Faculty of Sciences, Technology and Communication

UNIVERSITÉ DU LUXEMBOURG
Research Unit in Engineering Sciences (RUES)

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYD

Discretisation, Multiscale Mechanics Problems & Surgical Simulation

Stéphane Bordas & Pierre Kerfriden

University of Luxembourg and Cardiff University

University of Limerick, Ireland

20140210

Interreg IV-A
Großregion - Grande Région

UNIVERSITÉ DU LUXEMBOURG

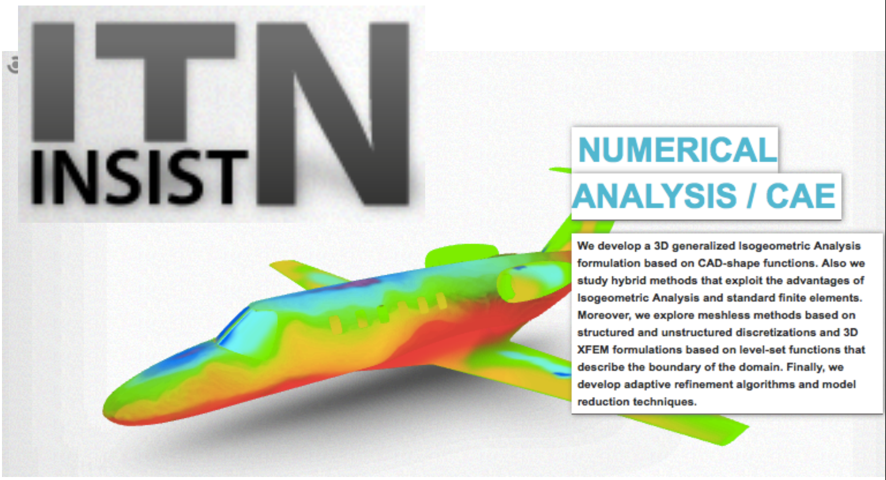
279578 - REALTCUT - Towards real time multiscale simulation of cutting in non-linear materials with applications to surgical simulation and computer guided surgery

UNIVERSITÉ DU LUXEMBOURG
Research Unit in Engineering Sciences (RUES)

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

- 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



Chicago, Illinois

IMAM
Institute of Mechanics
& Advanced Materials

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

IMAM
Institute of Mechanics
& Advanced Materials

Post-doc 2003-2006 -

Meshless/XFEM Geomechanics

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& Advanced Materials

Lecturer in civil engineering

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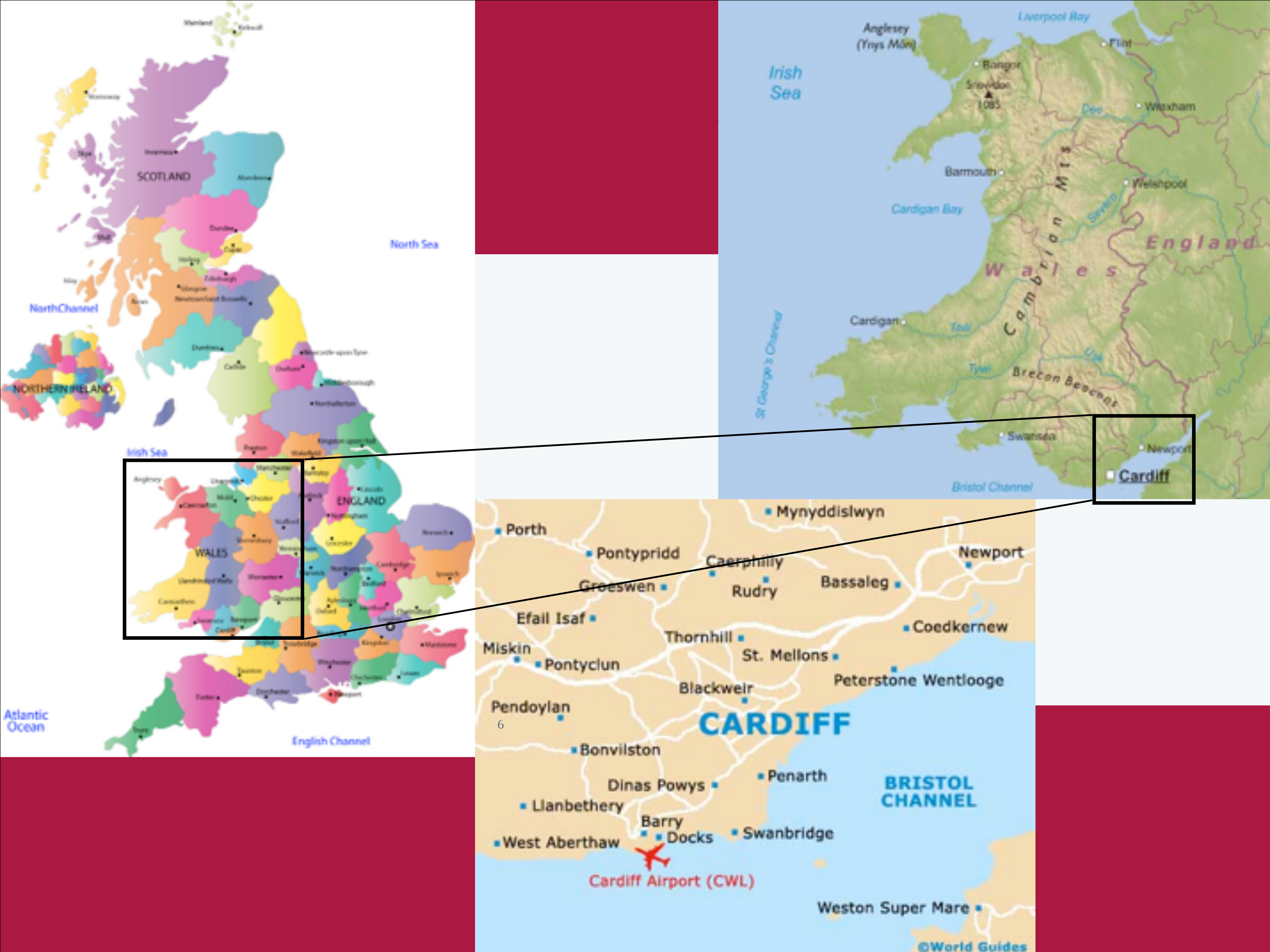
GLASGOW



SCOTLAND
North Sea
NorthChannel
NORTHERN IRELAND
Irish Sea
WALES
ENGLAND
Atlantic Ocean
English Channel
Liverpool Bay
Anglesey (Ynys Môn)
Irish Sea
Flint
Bangor
Snowdon 1085
Dee
Wrexham
Barmouth
Cambrian Mts
Welshpool
Cardigan Bay
Severn
England
Wales
Cardigan
Teifi
Usk
Tywi
Brecon Beacons
St George's Channel
Swansea
Newport
Cardiff
Bristol Channel
Mynyddislwyn
Porth
Pontypridd
Caerphilly
Newport
Groeswen
Rudry
Bassaleg
Efail Isaf
Coedkernew
Thornhill
Miskin
St. Mellons
Pontyclun
Peterstone Wentlooge
Blackweir
Pendoylan
CARDIFF
Bonvilston
Penarth
BRISTOL CHANNEL
Dinas Powys
Llanbethery
Barry
Docks
Swanbridge
West Aberthaw
Cardiff Airport (CWL)
Weston Super Mare
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Institute of mechanics and advanced materials

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

IMAM
Institute of Mechanics & Advanced Materials

Theoretical & Computational

Tribology & Contact Mechanics

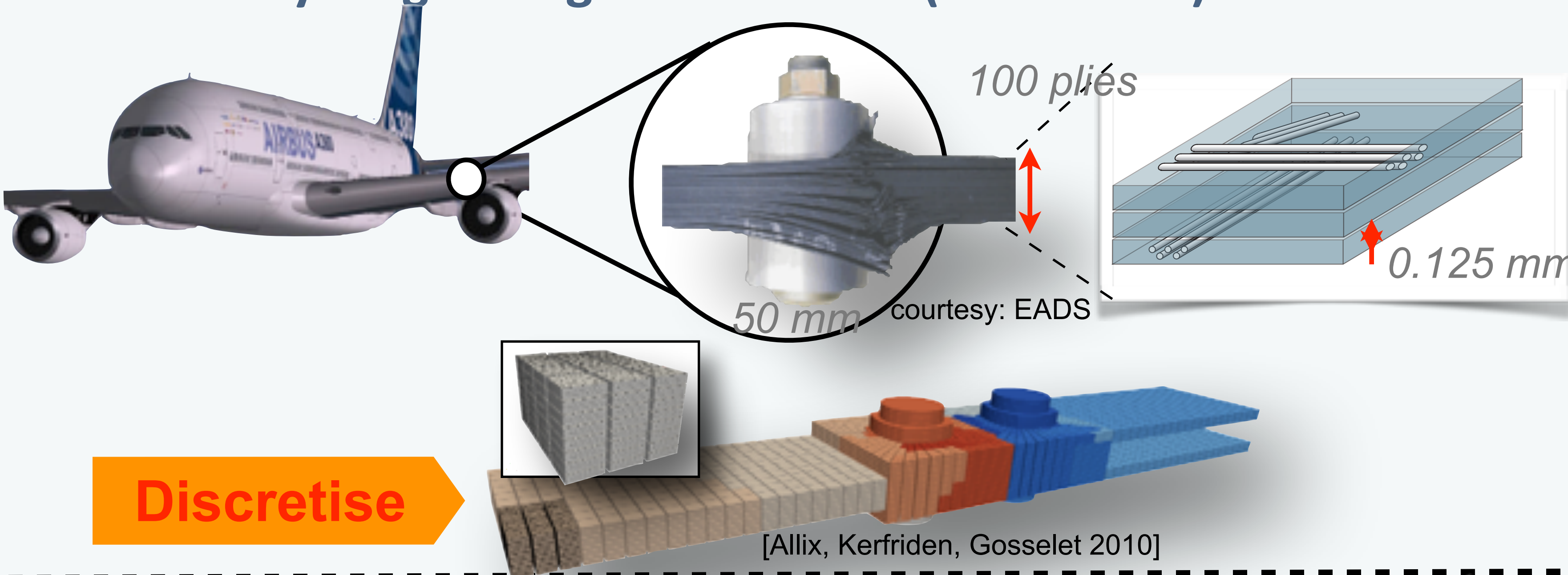
Experiments

Theory

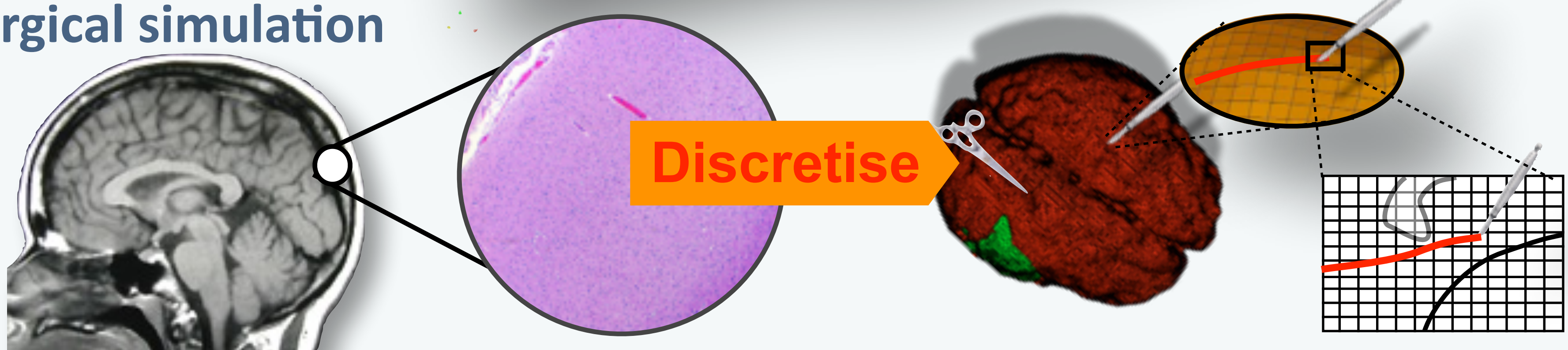
Computational Mechanics

Motivation: multiscale fracture of engineering structures and materials

Practical early-stage design simulations (interactive)



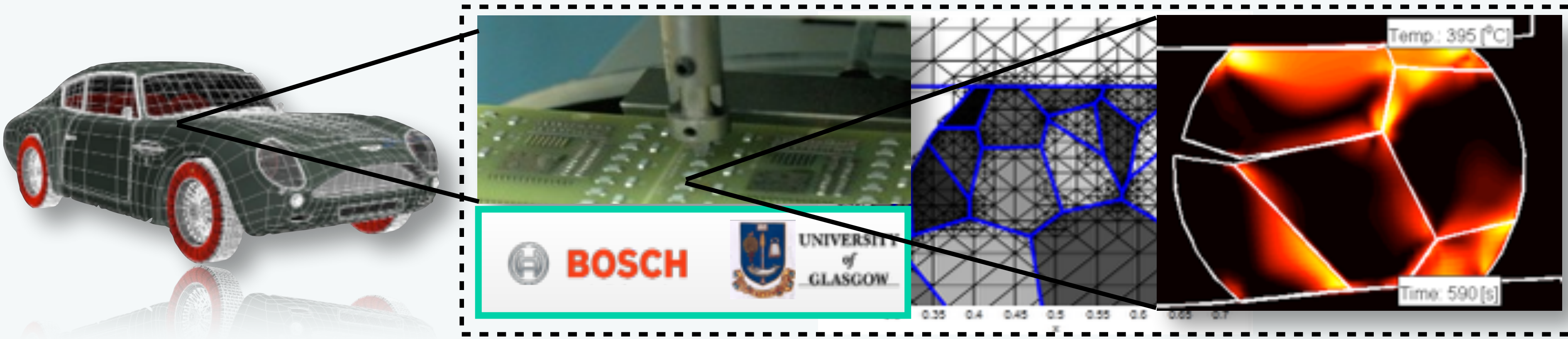
Surgical simulation

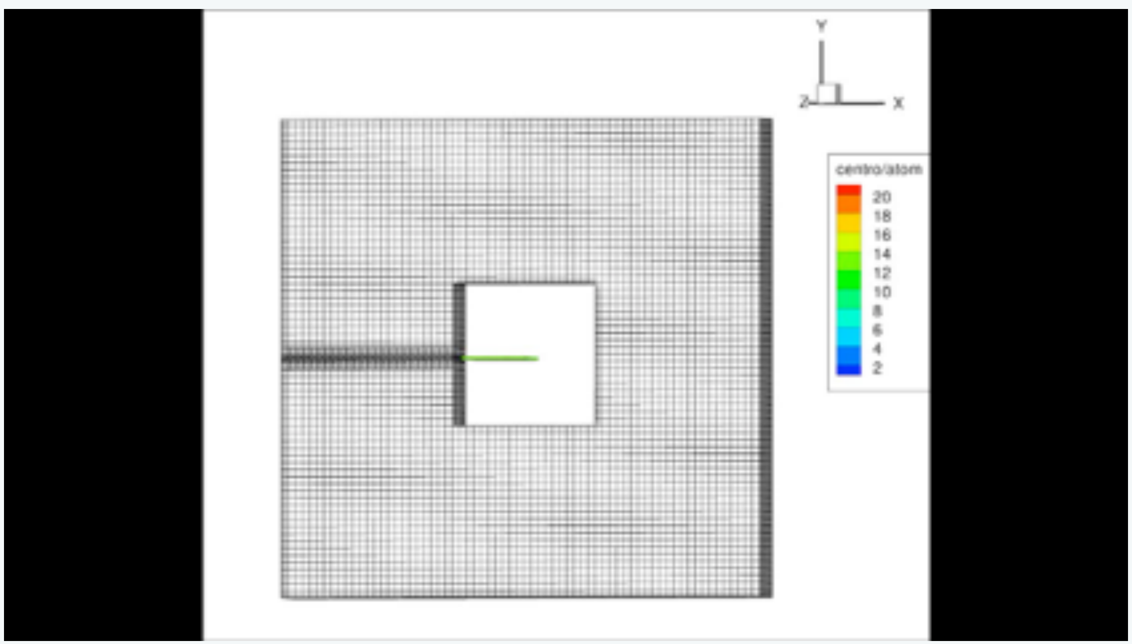


- Reduce the problem size while controlling the error (in QoI) when solving very large (multiscale) mechanics problems

Motivation: multiscale fracture of engineering structures and materials

Solder joint durability (microelectronics), Bosch GmbH





Model reduction

✓ multi-scale & homogenisation
✓ algebraic model reduction (using POD
✓ Newton-Krylov, "local/global", domai
decomposition

Discretization

➡ partition of unity enrichment
✓ ~~(enriched) meshless methods~~
✓ level sets

➡ isogeometric analysis
➡ implicit boundaries

Error control

✓ XFEM: goal-oriented error estimates
- used by CENAERO (Morfeo XFEM)

✓ meshless methods for fracture
✓ error estimation for reduced models

Part I. Streamlining the CAD-analysis transition

Part II. Some advances in enriched FEM

Part III. Application to H cutting of Si wafers

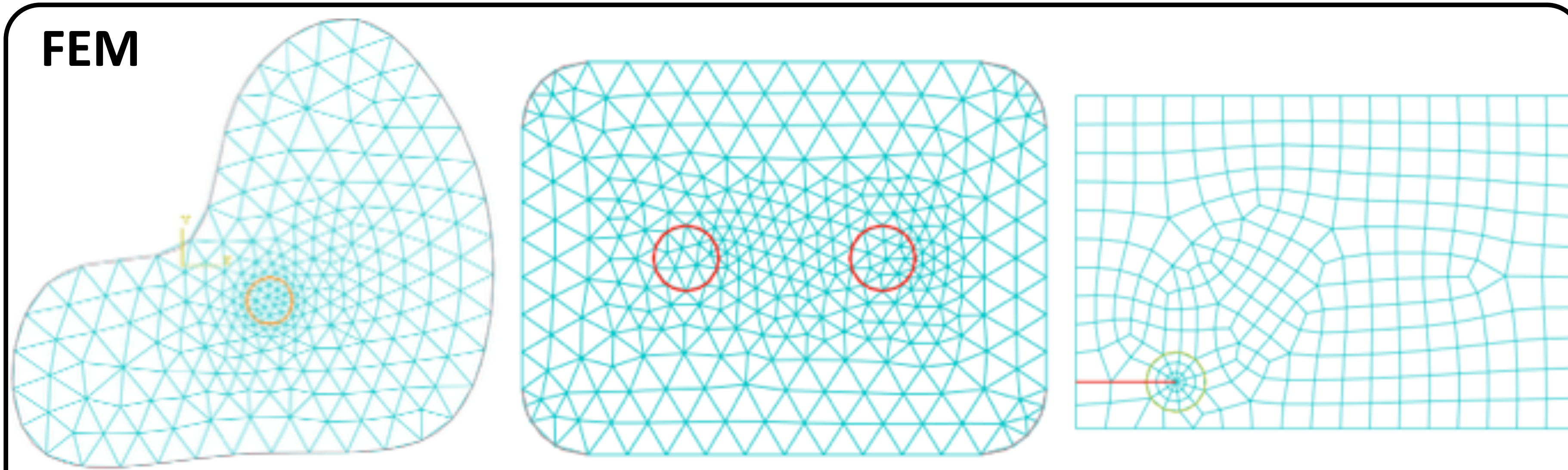
Part IV. Application to interactive cutting sim.

Part I. Streamlining the CAD-analysis transition

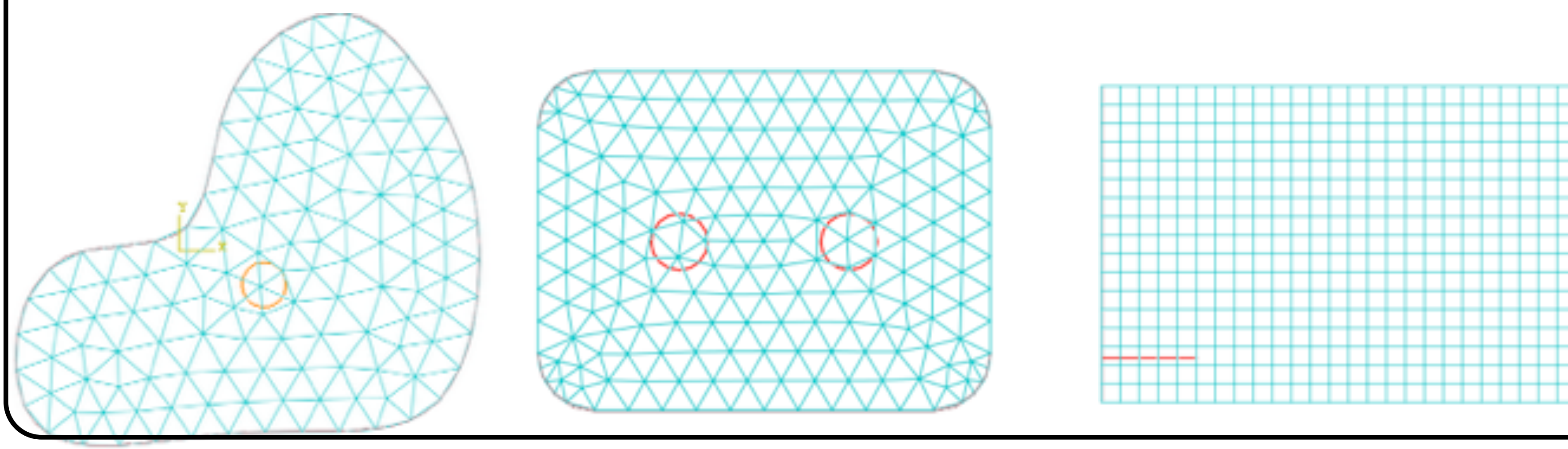
Coupling, or decoupling?

Motivation: free boundary problems - mesh burden

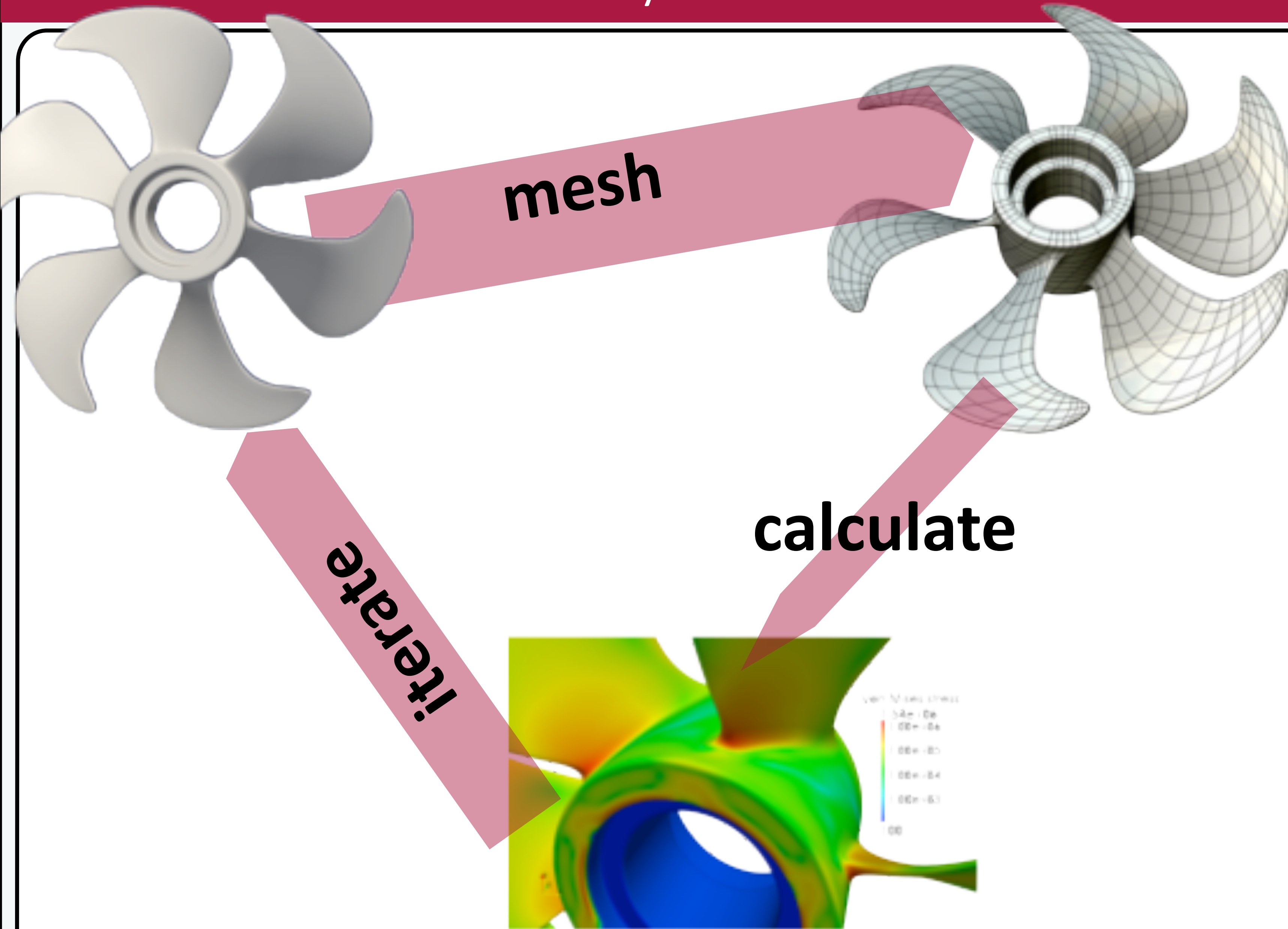
FEM



XFEM

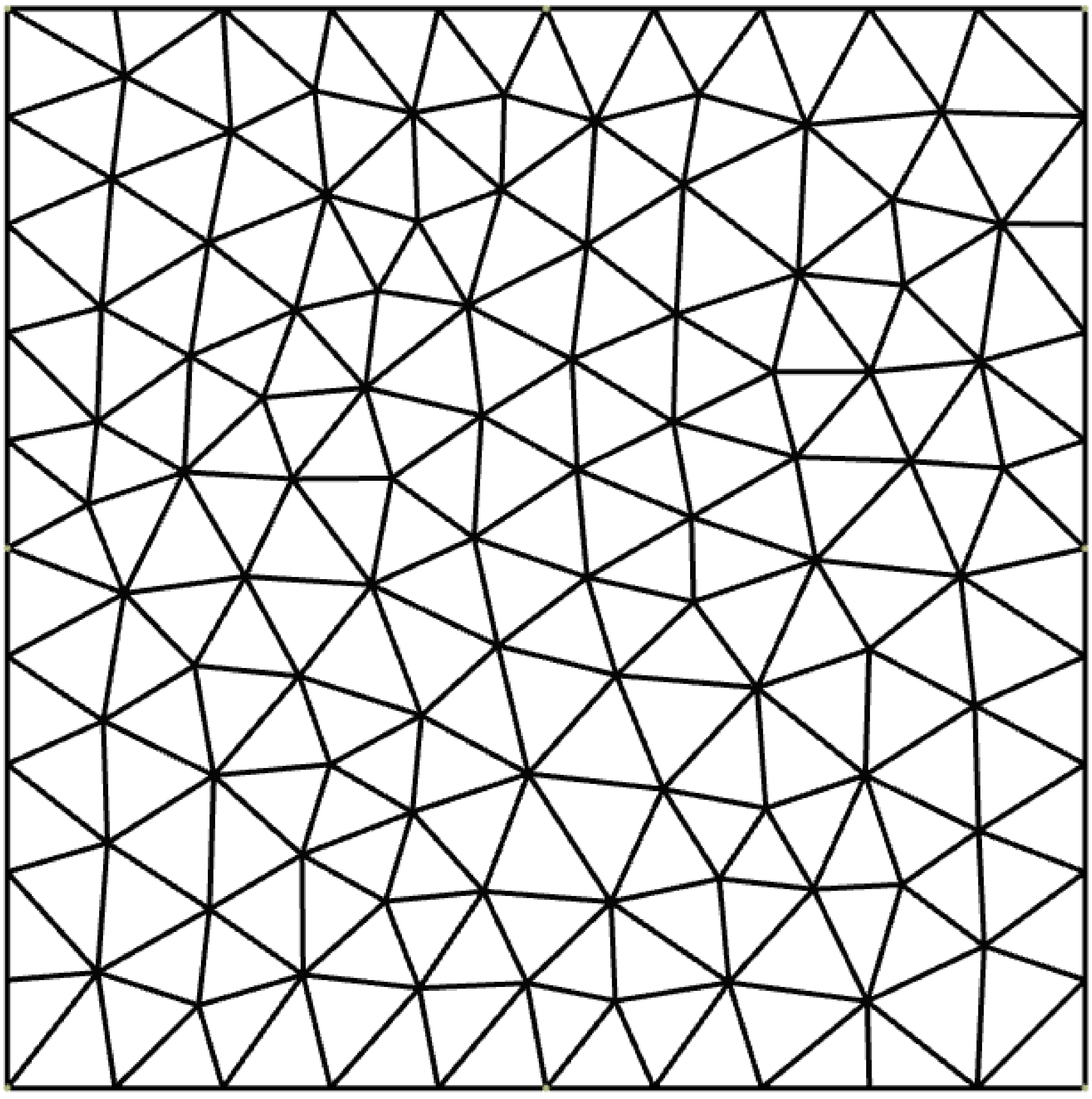


CAD to Analysis

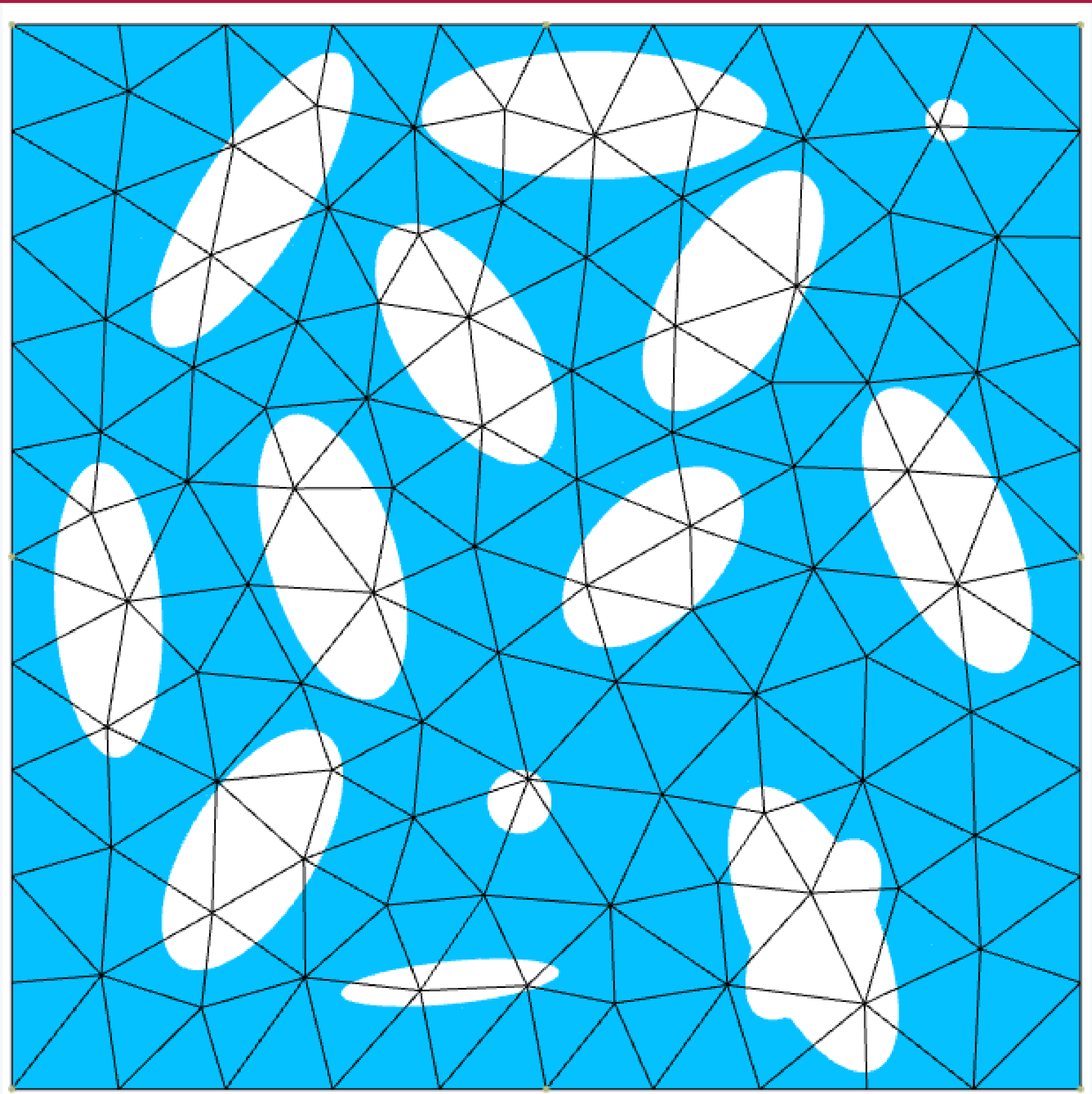


stress distribution

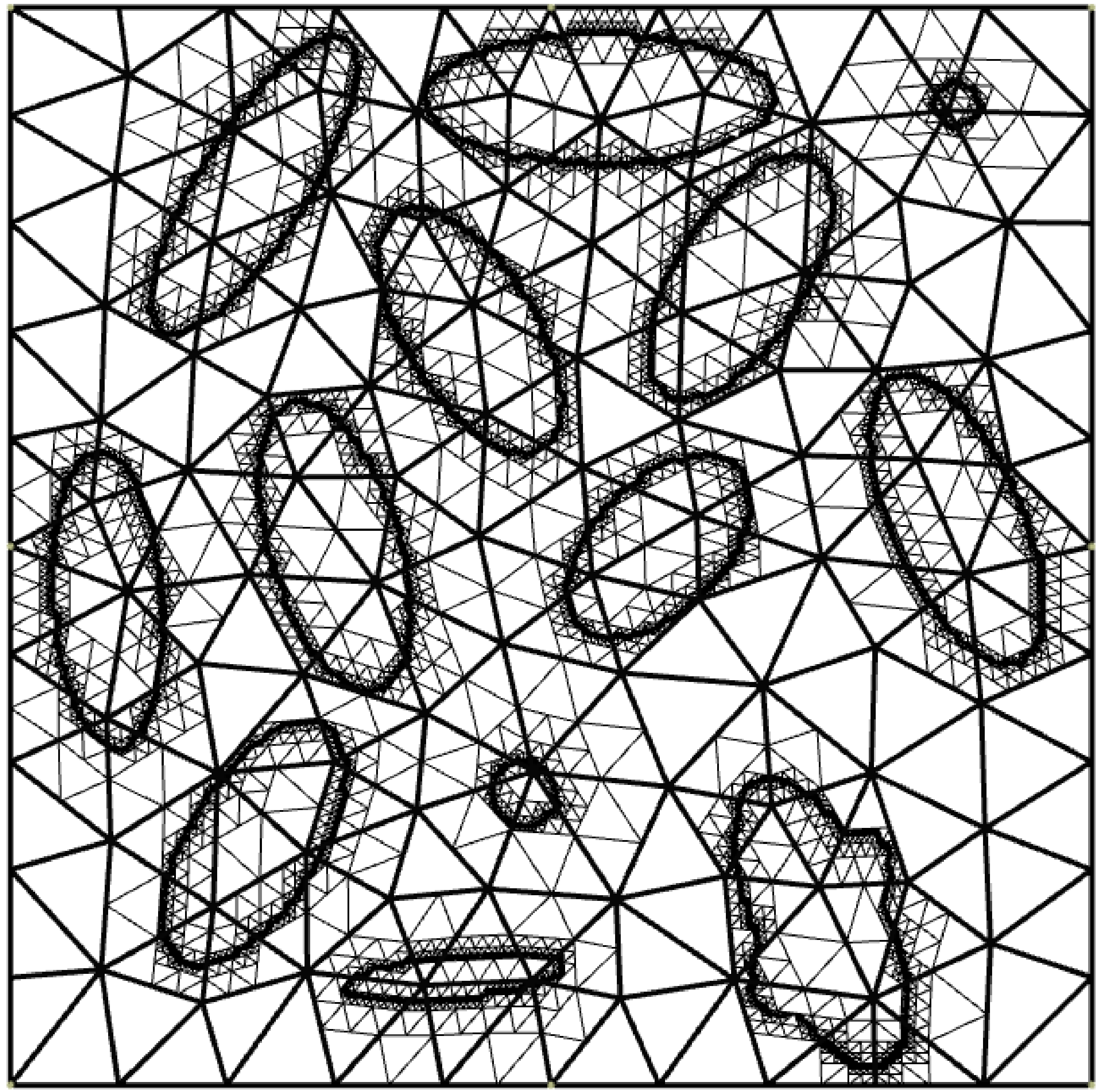
One would like to be able to use such a mesh



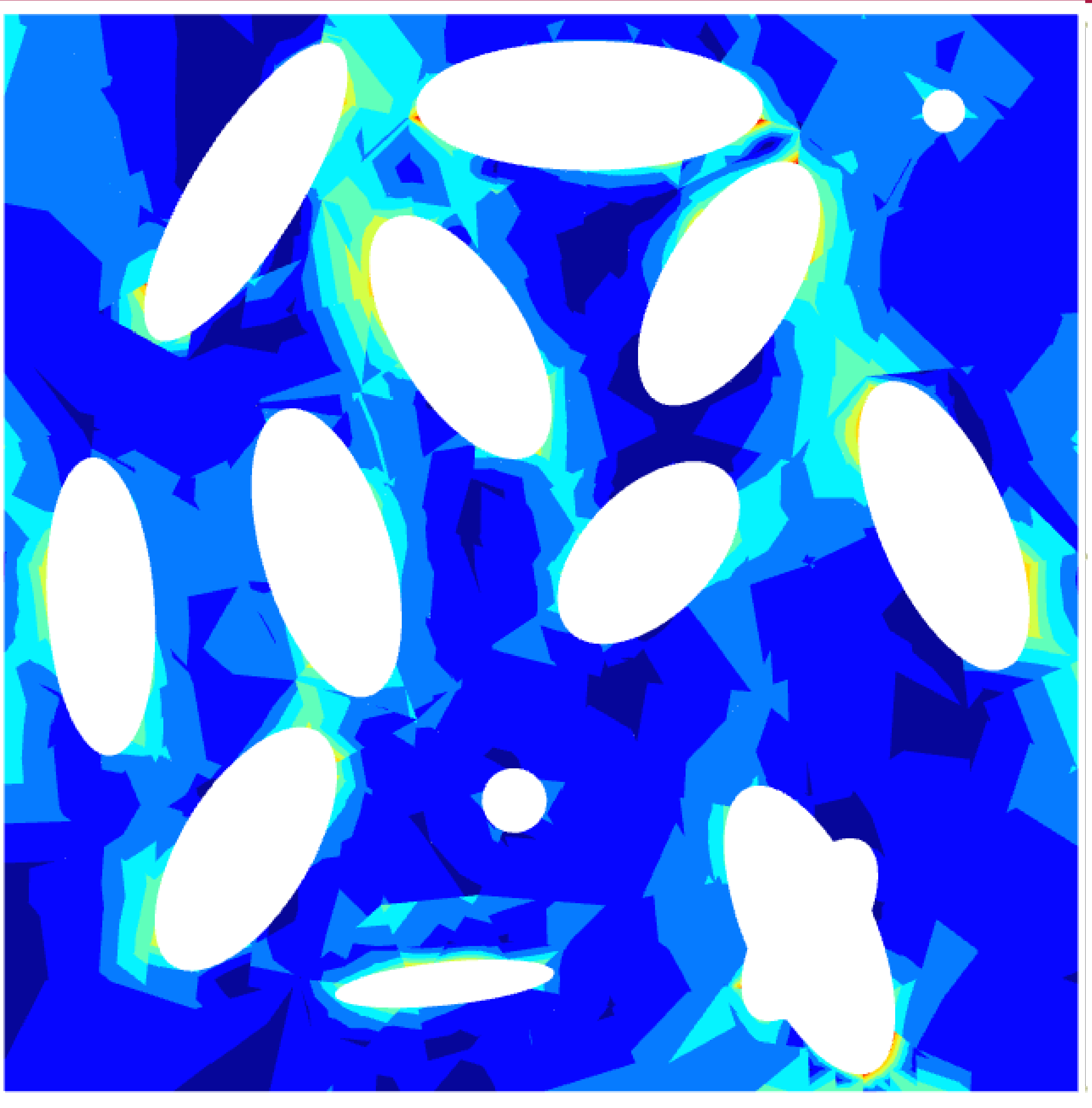
Superimpose the geometry onto an arbitrary background mesh



Compute interactions between the geometry and the mesh

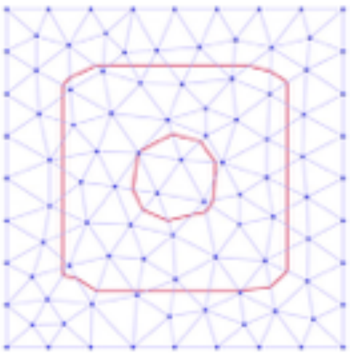


Perform the analysis



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)

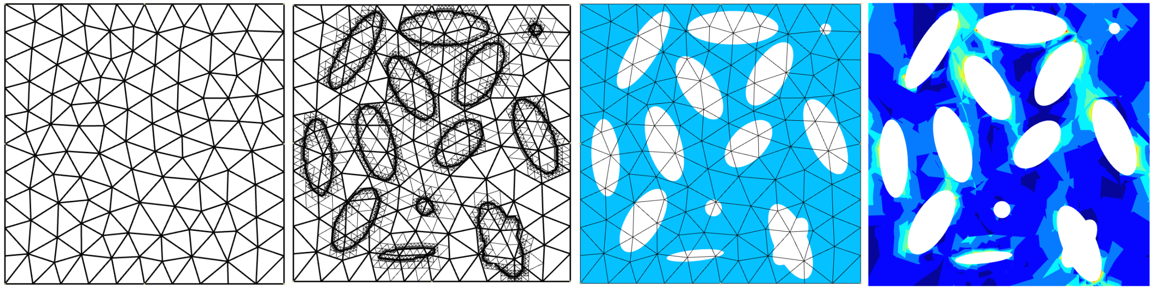


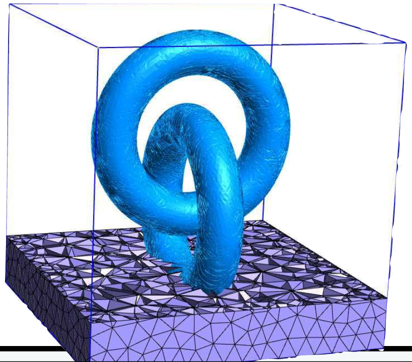
✓ Easy adaptive refinement + error estimation (Nadal, 2013)

✓ Flexibility of choosing basis functions

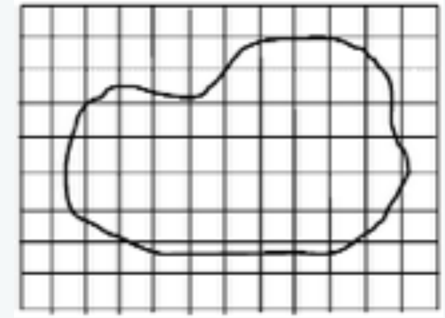
- Accuracy for complicated geometries? BCs on implicit surfaces?

➡ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi, *et al.* 2011)

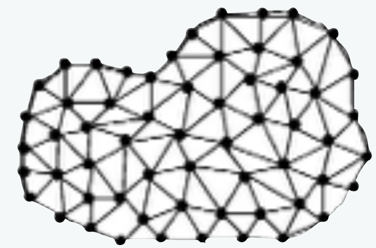


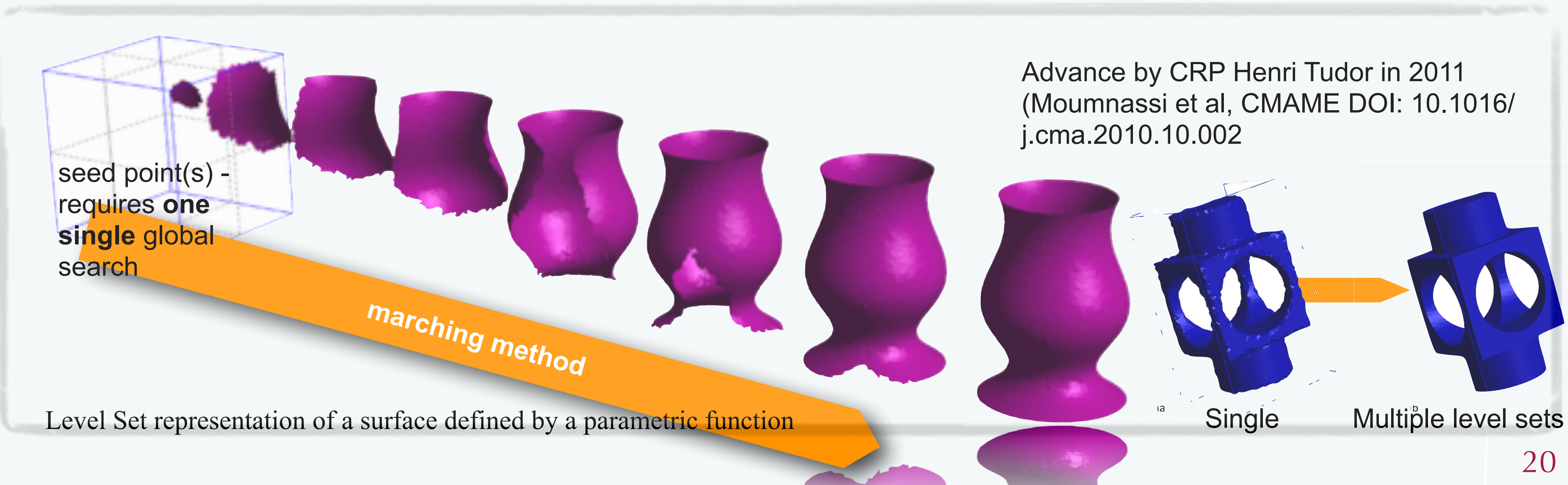


Ex: Moumnassi et al, CMAME DOI:10.1016/j.cma.2010.10.002



- 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



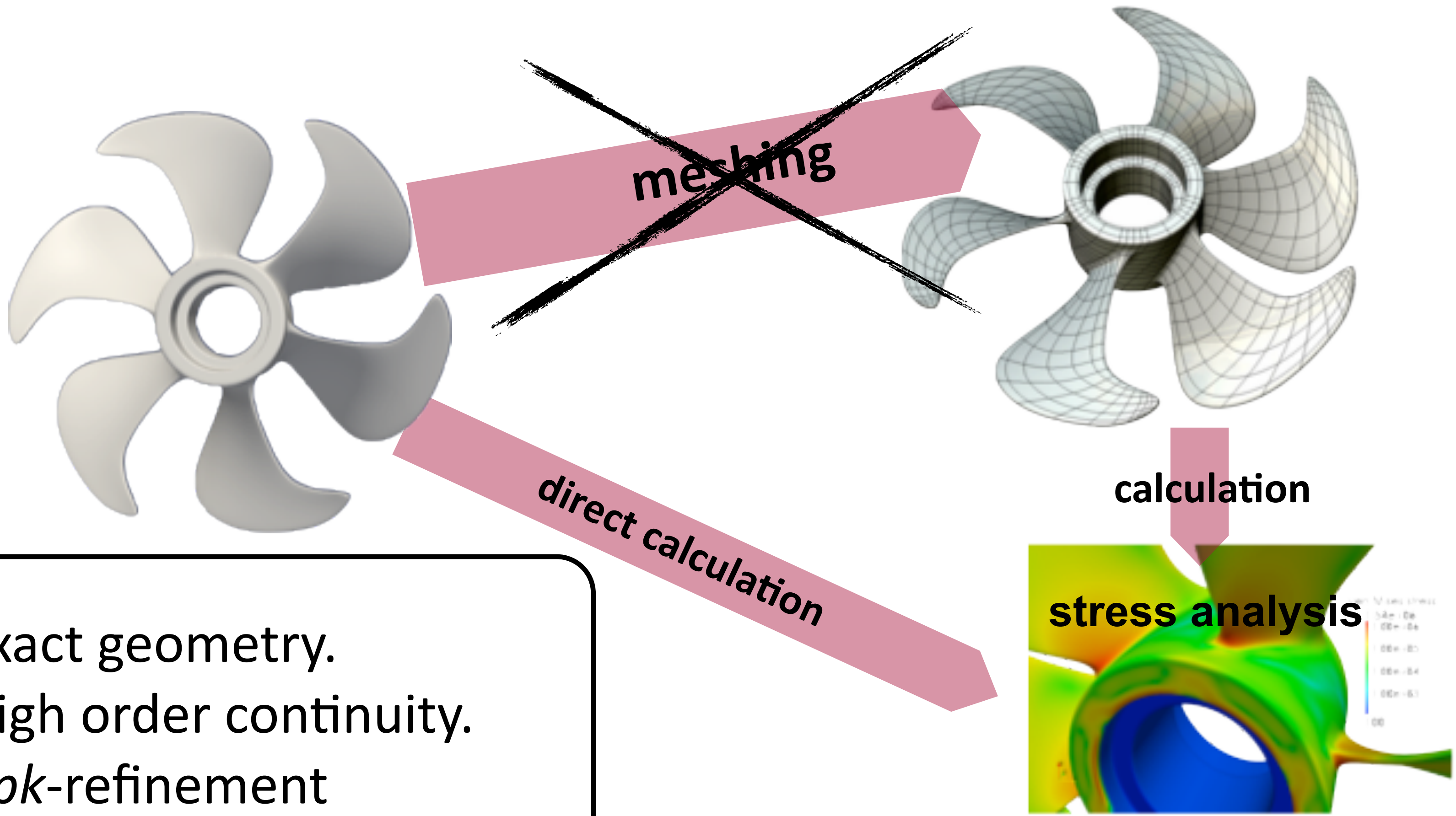


Level Set representation of a surface defined by a parametric function

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 **patch**es must be **glue**d 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).

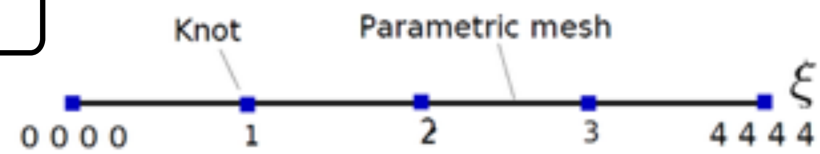
3. IGABEM with T-splines for 3D acoustic problems (Simpson, *et al*. 2013 - MAFELAP2013 TH1515).

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

Knot vector

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

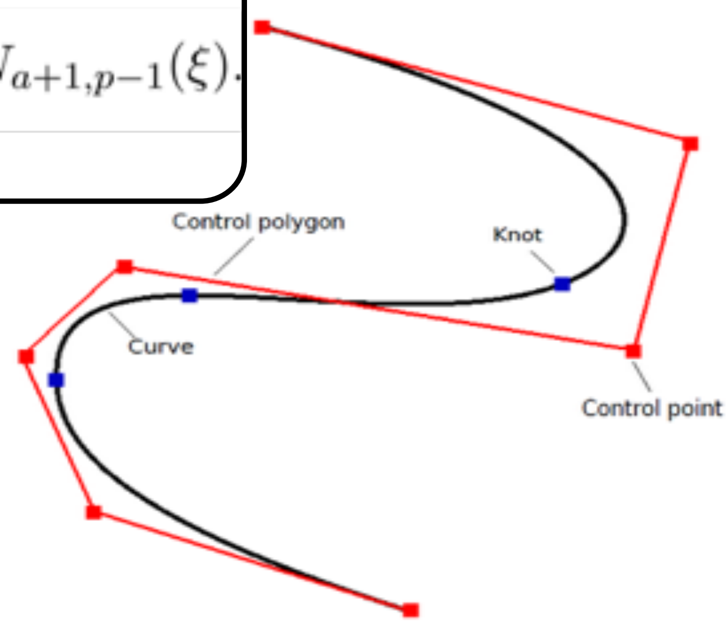
$$\Xi = \{\xi_1,\ \xi_2\ ,\ \cdots,\ \xi_{n+p+1}\}$$



B-spline basis function

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

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



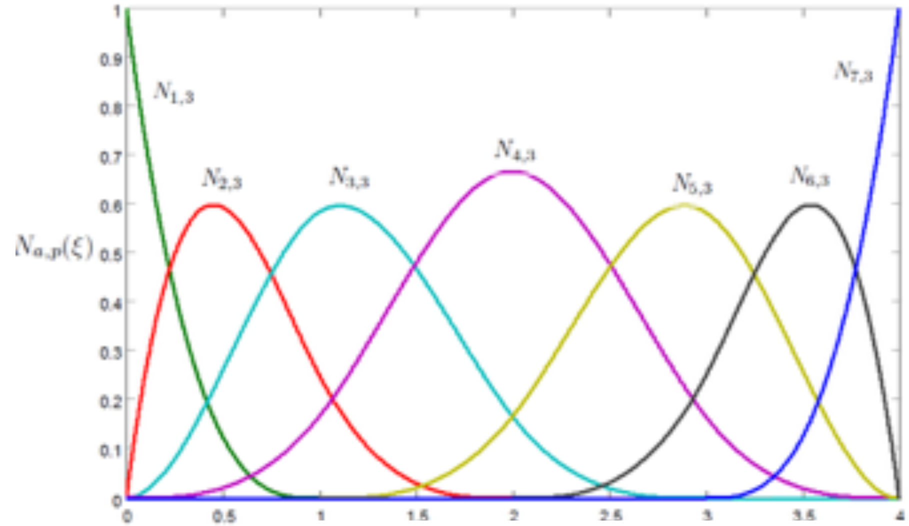
NURBS basis function

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

Properties of NURBS

- Partition of Unity

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



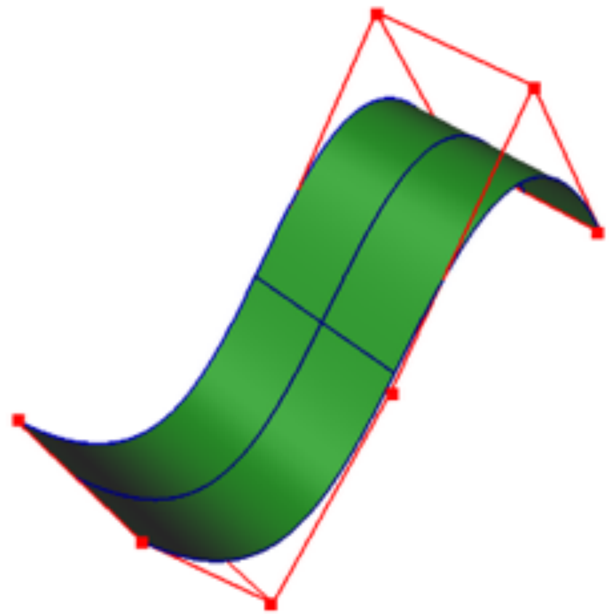
- Non-negative

- *p-1* continuous derivatives

- Tensor product property

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

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



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

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

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

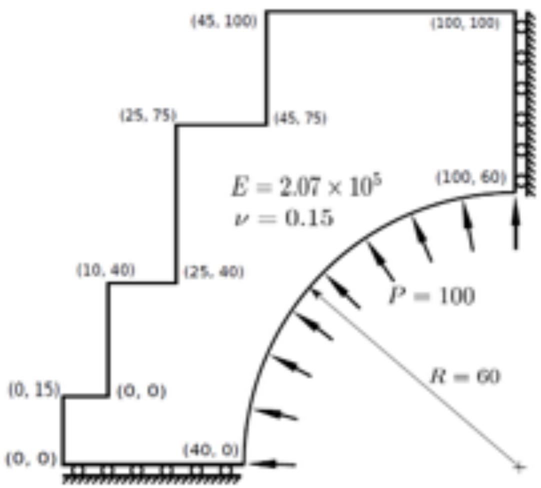
Discretise the geometry and solution field using NURBS

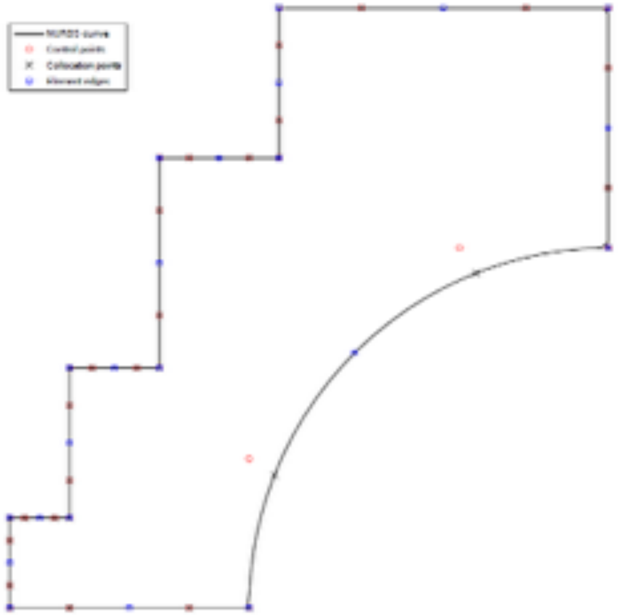
$$\mathbf{x} = \sum_{A=1}^{n_A} N_A(\xi)\mathbf{B}_A = N_A(\xi)\mathbf{B}_A$$

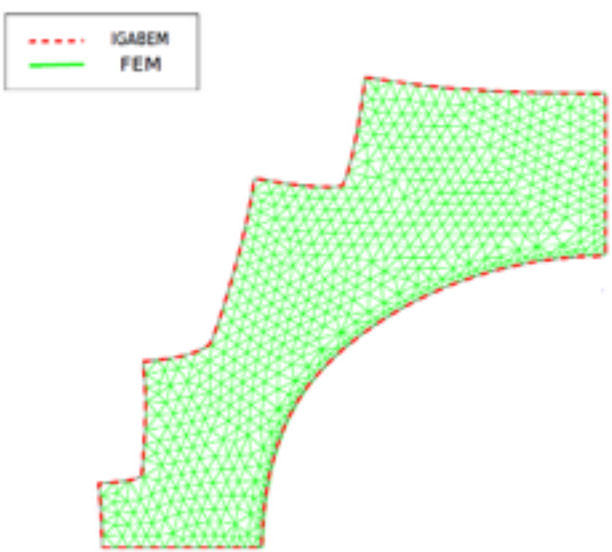
$$\mathbf{u} = \sum_{A=1}^{n_A} N_A(\xi)\mathbf{u}_A = N_A(\xi)\mathbf{u}_A$$

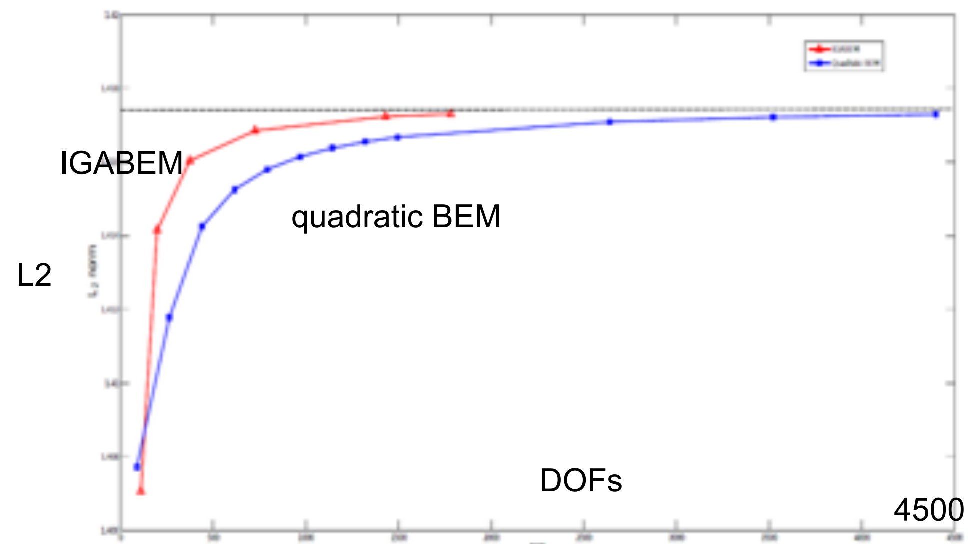
$$\mathbf{t} = \sum_{B=1}^{n_B} N_B(\xi)\mathbf{t}_B = N_B(\xi)\mathbf{t}_B$$

Nuclear reactor

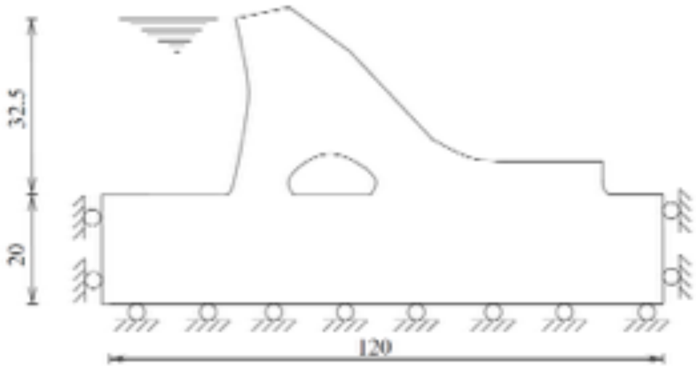


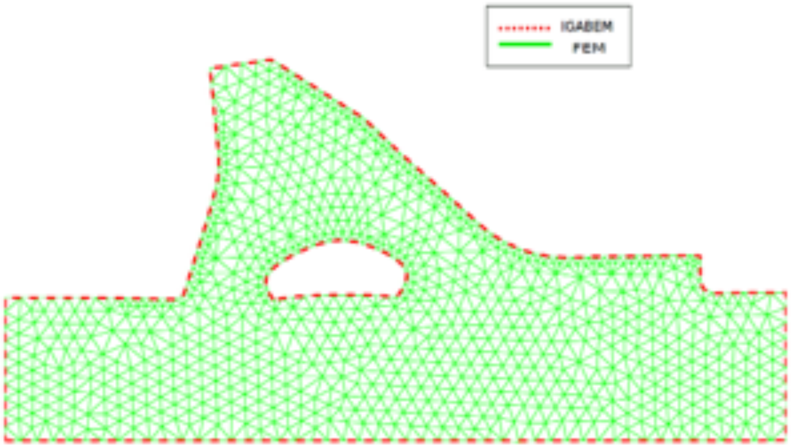


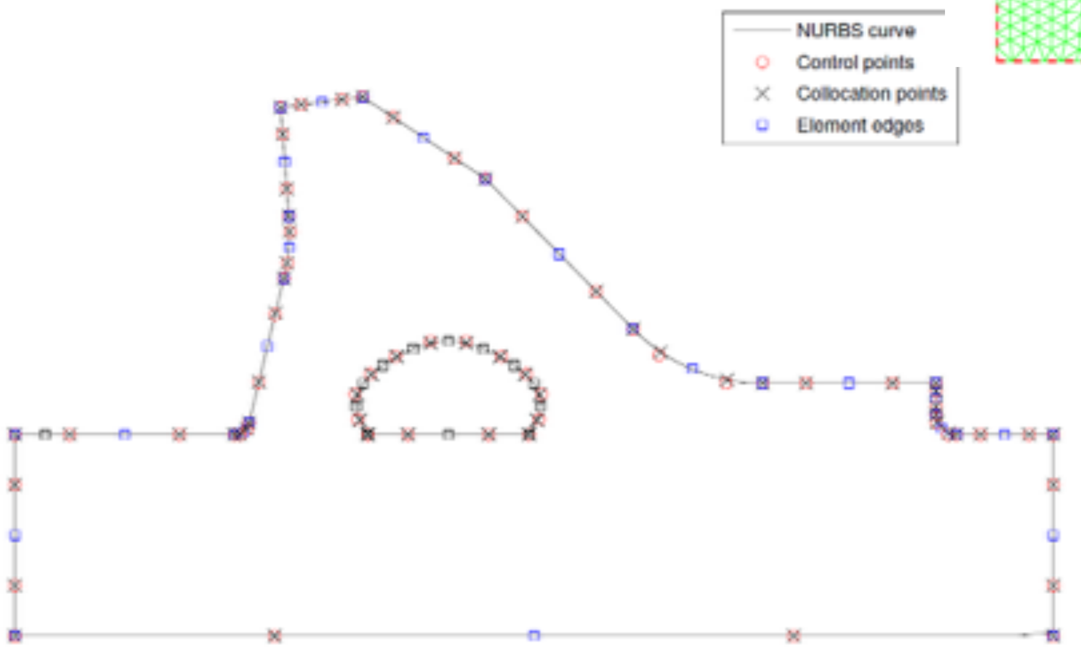




Dam



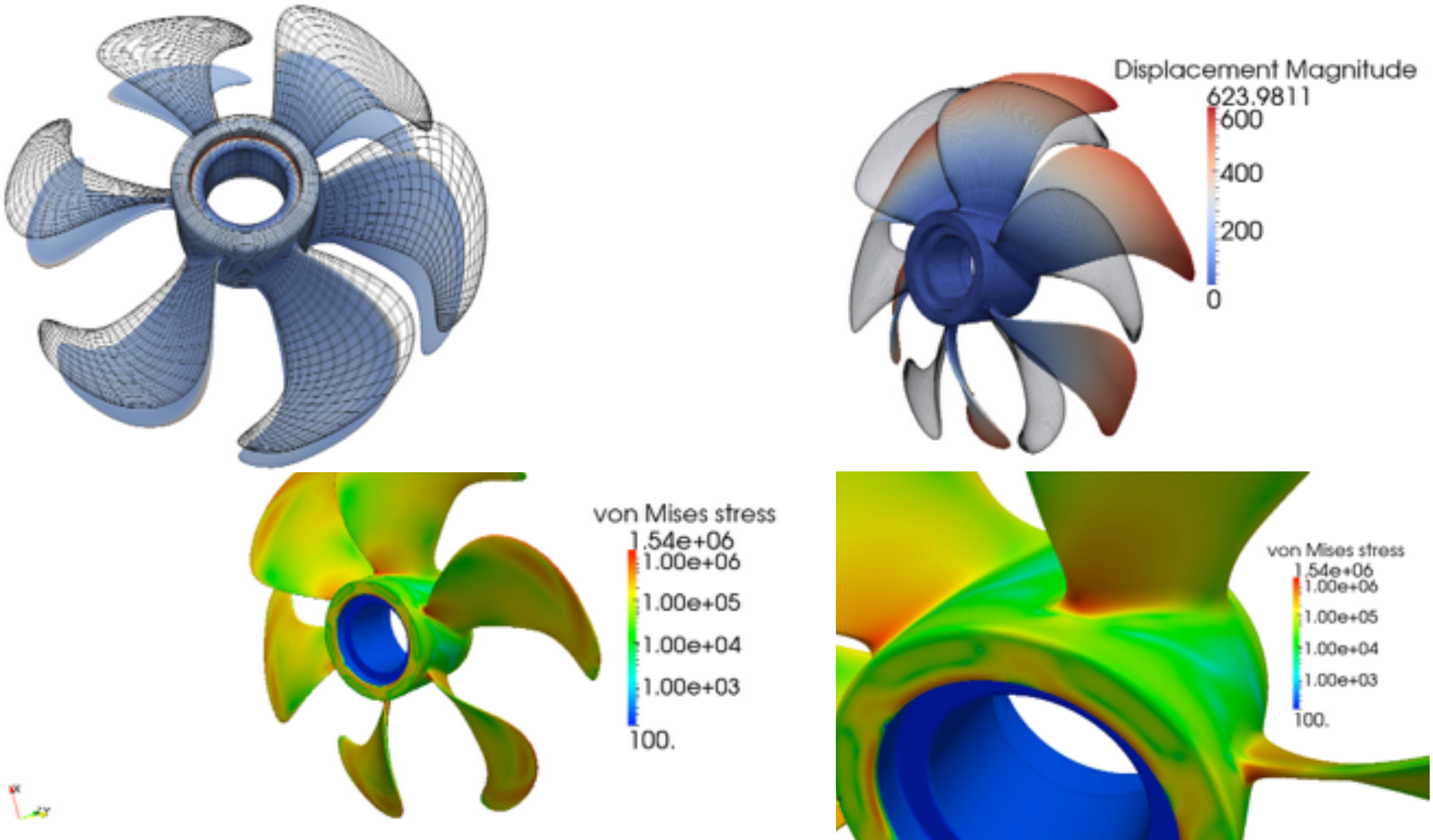




Stress analysis without meshing: isogeometric boundary-element method

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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ITN INSIST

Handling discontinuities in isogeometric formulations

Faculty of Sciences, Technology and Communication

erc

with Nguyen Vinh Phu, Marie Curie Fellow

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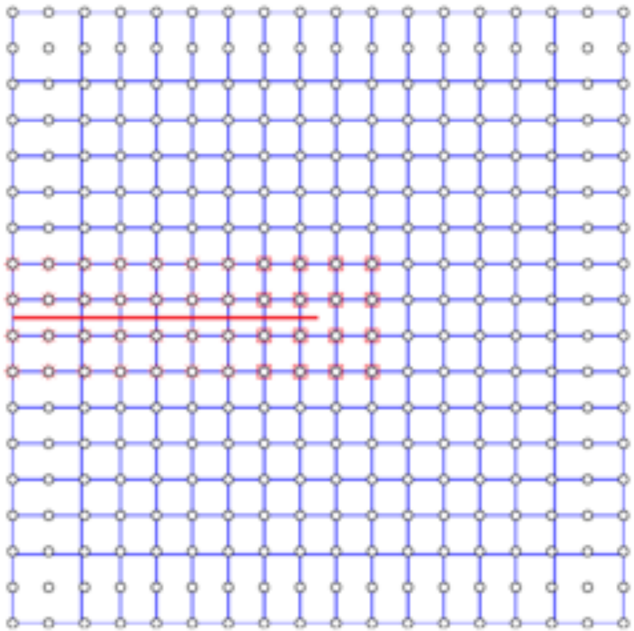
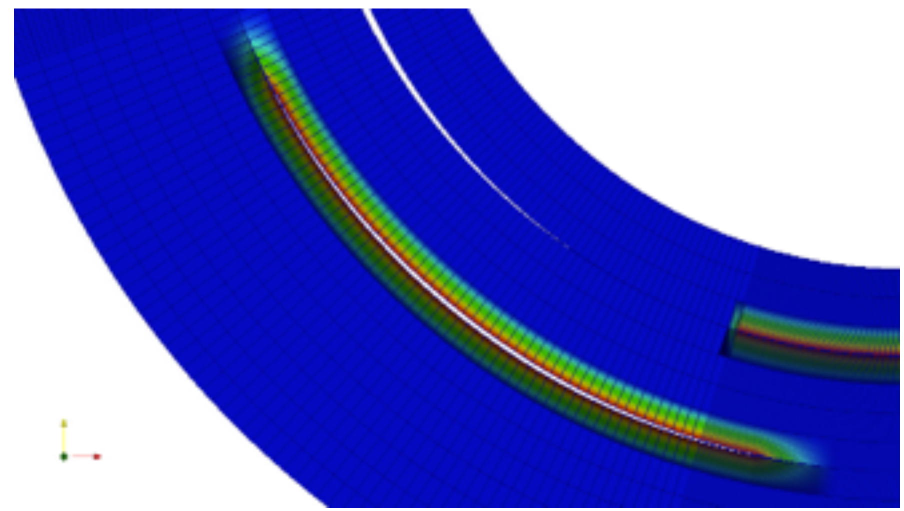
Discontinuities modeling

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

PUM enriched methods (XIGA)

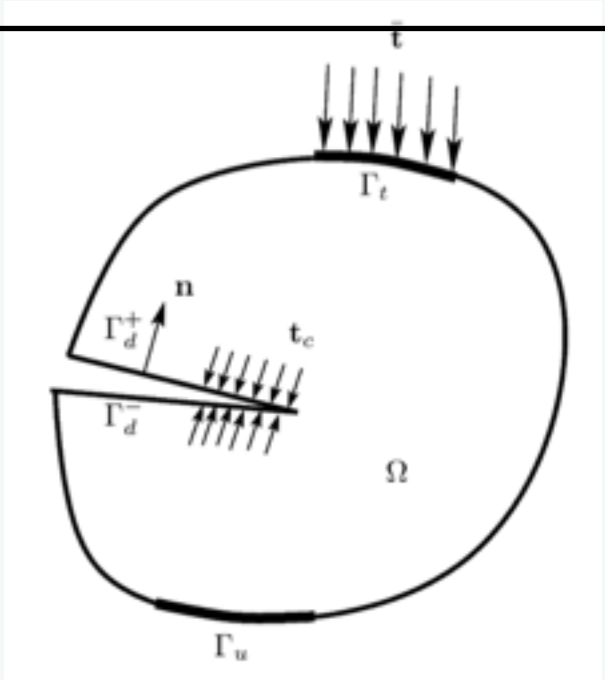
$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} R_I(\mathbf{x}) \mathbf{u}_I + \sum_{J \in \mathcal{S}^c} R_J(\mathbf{x}) \Phi(\mathbf{x}) \mathbf{a}_J$$

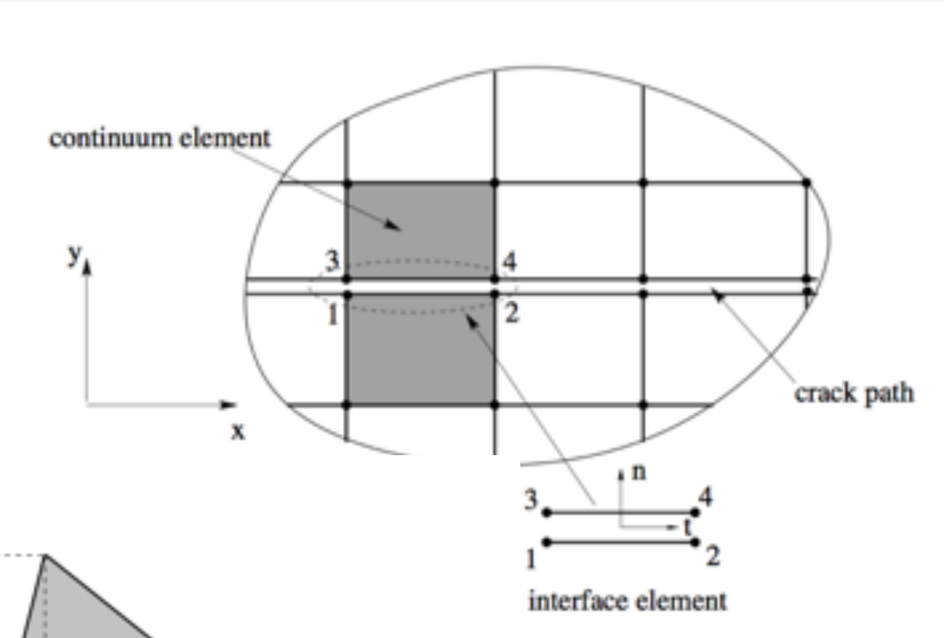
NURBS basis functions

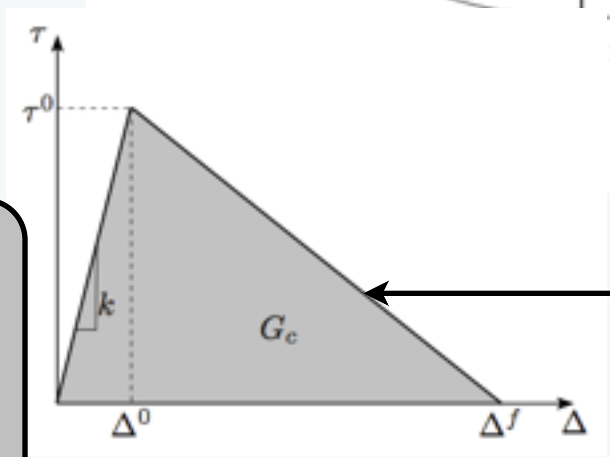
enrichment functions

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)



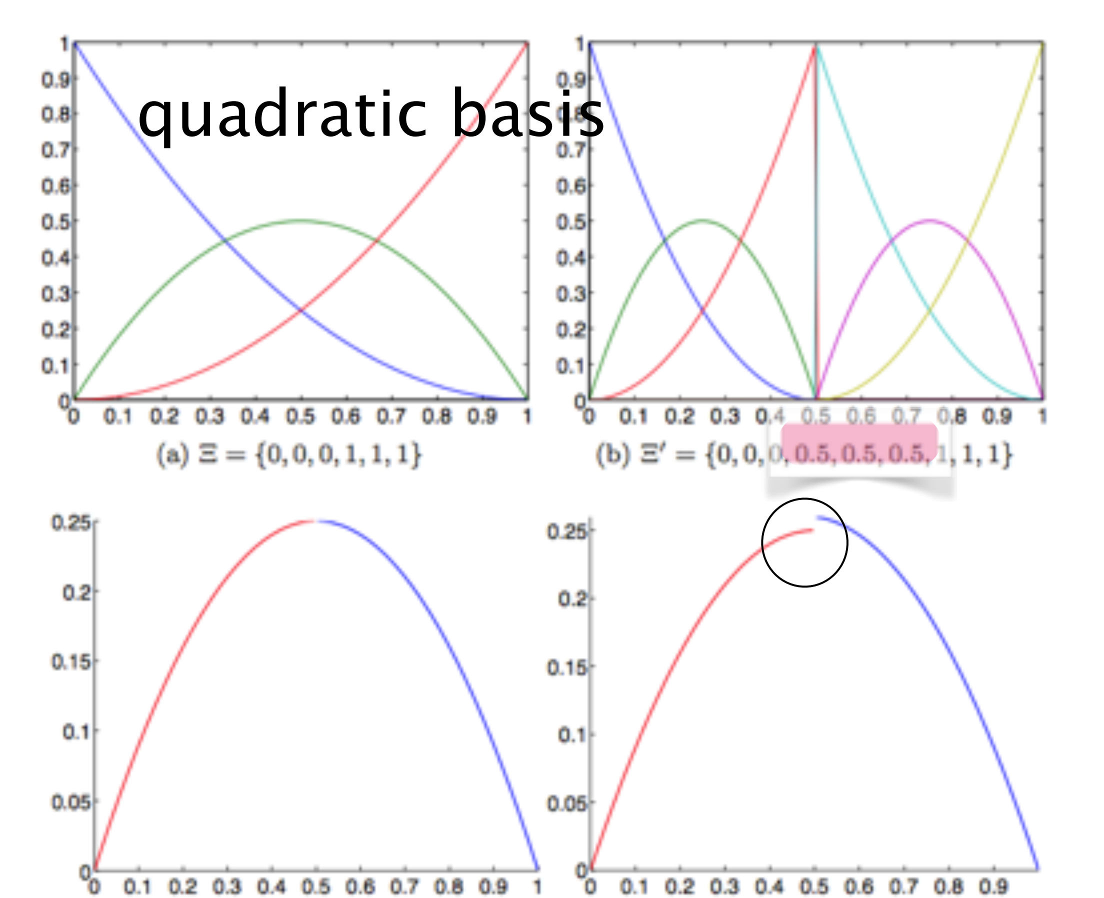


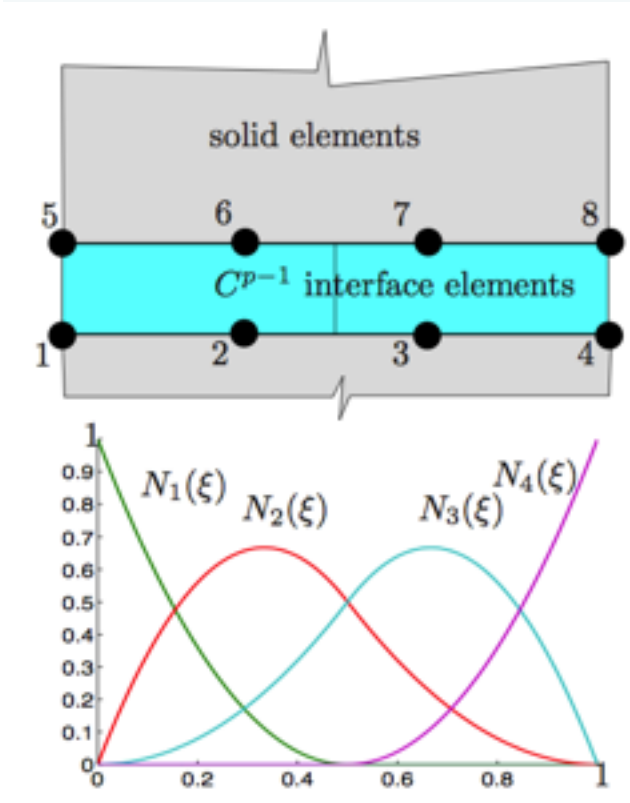


- No link to CAD
- Long preprocessing
- Refined meshes

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

Isogeometric cohesive elements



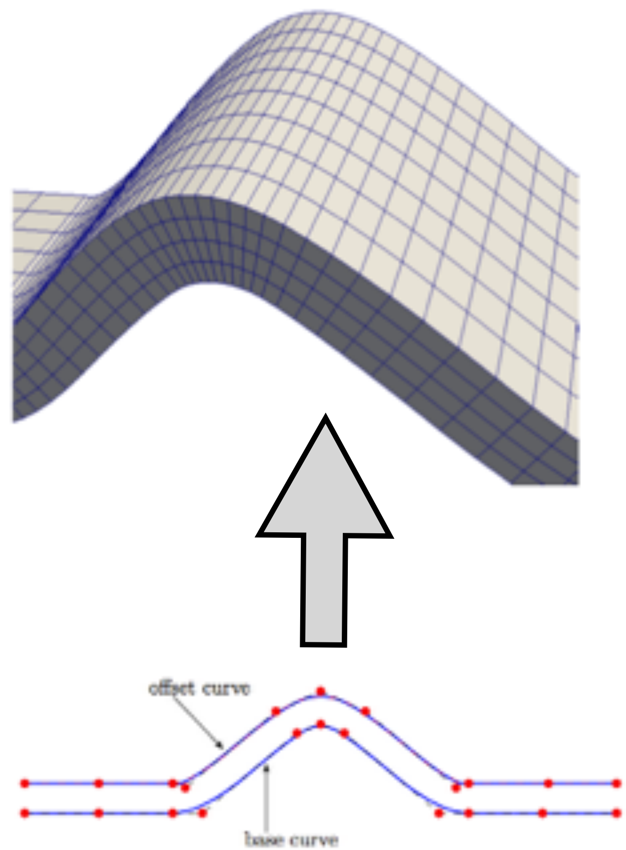


Knot insertion

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

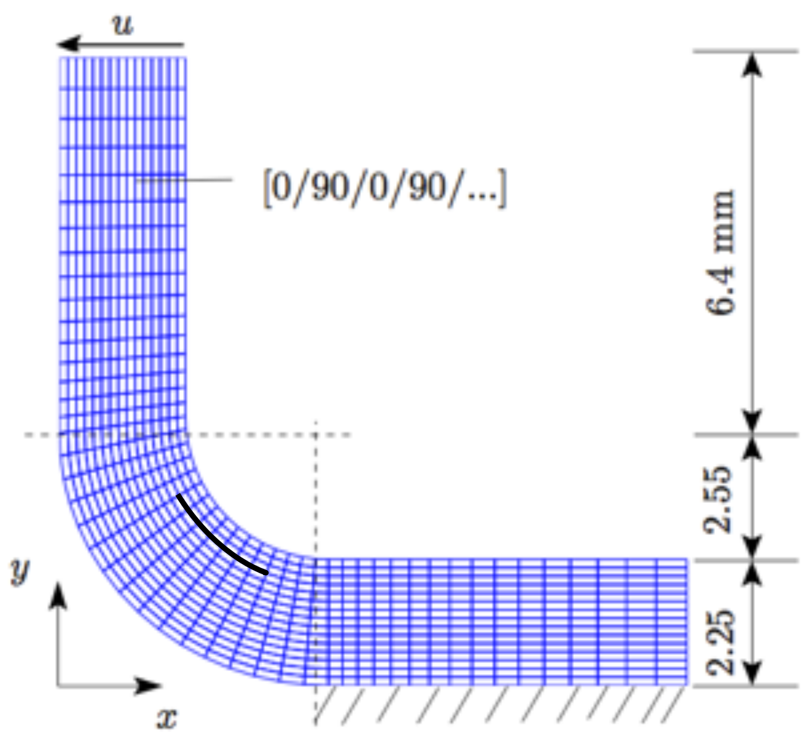
- Direct link to CAD
- Exact geometry
- Fast/straightforward generation of interface elements
- Accurate stress field
- Computationally cheaper

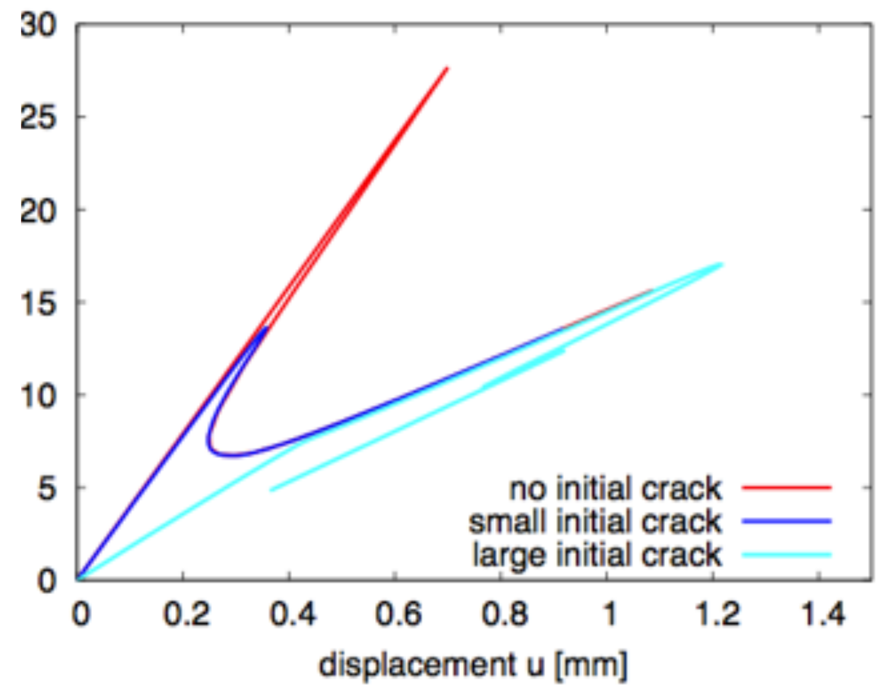


- 2D Mixed mode bending test (MMB)
- 2 x 70 quartic-linear B-spline elements
- Run time on a laptop 4GBi7: 6 s
- Energy arc-length control

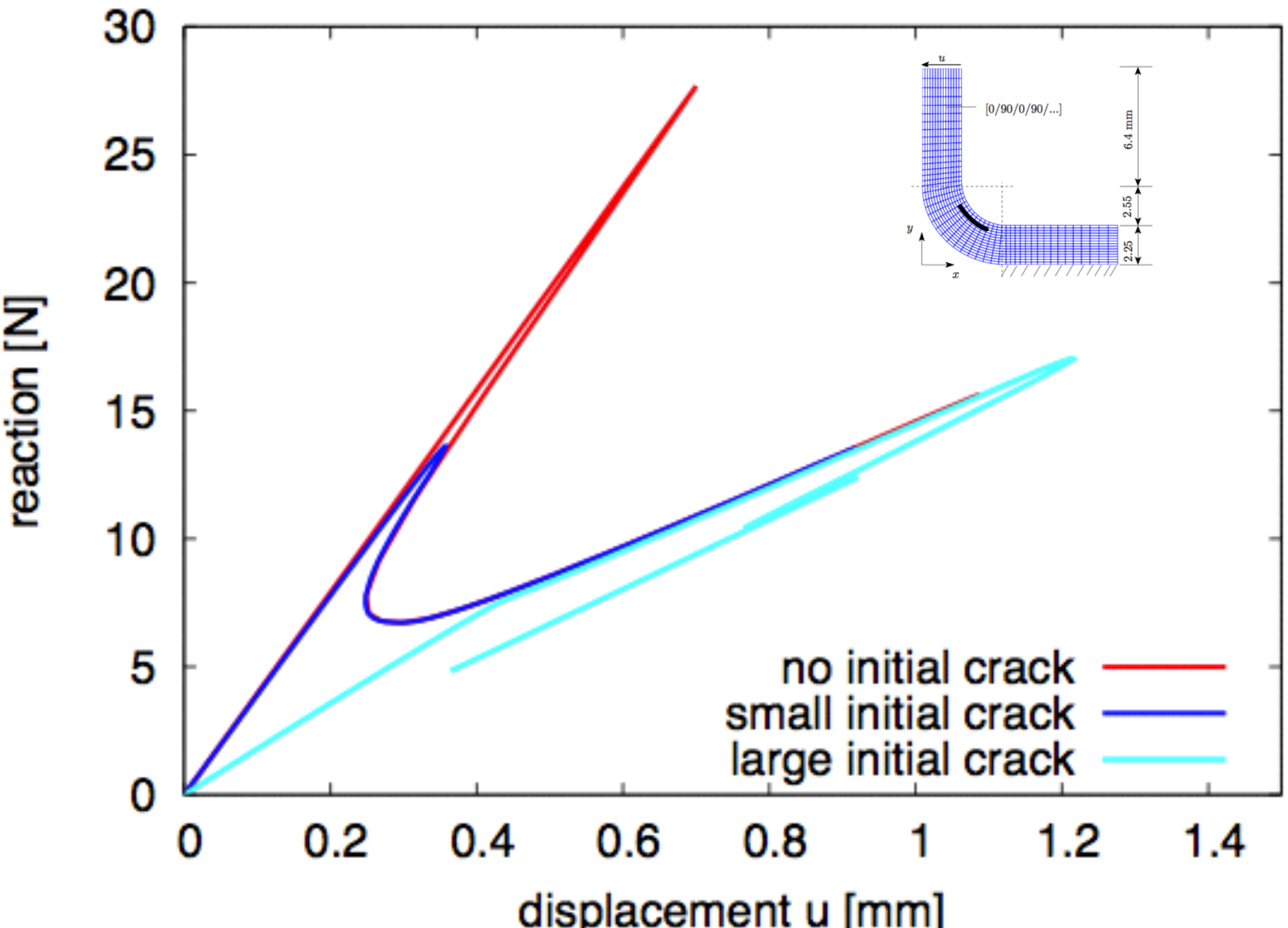
V. P. Nguyen and H. Nguyen-Xuan. High-order B-splines based finite elements for delamination analysis of laminated composites. Composite Structures, 102:261–275, 2013.

Isogeometric cohesive elements: 2D example



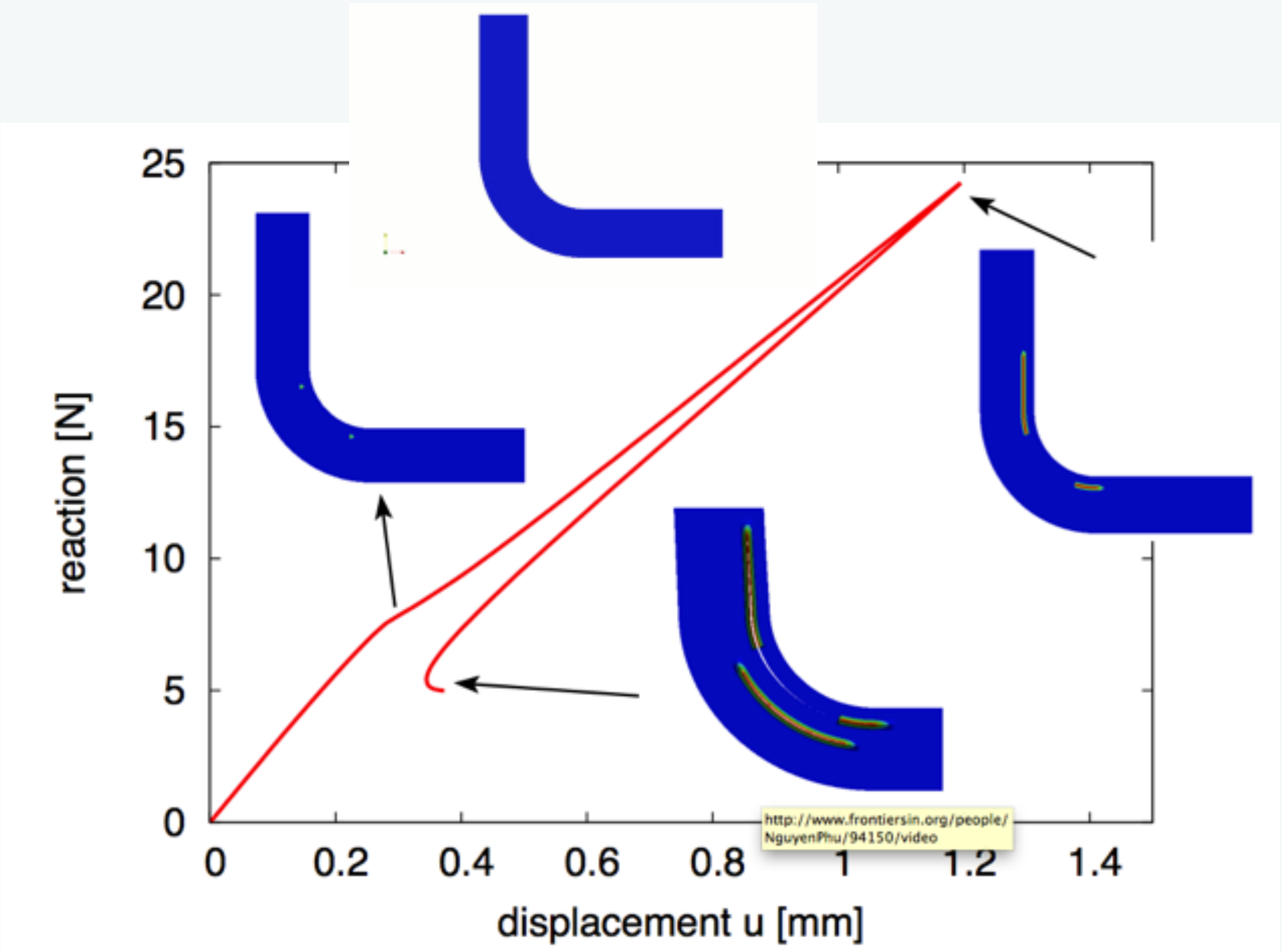


- Exact geometry by NURBS + direct link to CAD
- It is straightforward to vary
  (1) the number of plies and
  (2) # of interface elements:
- Suitable for parameter studies/design
- Solver: energy-based arc-length method (Gutierrez, 2007)

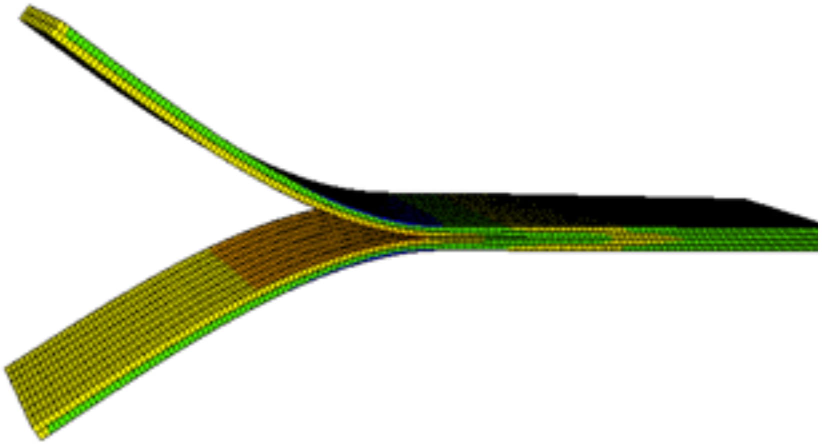


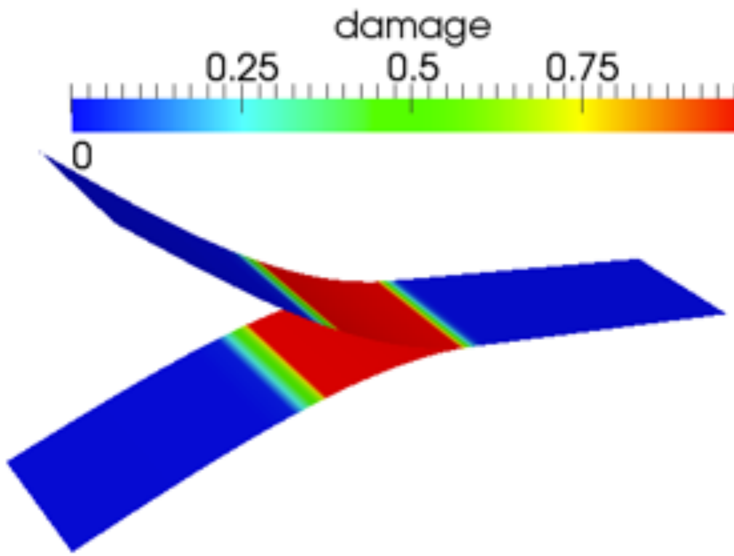
reaction [N]
30
25
20
15
10
5
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
displacement u [mm]
u
[0/90/0/90/...]
6.4 mm
2.55
2.25
y
x
no initial crack
small initial crack
large initial crack

Isogeometric cohesive elements: 2D example



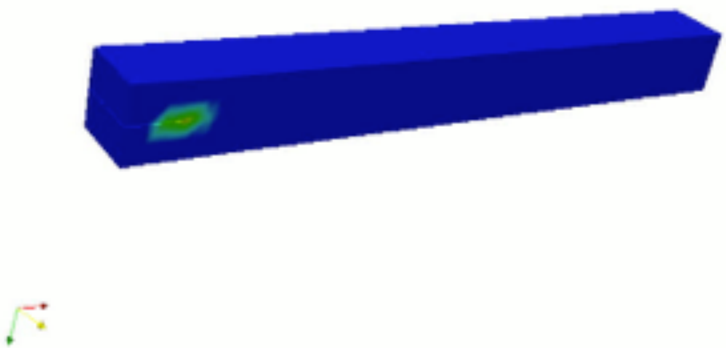
Isogeometric cohesive elements: 3D example with shells

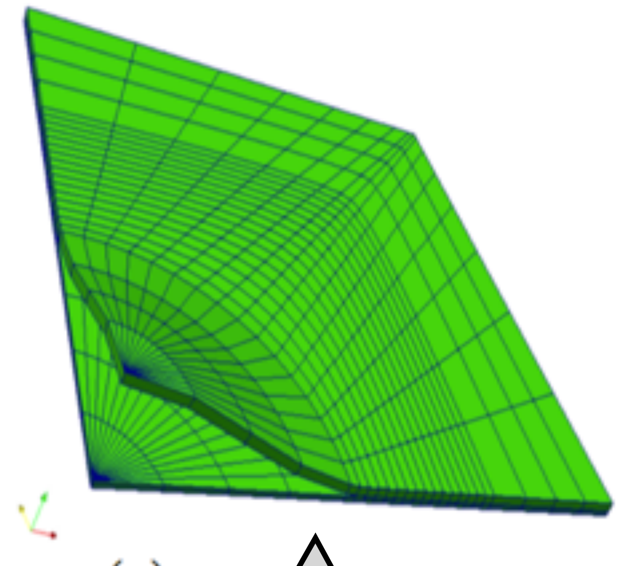




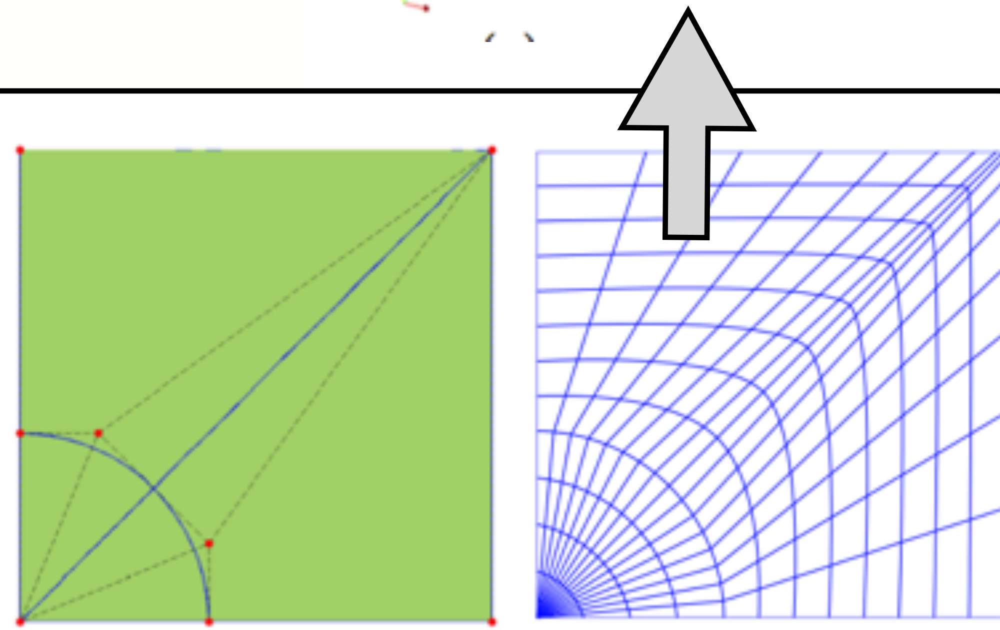
- Rotation free B-splines shell elements (Kiendl et al. CMAME)
- Two shells, one for each lamina
- Bivariate B-splines cohesive interface elements in between

Isogeometric cohesive elements: 3D examples

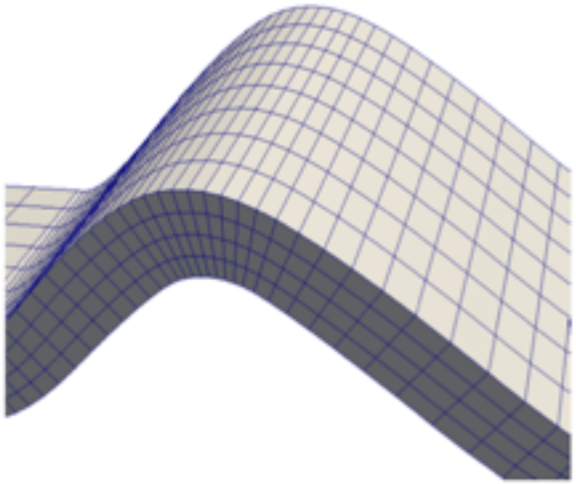




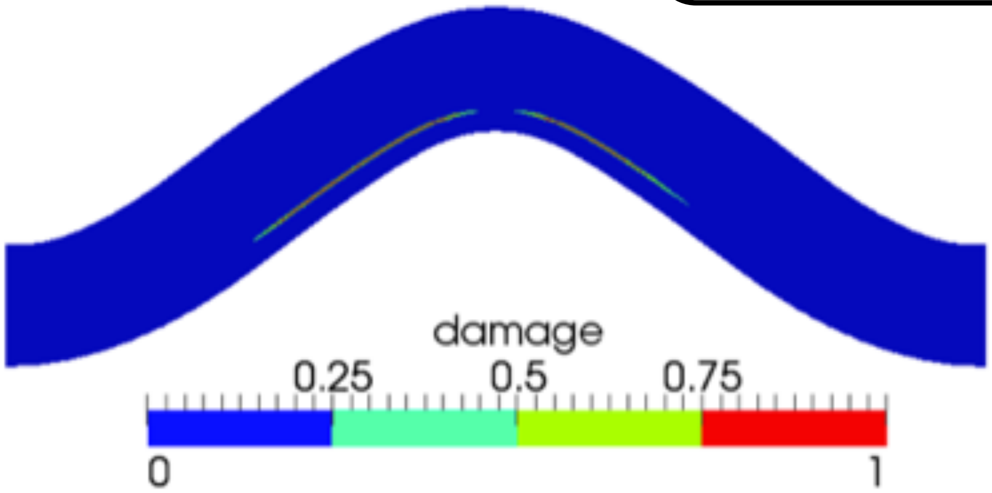
- cohesive elements for 3D meshes the same as 2D
- large deformations



Isogeometric cohesive elements



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



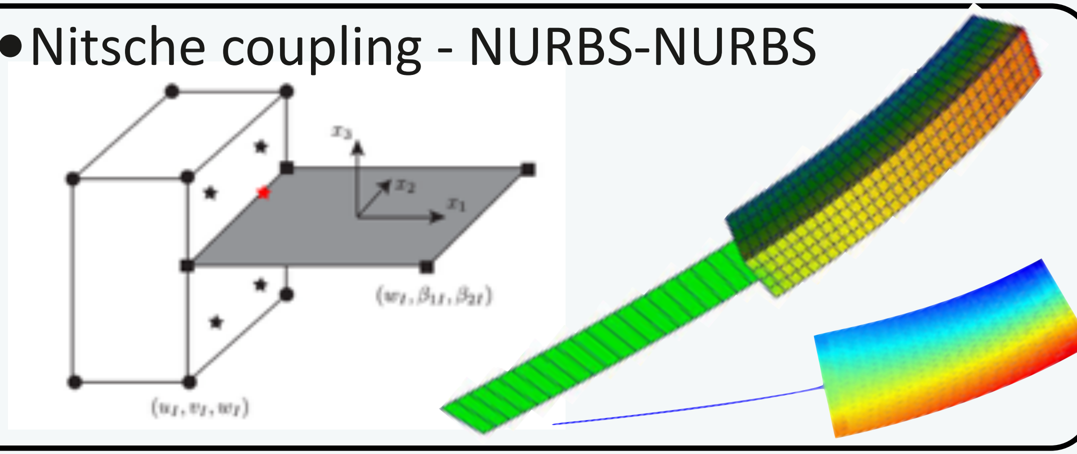
(*)V. P. Nguyen, P. Kerfriden, S.P.A. Bordas, and T. Rabczuk. An integrated design-analysis framework for three dimensional composite panels. Computer Aided Design, 2013. submitted.

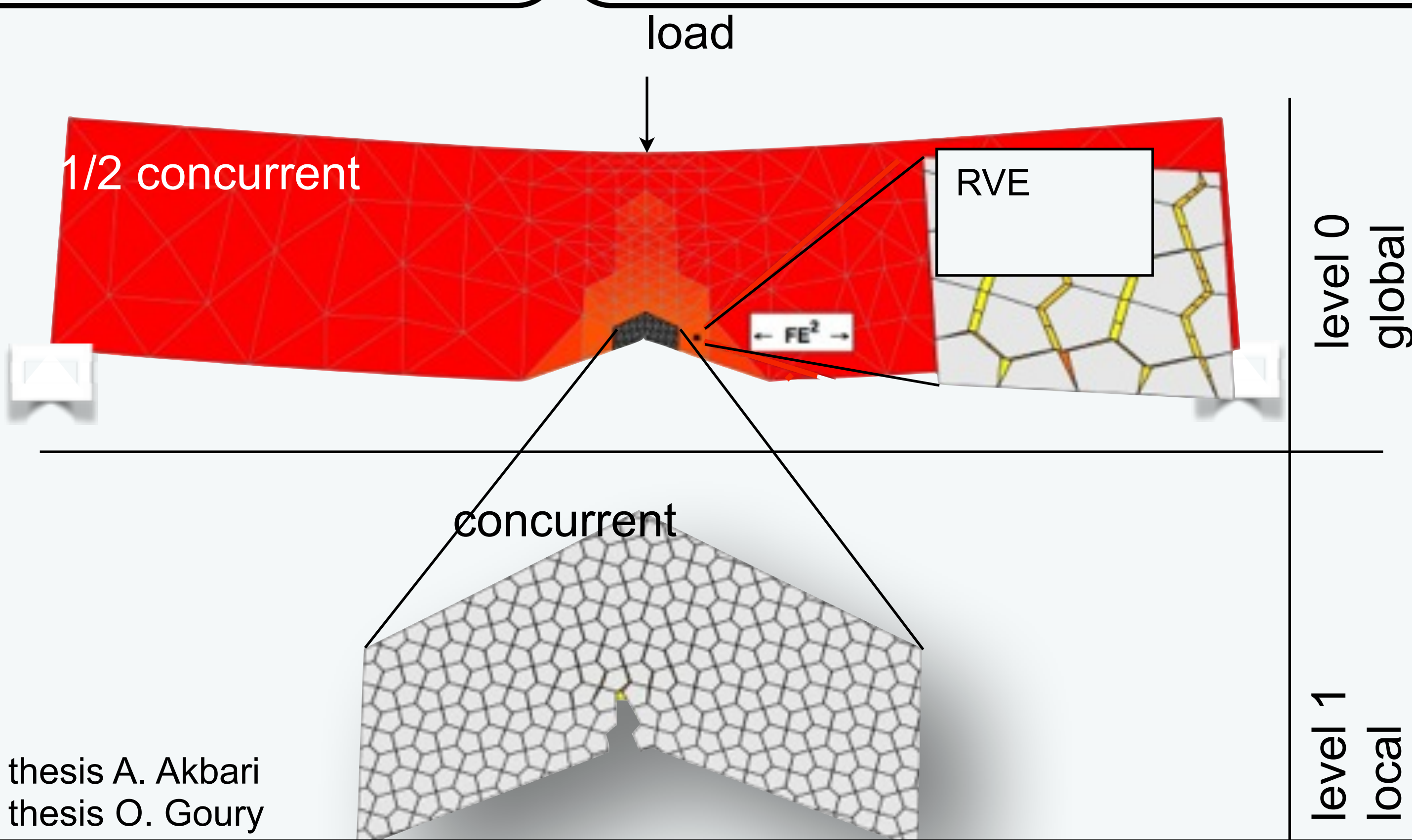
Future work: model selection (continuum, plate, beam, shell?)

Model selection

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

- Nitsche coupling - NURBS-NURBS





thesis A. Akbari
thesis O. Goury

Part III. Application to multi-crack propagation

with Danas Sutula, President Scholar

Faculty of Sciences, Technology and Communication

UNIVERSITÉ DU LUXEMBOURG

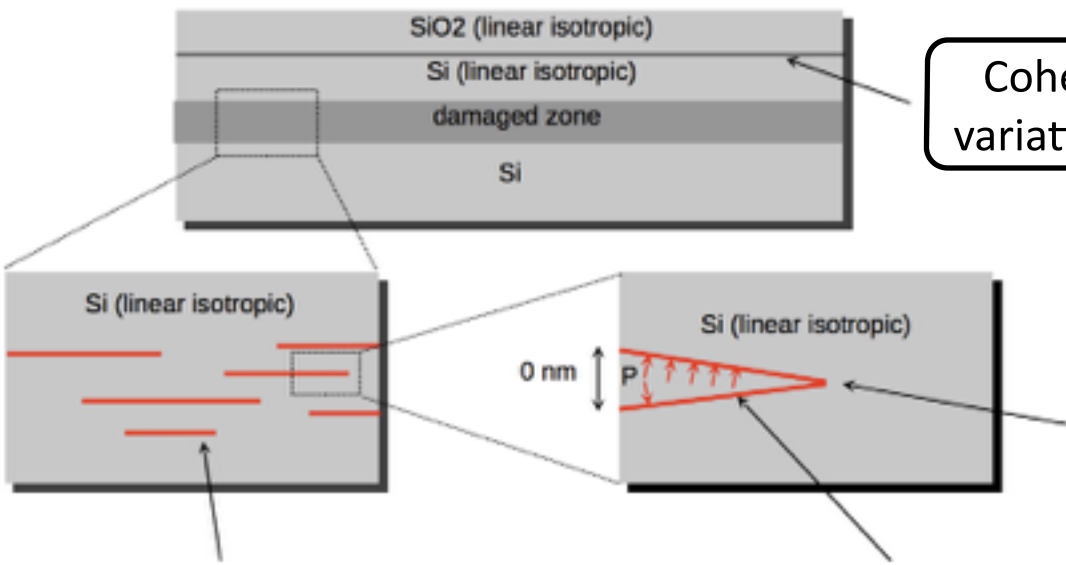
Model

Modeling cavities by zero thickness surfaces

- discontinuities in the displacement field

Linear elastic fracture mechanics (LEFM)

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



Cohesive interface with variation in surface energy

fracture criterion at the discontinuity tip

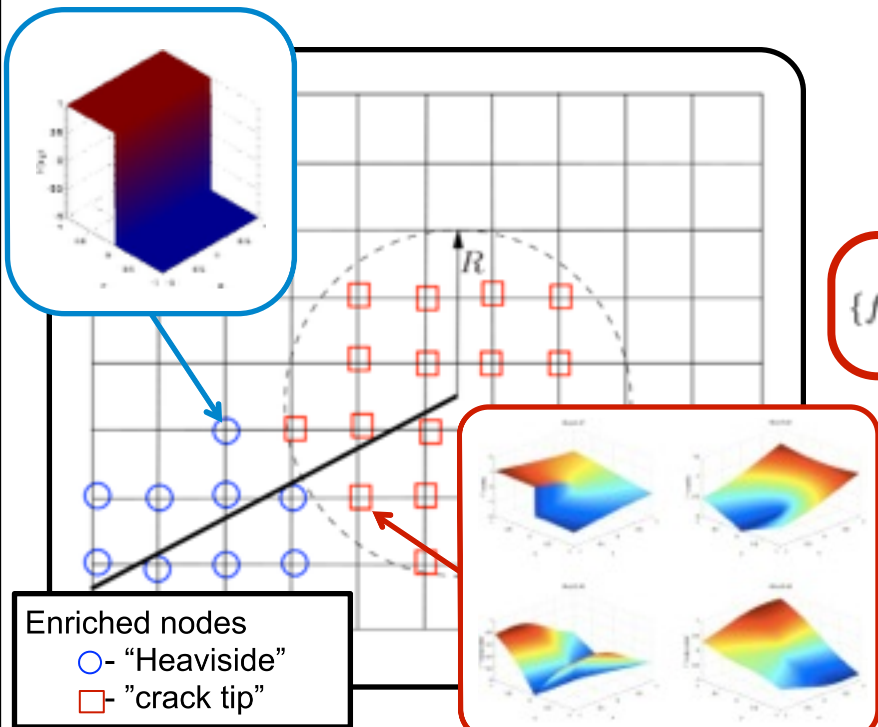
statistically distributed discontinuities

discontinuity subjected to H_2 pressure

XFEM formulation

Approximation function:

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

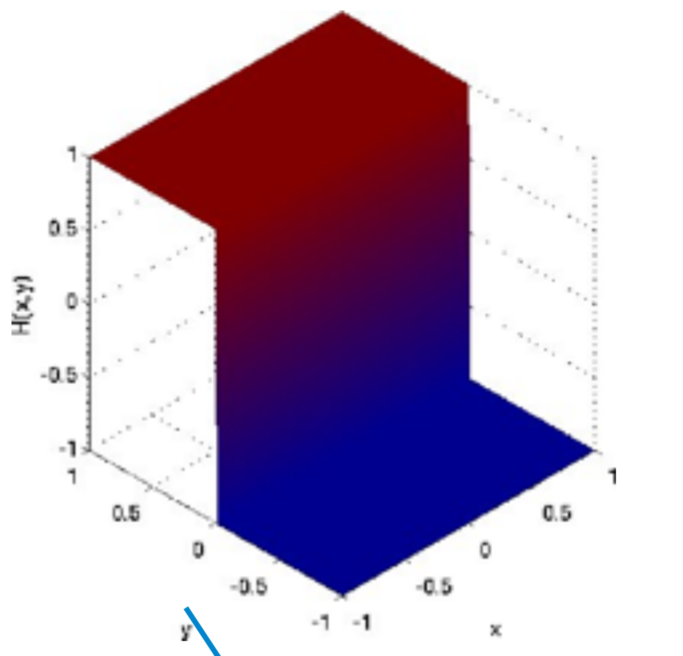


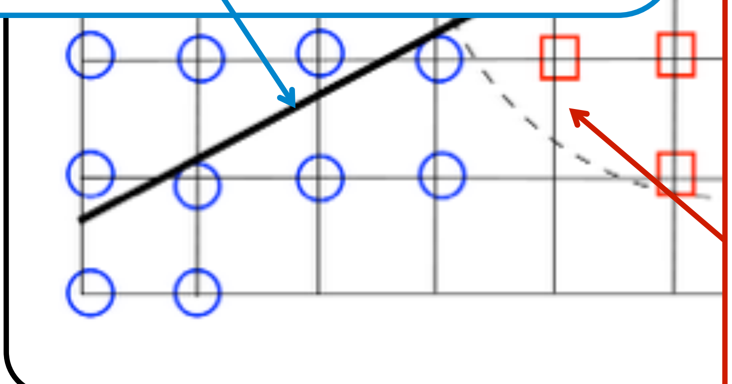
$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above crack} \\ -1 & \text{if } \mathbf{x} \text{ below crack} \end{cases}$$

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

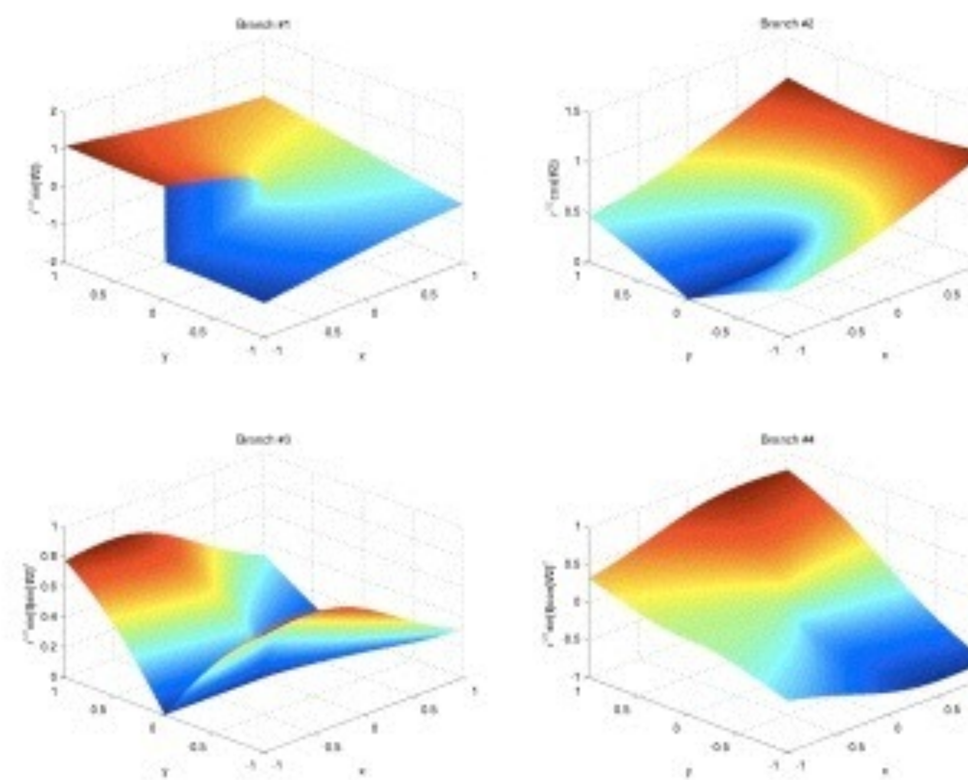
XFEM formulation

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





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



Extended Finite Element Method (XFEM)

- Introduced by Ted Belytschko (1999) for elastic problems

Fracture of “XFEM” using XFEM

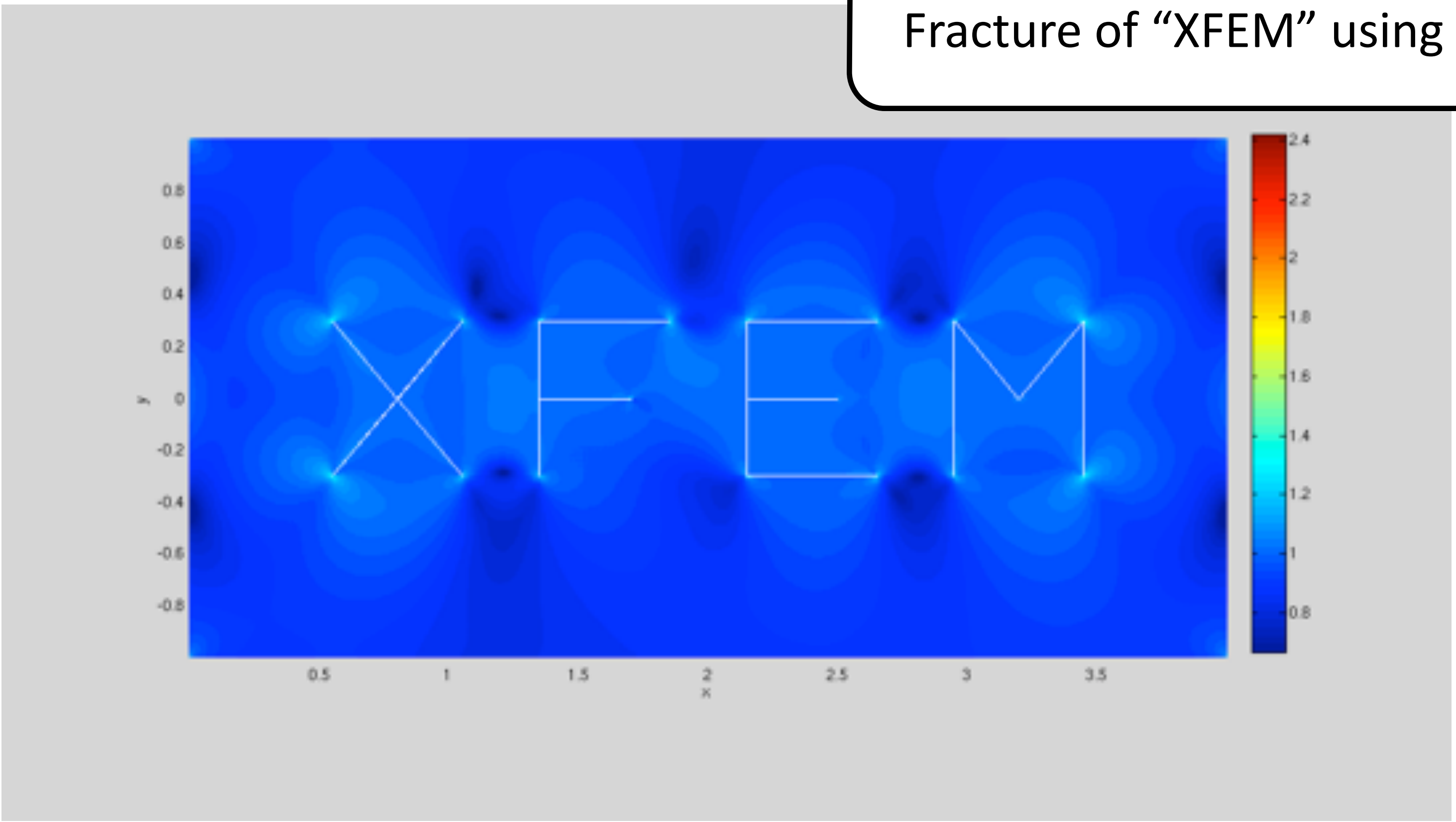
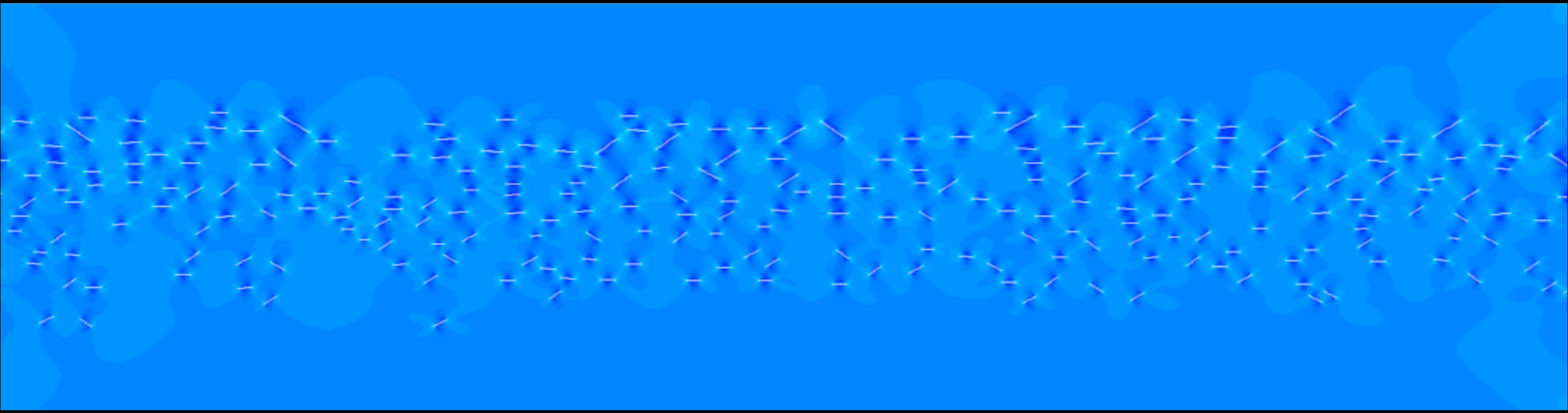


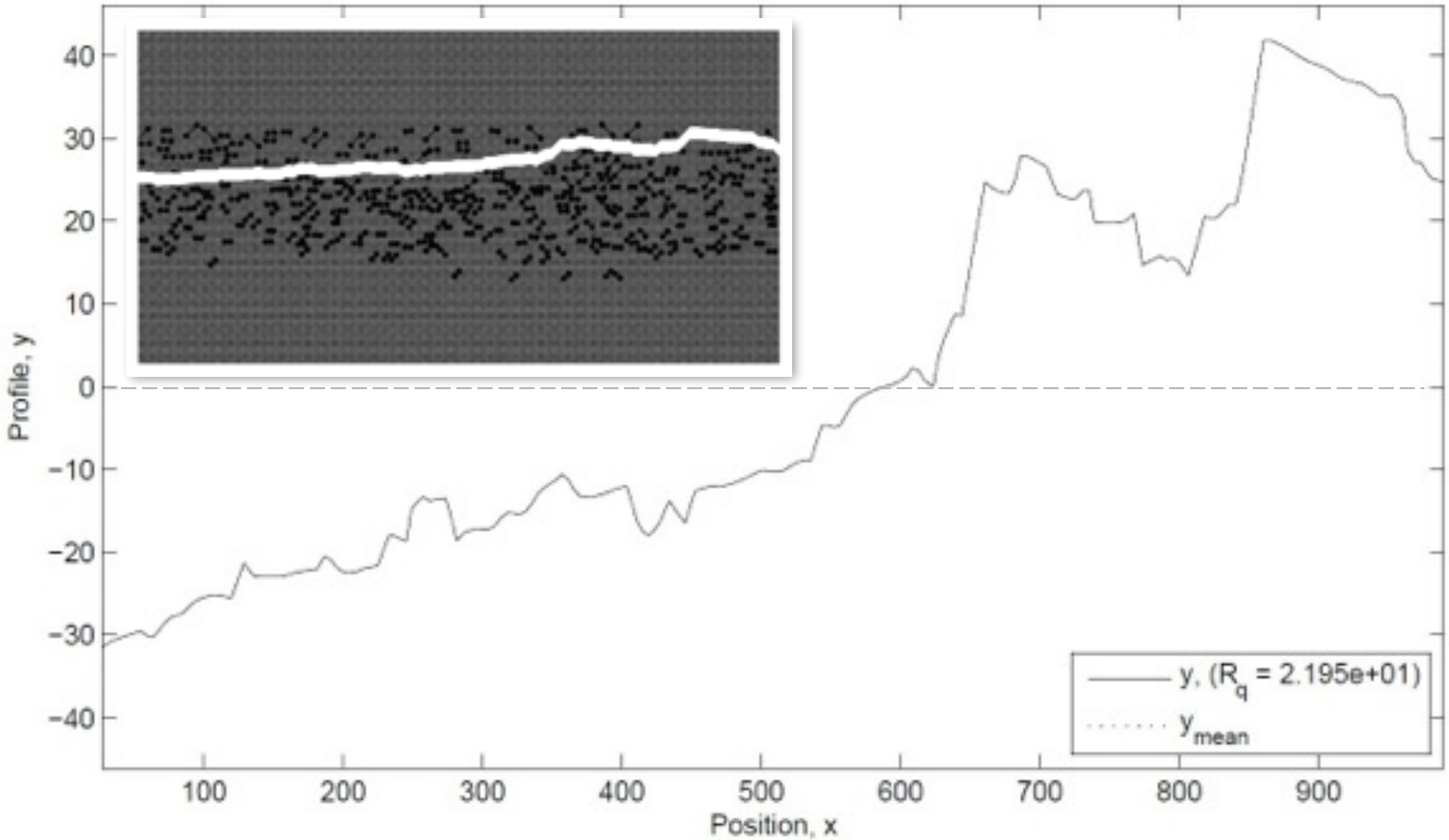
Plate with 300 cracks - vertical extension BCs



Example #1

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

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

Crack growth criterion for mixed mode fracture

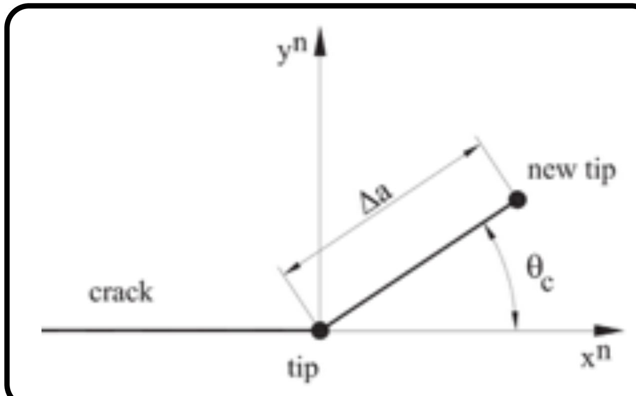
- Direction that maximises the energy release (Nuismer 1975)

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

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:**

$$Gs_i = -\frac{\partial \Pi}{\partial \theta_i}$$

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

$$Hs_{i,j} = \frac{\partial Gs_i}{\partial \theta_j} = -\frac{\partial^2 \Pi}{\partial \theta_i \partial \theta_j}$$

- **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:**

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

$$Gs_i = -\frac{1}{2}u'\delta_i Ku + u'\delta_i f$$

, where $\delta_i = \frac{\partial}{\partial\theta_i}$

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

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

, where $\delta_{ij} = \frac{\partial^2}{\partial\theta_i\theta_j}$

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ii}^2 Ku - u'\delta_{ii}^2 F\right) + (\delta_j Ku - \delta_j f)' K^{-1} (\delta_i Ku - \delta_i f)$$

Crack growth: optimization of direction

- **The discrete potential energy:**

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

- **The discrete energy release rate:**

$$Gs_i = -\frac{1}{2} u' \delta_i K u + u' \delta_i f - \delta_i u' (Ku - f)$$

$(Ku - f) \rightarrow \mathbf{0}$

$$Gs_i = -\frac{1}{2} u' \delta_i K u + u' \delta_i f$$

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

$$Hs_{ij} = -\left(\frac{1}{2} u' \delta^2_{ij} K u - u' \delta^2_{ij} f \right) - \delta_j u' (\delta_i K u - \delta_i f)$$

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

$$Hs_{ij} = -\left(\frac{1}{2} u' \delta^2_{ii} K u - u' \delta^2_{ii} F \right) + (\delta_j K u - \delta_j f)' K^{-1} (\delta_i K u - \delta_i f)$$

expensive: $K^{-1} (\delta_i K u - \delta_i f)$

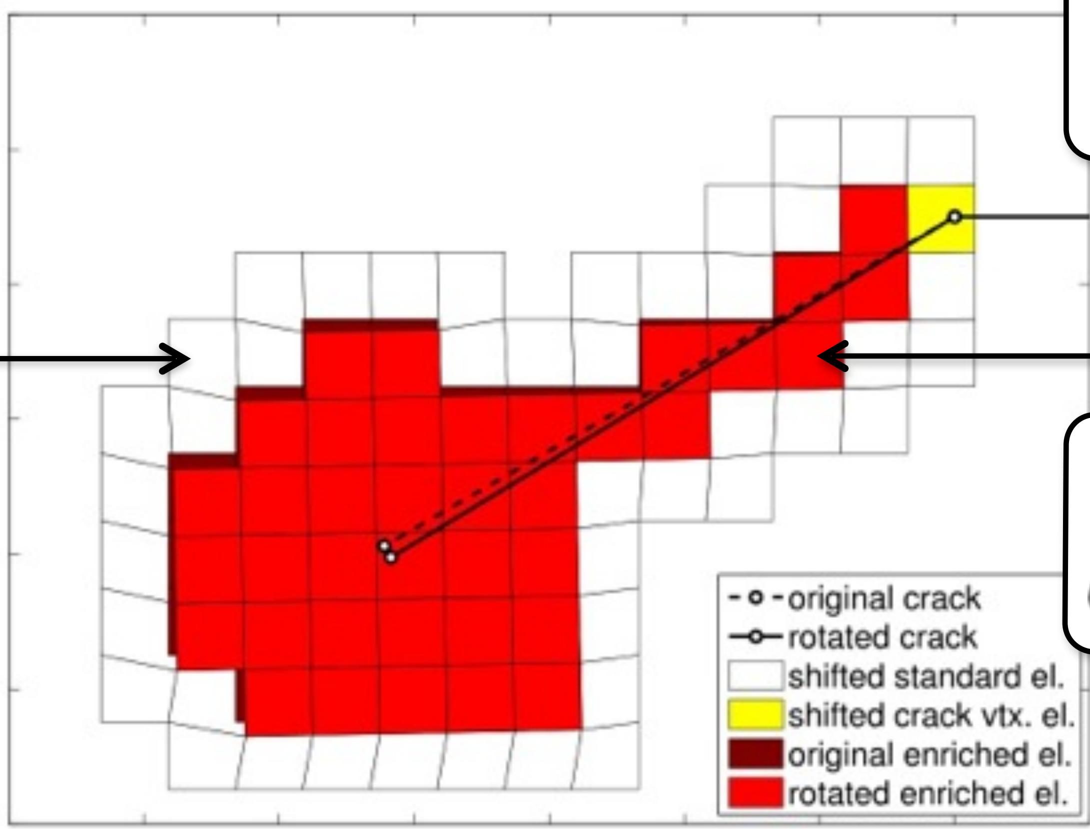
remote interaction: $(\delta_j K u - \delta_j f)' K^{-1} (\delta_i K u - \delta_i f)$

Crack growth: optimization of direction

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

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

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



$$\delta\mathbf{K_e} = \mathbf{T}^T\mathbf{K_e} + \mathbf{K_e}\mathbf{T}$$

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

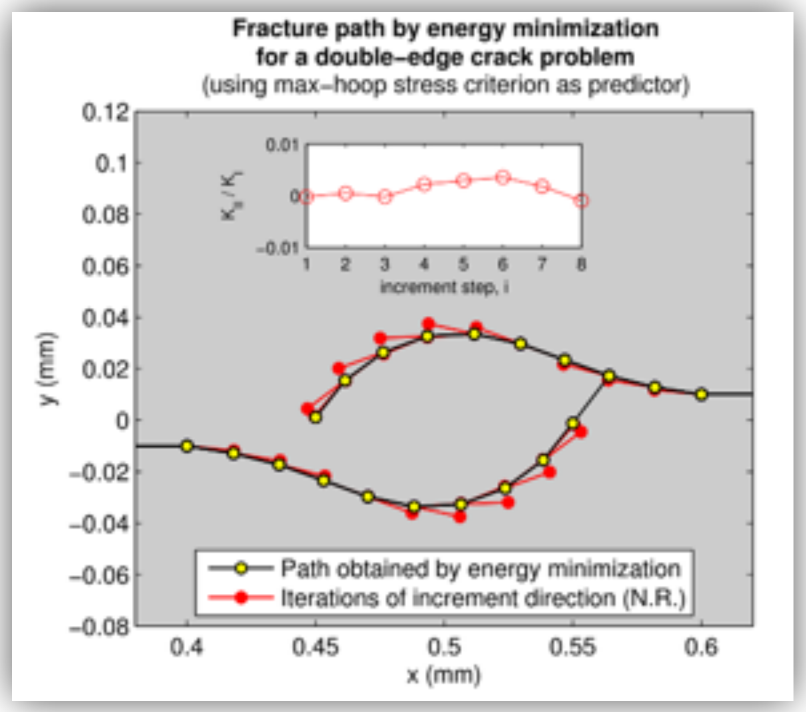
Updated directions:

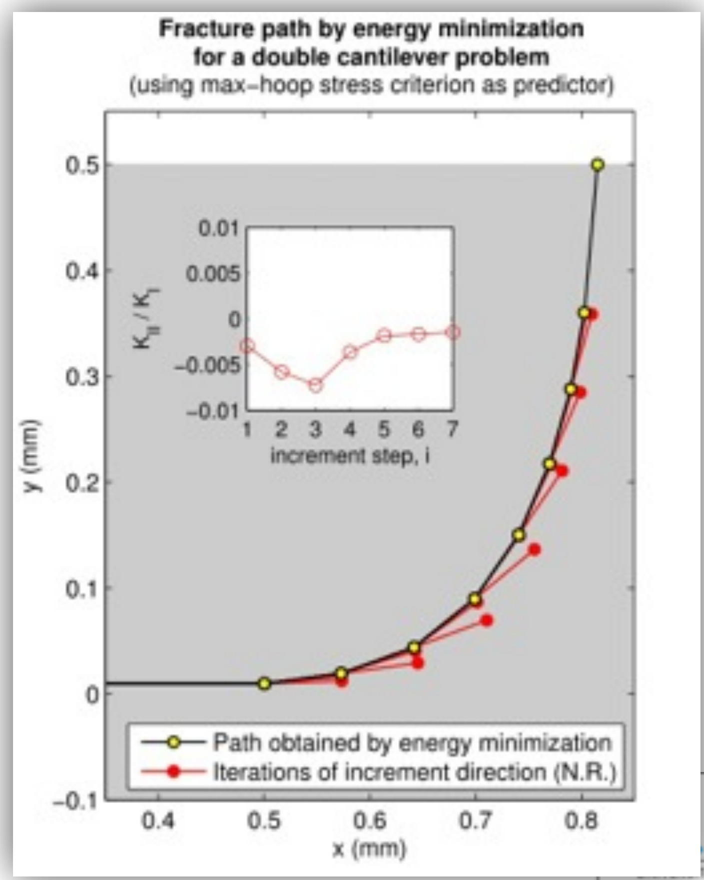
$$\theta^{k+1} = \theta^k - \mathbf{Hs}^{-1}\mathbf{Gs}$$

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

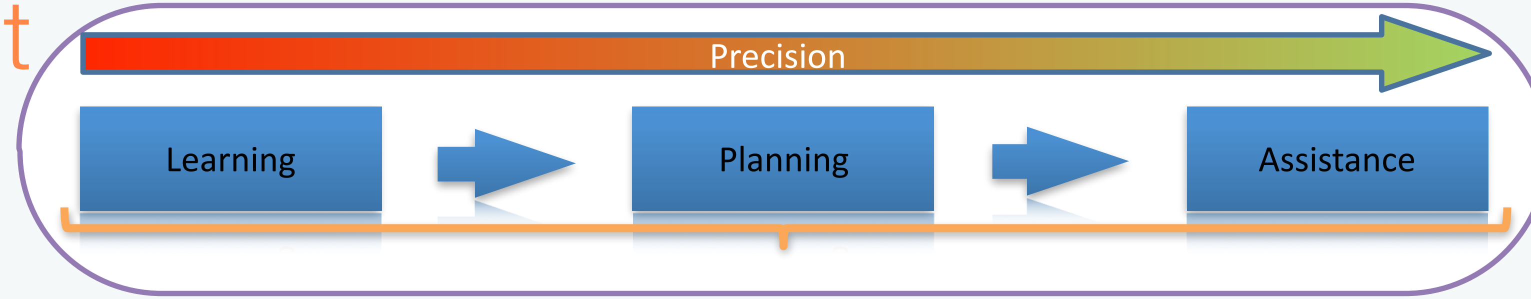
with Institue of Advanced Studies (iCube, University of Strasbourg, France: Hadrien Courtecuisse), INRIA, SHACRA Team (Stéphane Cotin, Christian Duriez); Karol Miller, UWA.

Faculty of Sciences, Technology and Communication

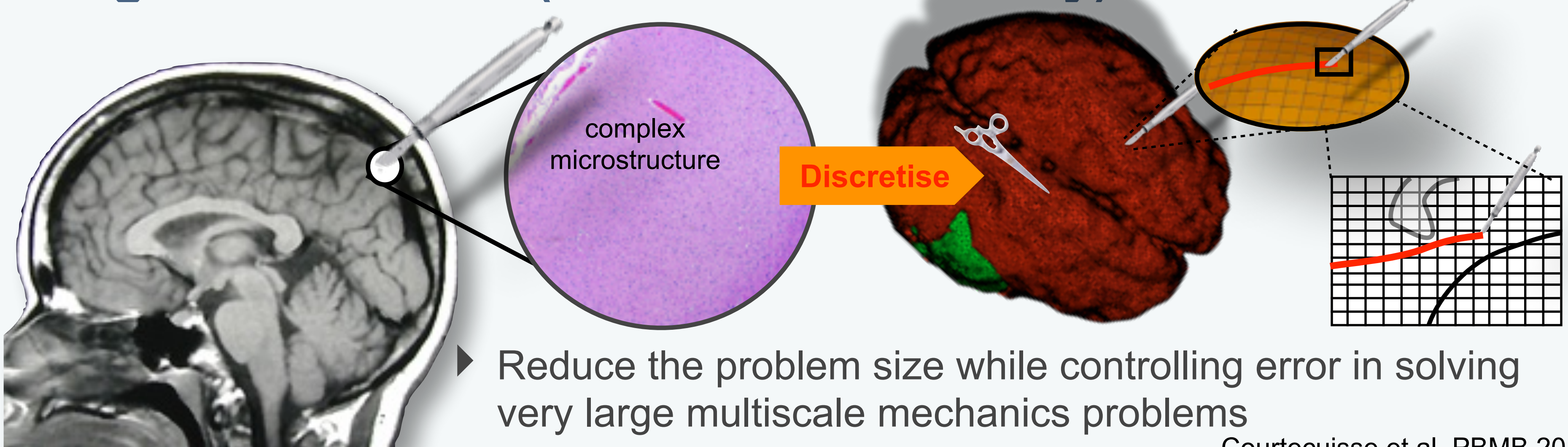
RealTcut

Interactive multiscale cutting simulations

RealTcut

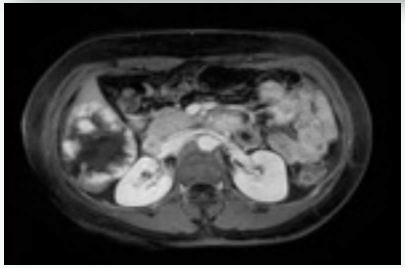


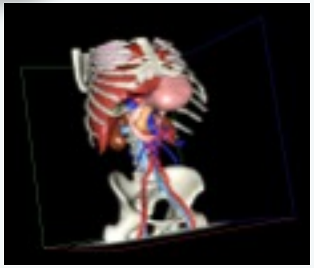
Surgical simulation (real time/interactivity)

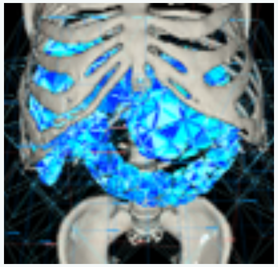


- Reduce the problem size while controlling error in solving very large multiscale mechanics problems

Courtecuisse et al. PBMB 2011





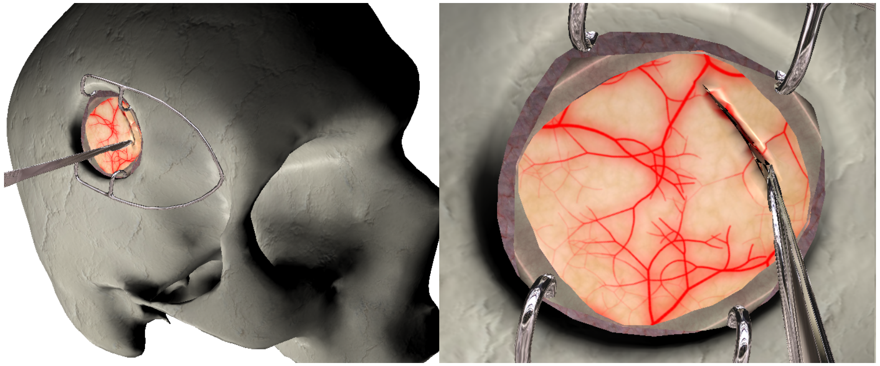


Concrete objective: compute the response of organs during surgical procedures (including cuts) in real time (50-500 solutions per second)

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

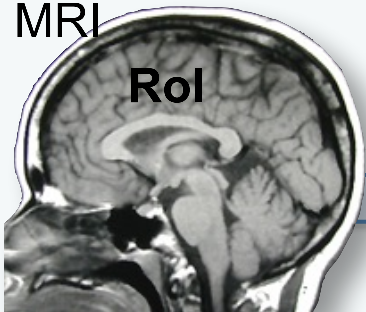
First implicit, interactive method for cutting with contact

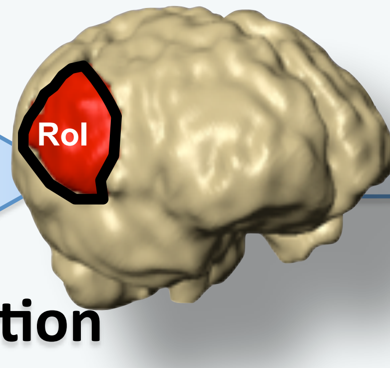


[Courtecuisse et al., MICCAI, 2013]
Collaboration INRIA

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

Complex geometries from medical images



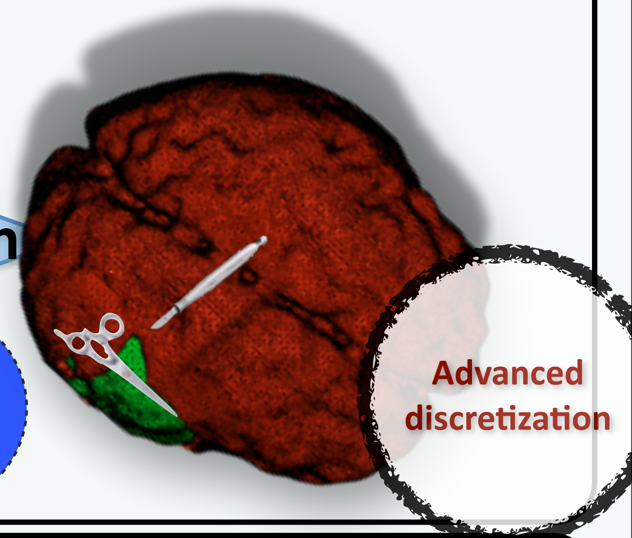


segmentation

Region of interest (RoI)

Topological changes & contact

discretization



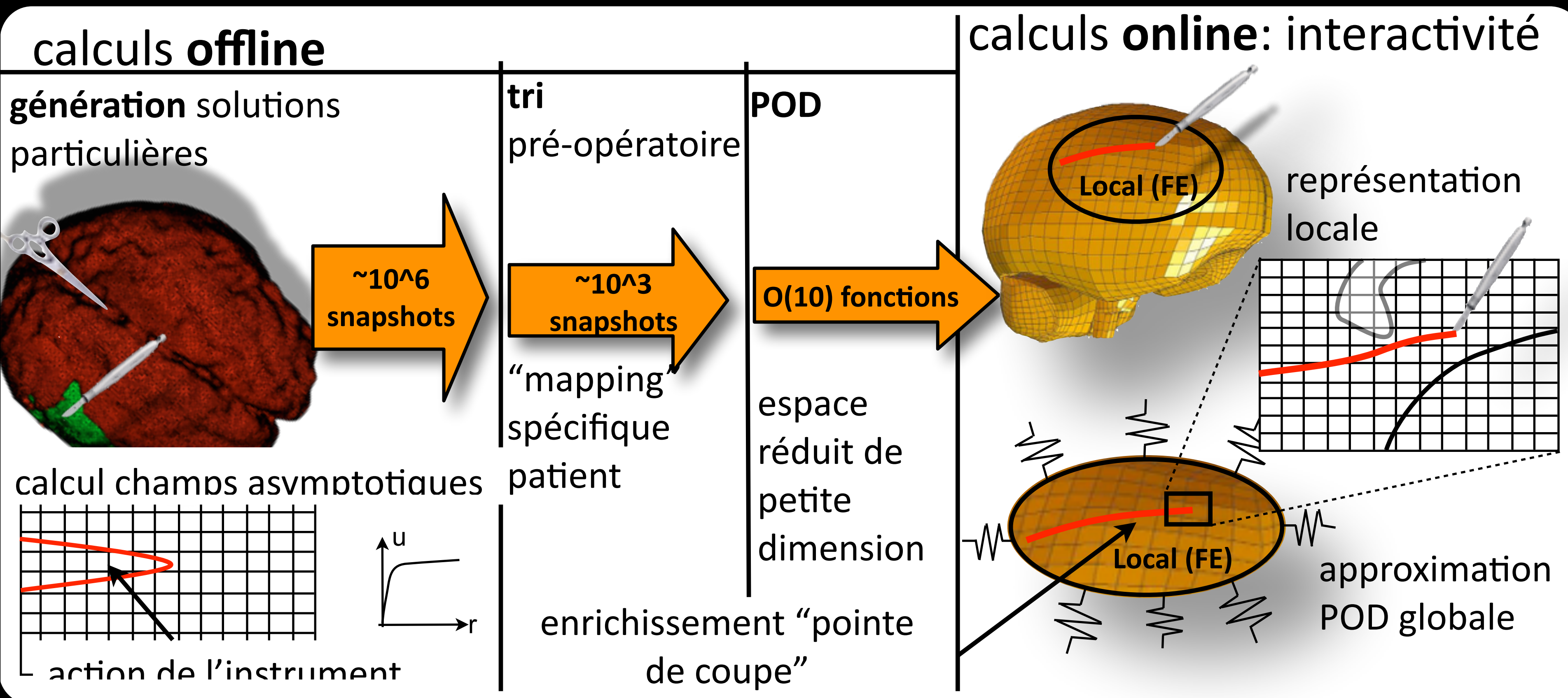
Model reduction

adaptivity

Error control

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

Verification & Validation


calculs **offline**
génération solutions particulières
~10^6 snapshots
calcul champs asymptotiques
u
r
action de l'instrument
tri pré-opératoire
~10^3 snapshots
"mapping" spécifique patient
POD
O(10) fonctions
espace réduit de petite dimension
enrichissement "pointe de coupe"
calculs **online**: interactivité
Local (FE)
représentation locale
Local (FE)
approximation POD globale

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

Paper ID : 269

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

IMAM
Institute of Mechanics & Advanced Materials

EPSRC
Pioneering research and skills

The Royal Academy of Engineering

Acknowledgements

THE ROYAL SOCIETY

Inria
INVENTEURS DU MONDE NUMÉRIQUE

hpc CYMRU WALES

SEVENTH FRAMEWORK PROGRAMME

The Leverhulme Trust

European Research Council
erc
IDEAS

CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

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SourceForge

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/

COMPUTATIONAL MECHANICS DISCUSSION GROUP

Request membership @
http://groups.google.com/group/computational_mechanics_discussion/about


the group…
November 2012
thank you

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
- http://orbilu.uni.lu/handle/10993/12159
- http://orbilu.uni.lu/handle/10993/14135
- http://orbilu.uni.lu/handle/10993/13847
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Damage tolerance analysis directly from CAD

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Reduce mesh burden

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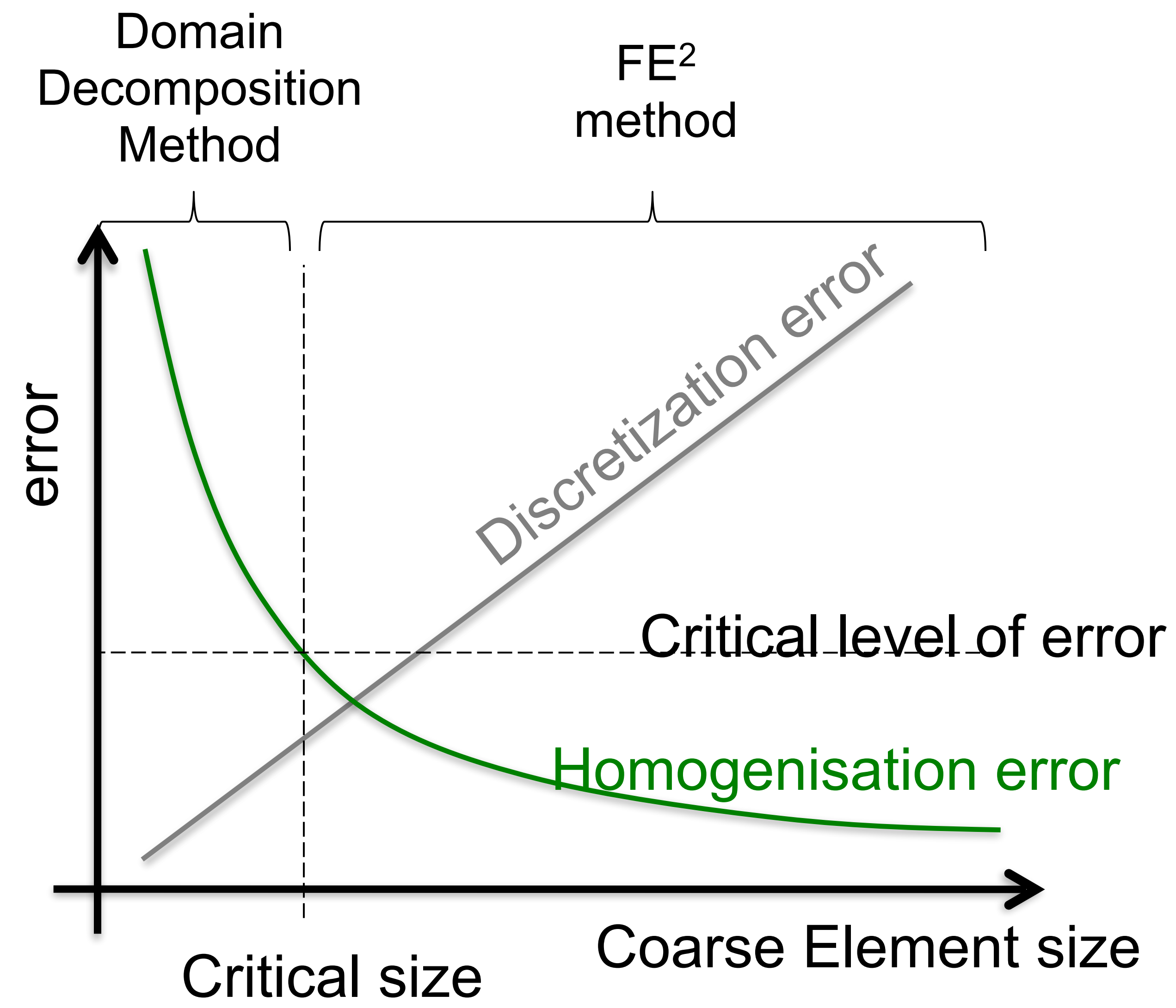
Outline

- ➢ Introduction: Multiscale methods for Fracture
- ➢ Adaptive multiscale method
  - Strategy
  - Fine scale problem
  - Coarse scale problem
    - FE^2 method
    - Adaptive mesh refinement
  - Coupling fine and coarse discretisations
  - Results
    - L-shape problem
    - Notched bar under Uni-axial tension

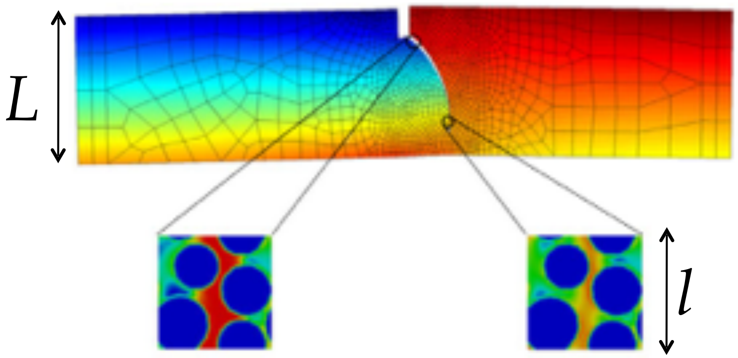
Error control in multiscale modelling



Multiscale methods for Fracture

- Non-concurrent

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

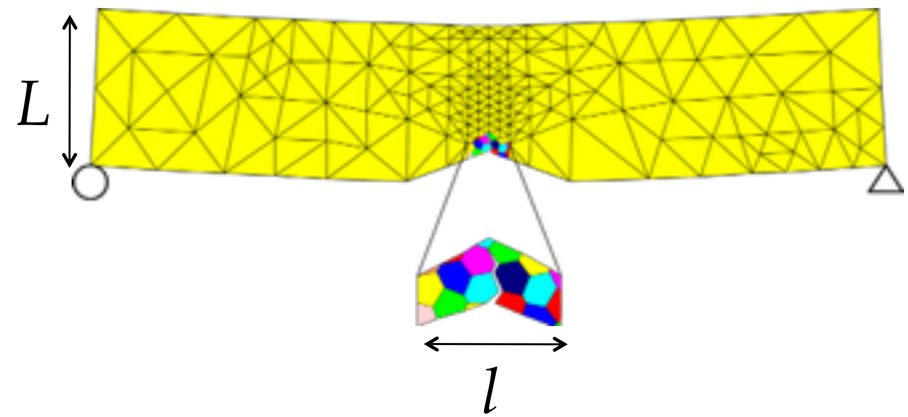


V.P. Nguyen 2012

$L/l >> 1$

- Concurrent

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

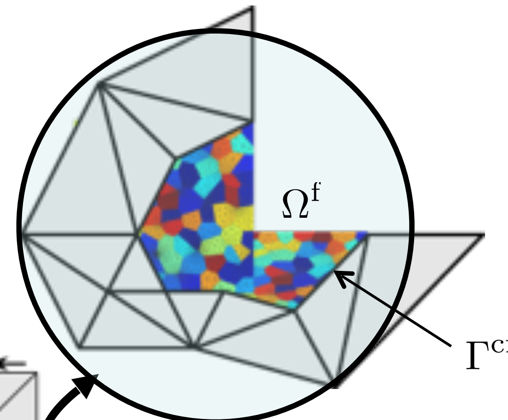


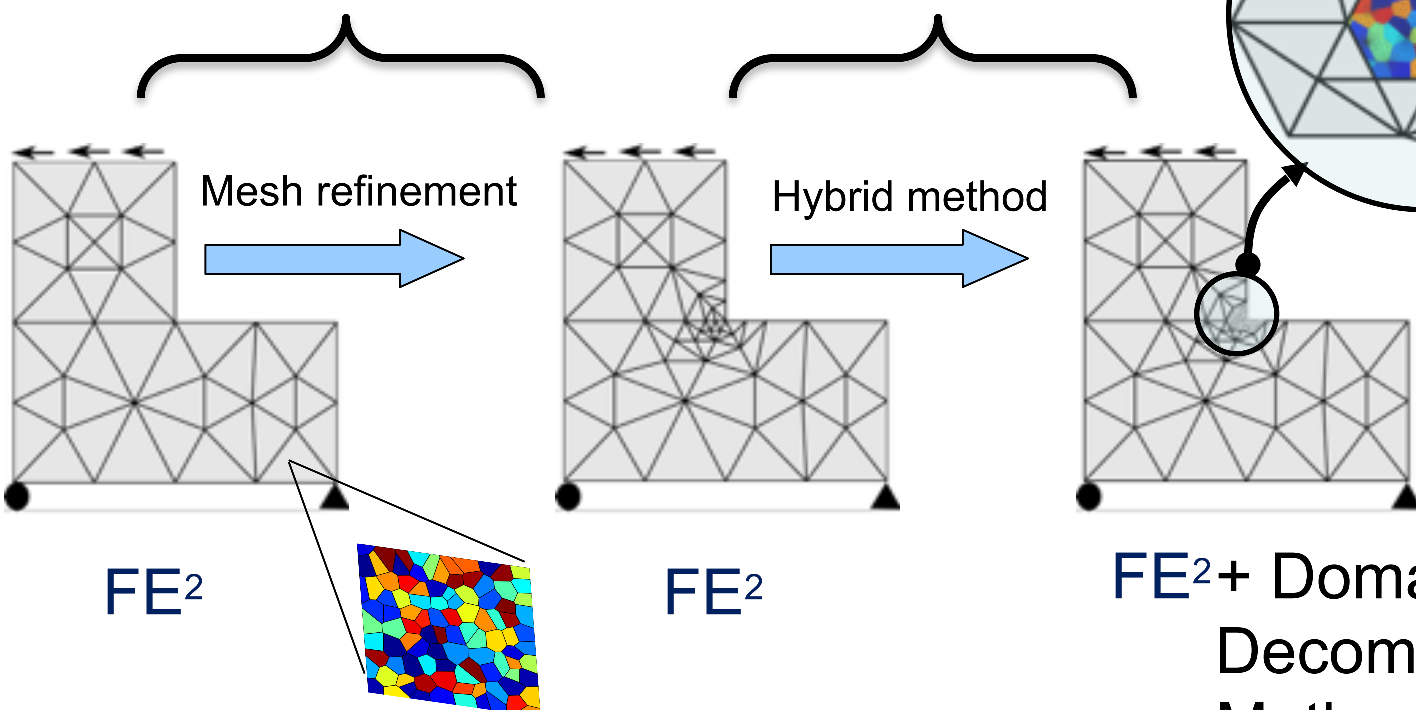
$L/l > 1$

Adaptive multiscale method: A Concurrent approach

➢Strategy:

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





Fine Scale: micro-structure

➢Microscale problem:

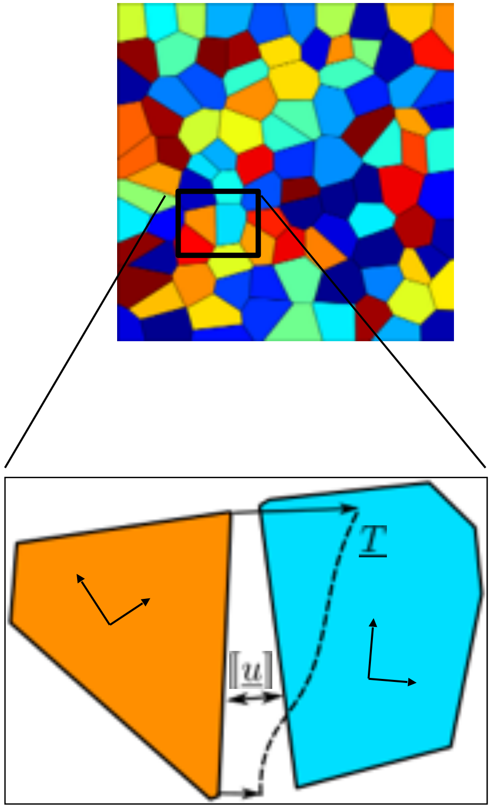
$$\int_{\Omega/\Gamma_c} \boldsymbol{\sigma}(\mathbf{u}) : \delta\varepsilon \, \mathrm{d}\Omega + \int_{\Gamma_c} \mathbf{T} \cdot [\![\delta \mathbf{u}]\!] \mathrm{d}\Omega = \int_{\partial\Omega} \mathbf{f} \cdot \delta \mathbf{u} \mathrm{d}\Gamma$$

- Orthotropic grains

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

- Cohesive interface

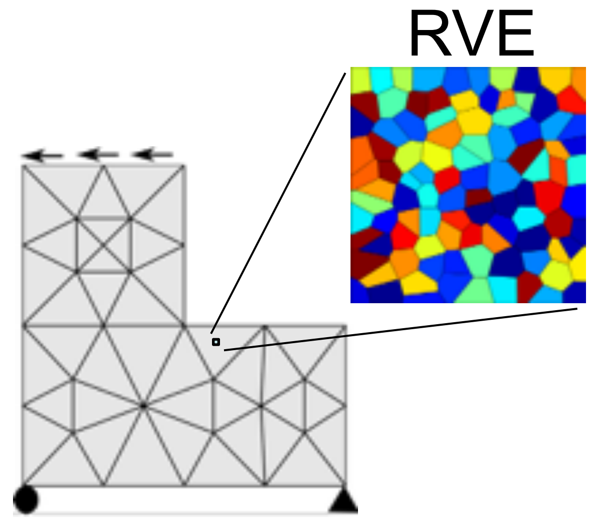
$$\forall \mathbf{x} \in \Gamma_c, \quad \mathbf{T}_{|t} = T\left(([\![\mathbf{u}]\!]_{|\tau})_{\tau \leq t} \right)$$



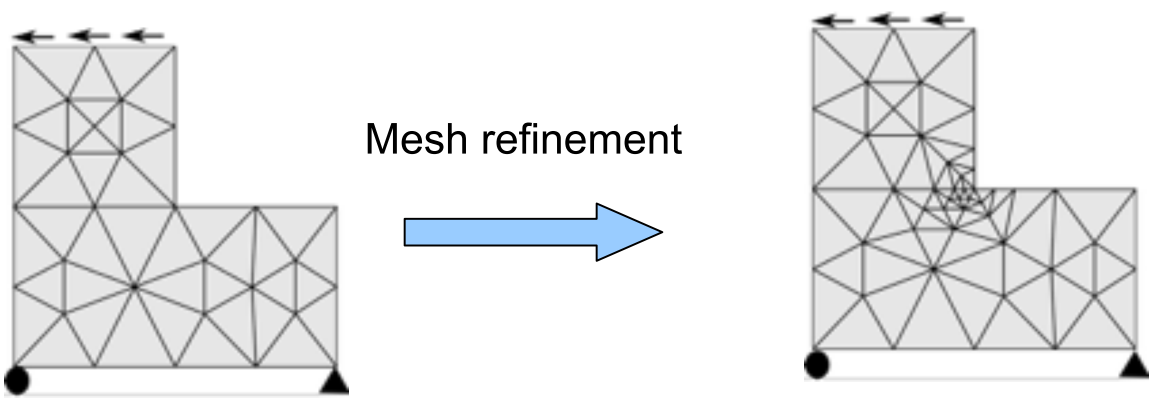
Coarse Scale

➢Macroscale problem:

- FE^2 Method
Based on averaging theorem
(computational homogenisation)

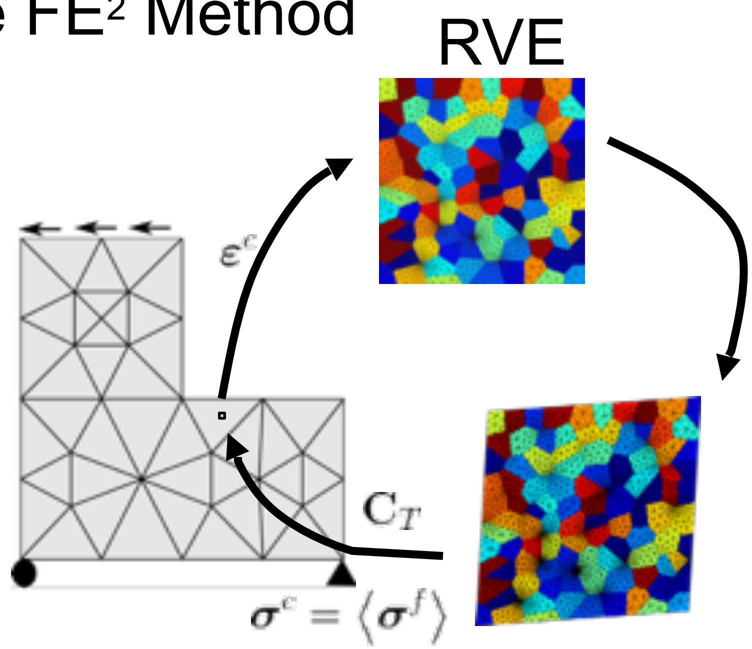


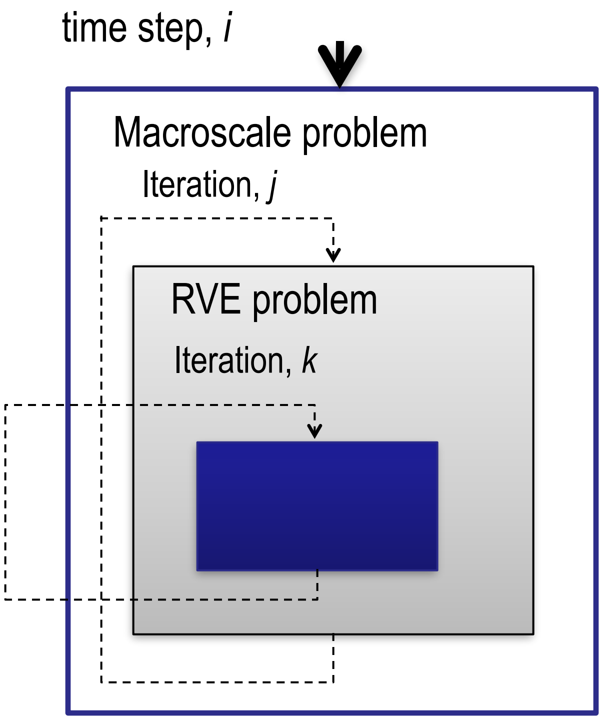
- Adaptive mesh refinement
Error estimation by Zienkiewicz-Zhu-type recovery technique



Coarse Scale: FE2

- The FE² Method





❖ Shortcoming of the FE² Method :

Lack of scale separation

RVE cannot be found in the **softening regime**

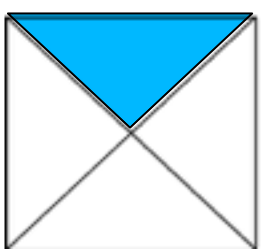
Coarse Scale: Adaptive mesh refinement

➢ **Coarse scale Adaptive mesh refinement**

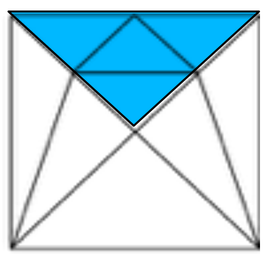
- Error estimation by Zienkiewicz-Zhu-type recovery technique

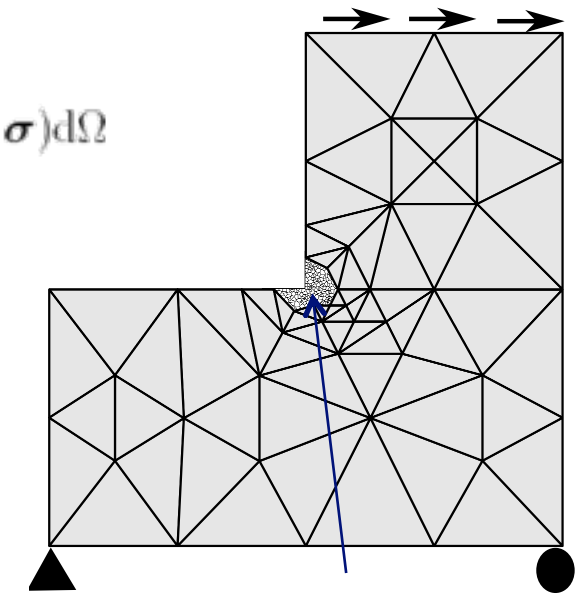
$$\|e\| = \int_{\Omega_e} (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}) : \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} \bigg|_{\mathbf{u}^c} \right)^{-1} : (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}) \mathrm{d}\Omega$$

Element to refine



Refined mesh



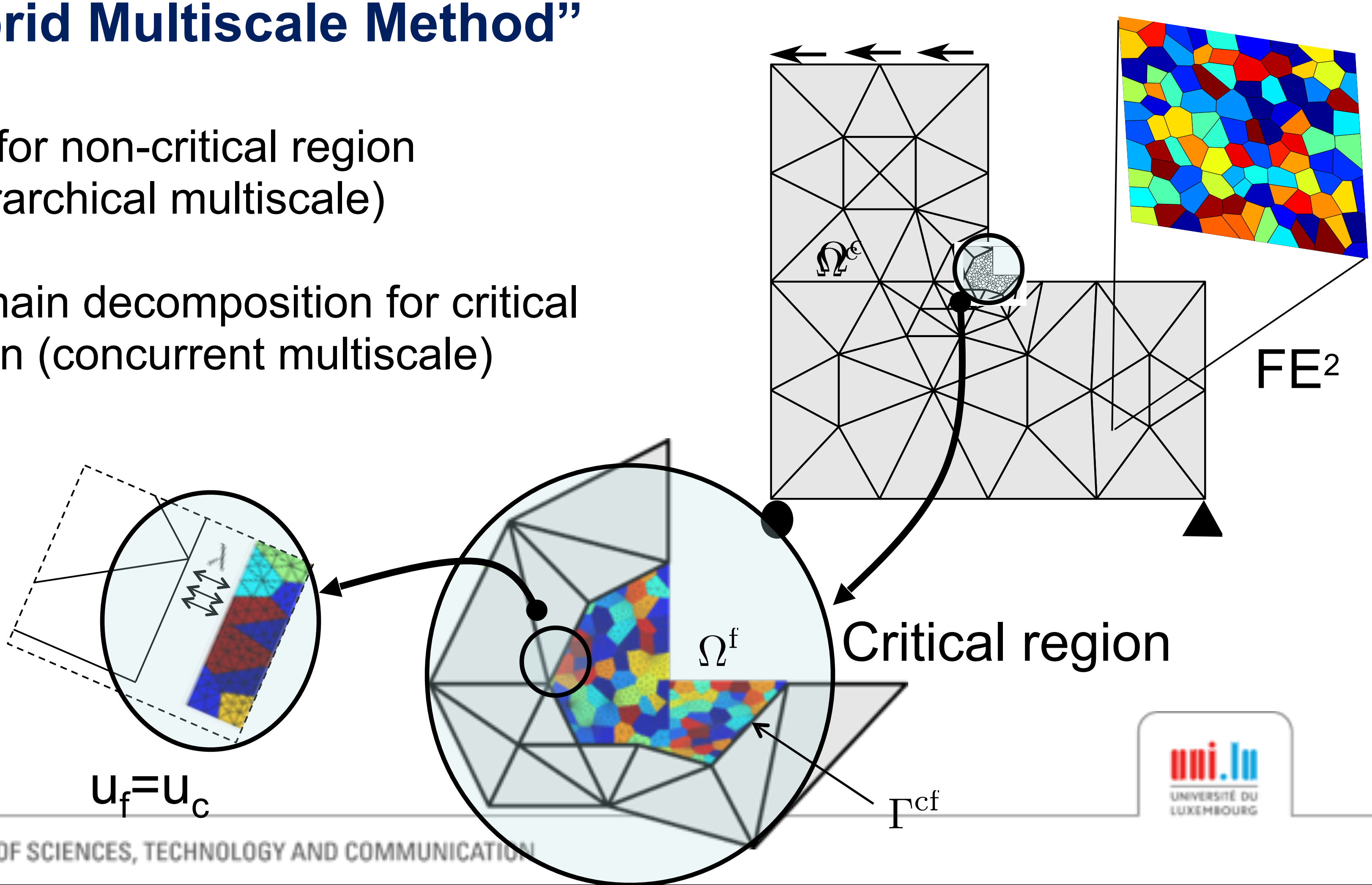


- Convergence criterion: $\frac{\|e\|}{\|\sigma\|} < Tol$

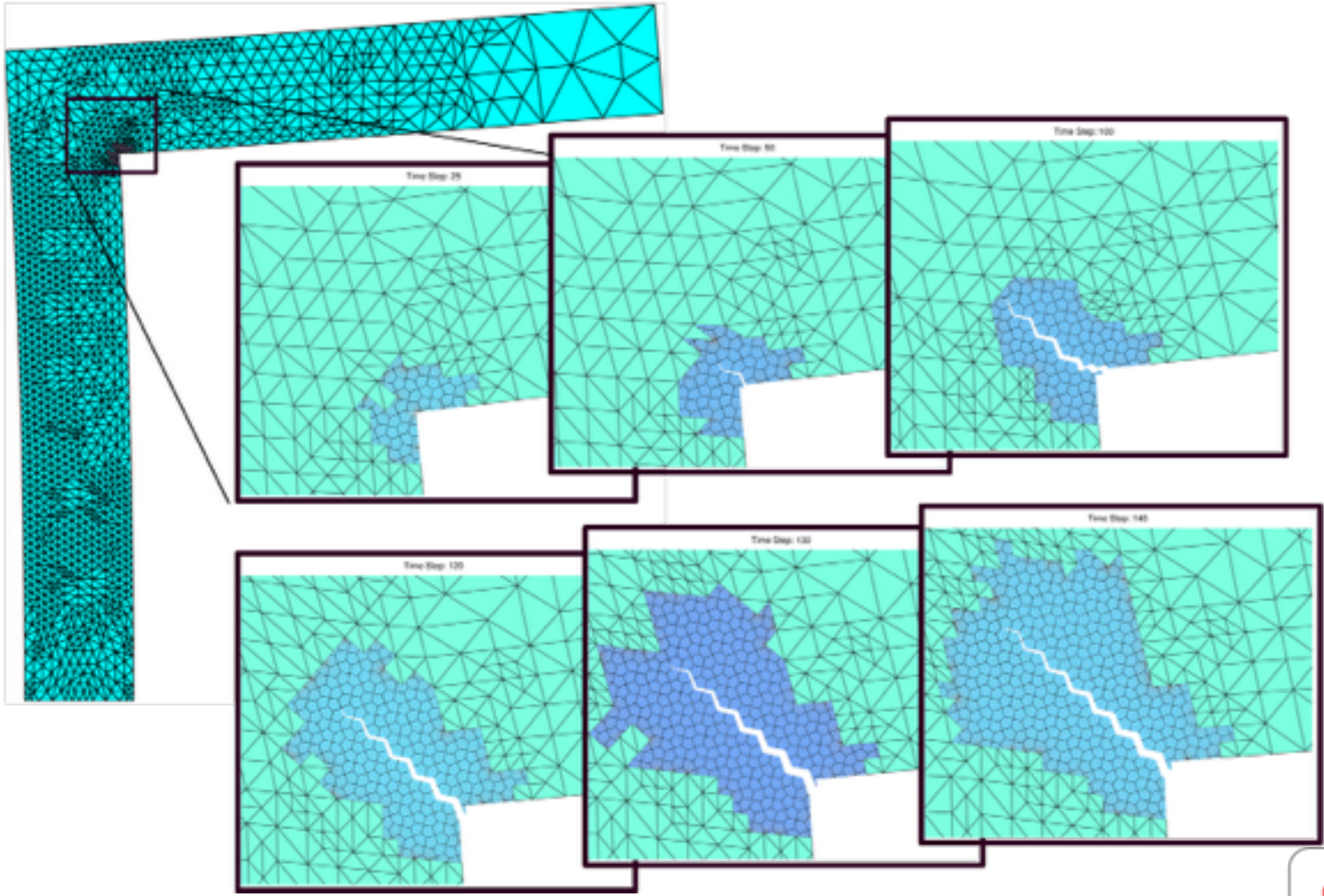
Fine-Coarse scales Coupling

What is the solution for the FE^2 **shortcoming:**
"Hybrid Multiscale Method"

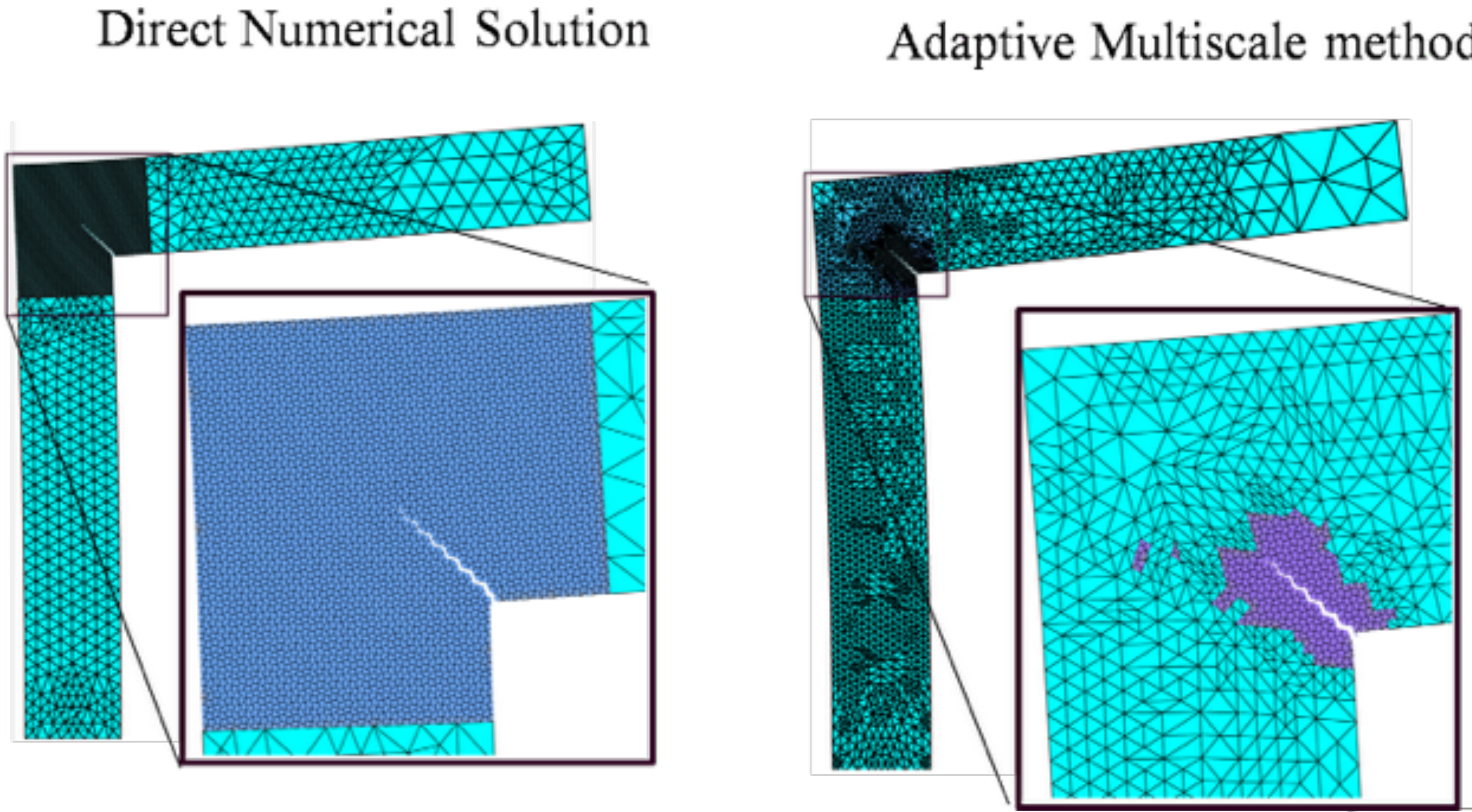
- FE^2 for non-critical region (hierarchical multiscale)
- Domain decomposition for critical region (concurrent multiscale)



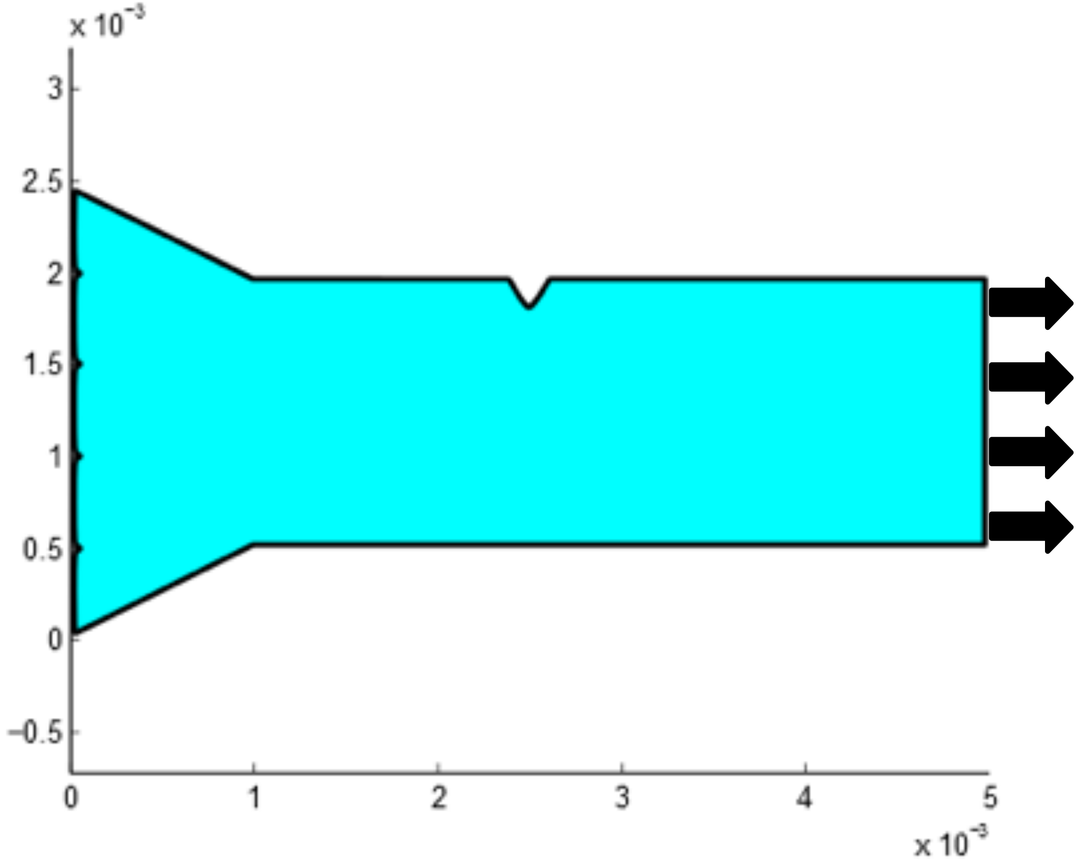
Results: L-shape



Results: L-shape



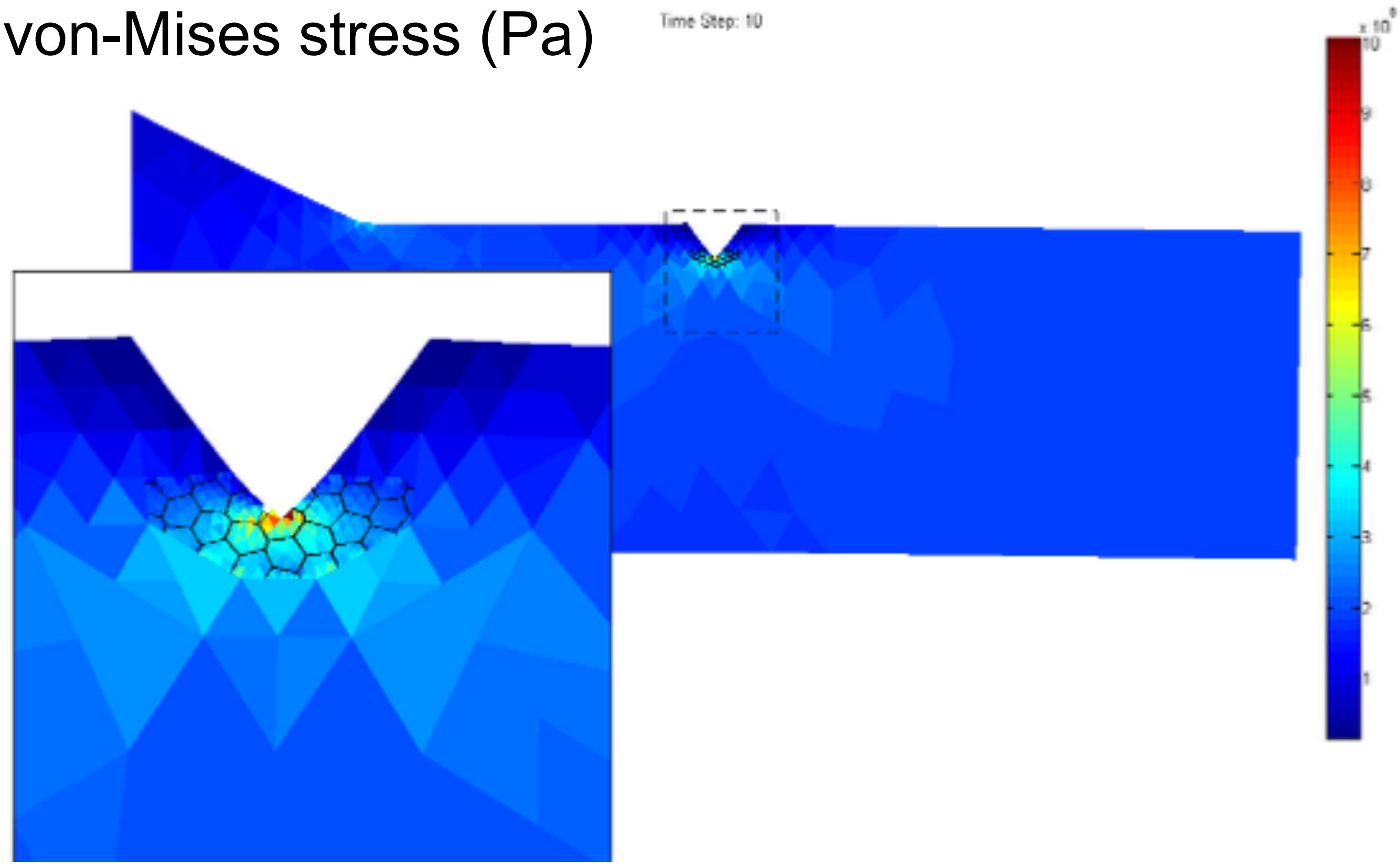
Results: uni-axial tension



- ❖ Sizes are in mm

Results: uni-axial tension

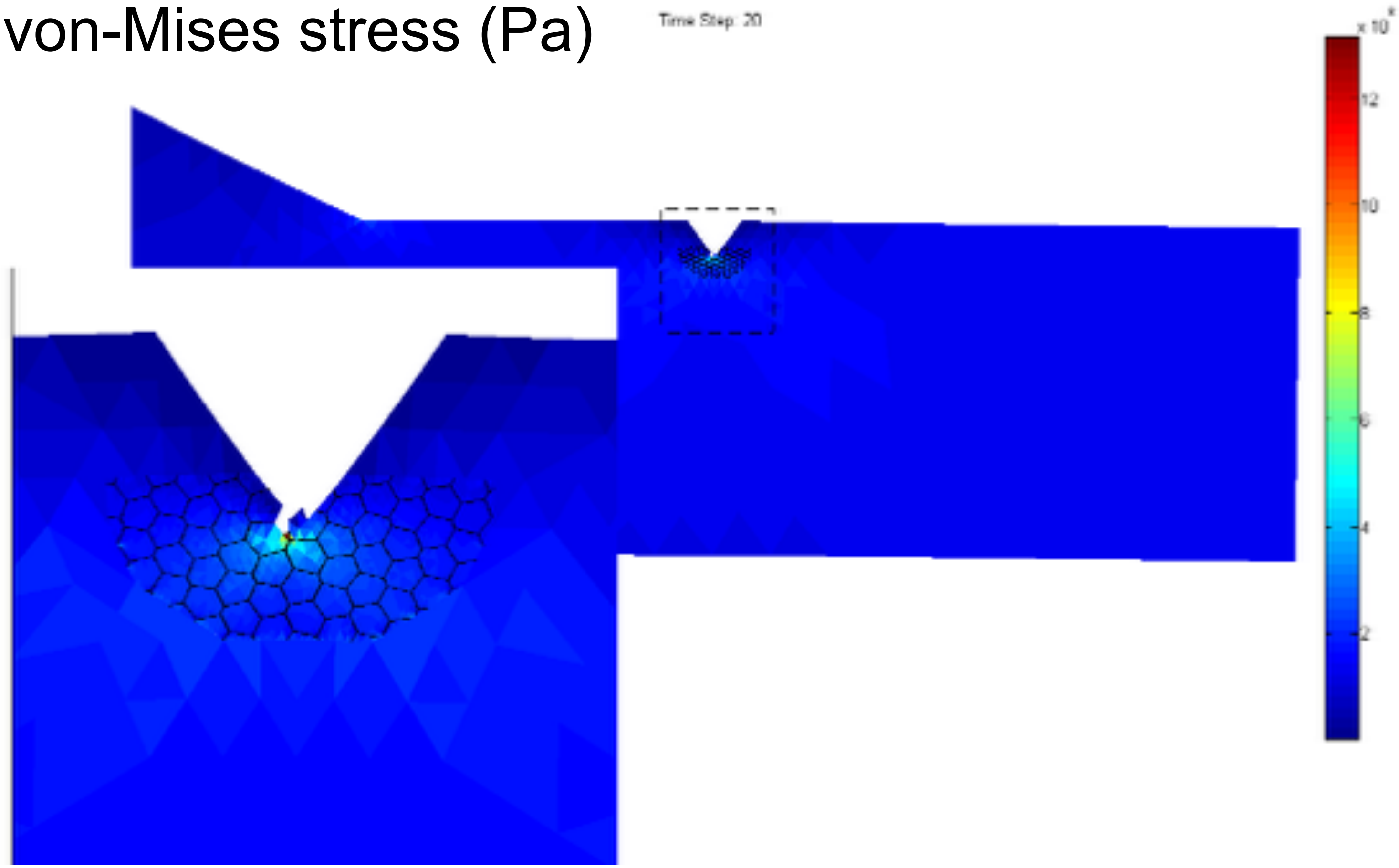
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)



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Results: uni-axial tension

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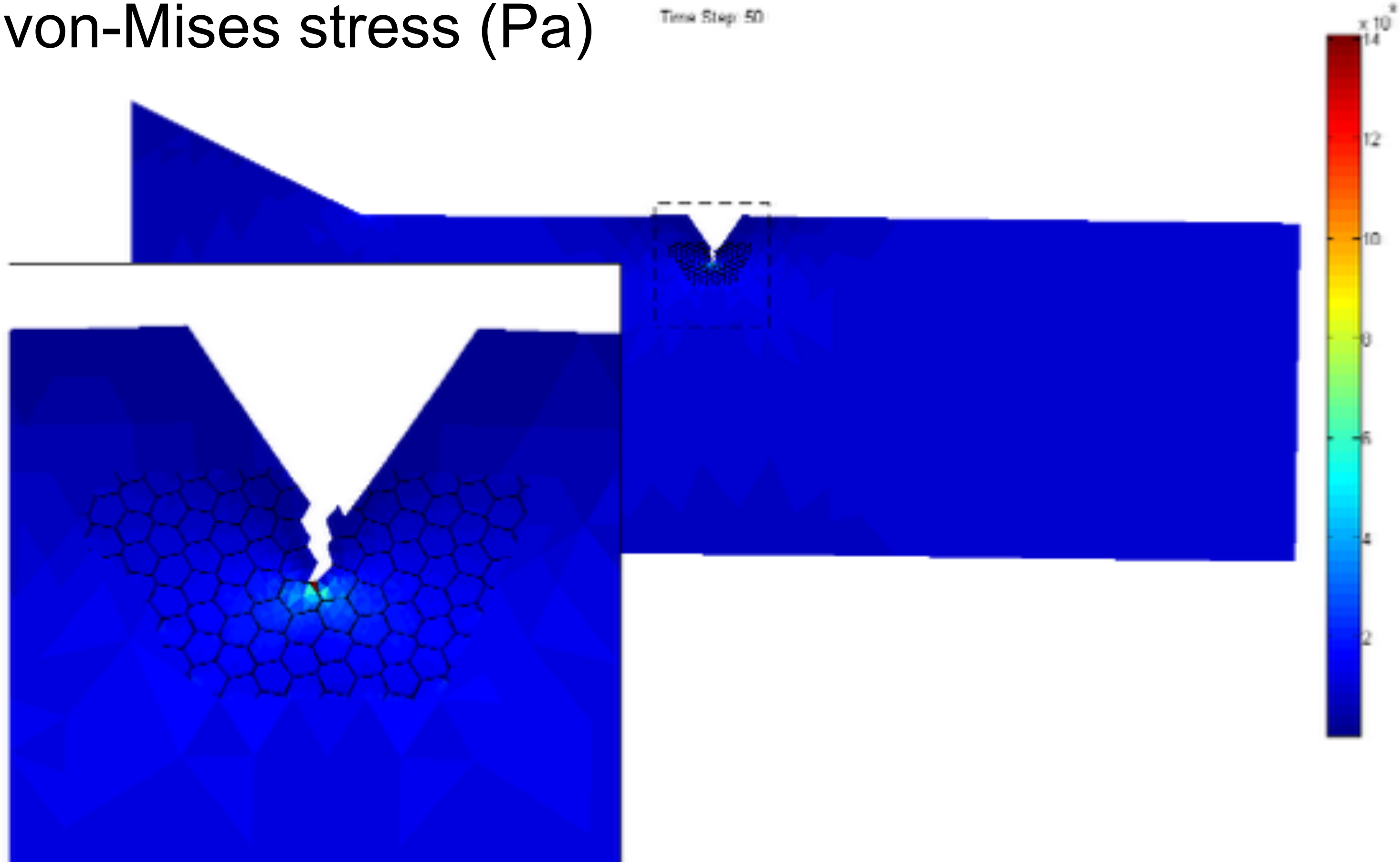
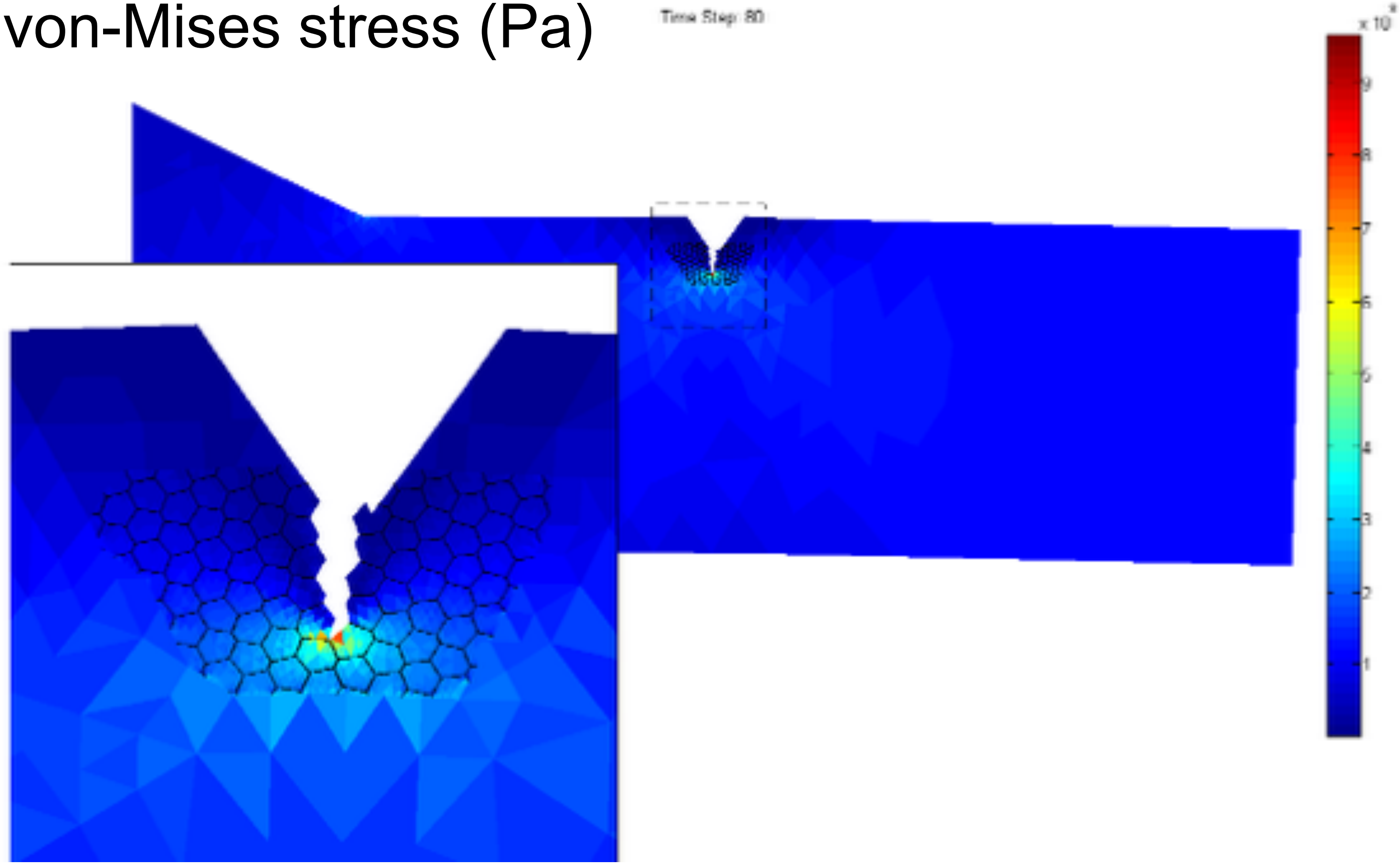


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)



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Results: uni-axial tension

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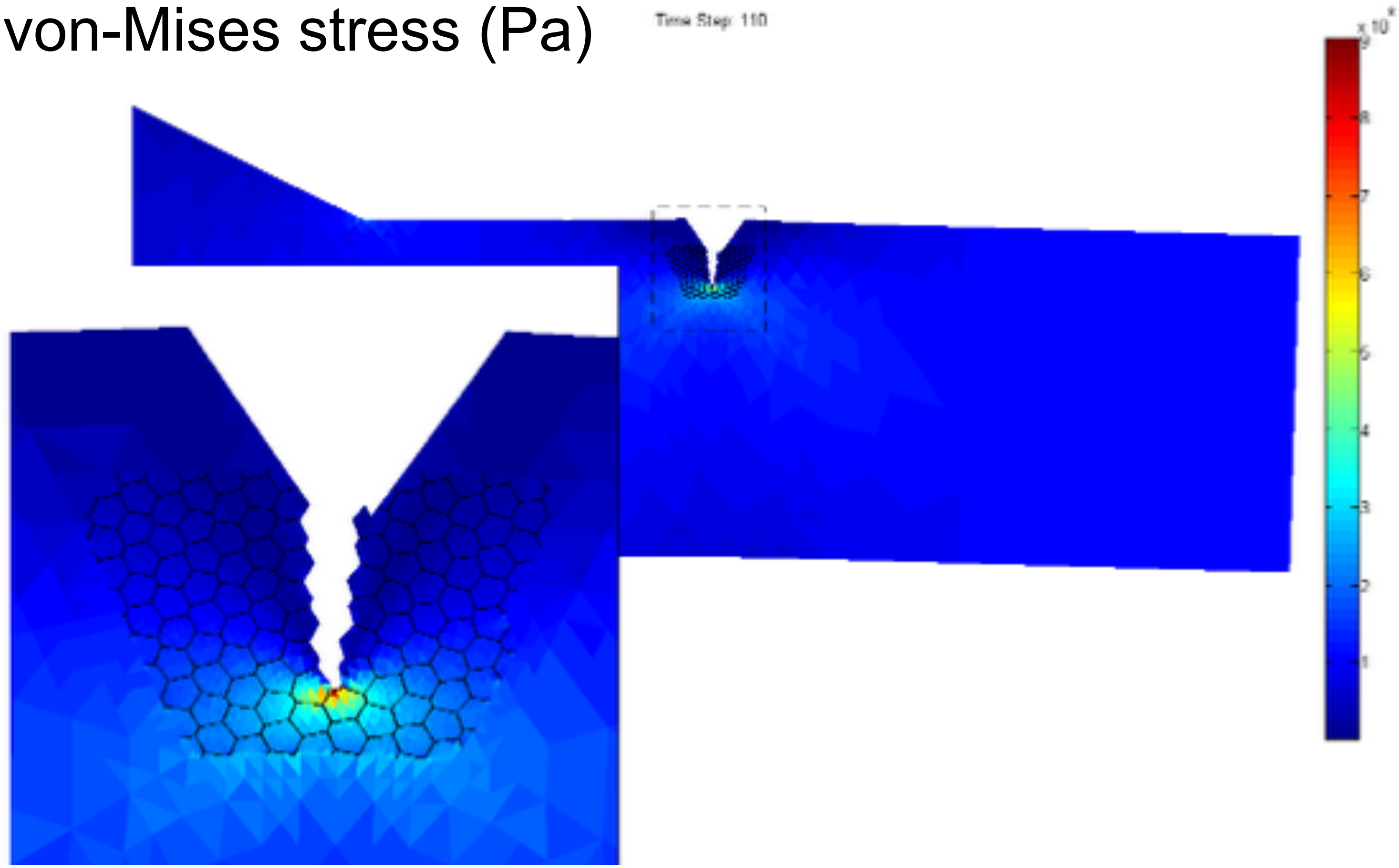


❖ 100X (magnification of displacement)

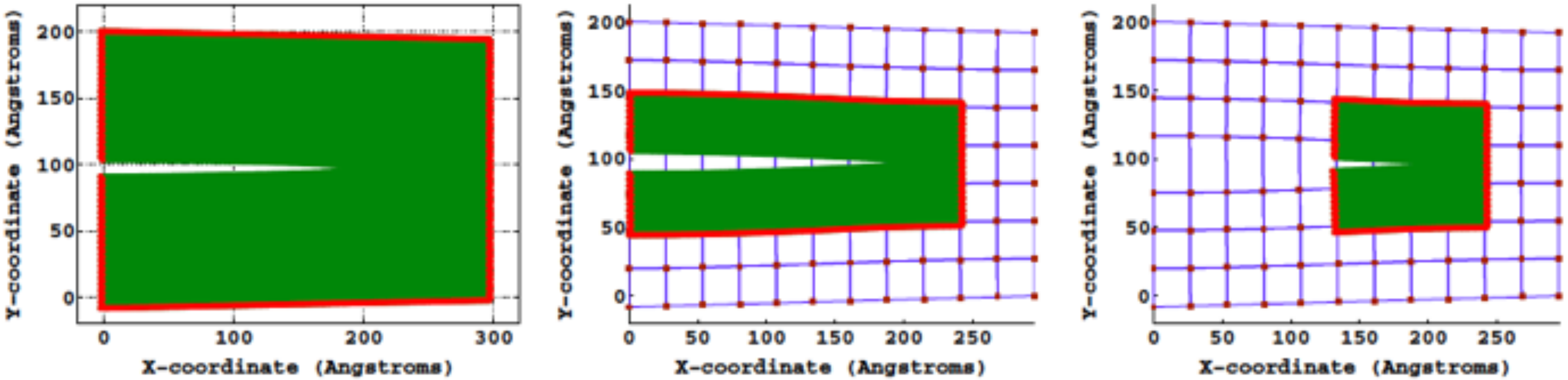
Adaptive Multiscale Method

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)

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SourceForge

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

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
- http://orbilu.uni.lu/handle/10993/12159
- http://orbilu.uni.lu/handle/10993/14135
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- http://orbilu.uni.lu/handle/10993/12157

Damage tolerance analysis directly from CAD

- http://orbilu.uni.lu/handle/10993/11850

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