.

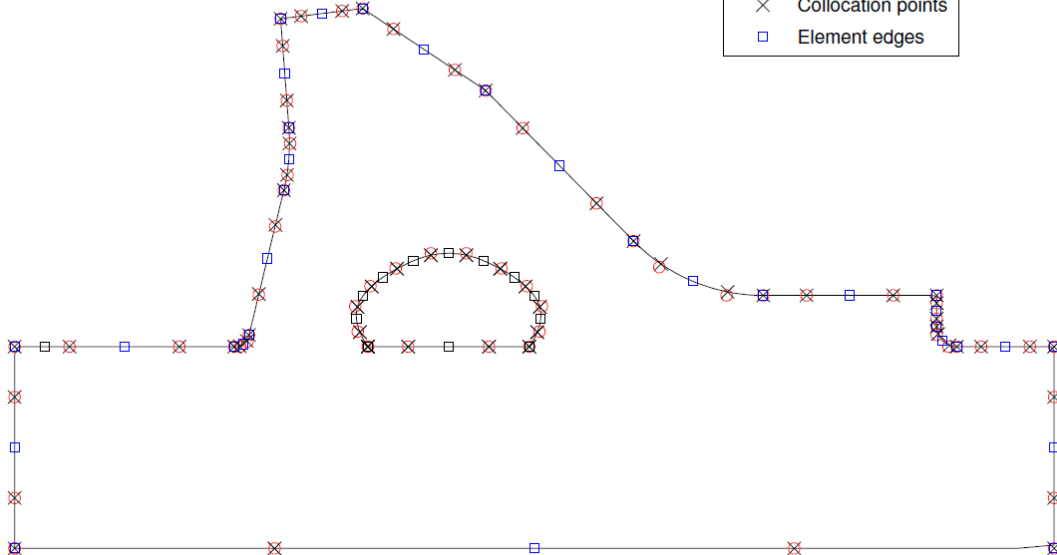
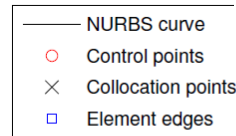
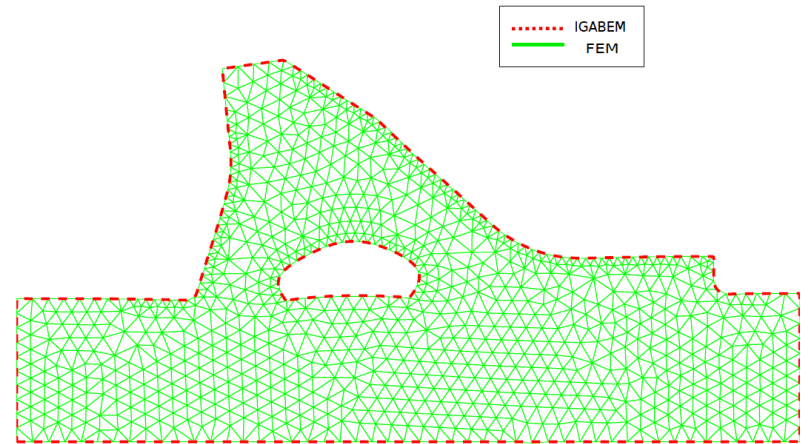
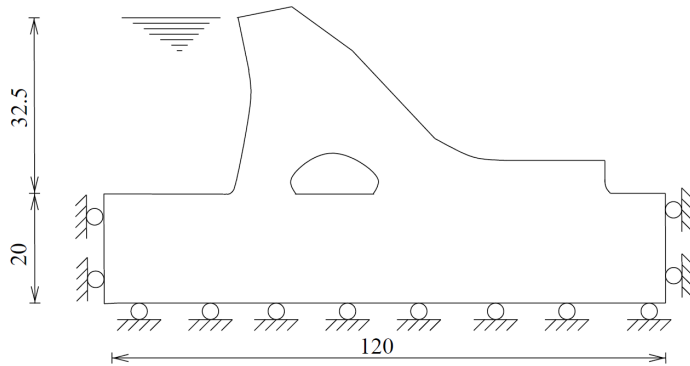
Discretise the geometry and solution field using NURBS

$$\mathbf{x} = \sum_{A=1}^{n_A} N_A(\xi) \mathbf{B}_A = N_A(\xi) \mathbf{B}_A$$
$$\mathbf{u} = \sum_{A=1}^{n_A} N_A(\xi) \mathbf{u}_A = N_A(\xi) \mathbf{u}_A$$
$$\mathbf{t} = \sum_{B=1}^{n_B} N_B(\xi) \mathbf{t}_B = N_B(\xi) \mathbf{t}_B$$

Nuclear reactor



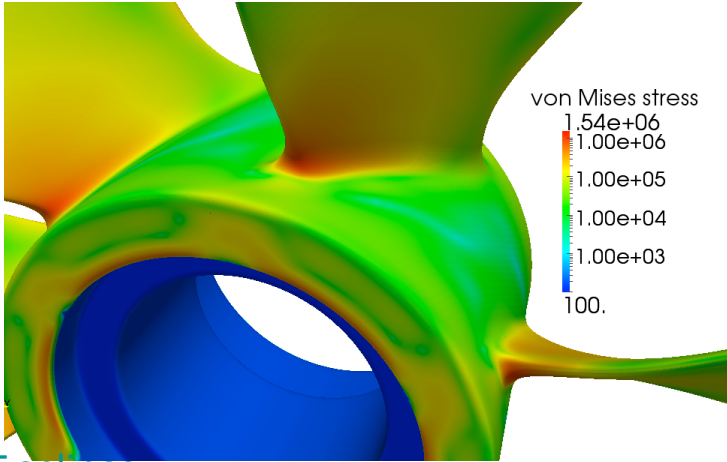
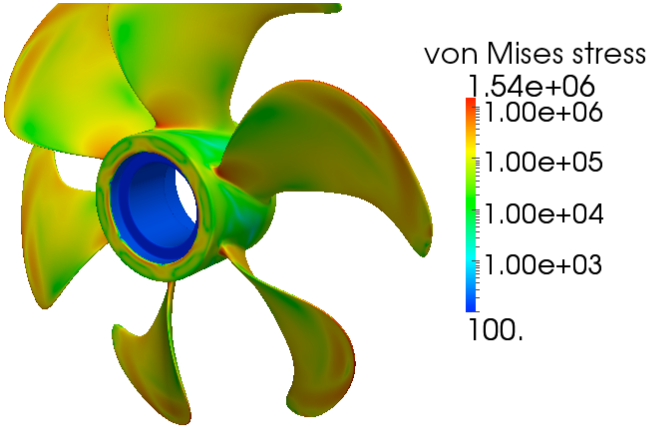
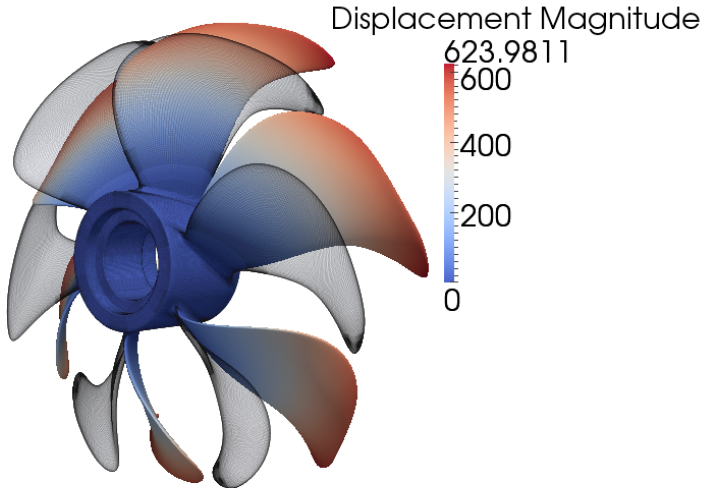
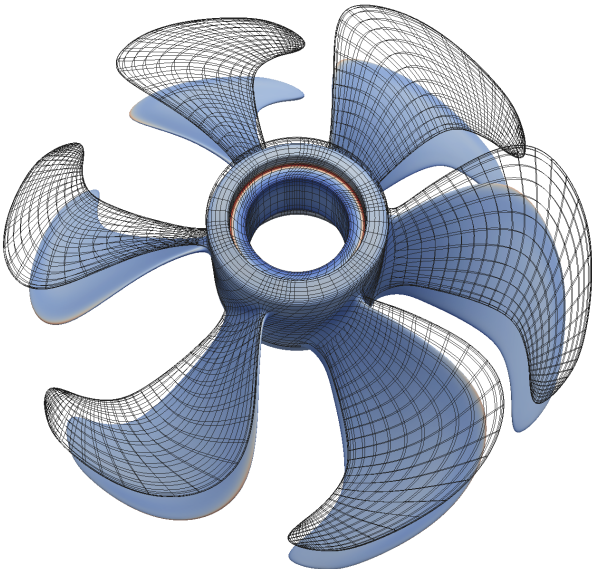
Dam



Stress analysis without meshing: isogeometric boundary-element method

ICE Proceeding, 2013, H Lian, RN Simpson, SPA Bordas

Propeller: NURBS would require several patches - single patch T-splines



Isogeometric boundary element analysis using unstructured T-splines

MA Scott, RN Simpson, JA Evans, S Lipton, SPA Bordas, TJR Hughes, TW Sederberg
CMAME, 2013.

Part II. Some recent advances in enriched FEM



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Handling discontinuities in isogeometric formulations

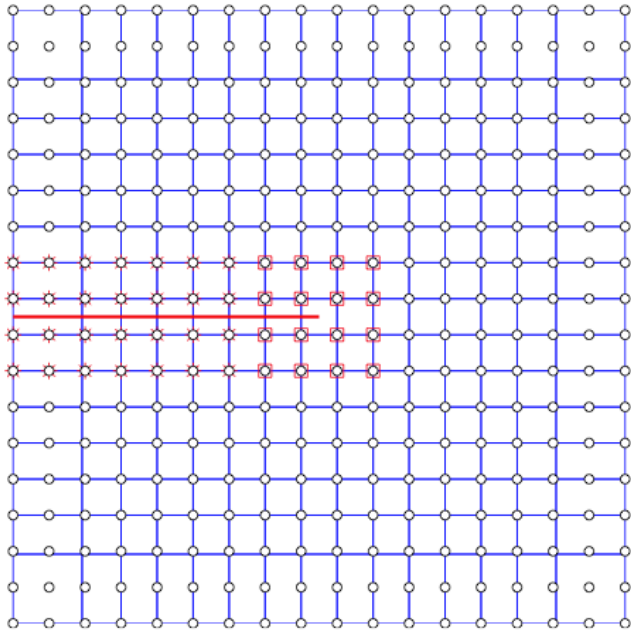
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and Communication

erc

with Nguyen Vinh Phu, Marie Curie Fellow

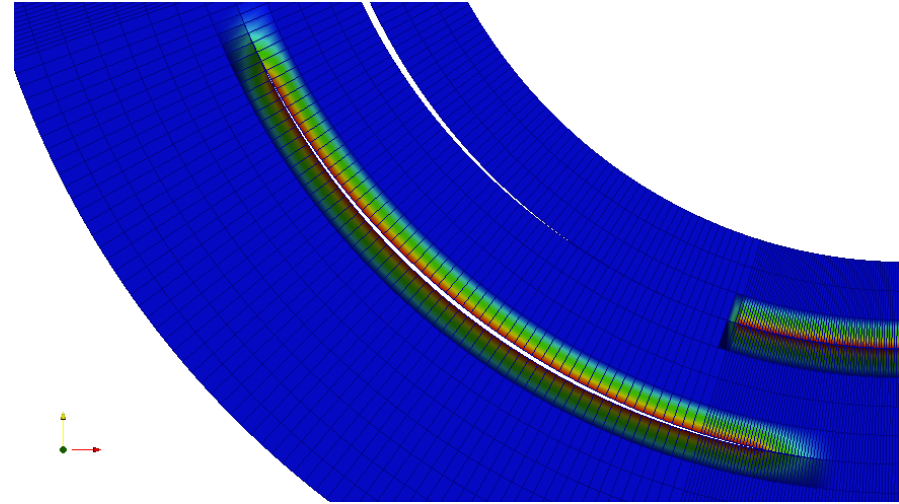


PUM enriched methods



- IGA: link to CAD and accurate stress fields
- XFEM: no remeshing

Mesh conforming methods



- IGA: link to CAD and accurate stress fields
- Apps: delamination



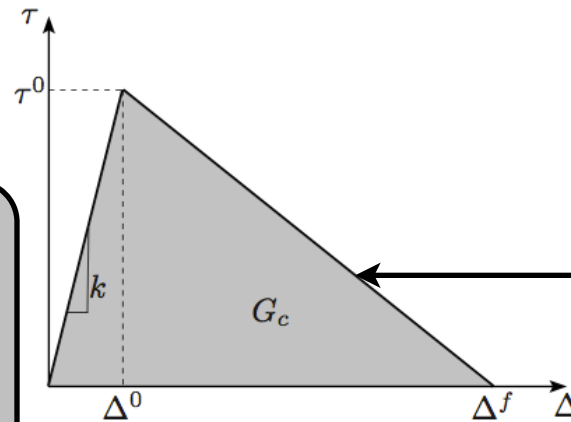
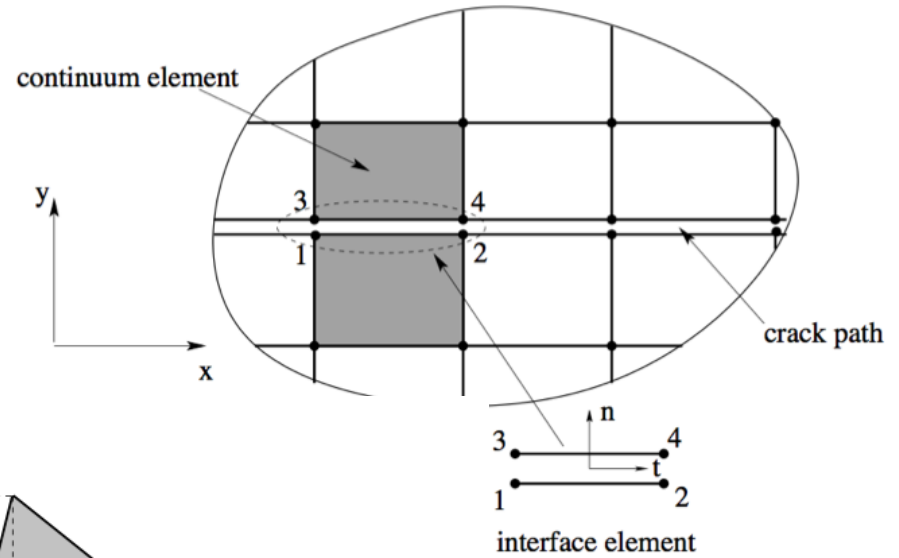
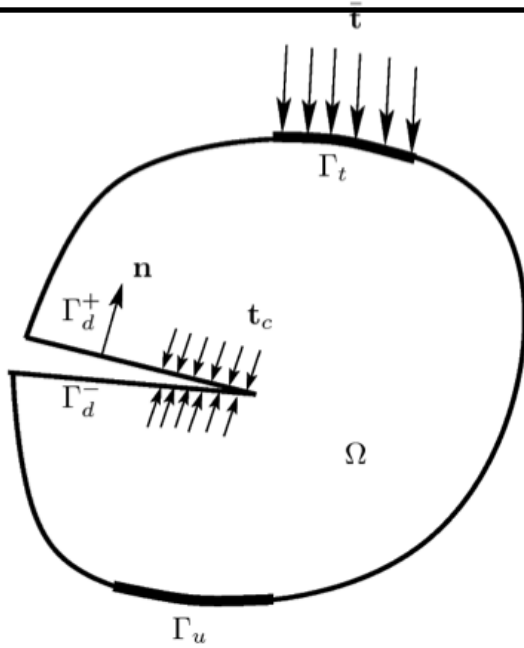
$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} R_I(\mathbf{x}) \mathbf{u}_I + \sum_{J \in \mathcal{S}^c} R_J(\mathbf{x}) \Phi(\mathbf{x}) \mathbf{a}_J$$

NURBS basis functions

enrichment functions

1. E. De Luycker, D. J. Benson, T. Belytschko, Y. Bazilevs, and M. C. Hsu. X-FEM in isogeometric analysis for linear fracture mechanics. *IJNME*, 87(6):541–565, 2011.
2. S. S. Ghorashi, N. Valizadeh, and S. Mohammadi. Extended isogeometric analysis for simulation of stationary and propagating cracks. *IJNME*, 89(9): 1069–1101, 2012.
3. D. J. Benson, Y. Bazilevs, E. De Luycker, M.-C. Hsu, M. Scott, T. J. R. Hughes, and T. Belytschko. A generalized finite element formulation for arbitrary basis functions: From isogeometric analysis to XFEM. *IJNME*, 83(6):765–785, 2010.
4. A. Tambat and G. Subbarayan. Isogeometric enriched field approximations. *CMAME*, 245–246:1 – 21, 2012.

Delamination analysis with cohesive elements (standard approach)

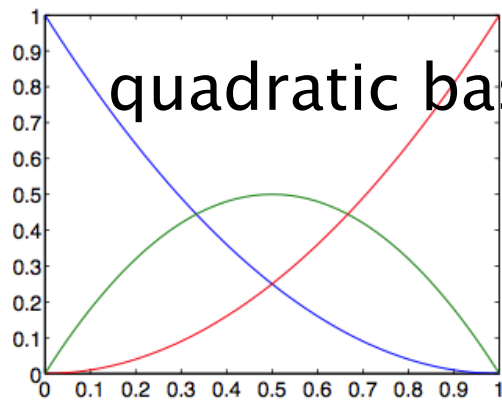


- No link to CAD
- Long preprocessing
- Refined meshes

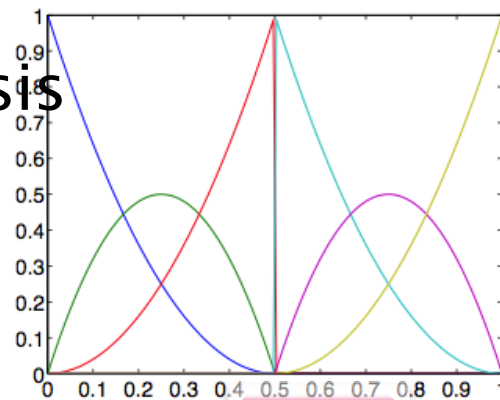
$$\int_{\Omega} \delta \mathbf{u} \cdot \mathbf{b} d\Omega + \int_{\Gamma_t} \delta \mathbf{u} \cdot \bar{\mathbf{t}} d\Gamma_t = \int_{\Omega} \delta \boldsymbol{\epsilon} : \boldsymbol{\sigma}(\mathbf{u}) d\Omega + \int_{\Gamma_d} \delta [[\mathbf{u}]] \cdot \mathbf{t}^c([[\mathbf{u}]]) d\Gamma_d$$

Isogeometric cohesive elements

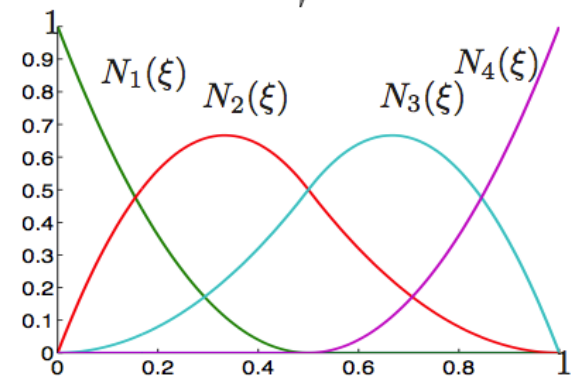
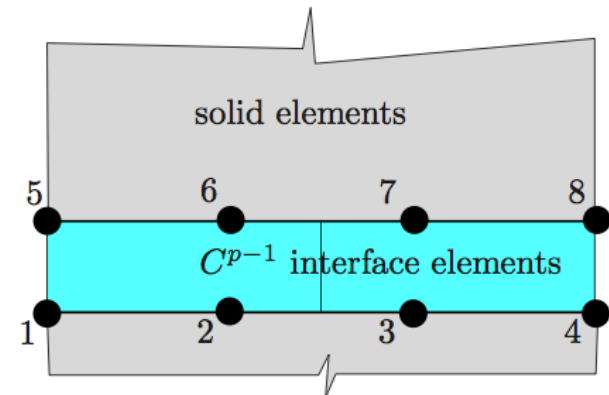
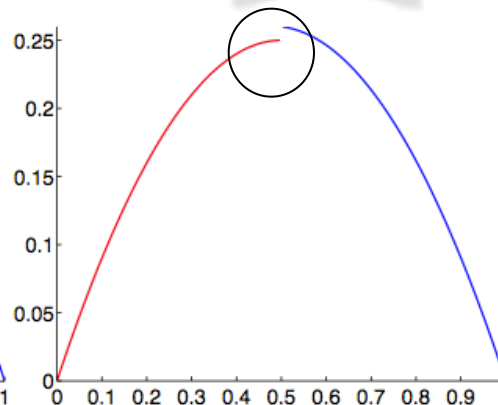
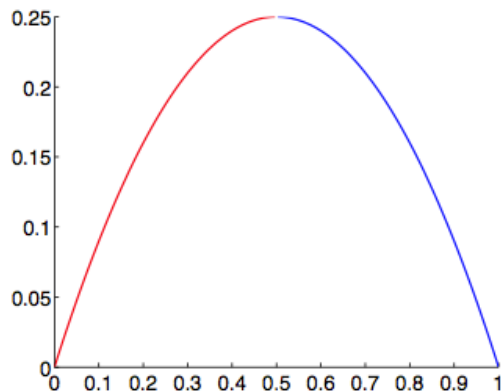
quadratic basis



(a) $\Xi = \{0, 0, 0, 1, 1, 1\}$



(b) $\Xi' = \{0, 0, 0, 0.5, 0.5, 0.5, 1, 1, 1\}$



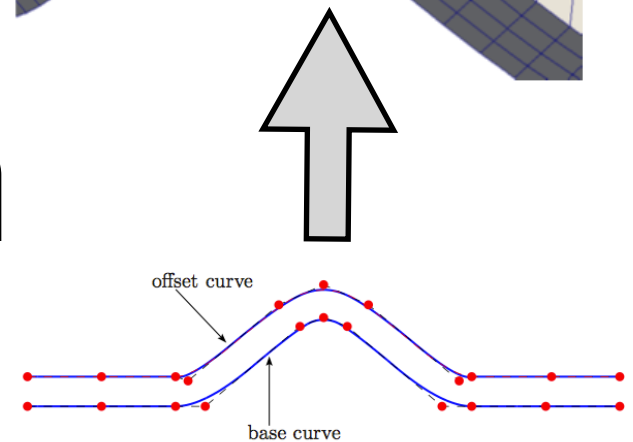
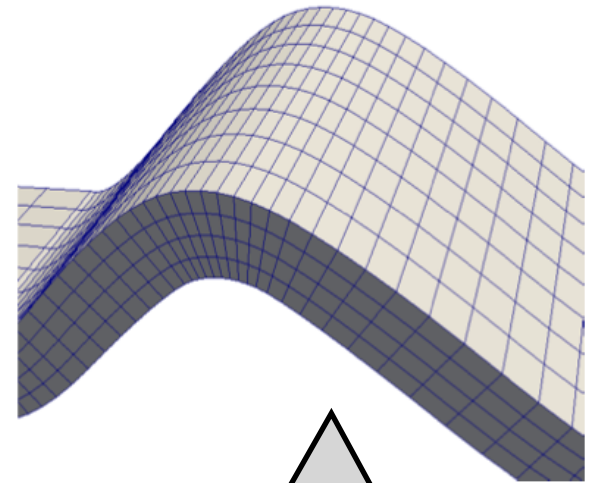
Knot insertion

1. C. V. Verhoosel, M. A. Scott, R. de Borst, and T. J. R. Hughes. An isogeometric approach to cohesive zone modeling. *IJNME*, 87(15):336–360, 2011.
2. V.P. Nguyen, P. Kerfriden, S. Bordas. Isogeometric cohesive elements for two and three dimensional composite delamination analysis, 2013, Arxiv.

Isogeometric cohesive elements: advantages

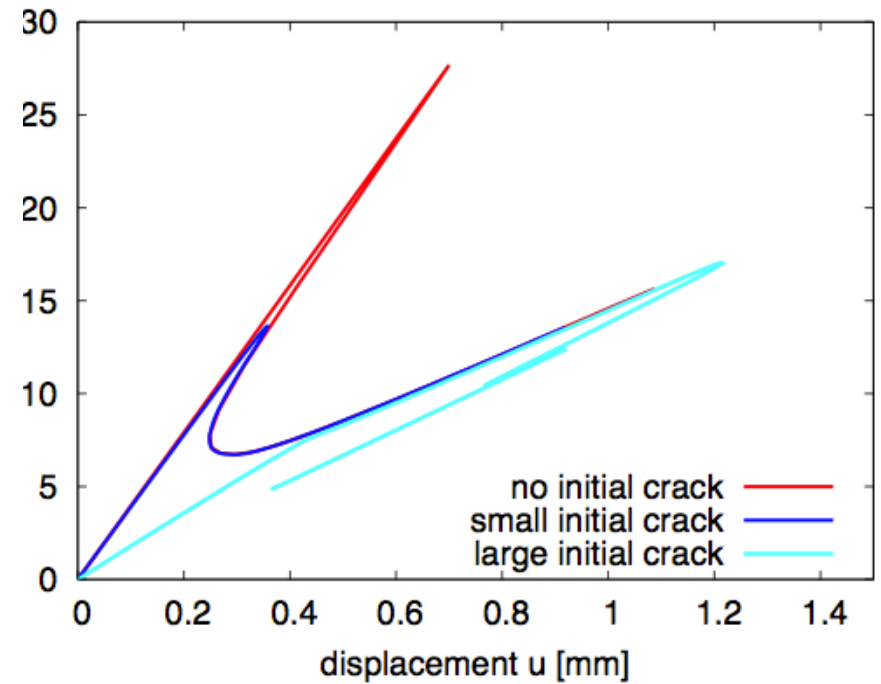
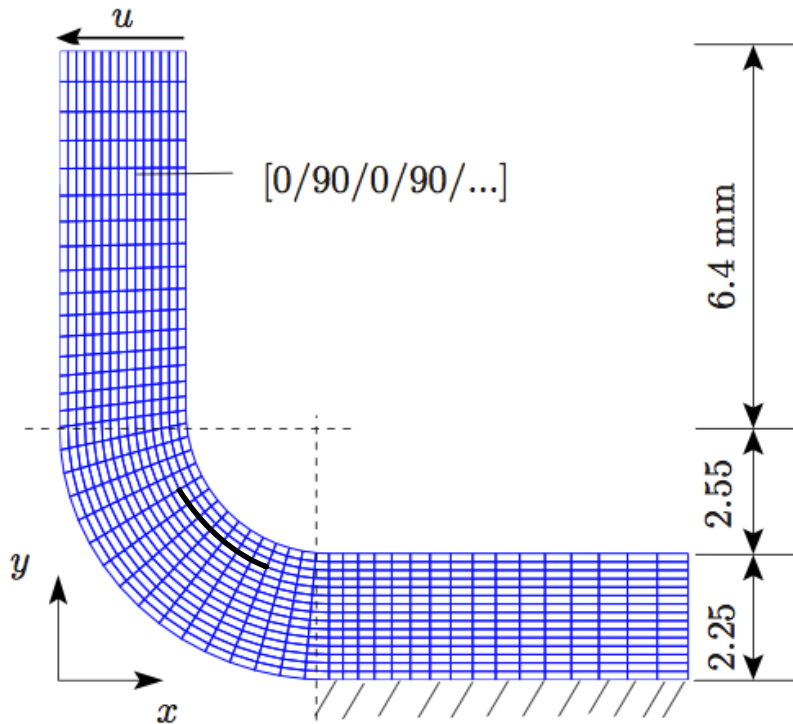
- Direct link to CAD
- Exact geometry
- Fast/straightforward generation of interface elements
- Accurate stress field
- Computationally cheaper

- 2D Mixed mode bending test (MMB)
- 2 x 70 quartic-linear B-spline elements
- Run time on a laptop 4GBi7: 6 s
- Energy arc-length control

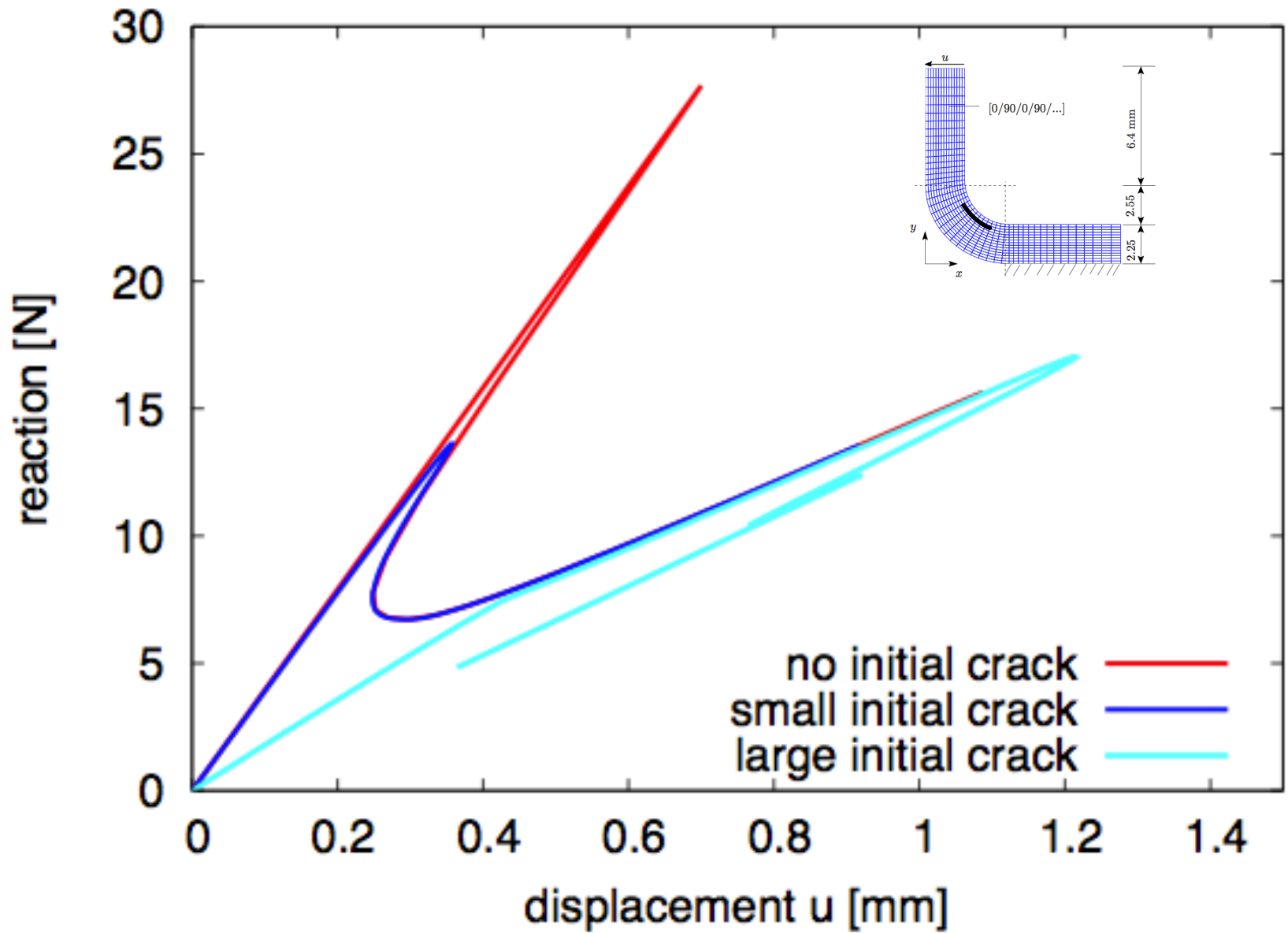


V. P. Nguyen and H. Nguyen-Xuan. High-order B-splines based finite elements for delamination analysis of laminated composites. *Composite Structures*, 102:261–275, 2013.

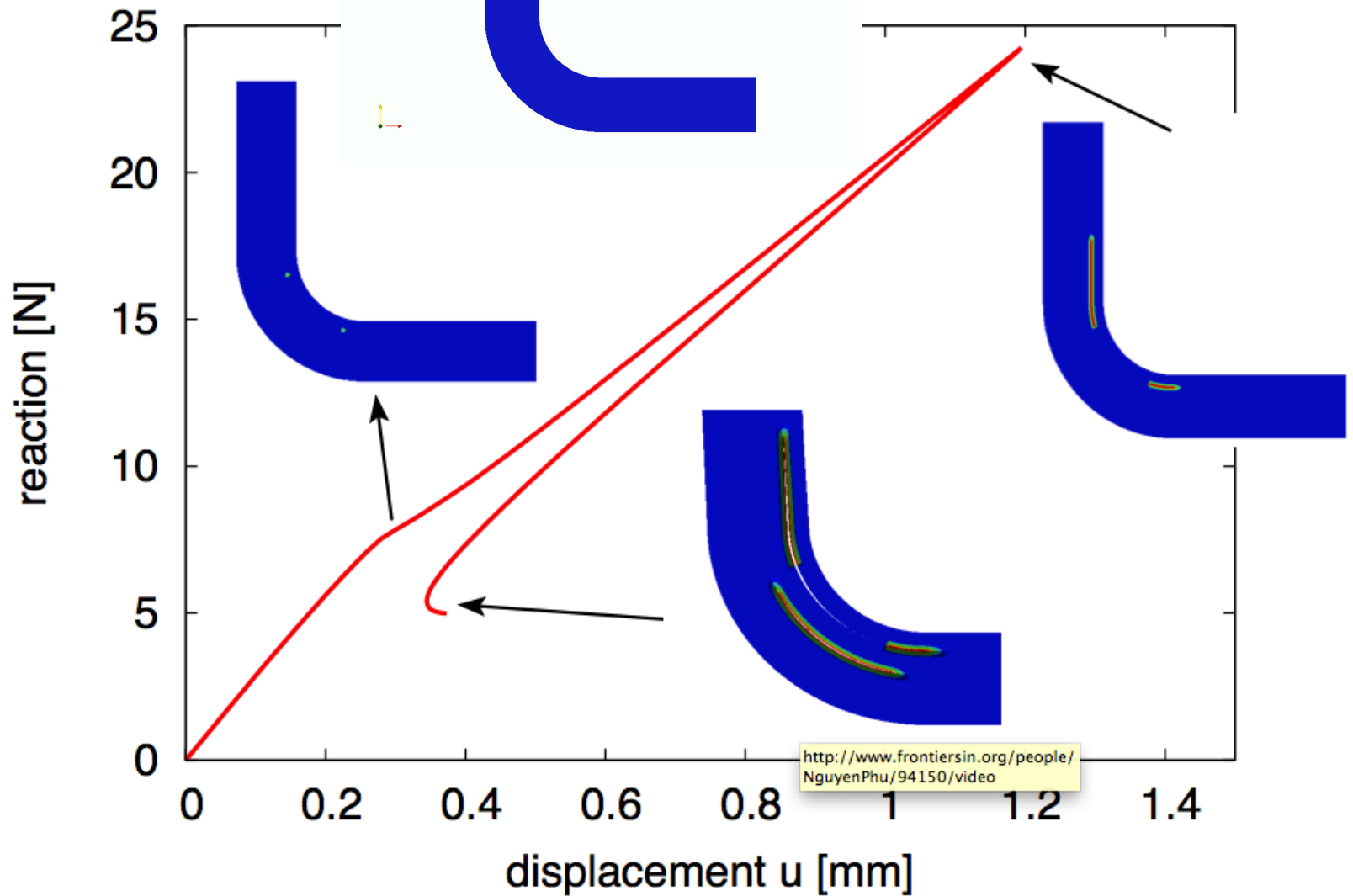
Isogeometric cohesive elements: 2D example



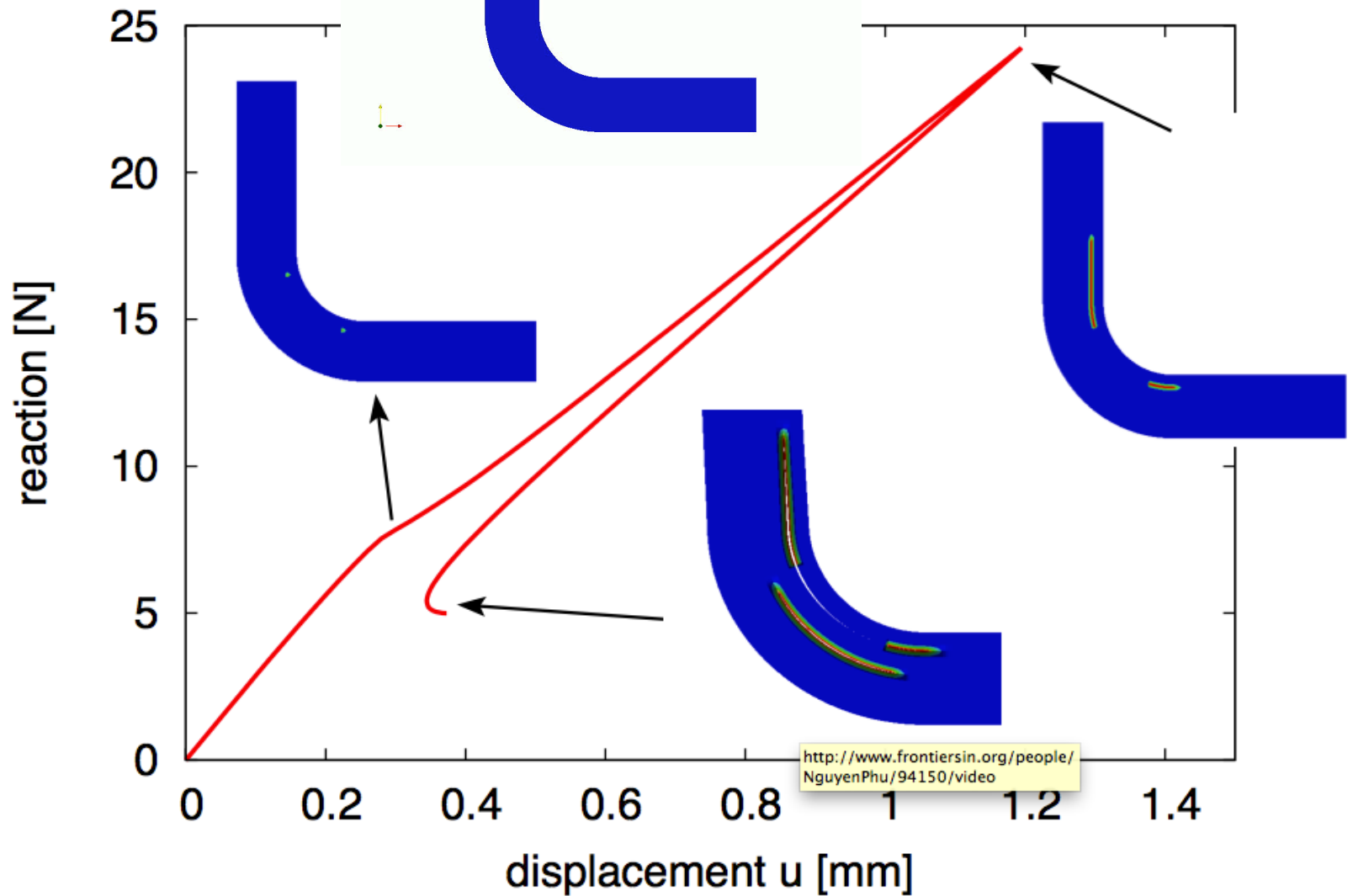
- Exact geometry by NURBS + direct link to CAD
- It is straightforward to vary
 - (1) the number of plies and
 - (2) # of interface elements:
- Suitable for parameter studies/design
- Solver: energy-based arc-length method (Gutierrez, 2007)



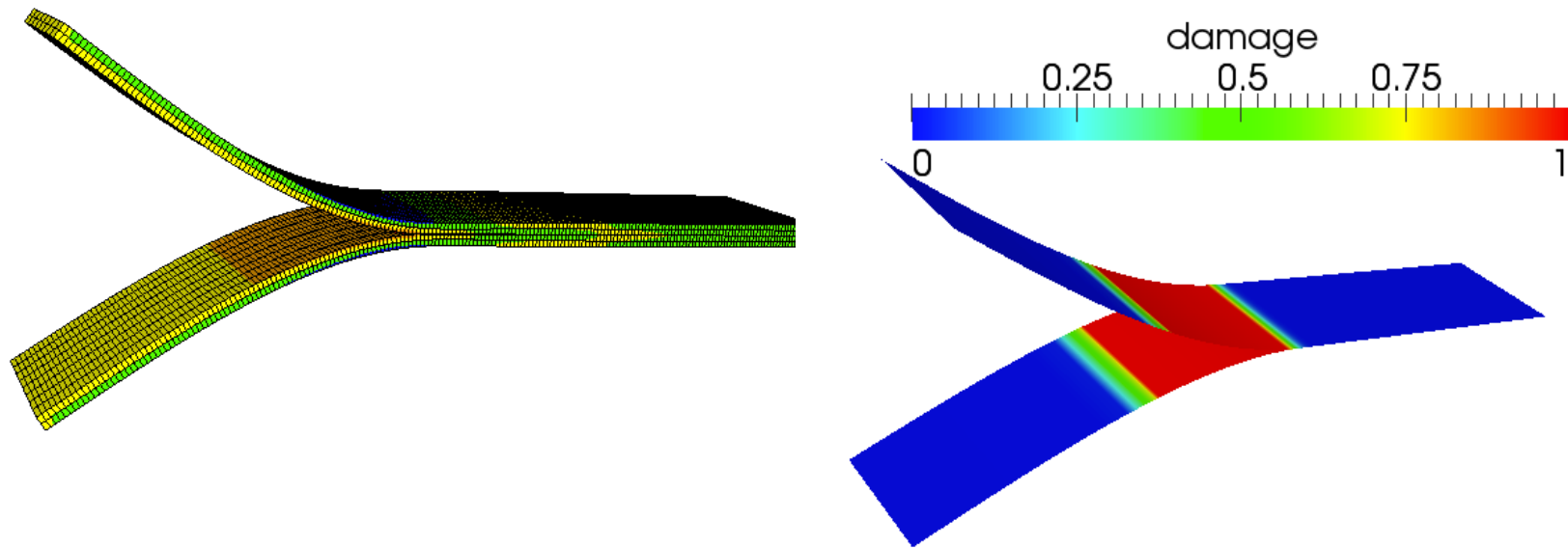
Isogeometric cohesive elements: 2D example



Isogeometric cohesive elements: 2D example

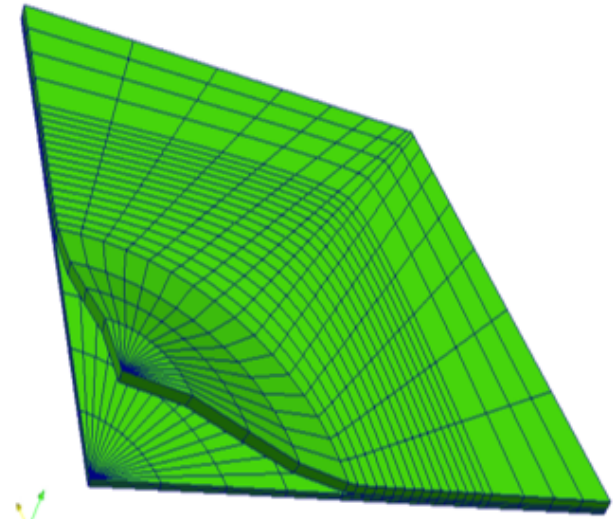
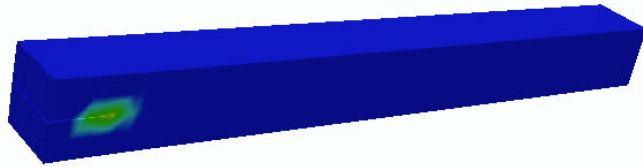


Isogeometric cohesive elements: 3D example with shells

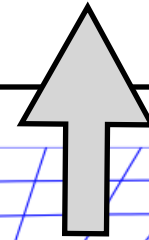
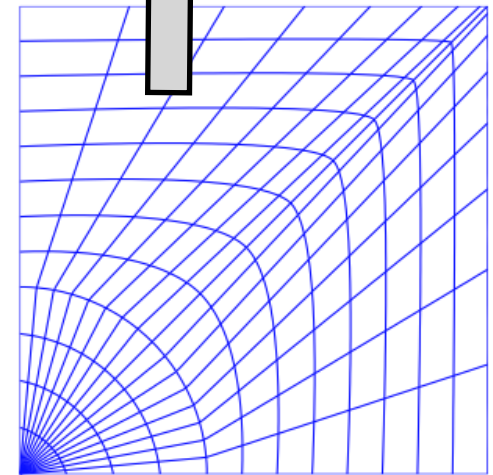
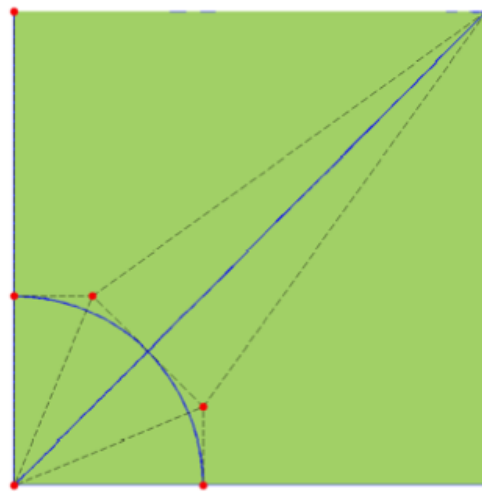


- Rotation free B-splines shell elements (Kiendl et al. CMAME)
- Two shells, one for each lamina
- Bivariate B-splines cohesive interface elements in between

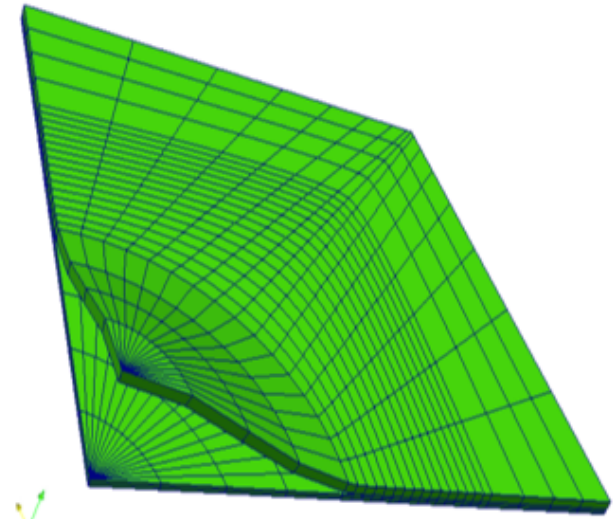
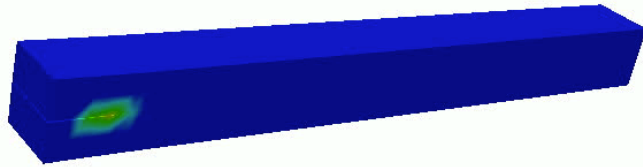
Isogeometric cohesive elements: 3D examples



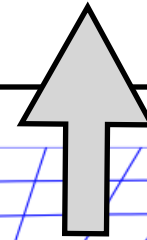
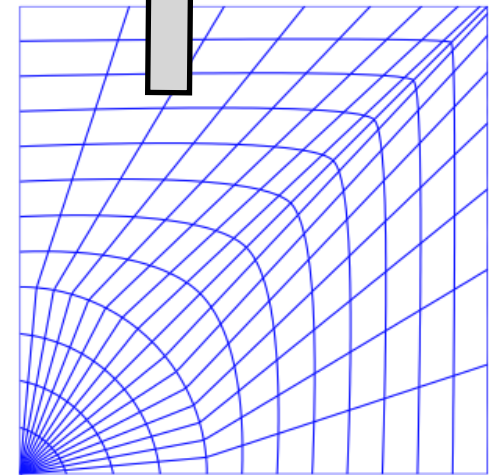
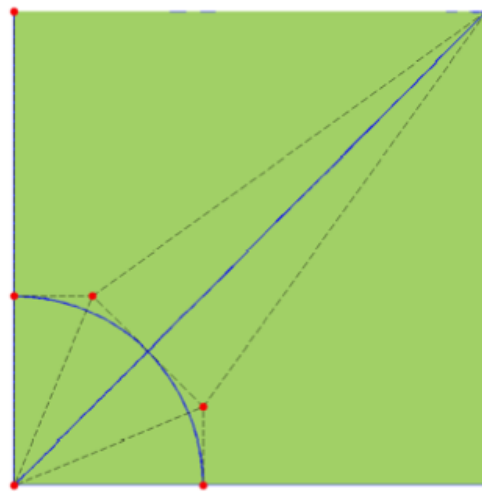
- cohesive elements for 3D meshes the same as 2D
- large deformations



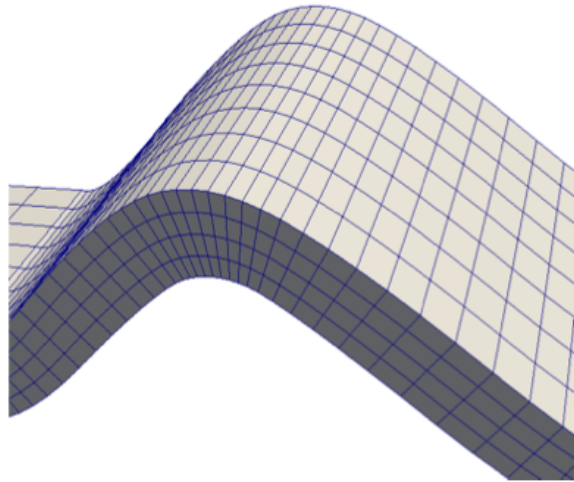
Isogeometric cohesive elements: 3D examples



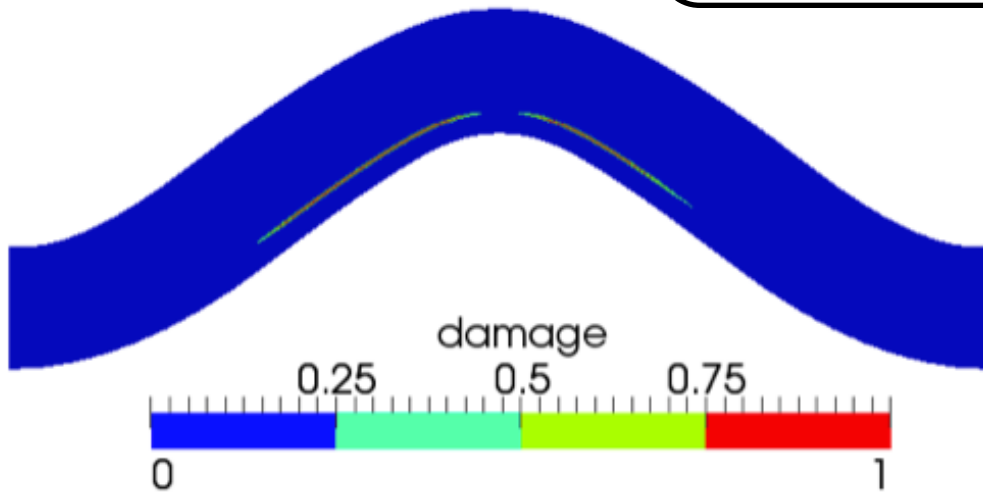
- cohesive elements for 3D meshes the same as 2D
- large deformations



Isogeometric cohesive elements



- singly curved thick-wall laminates
- geometry/displacements: NURBS
- trivariate NURBS from NURBS surface(*)
- cohesive surface interface elements



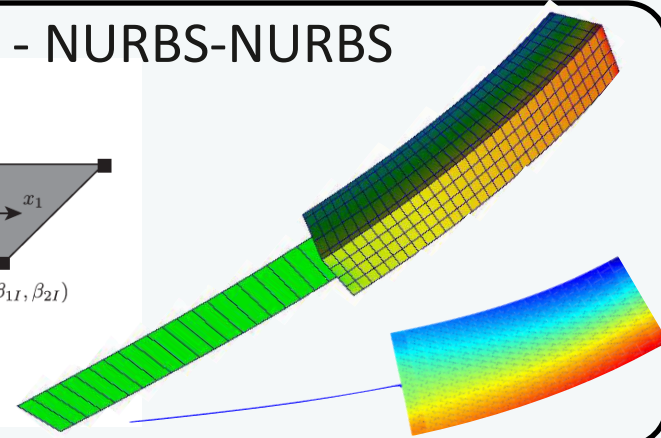
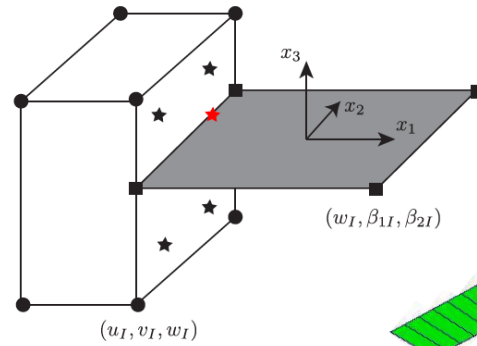
(*)V. P. Nguyen, P. Kerfriden, S.P.A. Bordas, and T. Rabczuk. An integrated design-analysis framework for three dimensional composite panels. Computer Aided Design, 2013. submitted.

Future work: model selection (continuum, plate, beam, shell?)

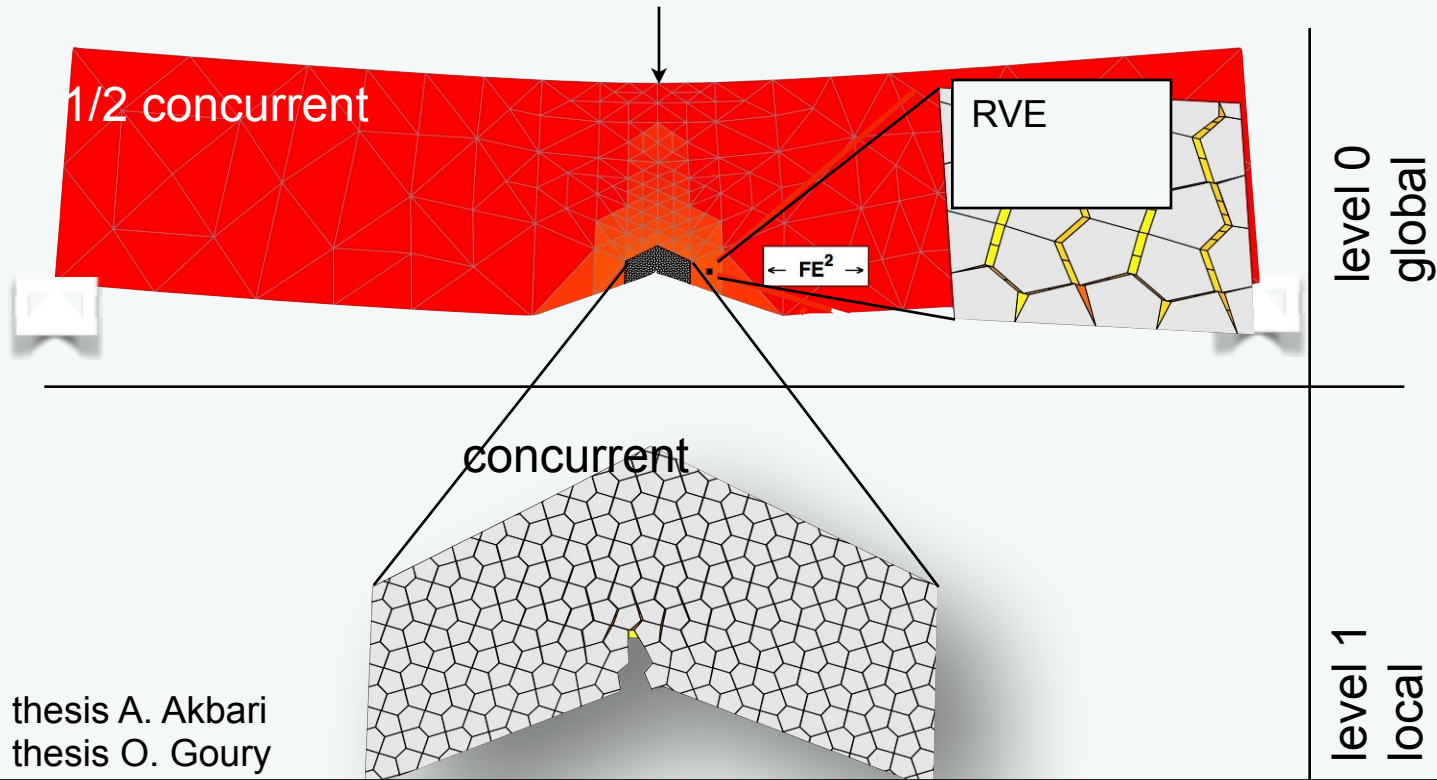
Model selection

- Model with shells
- Identify “hot spots” - dual
- Couple with continuum
- Coarse-grain

• Nitsche coupling - NURBS-NURBS



load



thesis A. Akbari
thesis O. Goury

Part III. Application to multi-crack propagation

with Danas Sutula, President Scholar



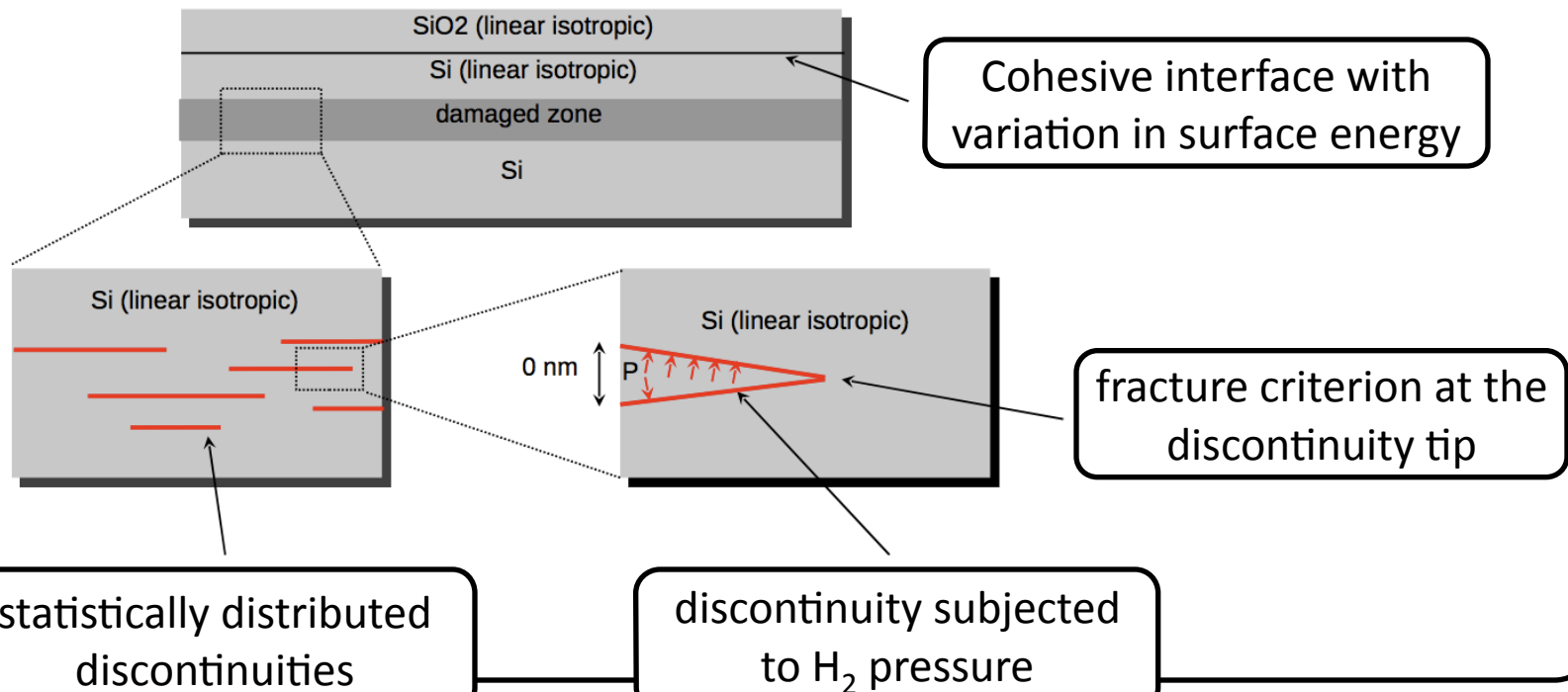
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Modeling cavities by zero thickness surfaces

- discontinuities in the displacement field

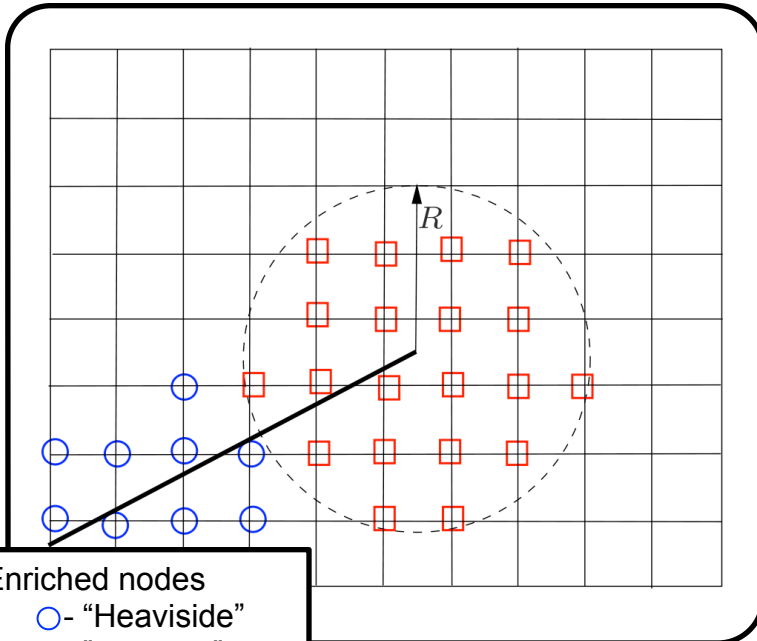
Linear elastic fracture mechanics (LEFM)

- infinite stress at crack tip, i.e. *singularity*



Approximation function:

$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) \mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K \in \mathcal{N}_K} N_K(\mathbf{x}) \sum_{\alpha=1}^4 f_\alpha(\mathbf{x}) \mathbf{b}^{K\alpha}}_{\text{singular tip enrichment}}$$

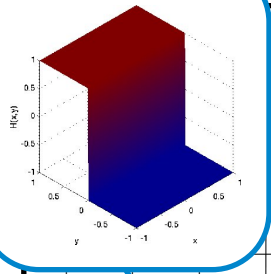


$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above crack} \\ -1 & \text{if } \mathbf{x} \text{ below crack} \end{cases}$$

$$\{f_\alpha(r, \theta), \alpha = 1, 4\} = \left\{ \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2} \sin \theta, \sqrt{r} \cos \frac{\theta}{2} \sin \theta \right\}$$

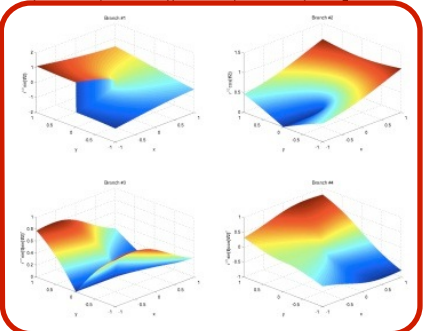
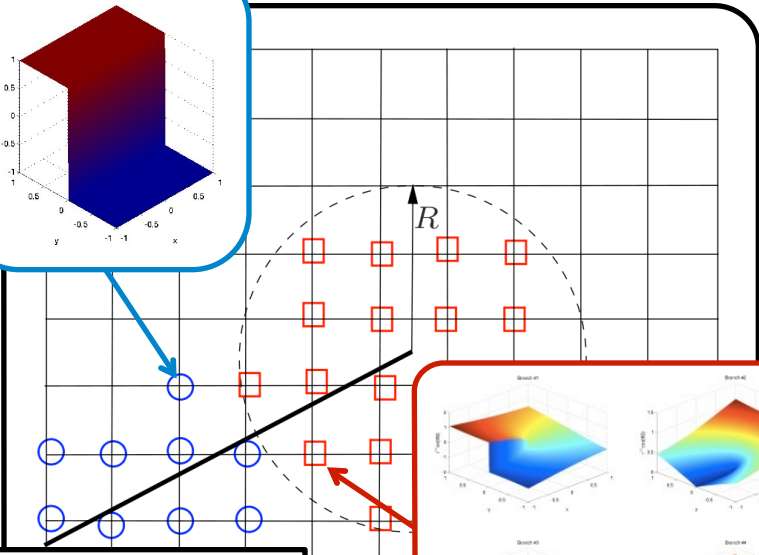
Approximation function:

$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) \mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K \in \mathcal{N}_K} N_K(\mathbf{x}) \sum_{\alpha=1}^4 f_\alpha(\mathbf{x}) \mathbf{b}^{K\alpha}}_{\text{singular tip enrichment}}$$



$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above crack} \\ -1 & \text{if } \mathbf{x} \text{ below crack} \end{cases}$$

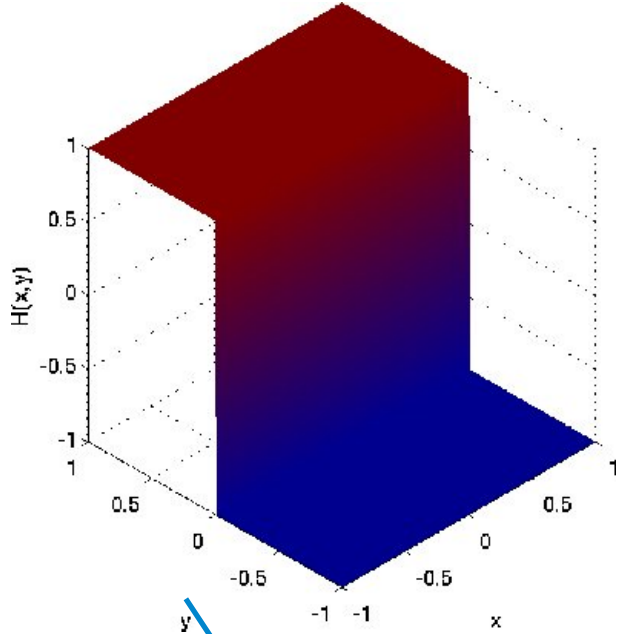
$$\{f_\alpha(r, \theta), \alpha = 1, 4\} = \left\{ \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2} \sin \theta, \sqrt{r} \cos \frac{\theta}{2} \sin \theta \right\}$$



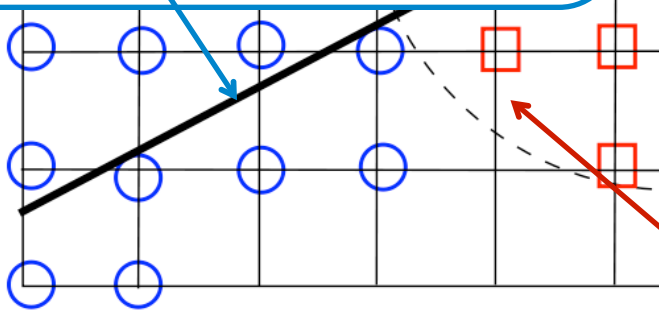
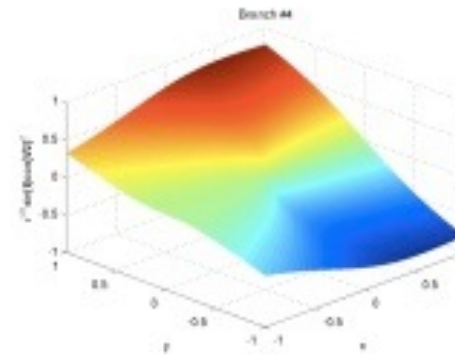
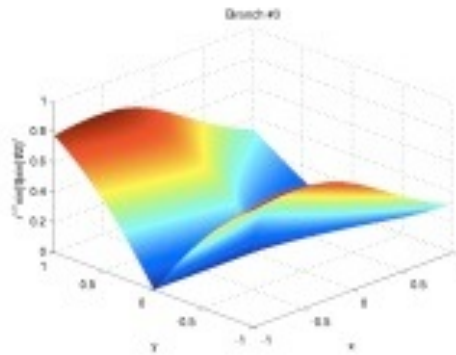
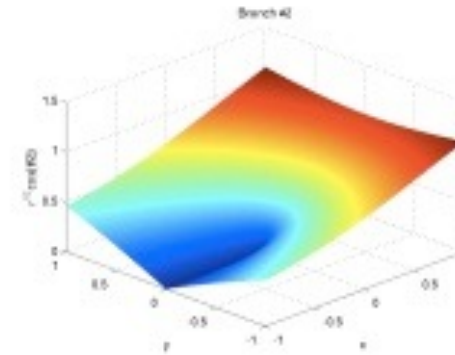
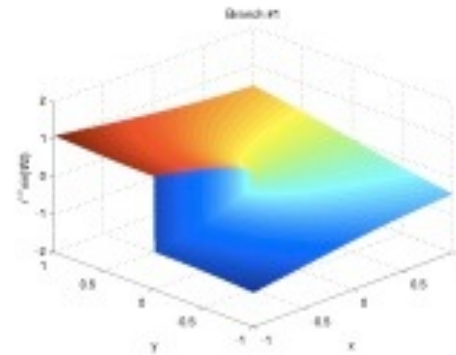
Enriched nodes
 ○ - "Heaviside"
 □ - "crack tip"

XFEM formulation

$$H(x) = \begin{cases} +1 & \text{if } x \text{ above crack} \\ -1 & \text{if } x \text{ below crack} \end{cases}$$



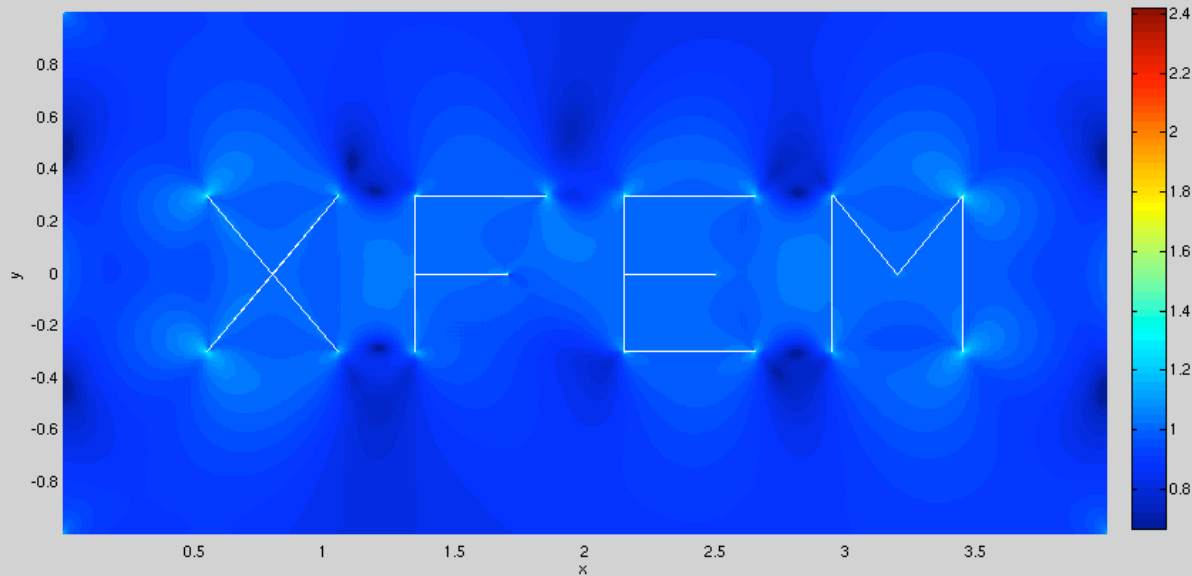
$$B(r,\theta) = \left\{ \sqrt{r} \cos \frac{\theta}{2} \quad \sqrt{r} \sin \frac{\theta}{2} \quad \sqrt{r} \sin \theta \sin \frac{\theta}{2} \quad \sqrt{r} \sin \theta \cos \frac{\theta}{2} \right\}$$



Extended Finite Element Method (XFEM)

- Introduced by Ted Belytschko (1999) for elastic problems

Fracture of “XFEM” using XFEM



Extended Finite Element Method (XFEM)

- Introduced by Ted Belytschko (1999) for elastic problems

Fracture of “XFEM” using XFEM

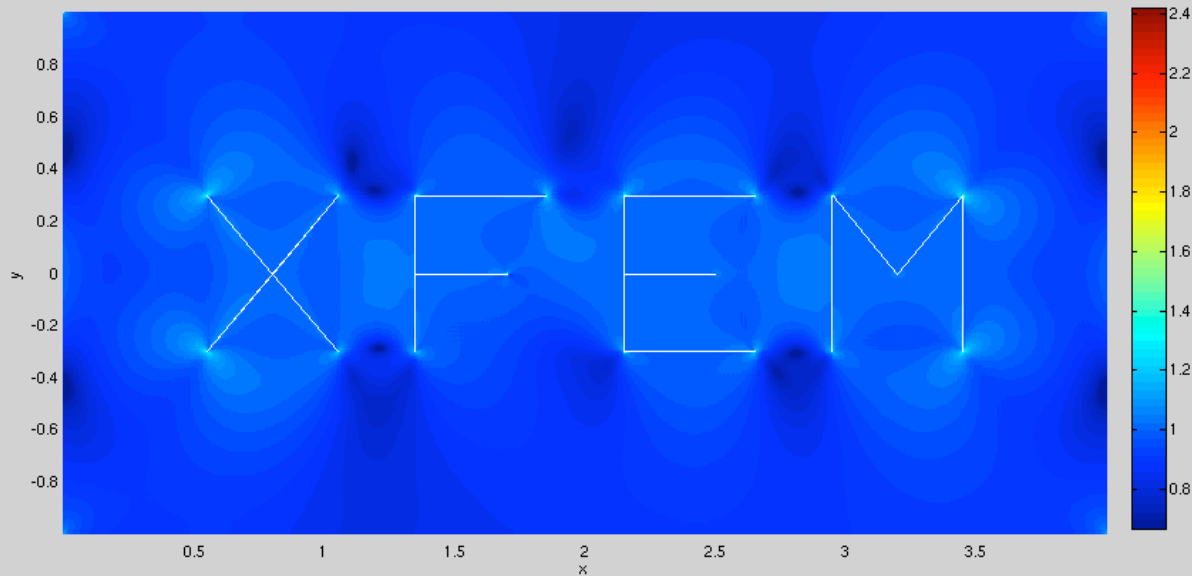


Plate with 300 cracks - vertical extension BCs

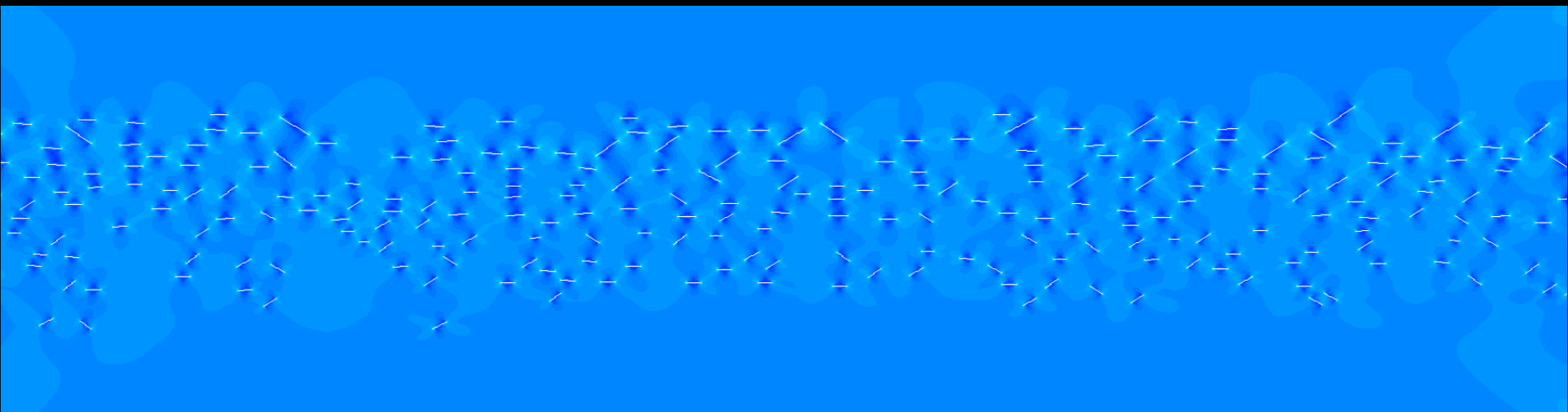
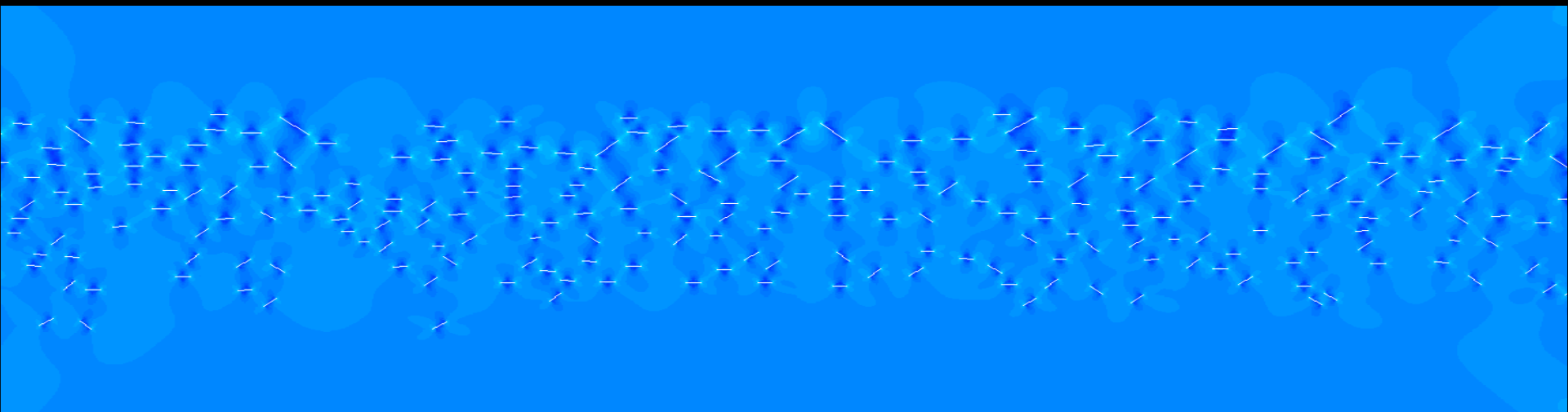
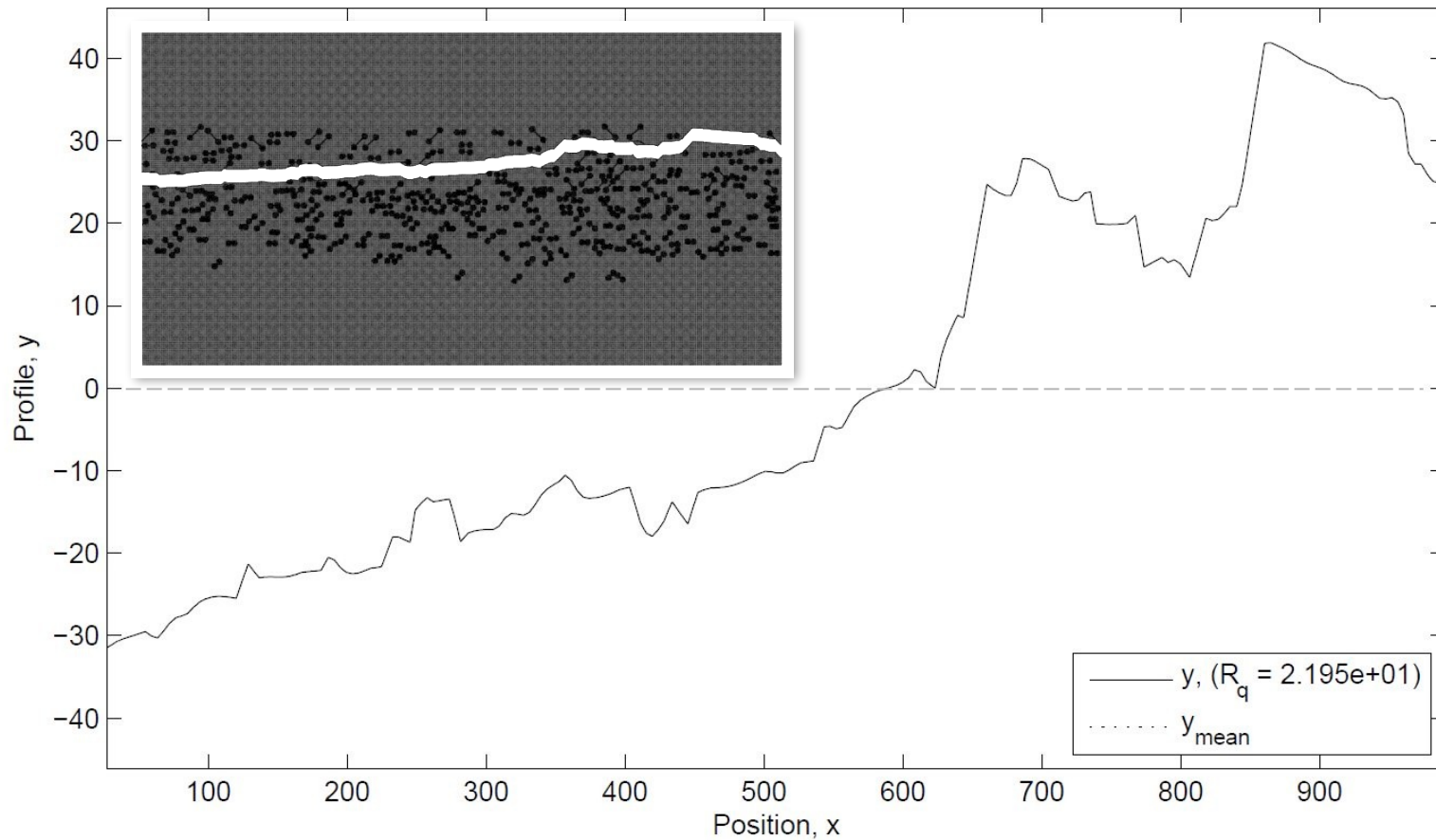


Plate with 300 cracks - vertical extension BCs



Vertical extension of a plate with 300 cracks

Post-split roughness



Crack growth: classical approach (LEFM)

Evaluation of stress intensity factors (SIF)

- The interaction integral (Yau 1980)

(1) – from current solution
(2) – known auxiliary solution

$$I^{(1+2)} = \int_{\Omega} \left(\sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} + \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} - W^{(1+2)} \delta_{1j} \right) \frac{\partial q}{\partial x_j} d\Omega = \frac{2}{E'} (K_I^{(1)} K_I^{(2)} + K_{II}^{(1)} K_{II}^{(2)})$$

Crack growth criterion for mixed mode fracture

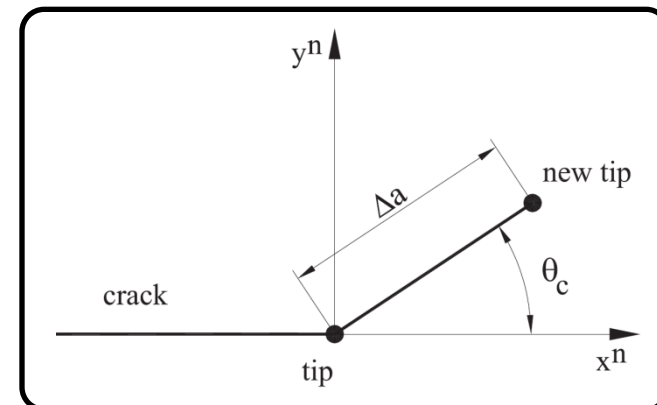
- Direction that maximises the energy release (Nuismer 1975)

$$\frac{k_I^2(K_I, K_{II}, \theta_{inc}) + k_{II}^2(K_I, K_{II}, \theta_{inc})}{E'} = G_c$$

Crack growth direction

- orthogonal to maximum hoop stress

$$\theta_c(K_I, K_{II}) = 2 \tan^{-1} \left[\frac{1}{4} \left(\frac{K_I}{K_{II}} - \text{sign}(K_{II}) \sqrt{\left(\frac{K_I}{K_{II}} \right)^2 + 8} \right) \right]$$



Crack growth: classical approach (LEFM)

- **Energy release rate w.r.t crack increment direction:**

$$G_{s_i} = -\frac{\partial \Pi}{\partial \theta_i}$$

- **The rates of the energy release rate are given by:**

$$H_{s_i,j} = \frac{\partial G_{s_i}}{\partial \theta_j} = -\frac{\partial^2 \Pi}{\partial \theta_i \partial \theta_j}$$

- **where, in a discrete setting, the potential energy is:**

$$\Pi = \frac{1}{2} u' K u - u' f$$

Crack growth: optimization of direction

- **The discrete potential energy:**

$$\Pi = \frac{1}{2}u'Ku - u'f$$

- **The discrete energy release rate:**

$$Gs_i = -\frac{1}{2}u'\delta_iKu + u'\delta_if - \delta_iu'(Ku - f)$$

$$Gs_i = -\frac{1}{2}u'\delta_iKu + u'\delta_if \quad , \text{ where } \delta_i = \frac{\partial}{\partial\theta_i}$$

- **The rates of the energy release rate**

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ij}^2Ku - u'\delta_{ij}^2f\right) - \delta_ju'(\delta_iKu - \delta_if) \quad , \text{ where } \delta_{ij} = \frac{\partial^2}{\partial\theta_i\theta_j}$$

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ii}^2Ku - u'\delta_{ii}^2F\right) + (\delta_jKu - \delta_jf)'K^{-1}(\delta_iKu - \delta_if)$$

Crack growth: optimization of direction

- The discrete potential energy:

$$\Pi = \frac{1}{2}u'Ku - u'f$$

- The discrete energy release rate:

$$Gs_i = -\frac{1}{2}u'\delta_iKu + u'\delta_if - \delta_iu'(Ku - f)$$

$$Gs_i = -\frac{1}{2}u'\delta_iKu + u'\delta_if$$

0

- The rates of the energy release rate

$$\delta u = -K^{-1}(\delta Ku - \delta f)$$

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ij}^2Ku - u'\delta_{ij}^2f\right) - \delta_ju'(\delta_iKu - \delta_if)$$

expensive

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ii}^2Ku - u'\delta_{ii}^2F\right) + (\delta_jKu - \delta_jf)'K^{-1}(\delta_iKu - \delta_if)$$

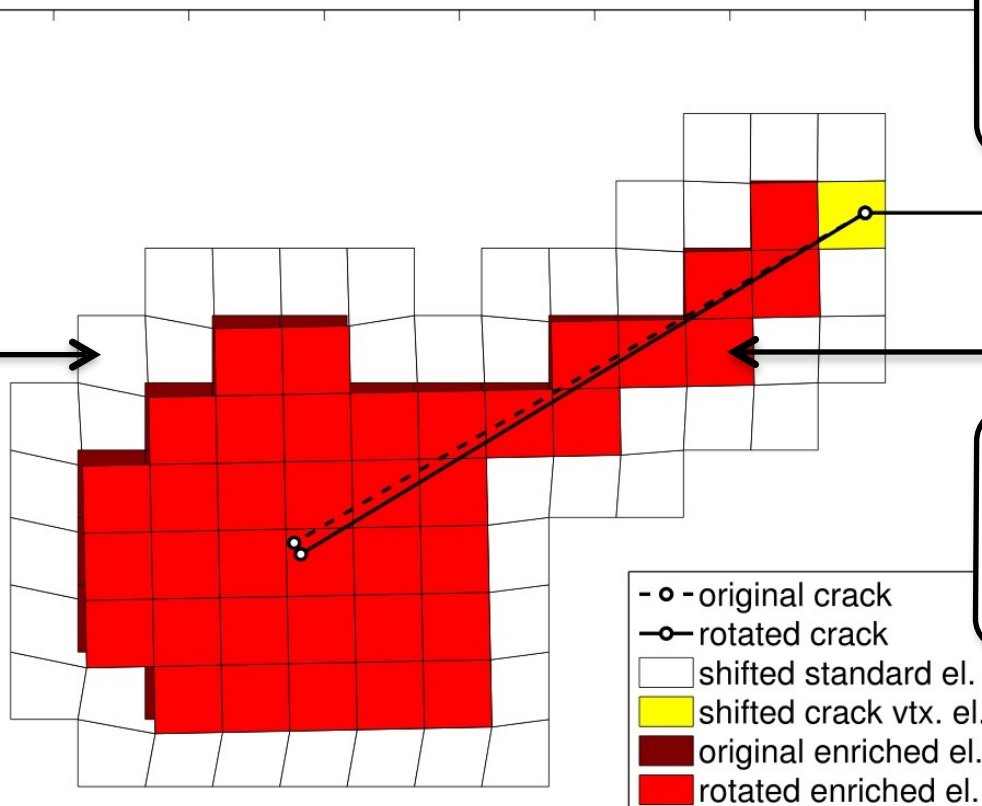
remote interaction

Crack growth: optimization of direction

$$\delta \mathbf{K}_e = \int_{\Omega_e} (\delta \mathbf{B}^T \mathbf{D} \mathbf{B} + \mathbf{B}^T \mathbf{D} \delta \mathbf{B}) \det(\mathbf{J}) d\bar{\Omega} + \int_{\Omega_e} \mathbf{B}^T \mathbf{D} \mathbf{B} \delta \det(\mathbf{J}) d\bar{\Omega}$$

$$\delta^2 \mathbf{K}_e = \int_{\Omega_e} (\delta^2 \mathbf{B}^T \mathbf{D} \mathbf{B} + 2\delta \mathbf{B}^T \mathbf{D} \delta \mathbf{B} + \mathbf{B}^T \mathbf{D} \delta^2 \mathbf{B}) \det(\mathbf{J}) d\bar{\Omega} + \int_{\Omega_e} 2(\delta \mathbf{B}^T \mathbf{D} \mathbf{B} + \mathbf{B}^T \mathbf{D} \delta \mathbf{B}) \delta \det(\mathbf{J}) d\bar{\Omega} + \int_{\Omega_e} \mathbf{B}^T \mathbf{D} \mathbf{B} \delta^2 \det(\mathbf{J}) d\bar{\Omega}$$

Differentiation of the stiffness matrix
w.r.t. crack increment direction



$$\delta \mathbf{K}_e = \mathbf{T}^T \mathbf{K}_e + \mathbf{K}_e \mathbf{T}$$

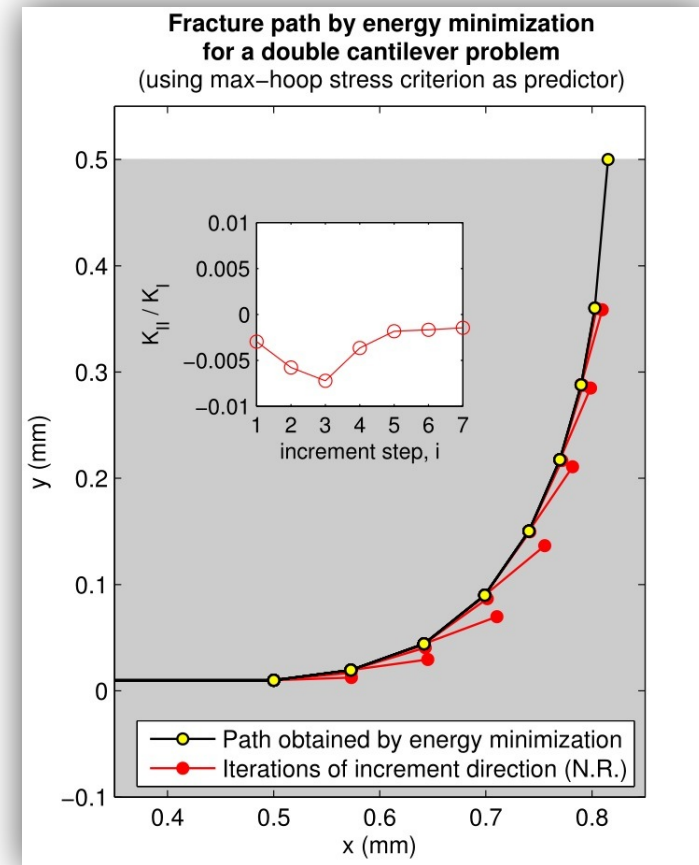
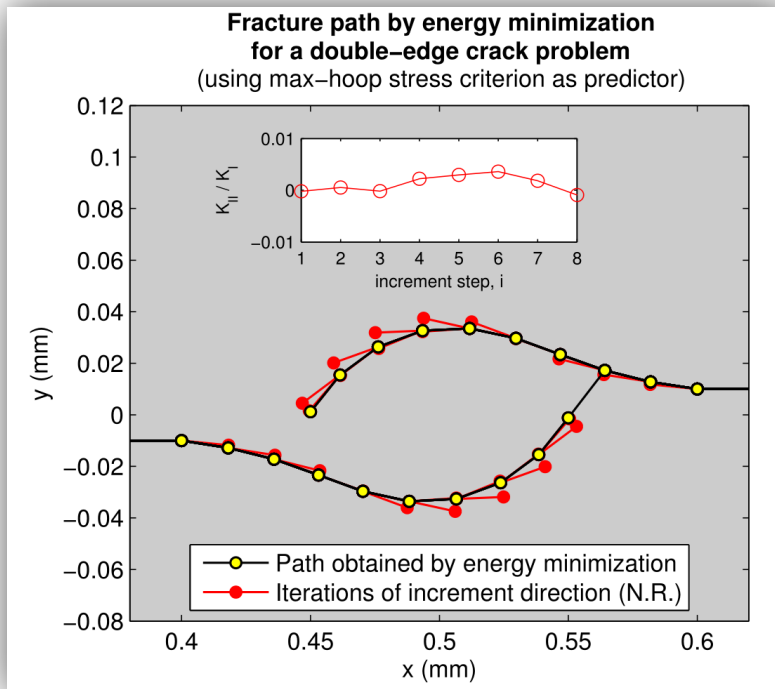
$$\delta^2 \mathbf{K}_e = 2(\mathbf{T}^T \mathbf{K}_e \mathbf{T} - \mathbf{K}_e)$$

Updated directions:

$$\theta^{k+1} = \theta^k - \mathbf{H}_s^{-1} \mathbf{G}_s$$

Crack growth: optimization of direction

- **Energy minimization w.r.t. to a finite crack propagation**
 - The growth direction is given by satisfying: $\partial\Pi/\partial\theta_i = 0$
 - Using the maximum hoop-stress criterion as initial guess
- **Numerical examples:**



Part IV. Application to surgical simulation

with Institute of Advanced Studies (iCube, University of Strasbourg, France: Hadrien Courtecuisse), INRIA, SHACRA Team (Stéphane Cotin, Christian Duriez); Karol Miller, UWA.



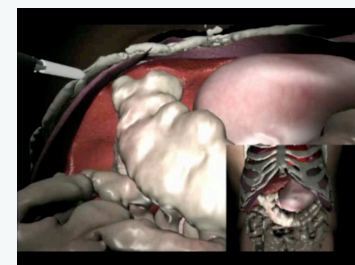
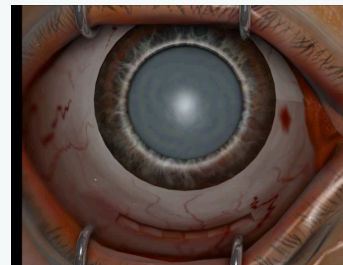
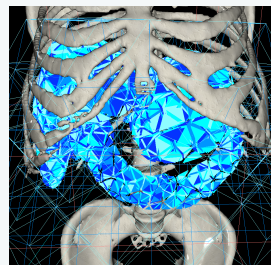
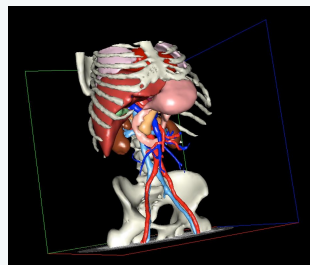
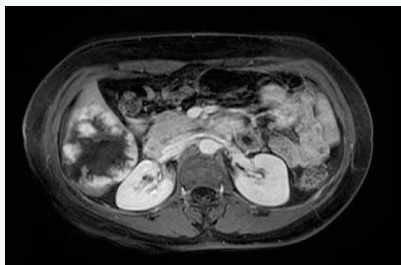
Faculty of Sciences,
Technology
and Communication

RealTcut

Interactive multiscale
cutting simulations

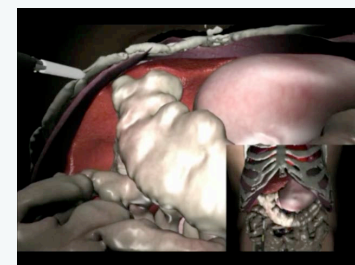
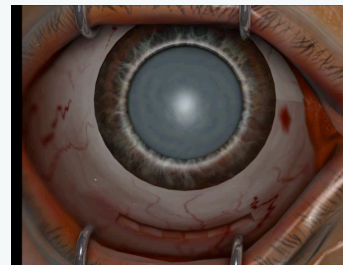
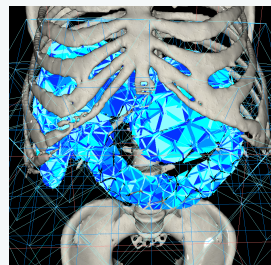
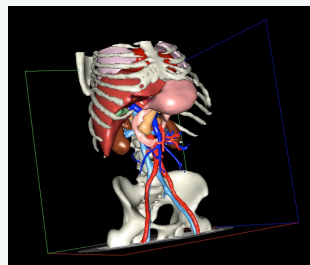


Courtecuisse et al. PBMB 2011



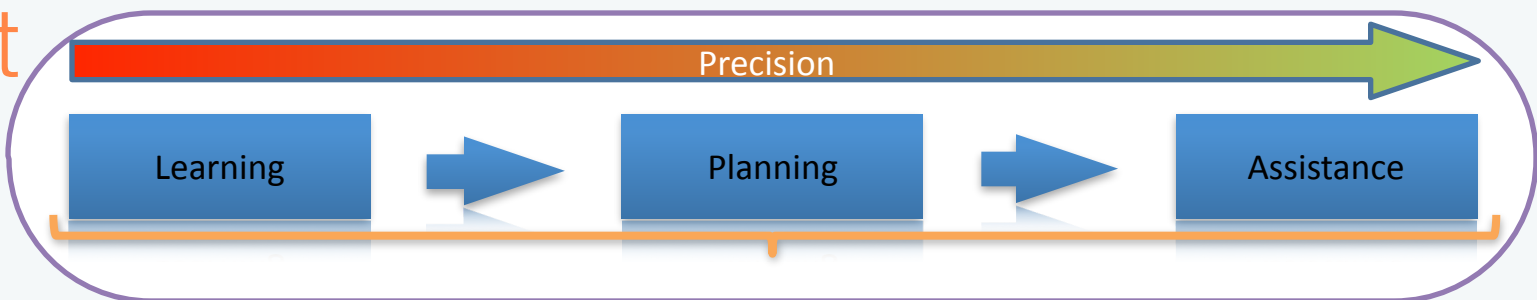


Courtecuisse et al. PBMB 2011



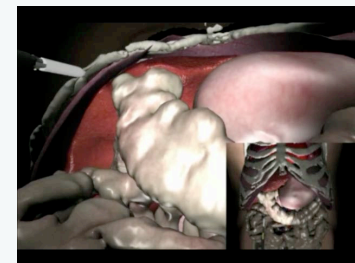
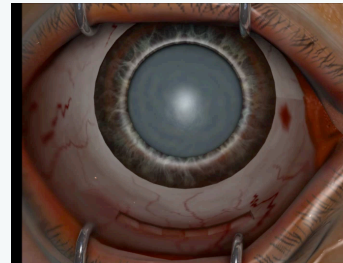
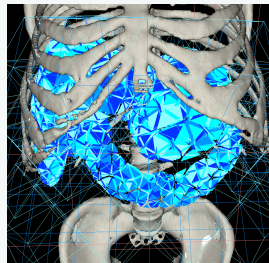
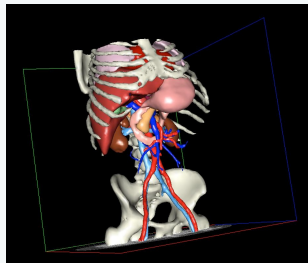
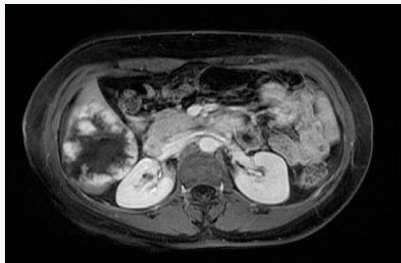


RealTcut



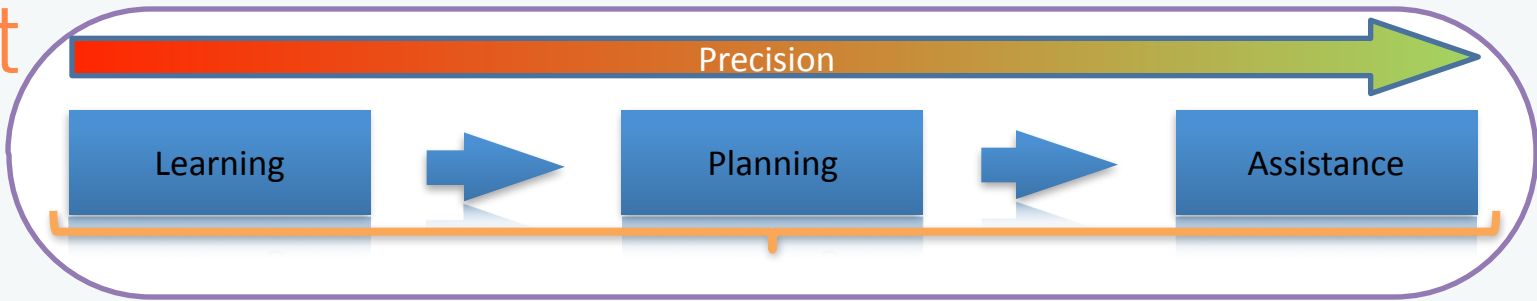
Surgical simulation (real time/interactivity)

Courtecuisse et al. PBMB 2011

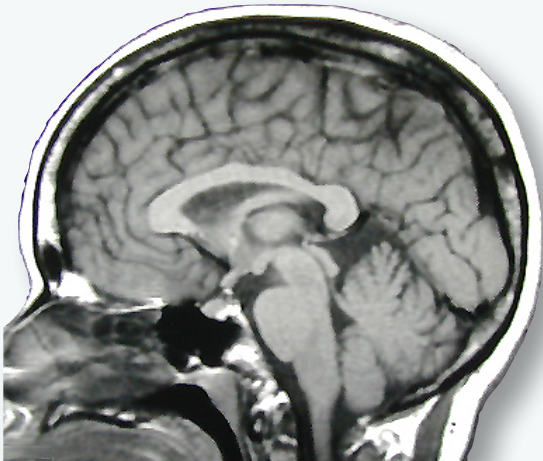




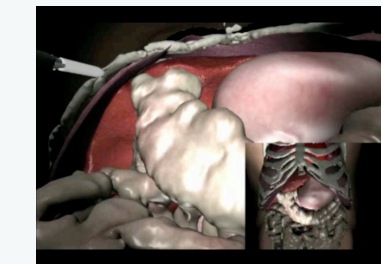
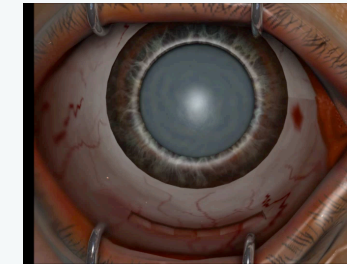
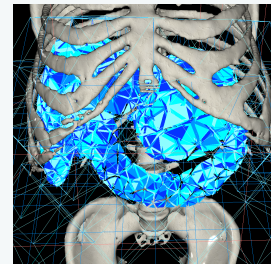
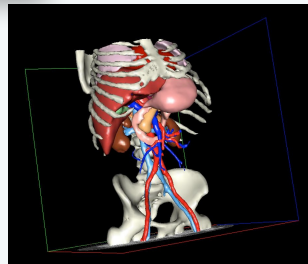
RealTcut



Surgical simulation (real time/interactivity)

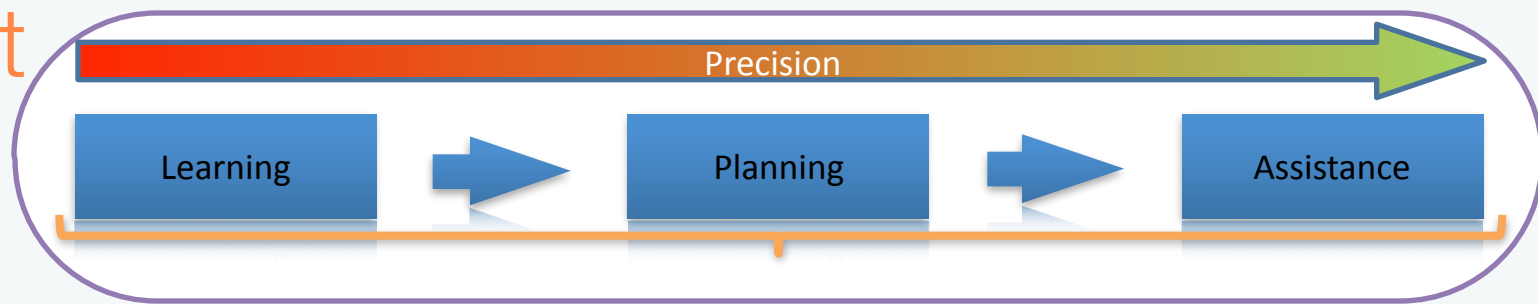


Courtecuisse et al. PBMB 2011

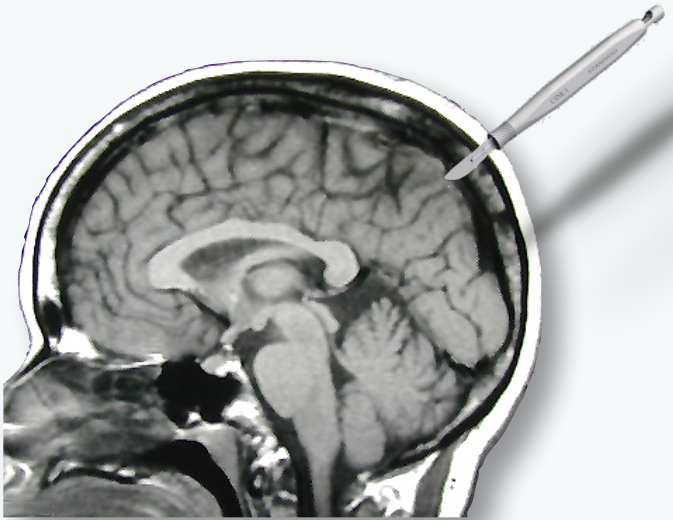




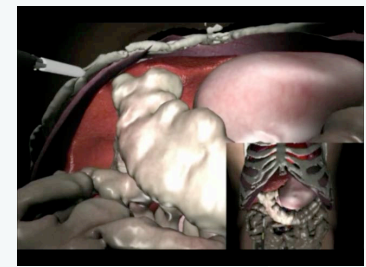
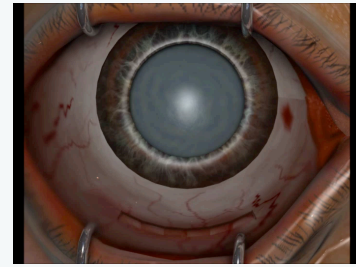
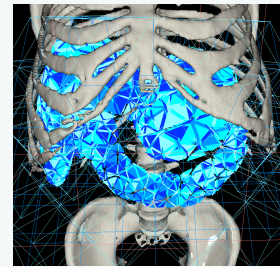
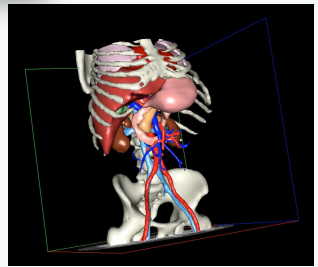
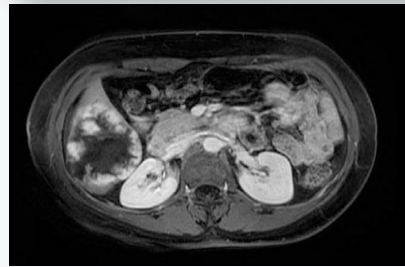
RealTcut



Surgical simulation (real time/interactivity)

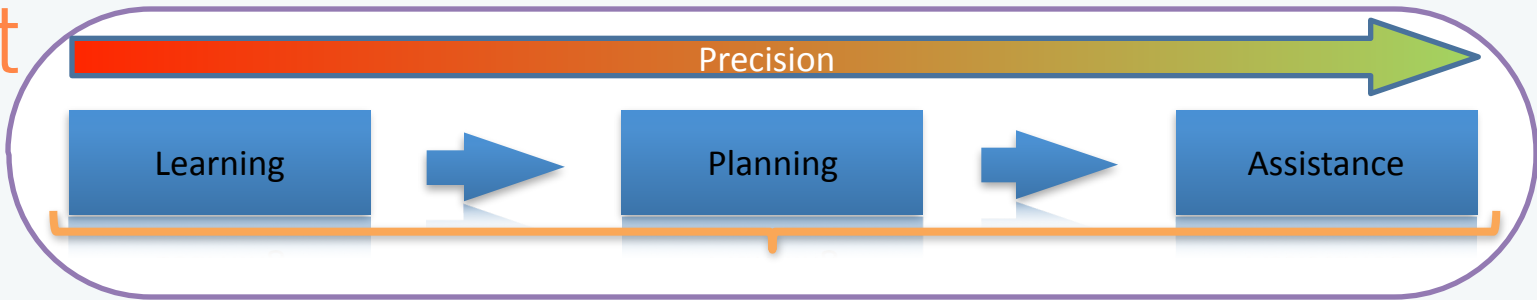


Courtecuisse et al. PBMB 2011

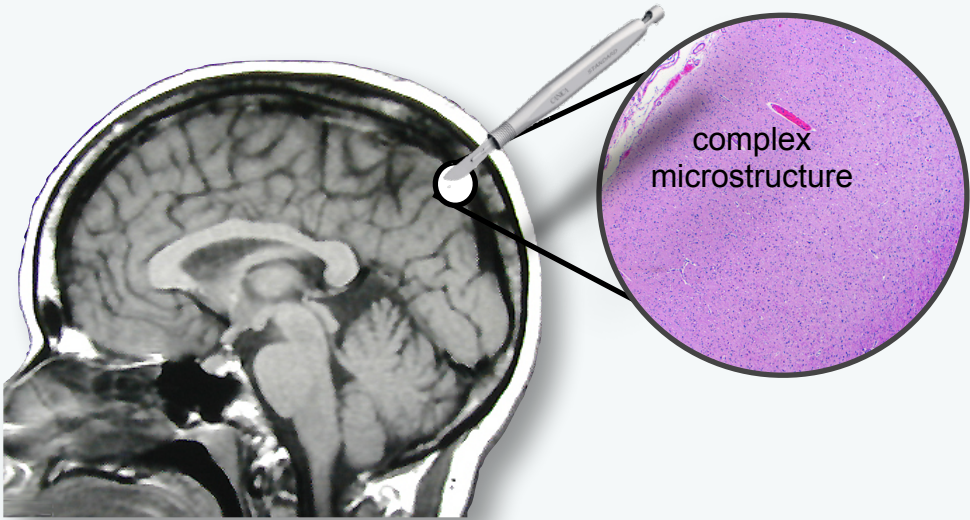




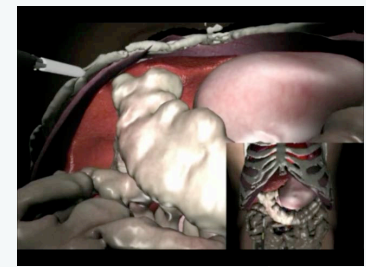
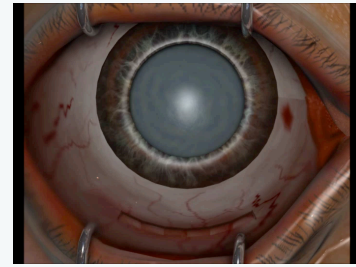
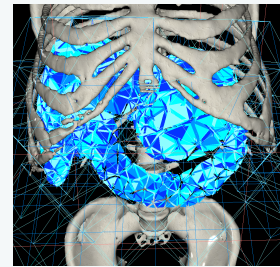
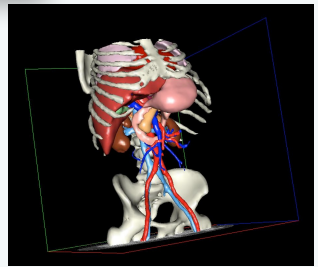
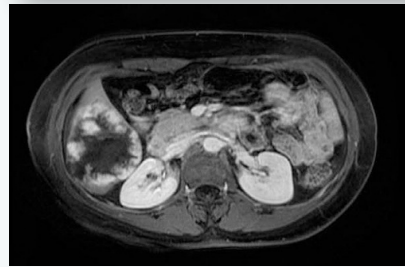
RealTcut



Surgical simulation (real time/interactivity)

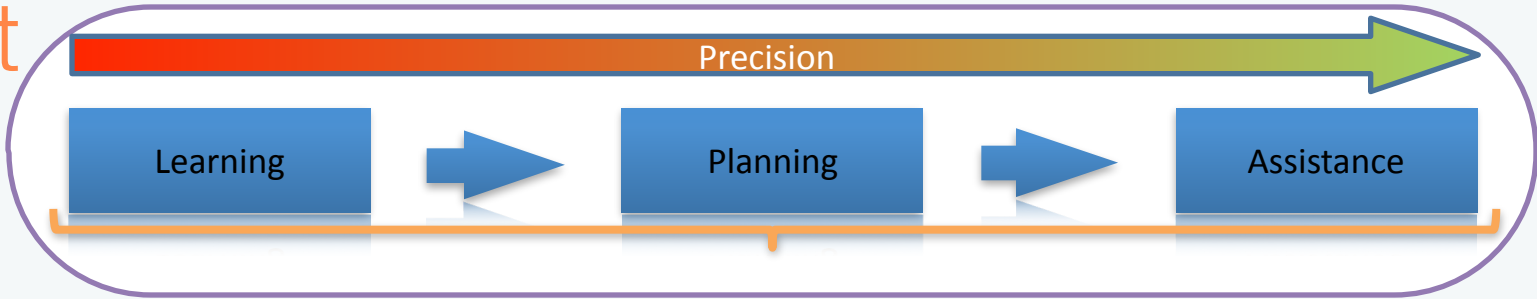


Courtecuisse et al. PBMB 2011

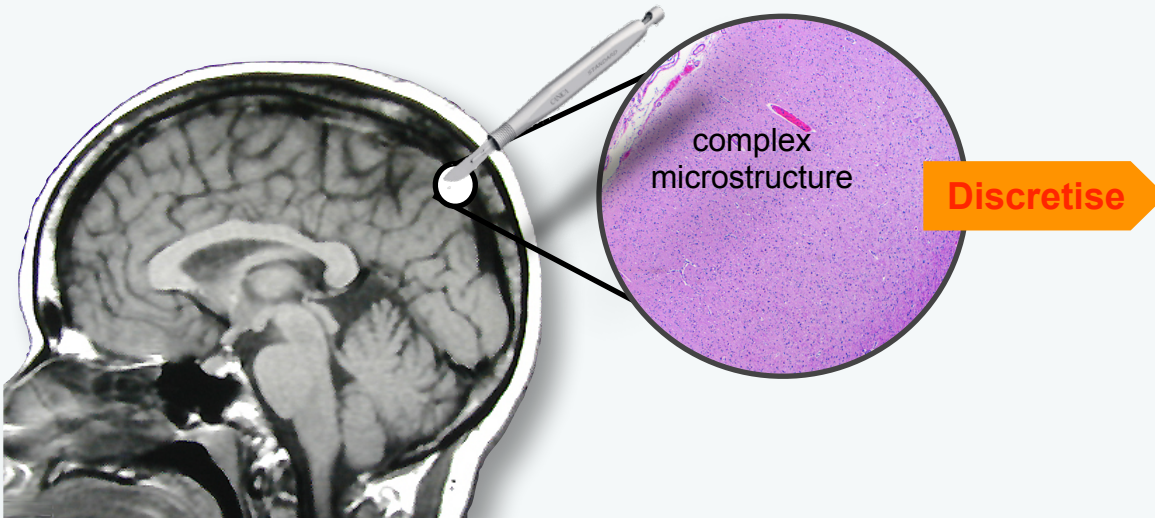




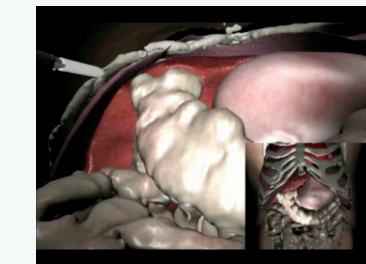
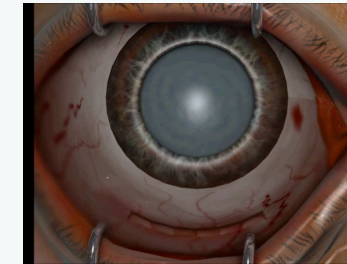
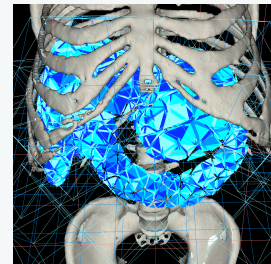
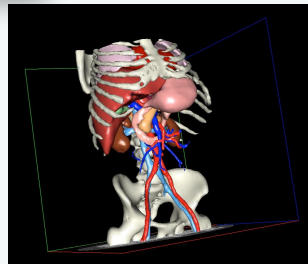
RealTcut



Surgical simulation (real time/interactivity)

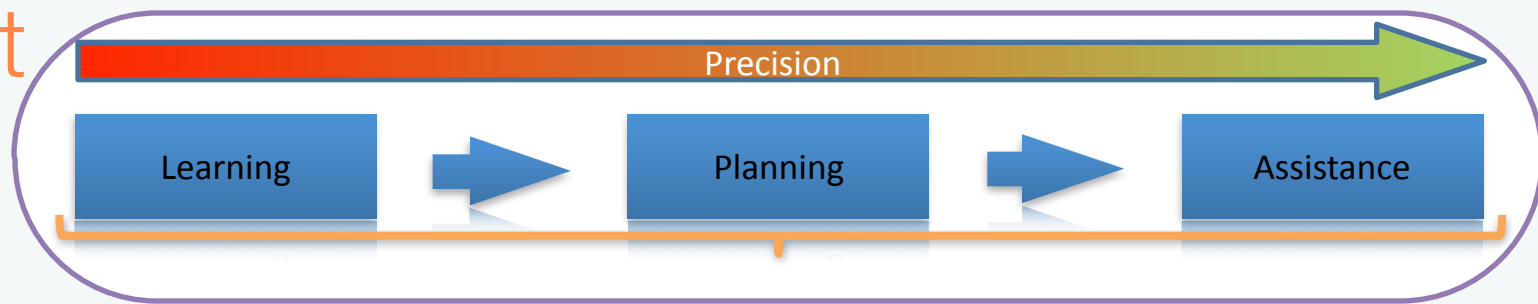


Courtecuisse et al. PBMB 2011

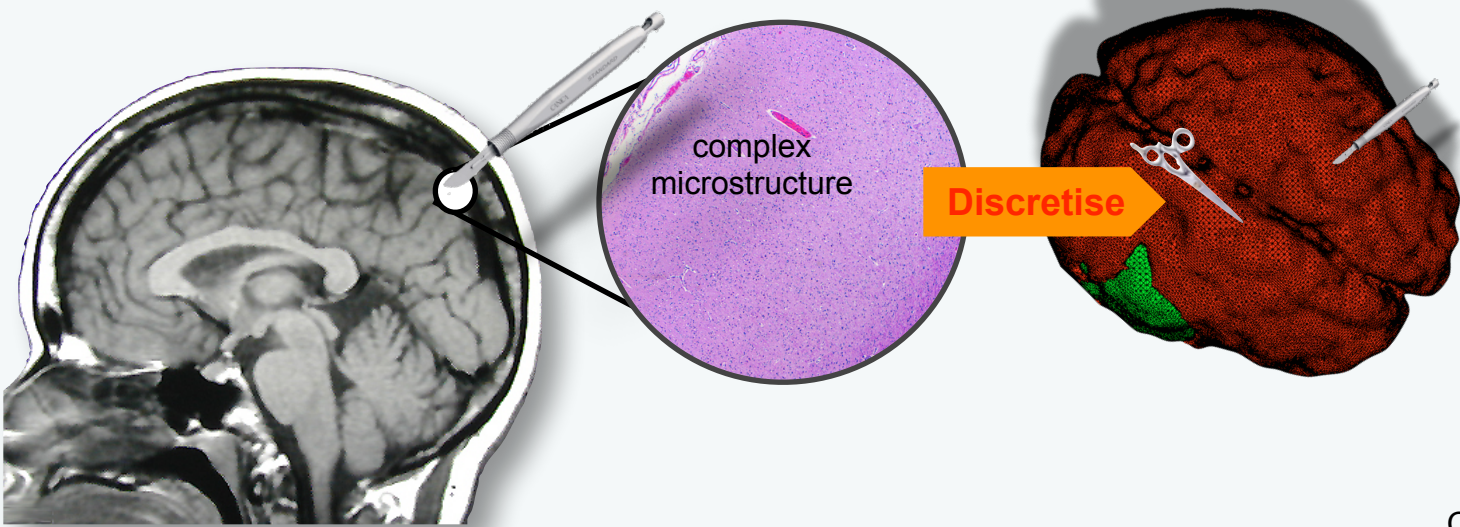




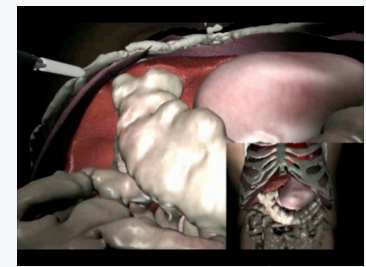
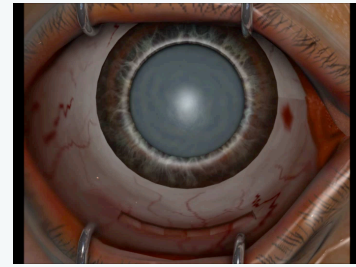
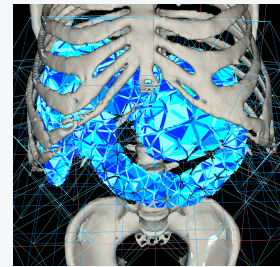
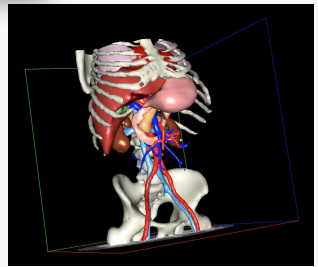
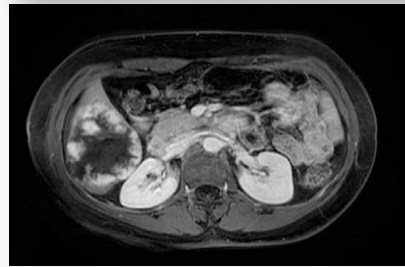
RealTcut



Surgical simulation (real time/interactivity)

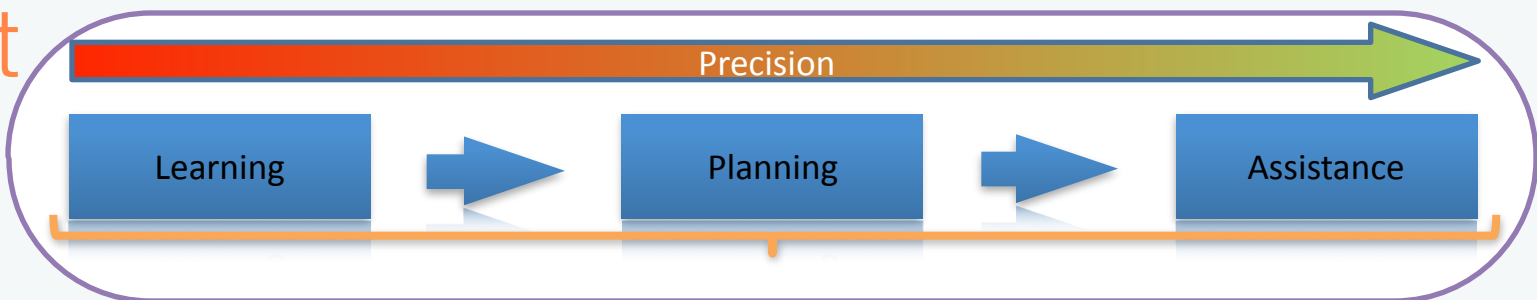


Courtecuisse et al. PBMB 2011

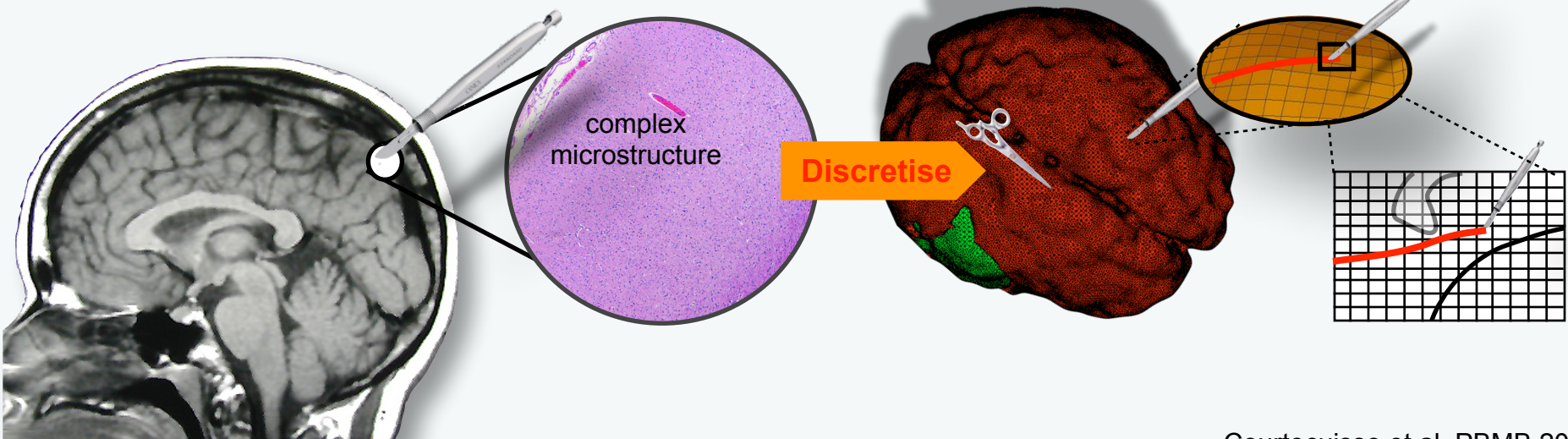




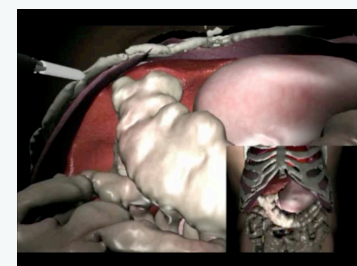
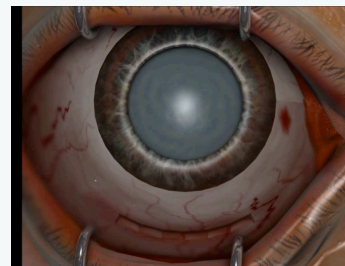
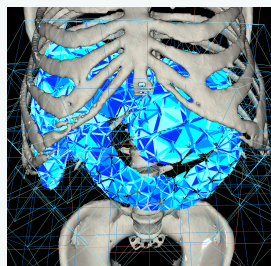
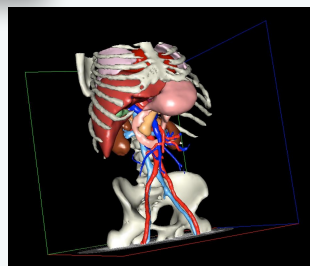
RealTcut



Surgical simulation (real time/interactivity)

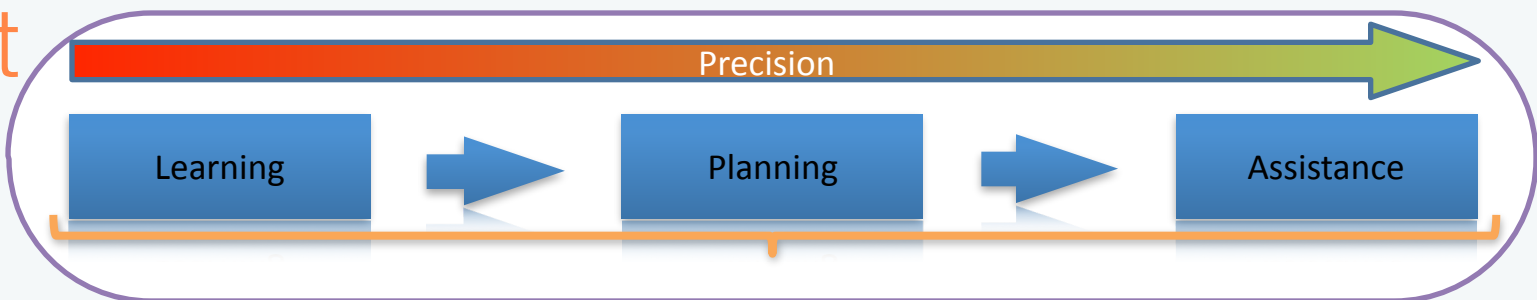


Courtecuisse et al. PBMB 2011

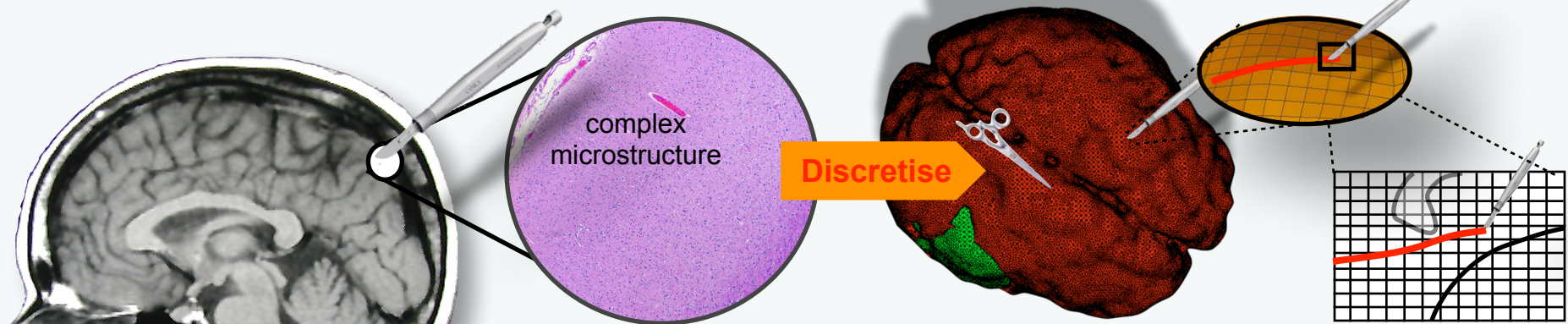




RealTcut

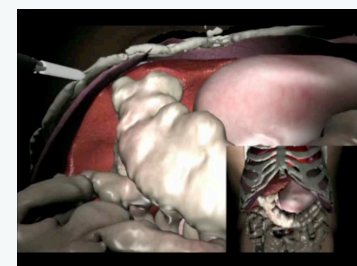
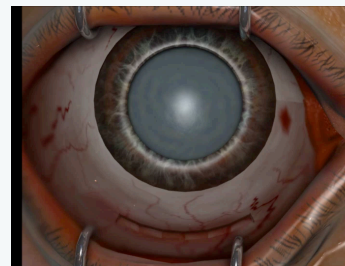
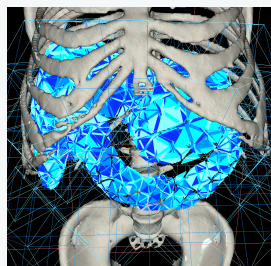
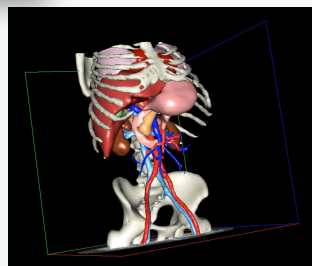


Surgical simulation (real time/interactivity)



- ▶ Reduce the problem size while controlling error in solving very large multiscale mechanics problems

Courteuisse et al. PBMB 2011

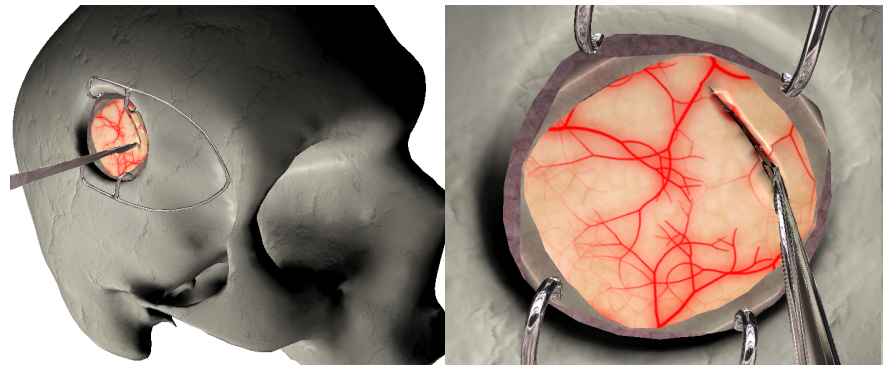


Concrete objective: compute the response of organs during surgical procedures (including cuts) in real time (50-500 solutions per second)

Two schools of thought

- ▶ constant time
 - ➔ accuracy often controlled visually only
- ▶ model reduction or “learning”
 - ➔ scarce development for biomedical problems
 - ➔ no results available for cutting

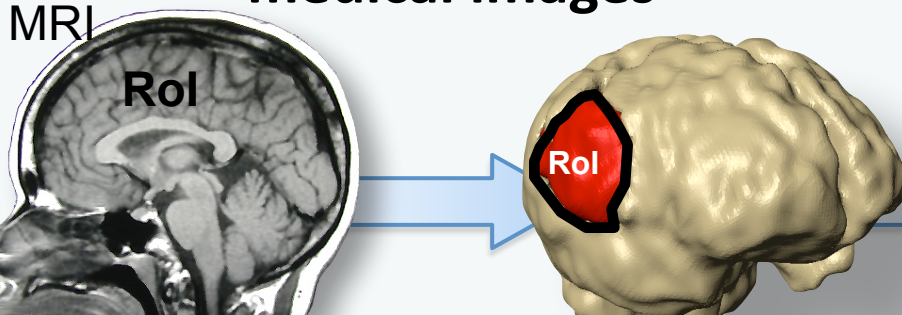
First implicit, interactive method for cutting with contact



[Courtecuisse et al., MICCAI, 2013]
Collaboration INRIA

Proposed approach: maximize accuracy for given computational time. Error control

Complex geometries from medical images



segmentation

Region of interest (RoI)

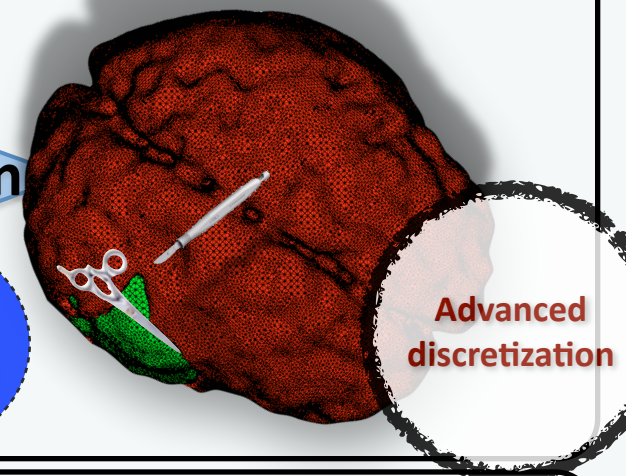
Topological changes & contact

discretization

Model reduction

Advanced discretization

adaptivity



Error control

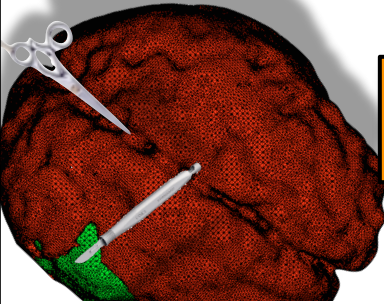
- interactivity
- space-time discretization?
- optimize use of compute resources

Verification & Validation



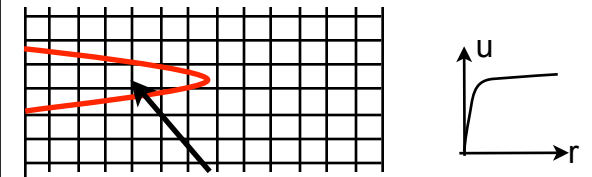
calculs offline

génération solutions particulières



~10⁶ snapshots

calcul champs asymptotiques



action de l'instrument

tri pré-opérateur

~10³ snapshots

"mapping" spécifique patient

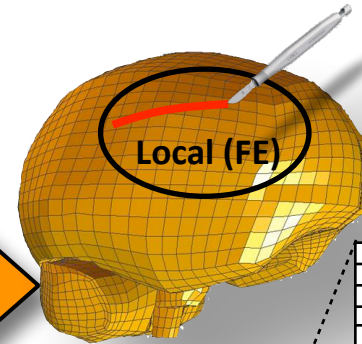
enrichissement "pointe de coupe"

POD

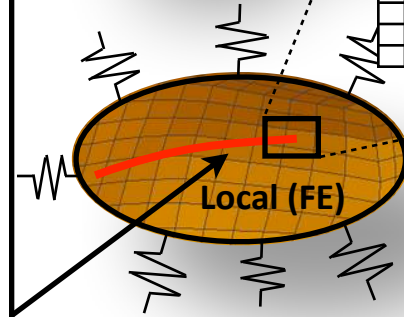
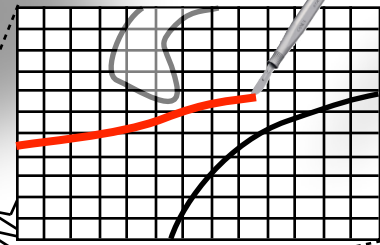
O(10) fonctions

espace réduit de petite dimension

calculs online: interactivité



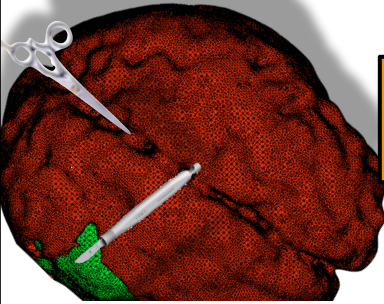
représentation locale



approximation POD globale

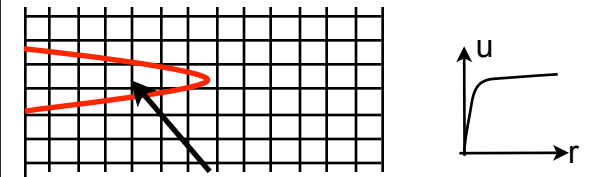
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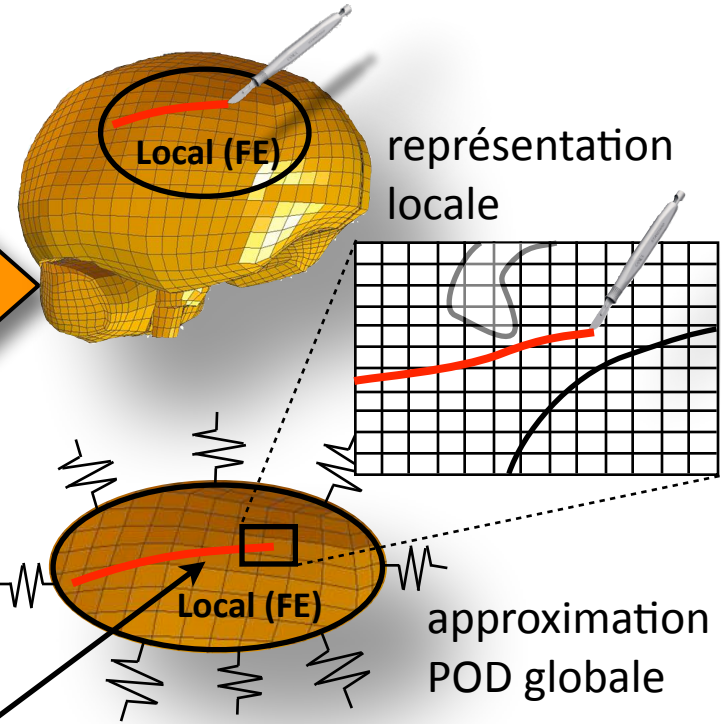
enrichissement "pointe de coupe"

POD

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espace réduit de petite dimension

calculs online: interactivité



A semi-implicit method for real-time deformation, topological changes, and contact of soft tissues

Paper ID : 269

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EPSRC

Pioneering research
and skills

THE ROYAL
SOCIETY

hpc
CYMRU WALES

SEVENTH FRAMEWORK
PROGRAMME

Acknowledgements

The Leverhulme Trust

The Royal Academy
of Engineering



INVENTEURS DU MONDE NUMÉRIQUE

European Research Council

erc

IDEAS

**TWO POST DOCS
TWO FACULTY POSITIONS AVAILABLE**

OPEN SOURCE CODES

PERMIX: Multiscale, XFEM, large deformation, coupled 2 LAMMPS, ABAQUS, OpenMP -
Fortran 2003, C++

MATLAB Codes: XFEM, 3D ISOGOMETRIC XFEM, 2D ISOGOMETRIC BEM, 2D MESHLESS
DOWNLOAD @ <http://cmechanicsos.users.sourceforge.net/>

72

COMPUTATIONAL MECHANICS DISCUSSION GROUP

Request membership @

http://groups.google.com/group/computational_mechanics_discussion/about

the group...
November 2012



73

thank you

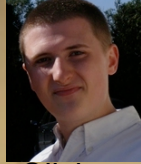


Yusuf Ghaffari
Stlagh

Chi Hoang



Hadrien
Courtecuisse



Olivier
Goury

Daniel Paladim



Xuan Peng



Haojie
Liang

Danas
Sutula



Dr. Nguyen
Vinh Phu



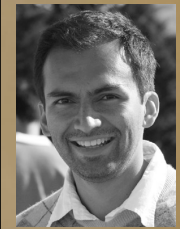
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Estrada

Dr. Sundararajan
Natarajan

Ahmad
Akbari

Nguyen-Tanh
Nhon

Chang-
Lee



Dr. Robert Simpson



Dr. Pierre Kerfriden

Publications - model reduction

- <http://orbilu.uni.lu/handle/10993/12024>
- <http://orbilu.uni.lu/handle/10993/12012>
- <http://orbilu.uni.lu/handle/10993/10207>
- <http://orbilu.uni.lu/handle/10993/12454>
- <http://orbilu.uni.lu/handle/10993/12453>
- <http://orbilu.uni.lu/handle/10993/14475>
- <http://orbilu.uni.lu/handle/10993/10206>

Mesh-burden reduction

- <http://orbilu.uni.lu/handle/10993/12159>
- <http://orbilu.uni.lu/handle/10993/14135>
- <http://orbilu.uni.lu/handle/10993/13847>
- <http://orbilu.uni.lu/handle/10993/12157>
- <http://orbilu.uni.lu/handle/10993/11850>

Demos

- Surgical simulation
 - <http://www.youtube.com/watch?v=KqM7rh6sE8s>
 - <http://www.youtube.com/watch?v=DYBRKbEiHj8>
- Multi-crack growth
 - <http://www.youtube.com/watch?v=6yPb6NXnex8>
 - <http://www.youtube.com/watch?v=7U2o5bFvj8E>

Demos

- <http://www.youtube.com/watch?v=90NAq76mVmQ>
- Solder joint durability
 - <http://www.youtube.com/watch?v=Ri96Wv6zBNU>
 - http://www.youtube.com/watch?v=1g3Pe_9XN9I

Damage tolerance assessment directly from CAD

- <http://www.youtube.com/watch?v=RV0gidOT0-U>
- <http://www.youtube.com/watch?v=cYhaj6SPLTE>
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- F. Cirak, M. Ortiz, and P. Schröder. Subdivision surfaces: a new paradigm for thin-shell finite-element analysis. *IJNME*, 47(12): 2039–2072, 2000.
- Constructive solid analysis: a hierarchical, geometry-based meshless analysis procedure for integrated design and analysis. D. Natekar, S. Zhang, and G. Subbarayan. *CAD*, 36(5): 473--486, 2004.
- T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *CMAME*, 194(39-41):4135–4195, 2005.
- J. A. Cottrell, T. J.R. Hughes, and Y. Bazilevs. *Isogeometric Analysis: Toward Integration of CAD and FEA*. Wiley, 2009.



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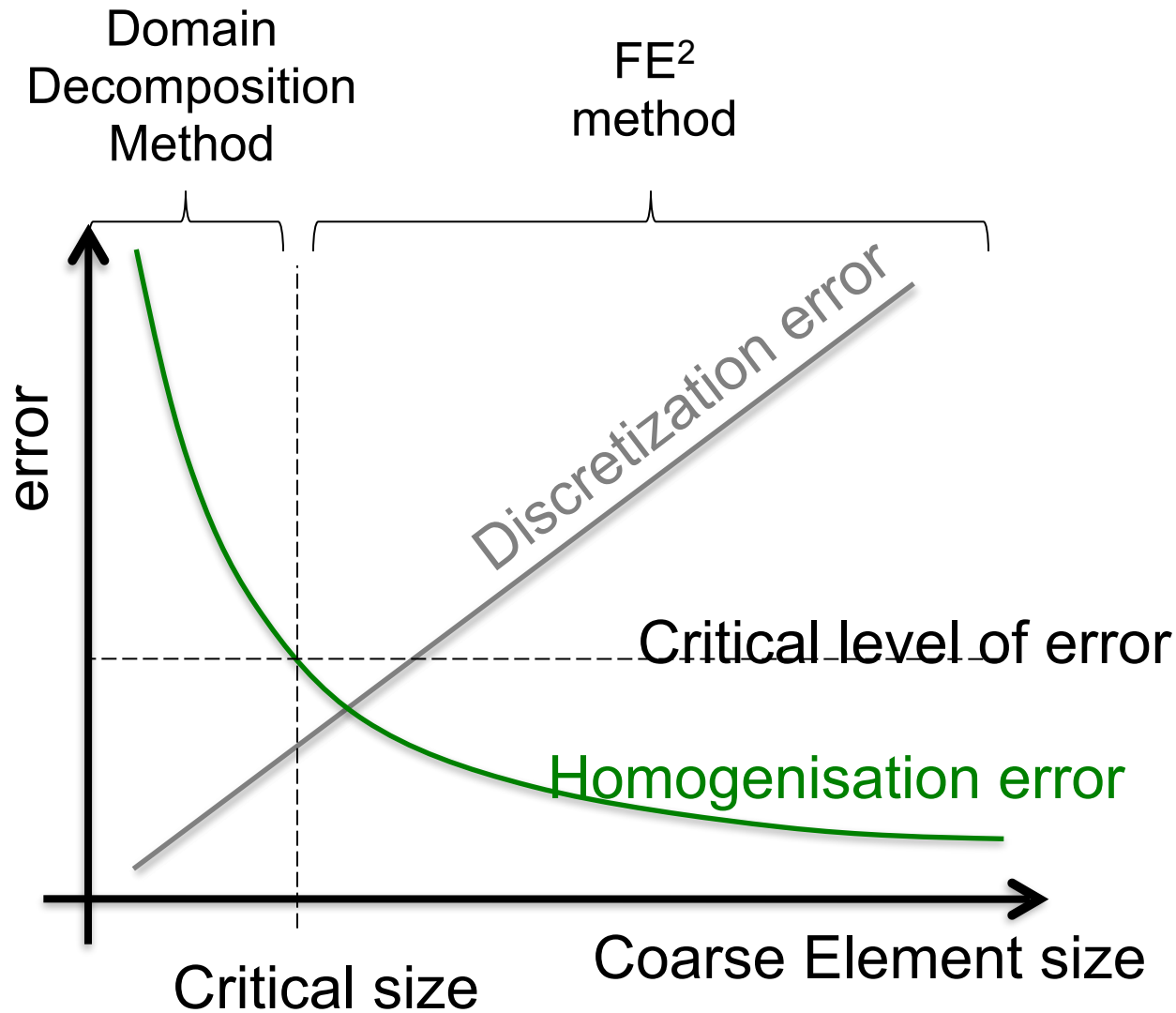
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Outline

- Introduction: Multiscale methods for Fracture
- Adaptive multiscale method
 - Strategy
 - Fine scale problem
 - Coarse scale problem
 - FE² method
 - Adaptive mesh refinement
 - Coupling fine and coarse discretisations
 - Results
 - L-shape problem
 - Notched bar under Uni-axial tension

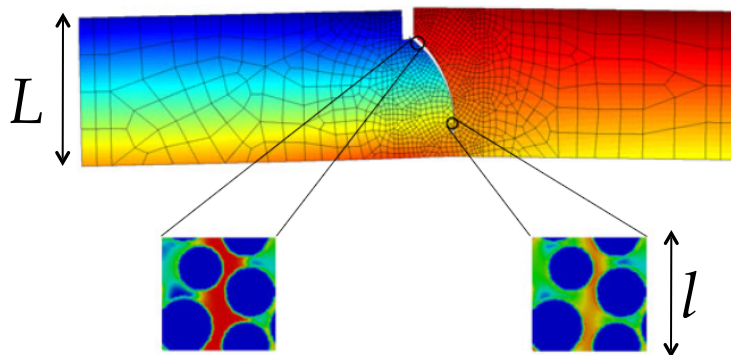
Error control in multiscale modelling



Multiscale methods for Fracture

■ Non-concurrent

Damage zone is modelled by a macroscopic cohesive crack that homogenises the failure zone.

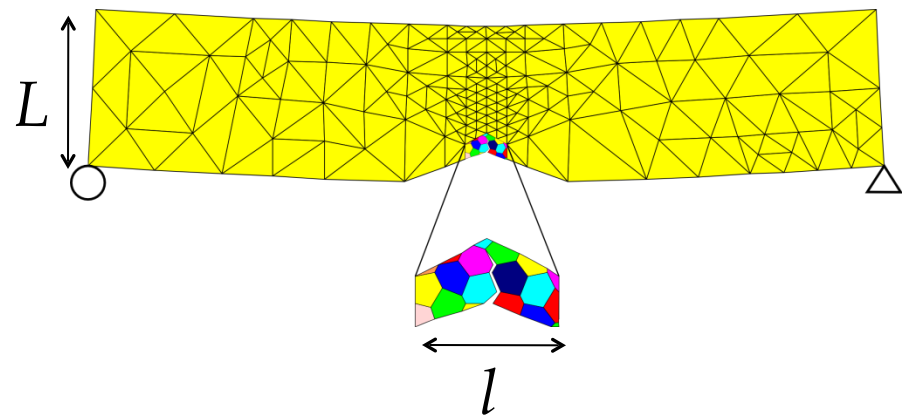


V.P. Nguyen 2012

$$L/l \gg 1$$

■ Concurrent

Damage zone is modelled directly at the microscale and coupled to the coarse scale.

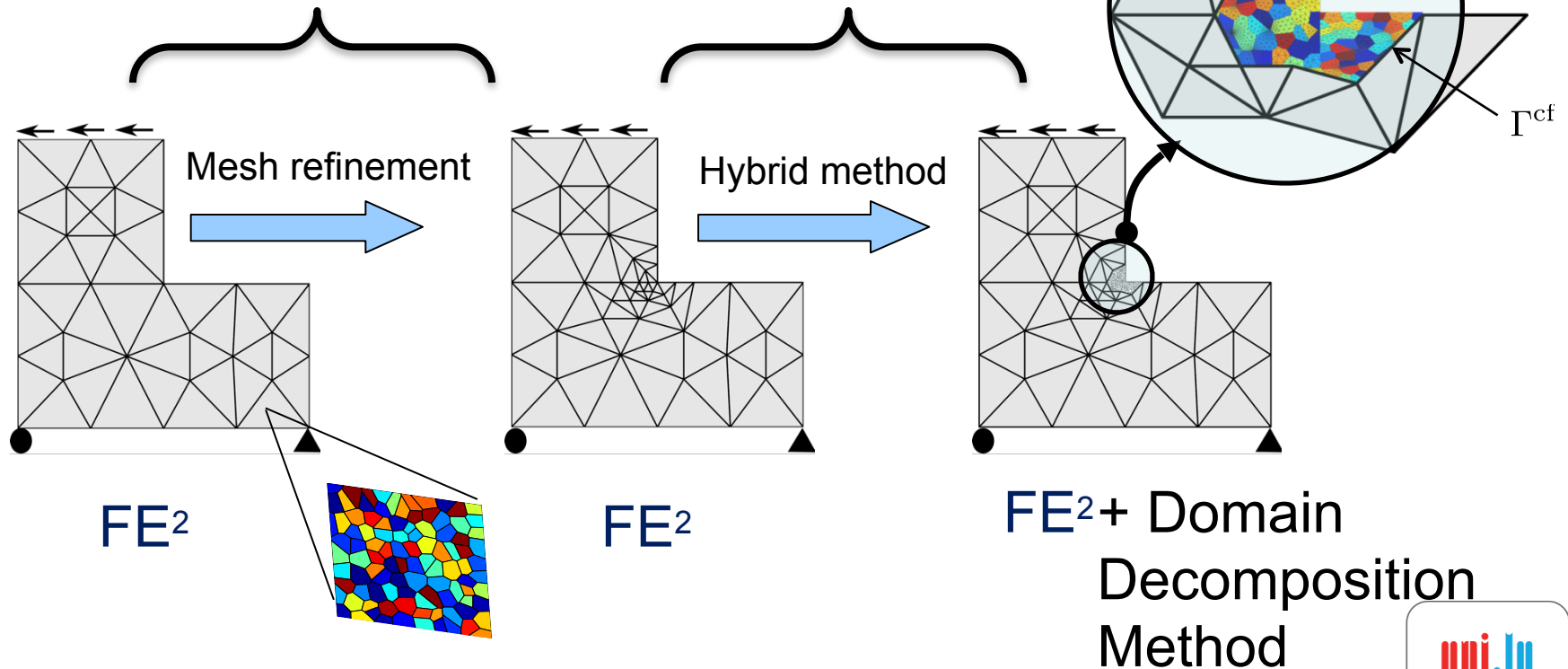


$$L/l > 1$$

Adaptive multiscale method: A Concurrent approach

➤ Strategy:

- control the coarse scale discretization error
- control the modelling error



Fine Scale: micro-structure

➤ Microscale problem:

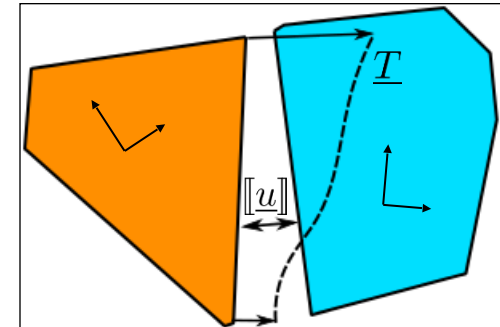
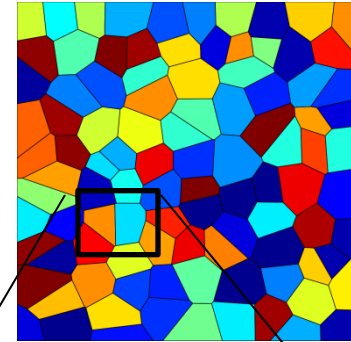
$$\int_{\Omega/\Gamma_c} \boldsymbol{\sigma}(\mathbf{u}) : \delta \boldsymbol{\varepsilon} \, d\Omega + \int_{\Gamma_c} \mathbf{T} \cdot [[\delta \mathbf{u}]] \, d\Omega = \int_{\partial\Omega} \mathbf{f} \cdot \delta \mathbf{u} \, d\Gamma$$

- Orthotropic grains

$$\forall \mathbf{x} \in \Omega/\Gamma_c, \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}$$

- Cohesive interface

$$\forall \mathbf{x} \in \Gamma_c, \quad \mathbf{T}|_t = T \left(([\mathbf{u}]|_T)_{T \leq t} \right)$$



Coarse Scale

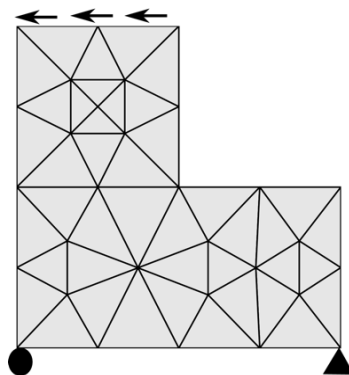
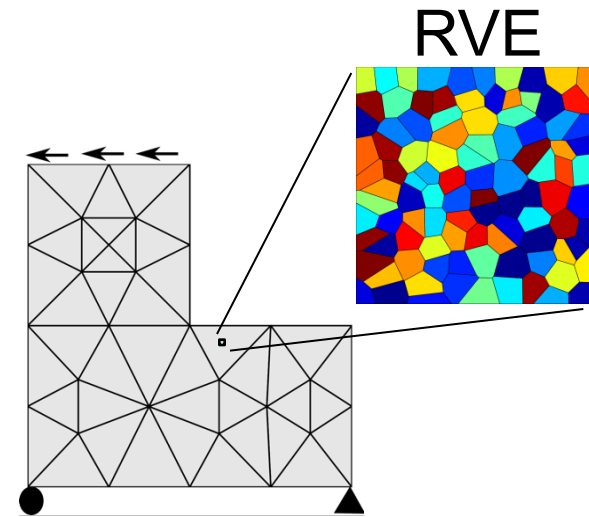
➤ Macroscale problem:

- FE² Method

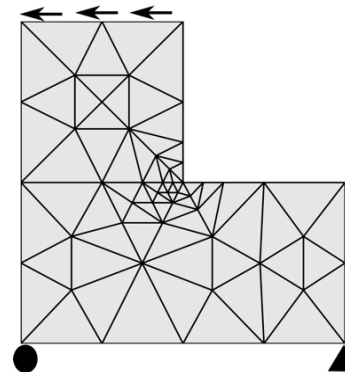
Based on averaging theorem
(computational homogenisation)

- Adaptive mesh refinement

Error estimation by Zienkiewicz-Zhu-type recovery technique

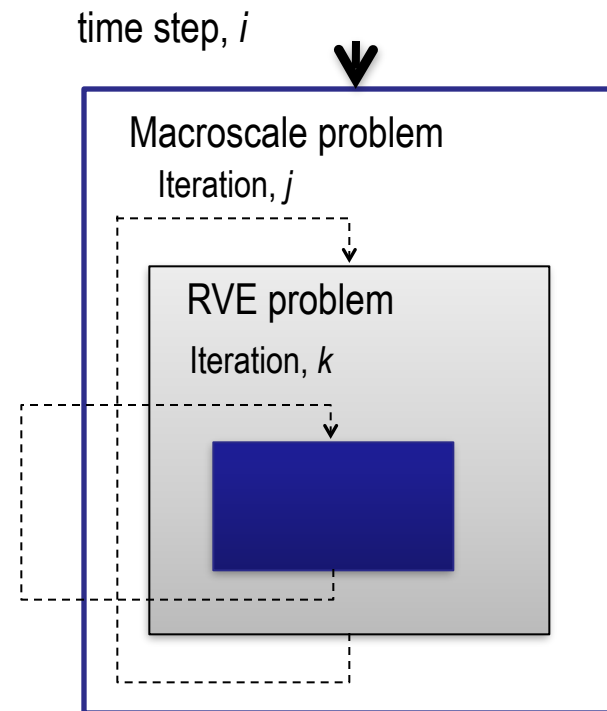
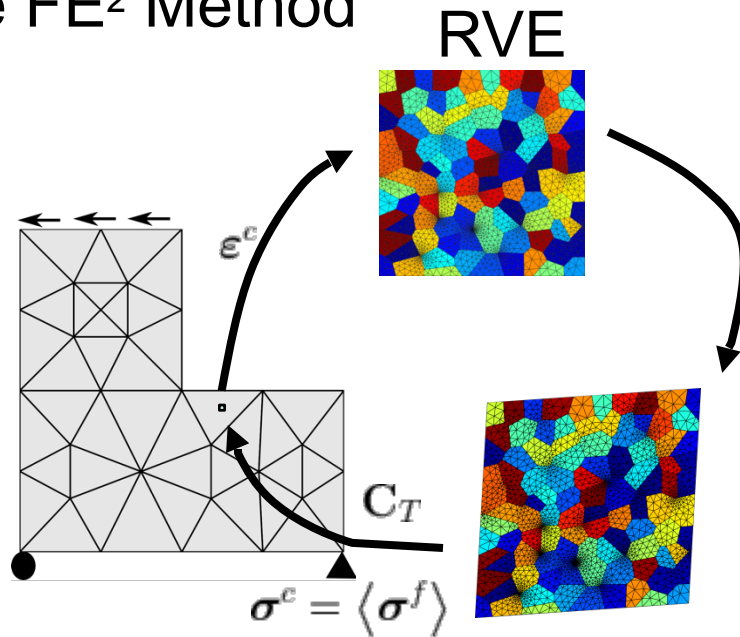


Mesh refinement



Coarse Scale: FE2

- The FE² Method



❖ Shortcoming of the FE² Method :

Lack of scale separation
RVE cannot be found in the **softening regime**

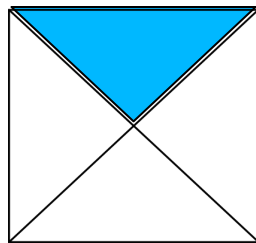
Coarse Scale: Adaptive mesh refinement

➤ Coarse scale Adaptive mesh refinement

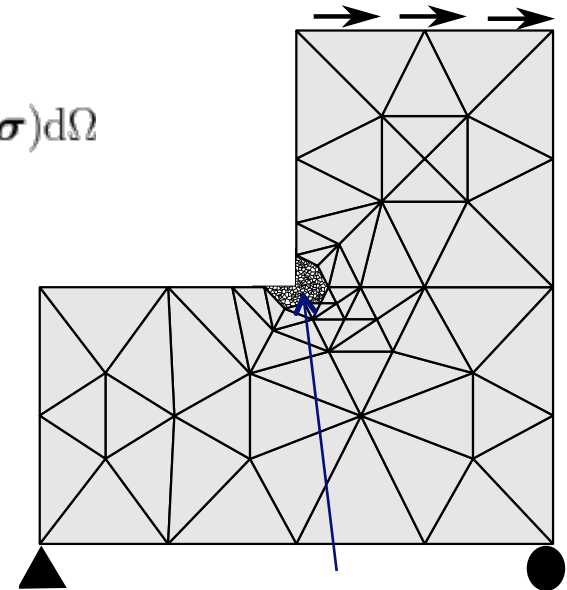
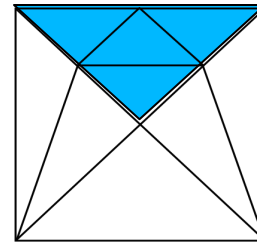
- Error estimation by Zienkiewicz-Zhu-type recovery technique

$$\|e\| = \int_{\Omega_c} (\sigma^* - \sigma) : \left(\frac{\partial \sigma}{\partial \varepsilon} \Big|_{u^c} \right)^{-1} : (\sigma^* - \sigma) d\Omega$$

Element to refine



Refined mesh



Error due to the discretisation of Ω^f neglected

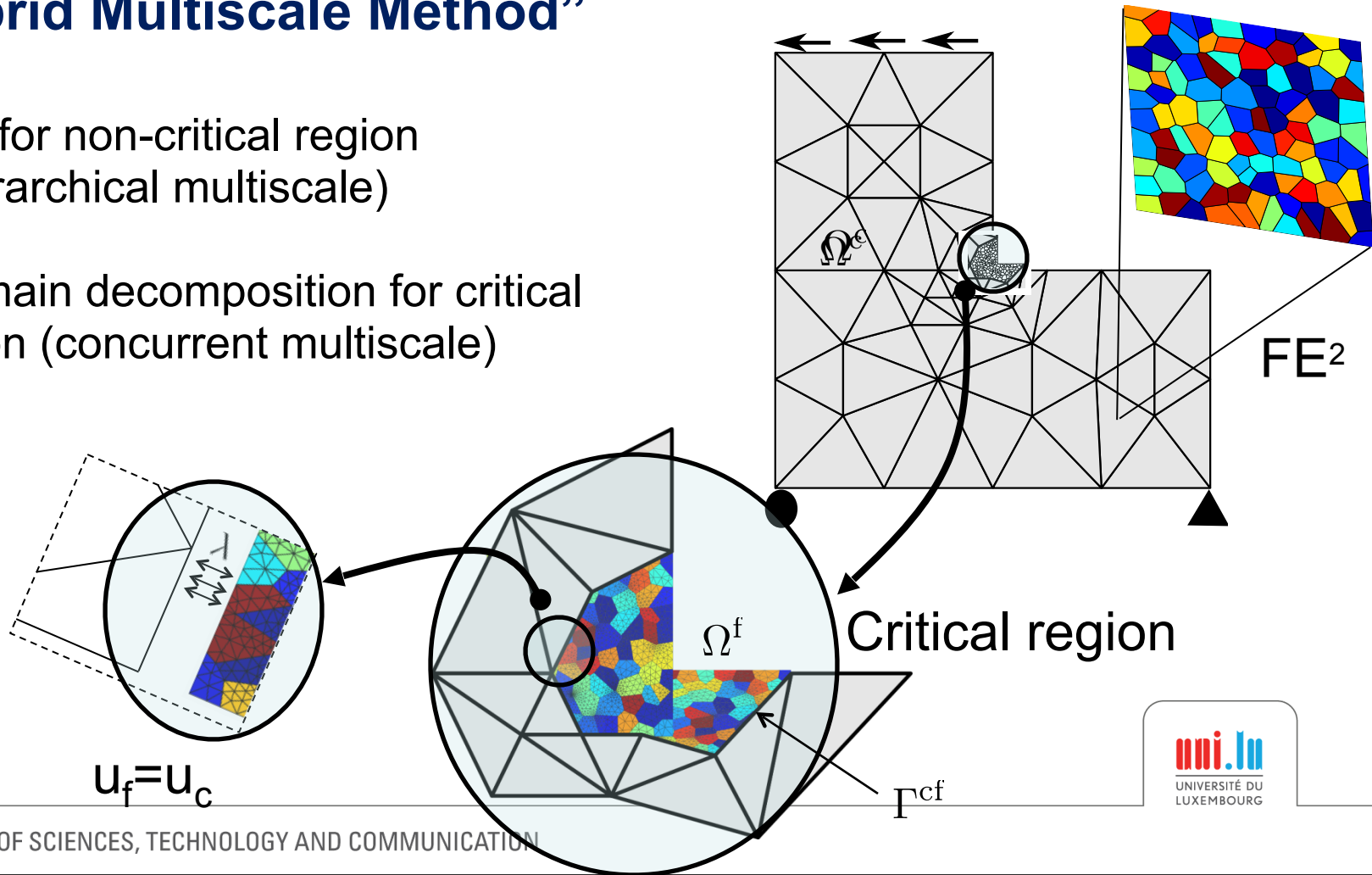
- Convergence criterion: $\frac{\|e\|}{\|\sigma\|} < Tol$

Fine-Coarse scales Coupling

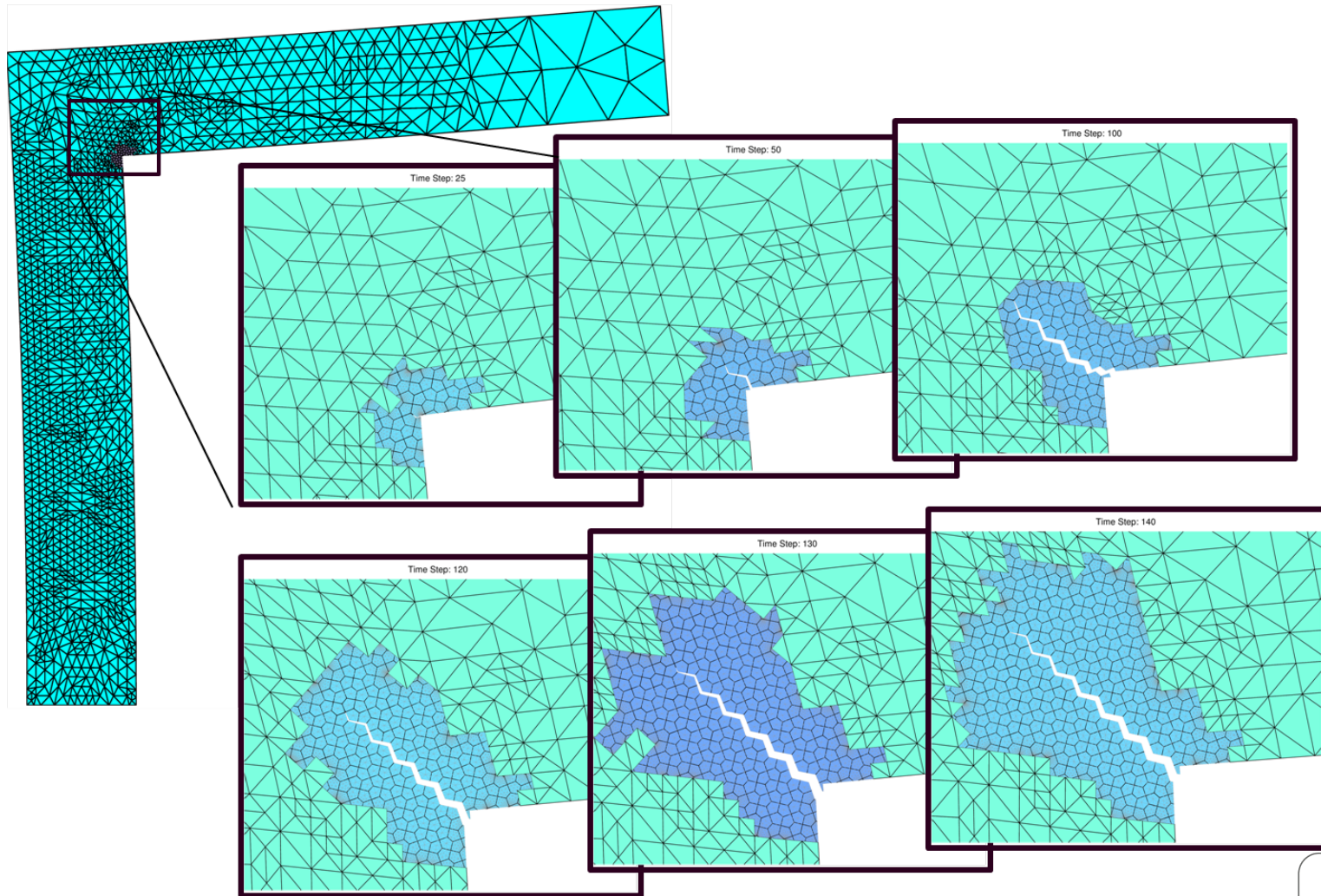
What is the solution for the FE² shortcoming:

“Hybrid Multiscale Method”

- FE² for non-critical region (hierarchical multiscale)
- Domain decomposition for critical region (concurrent multiscale)

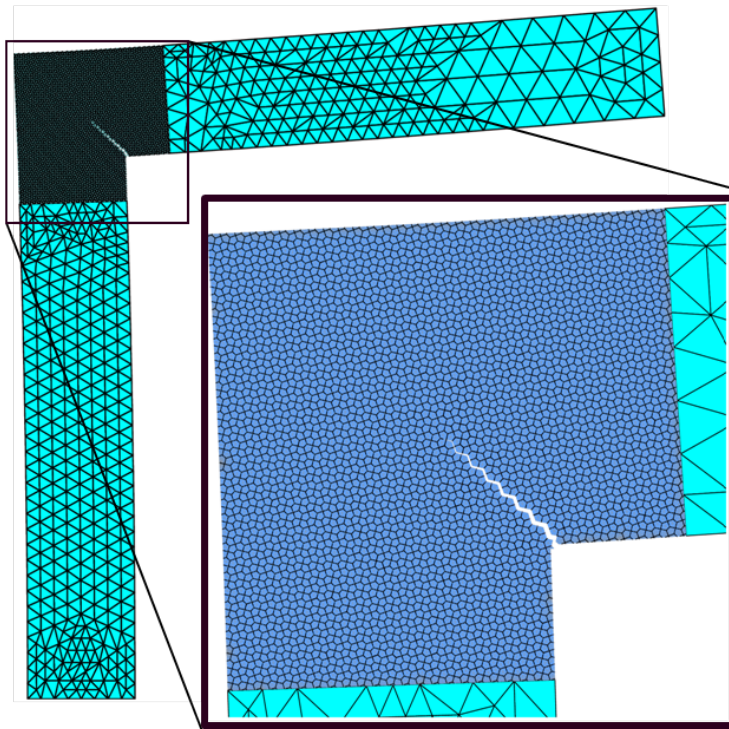


Results: L-shape

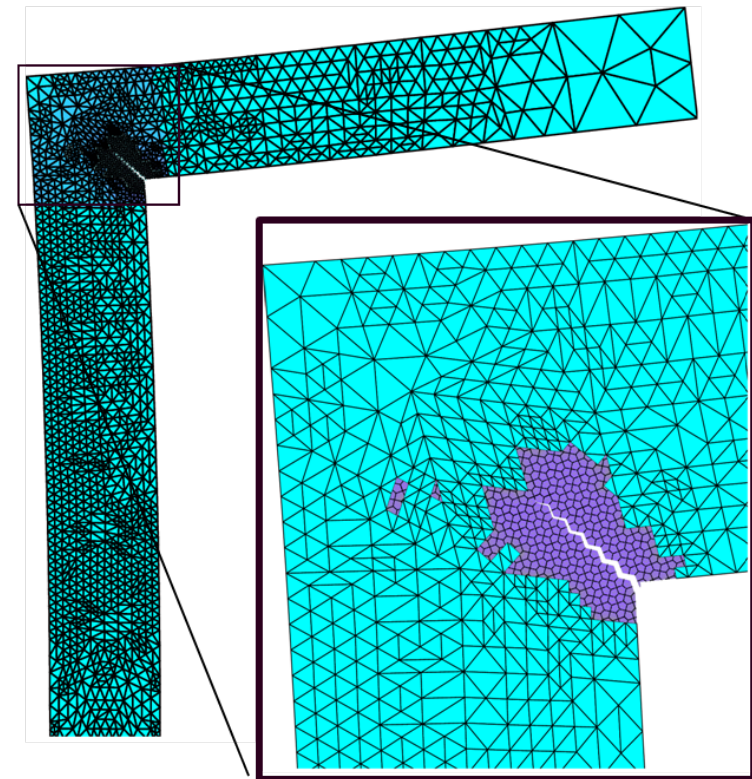


Results: L-shape

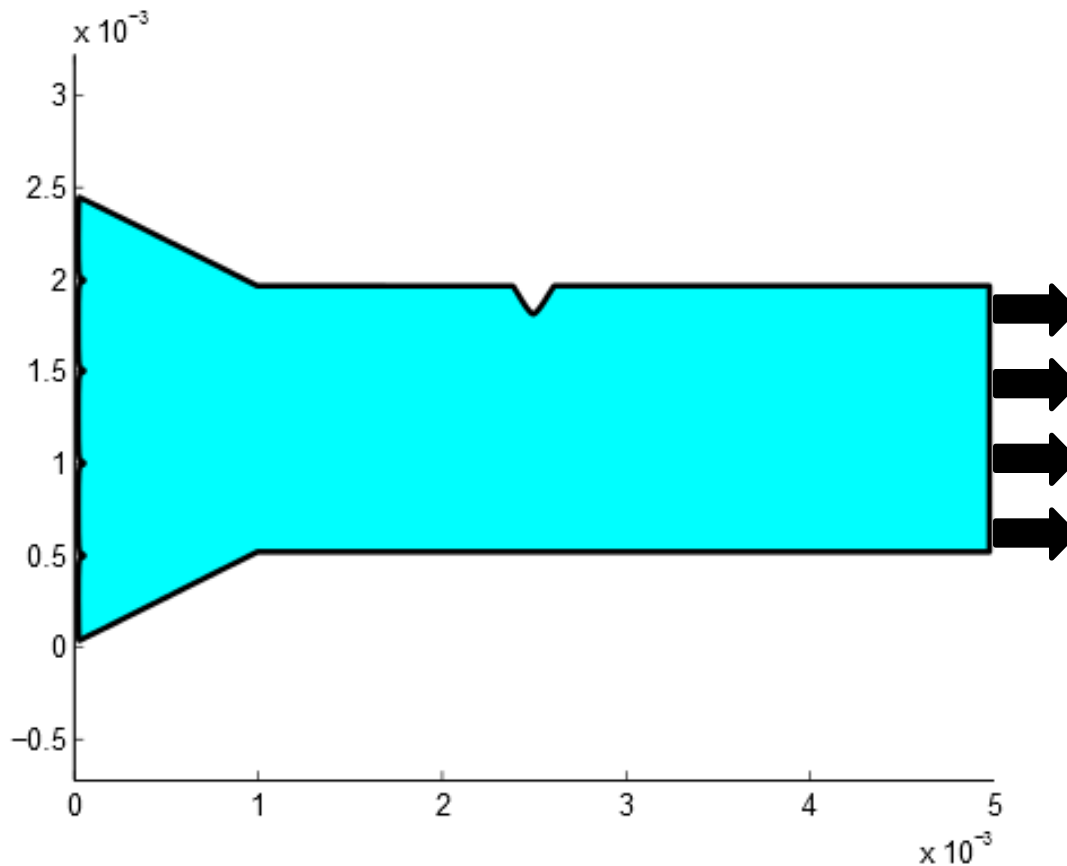
Direct Numerical Solution



Adaptive Multiscale method



Results: uni-axial tension

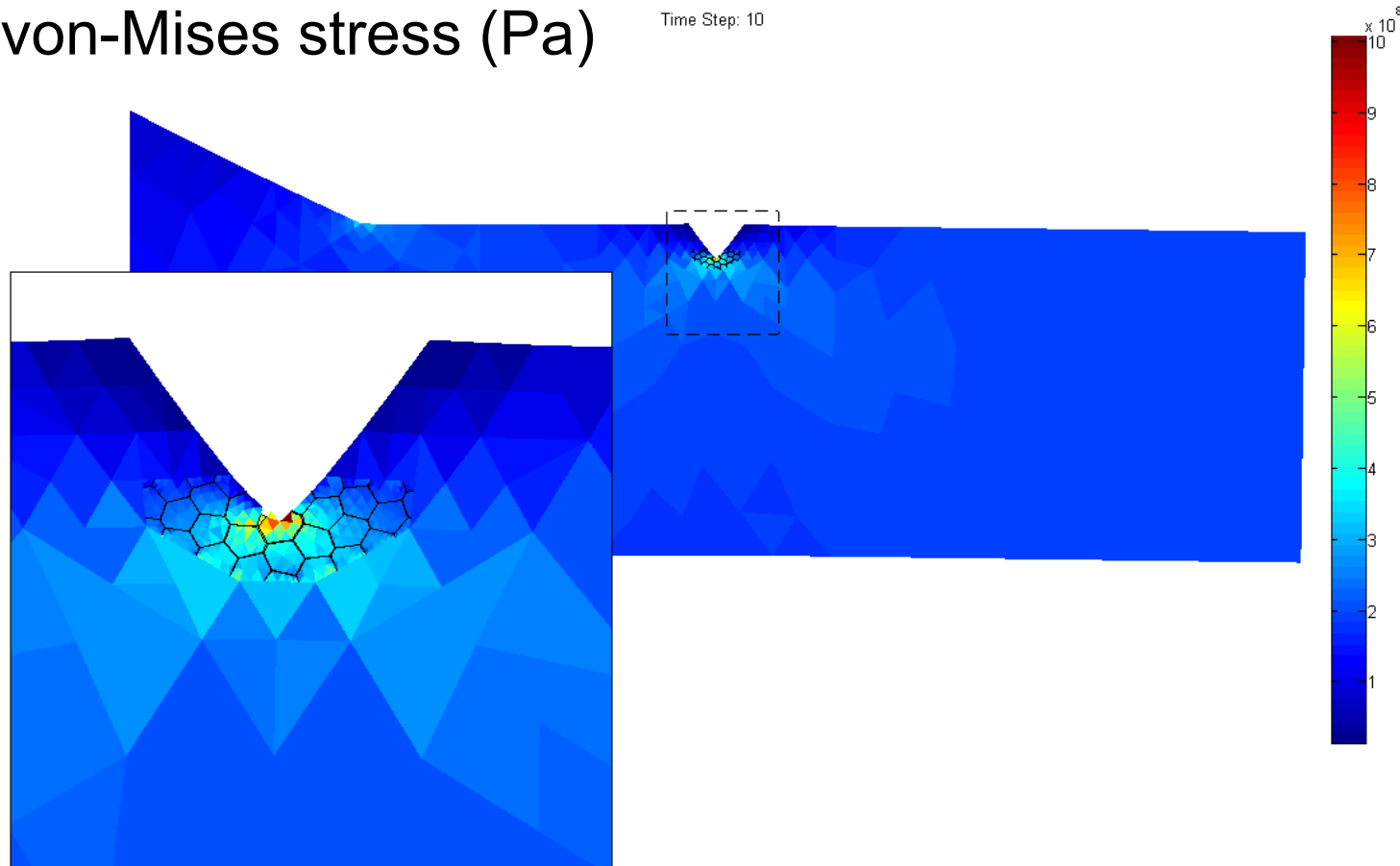


❖ Sizes are in mm

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 10

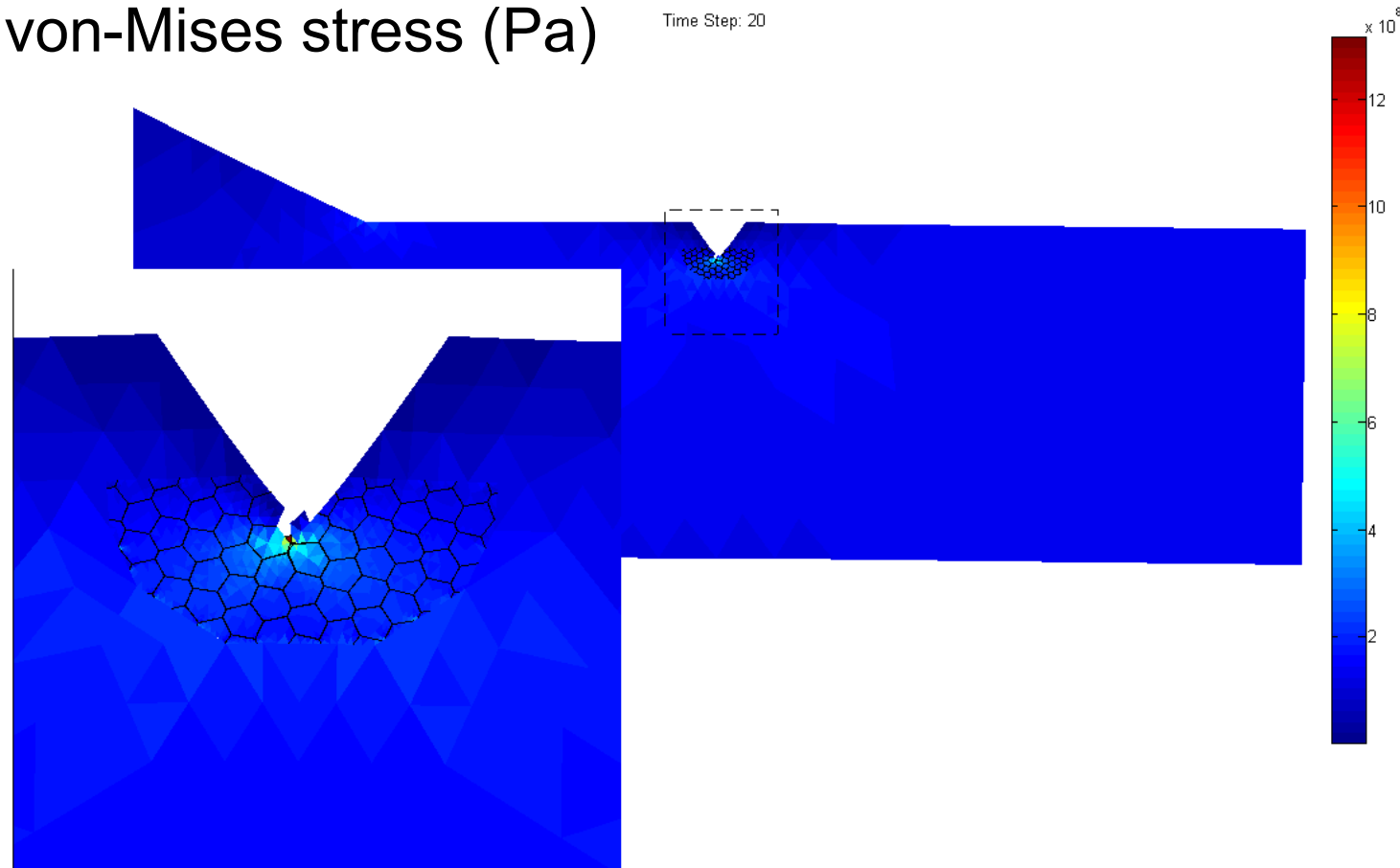


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 20

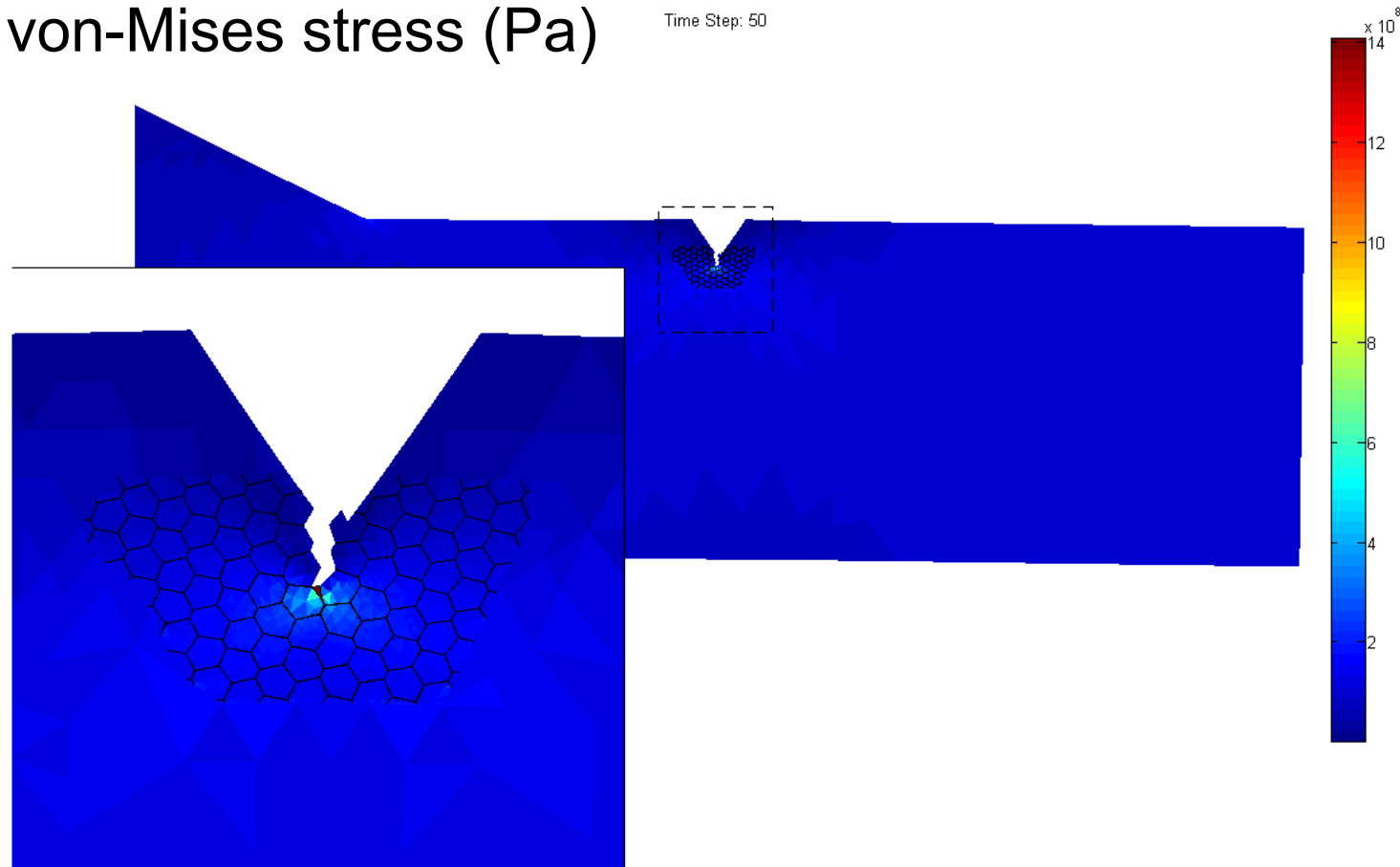


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 50

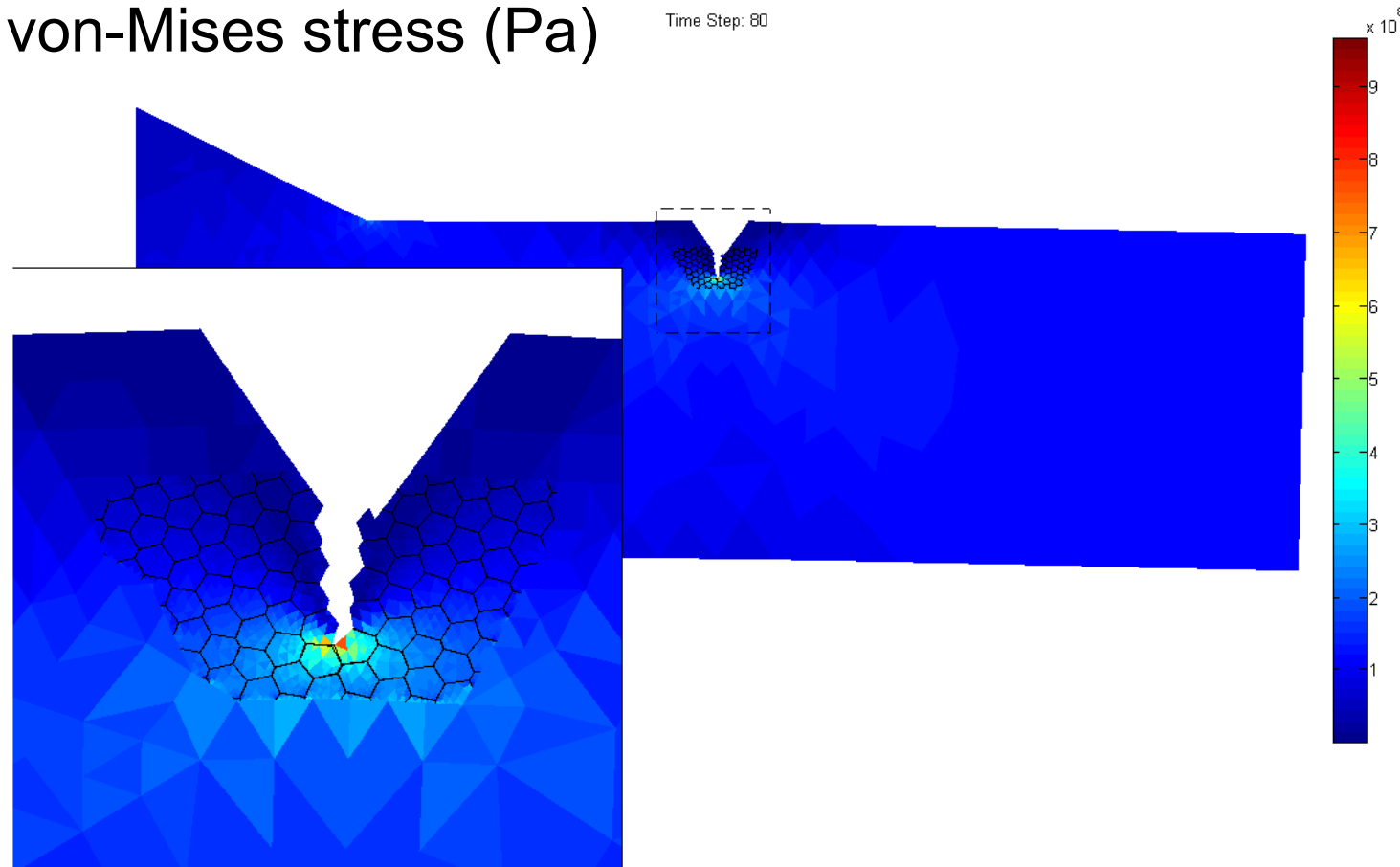


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 80

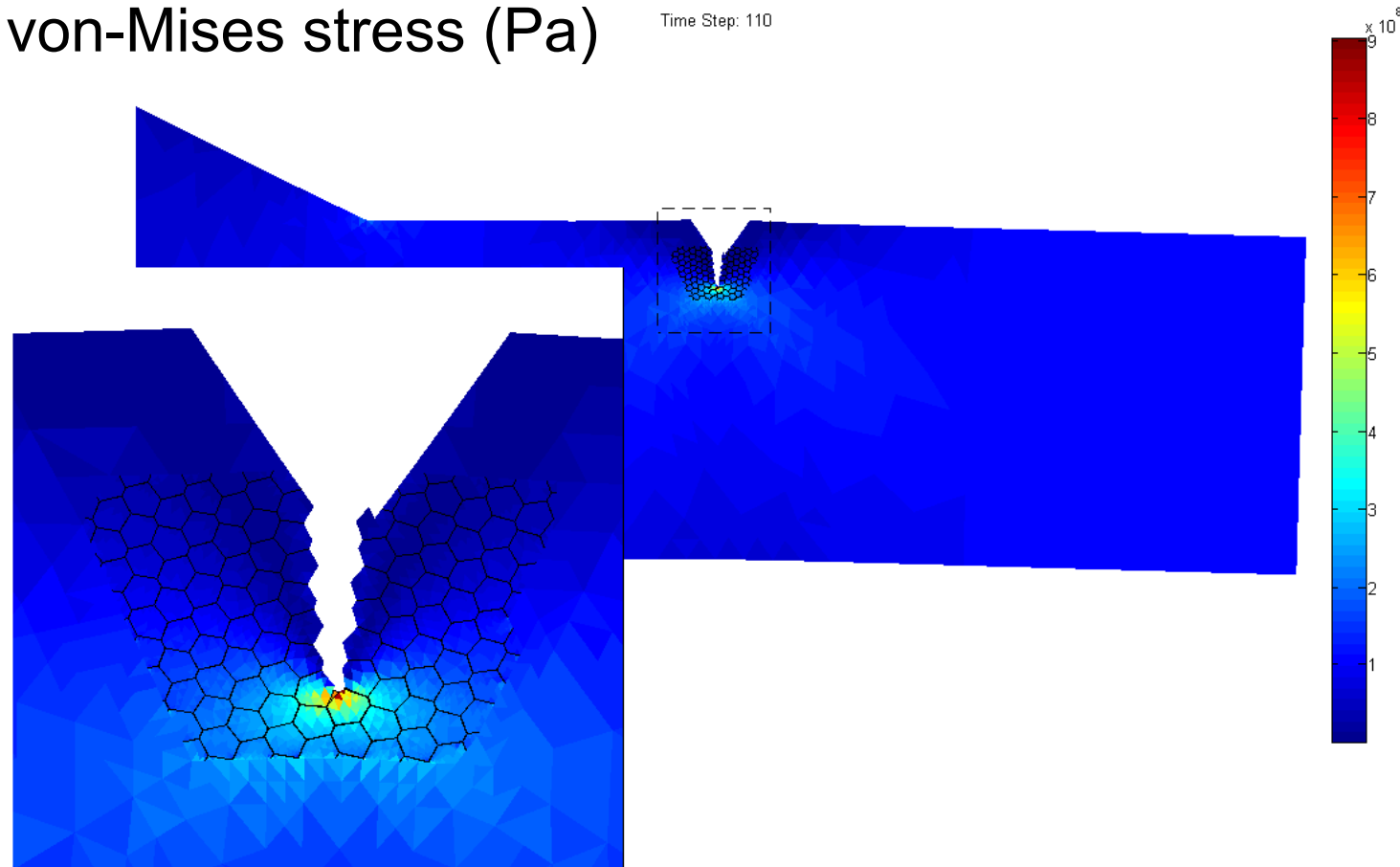


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 110



❖ 100X (magnification of displacement)

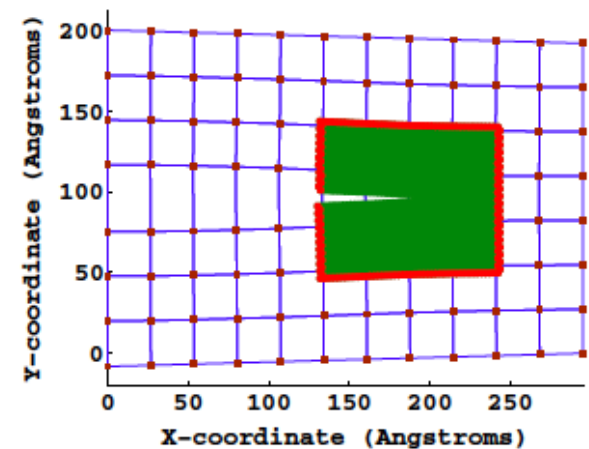
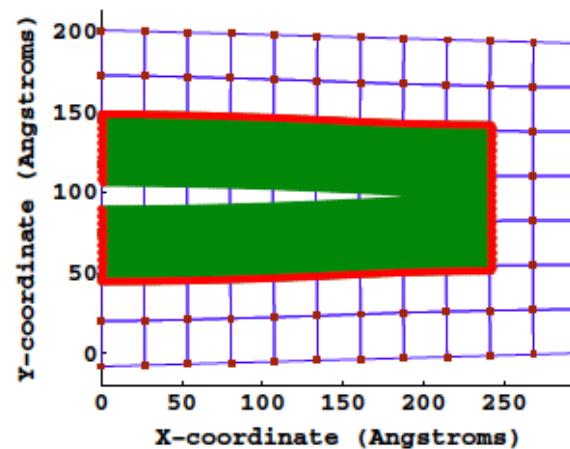
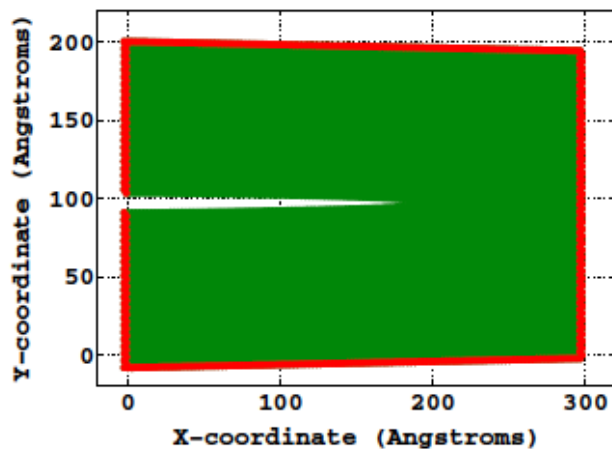
Adaptive Multiscale Method

An adaptive multiscale method was developed for discrete fracture in polycrystalline materials:

- An unstructured mesh is used for the coarse scale problem
- A local arc-length was used to control crack speed in the fully resolved region.
- A recovery based error indicator was employed to limit discretization error at each time step.

Perspectives

- coarsening once the crack is open
- molecular dynamics at the fine scale



- real-life problems! :)
- coupling with algebraic model reduction (POD)



TWO POST DOCS TWO FACULTY POSITIONS AVAILABLE

OPEN SOURCE CODES

PERMIX: Multiscale, XFEM, large deformation, coupled 2 LAMMPS, ABAQUS, OpenMP -
Fortran 2003, C++

MATLAB Codes: XFEM, 3D ISOGEOMETRIC XFEM, 2D ISOGEOMETRIC BEM, 2D MESHLESS
DOWNLOAD @ <http://cmechanicsos.users.sourceforge.net/>

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COMPUTATIONAL MECHANICS DISCUSSION GROUP

Request membership @

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IGA delamination and multi-patch coupling

- Nitsche: <http://orbilu.uni.lu/handle/10993/14460>
- IGA review and implementation: <http://orbilu.uni.lu/handle/10993/14191>
- Delamination: <http://orbilu.uni.lu/handle/10993/14468>

Meshless methods

- review and implementation: <http://orbilu.uni.lu/handle/10993/13726>