

+



Computed in Luxembourg

## Computational Sciences Luxembourg

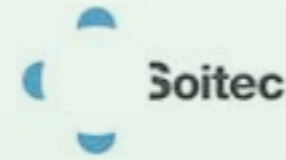
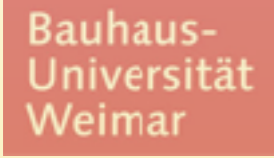


12th International Conference on Damage Assessment of Structures  
2017, Kitakyushu, Japan, 10-12 July 2017  
<http://www.damas.ugent.be/>



MAIN PARTNERS

MAIN FUNDERS since 2006 (10M)



UNIVERSITÉ DE STRASBOURG



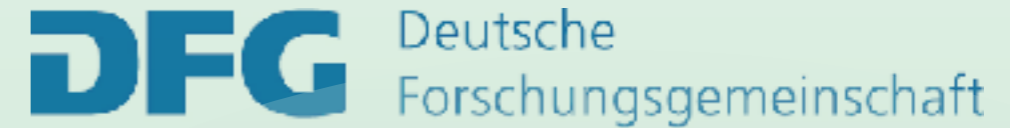
ArcelorMittal



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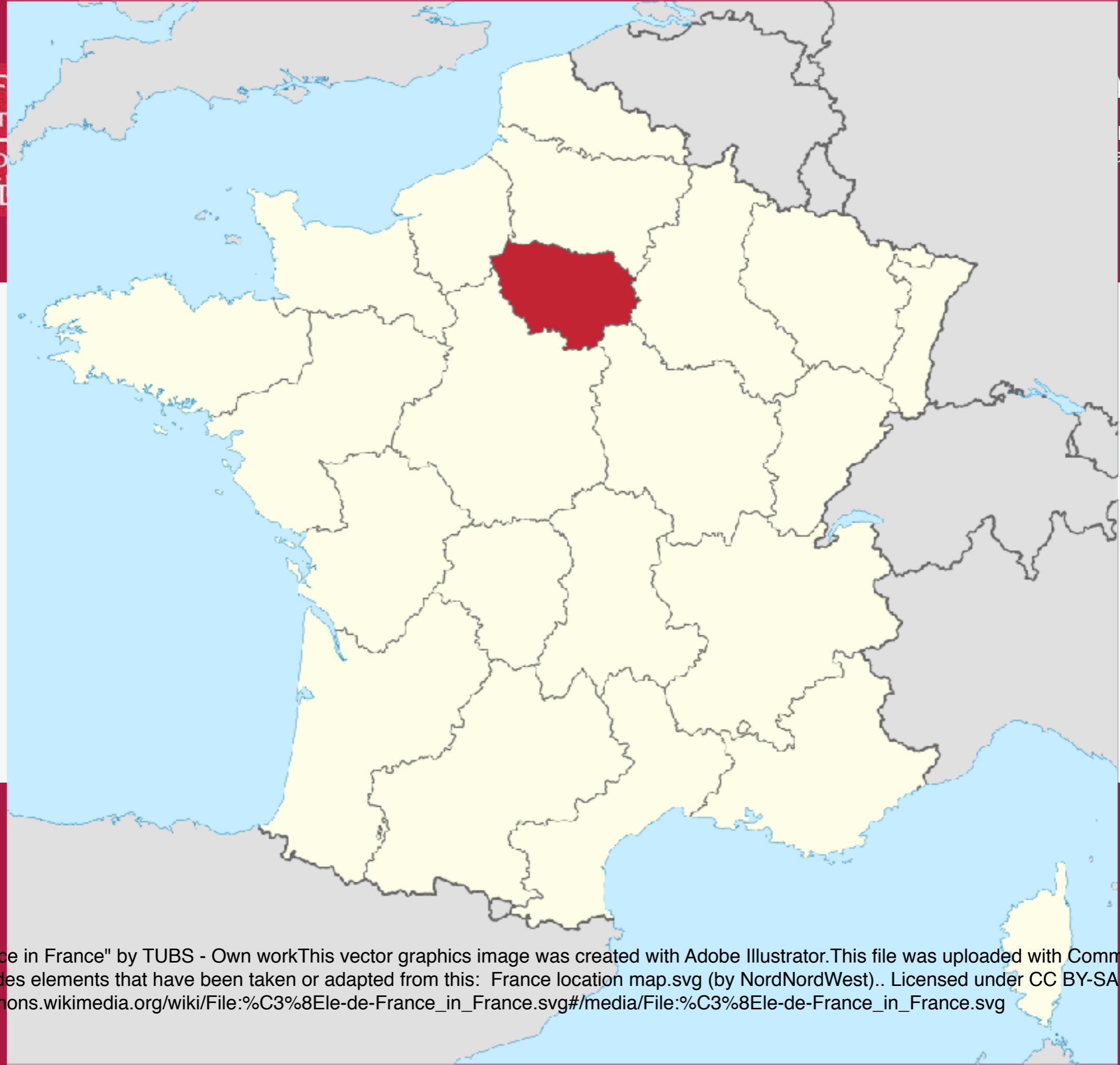
Funding

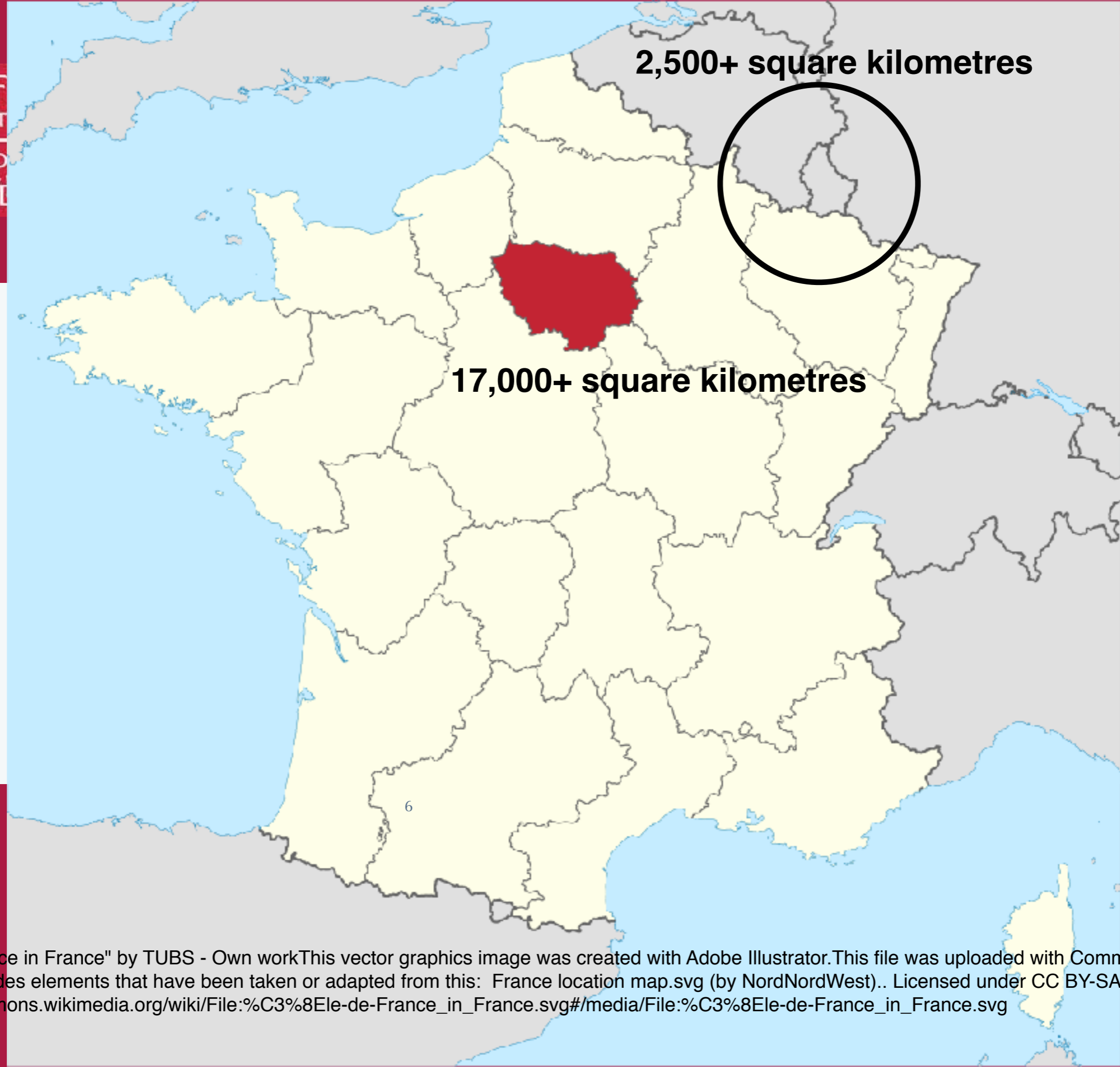
Industry















Tokyo 13,572 km<sup>2</sup> 13.5 million people...  
Luxembourg 2,500 km<sup>2</sup> 500,000 people...





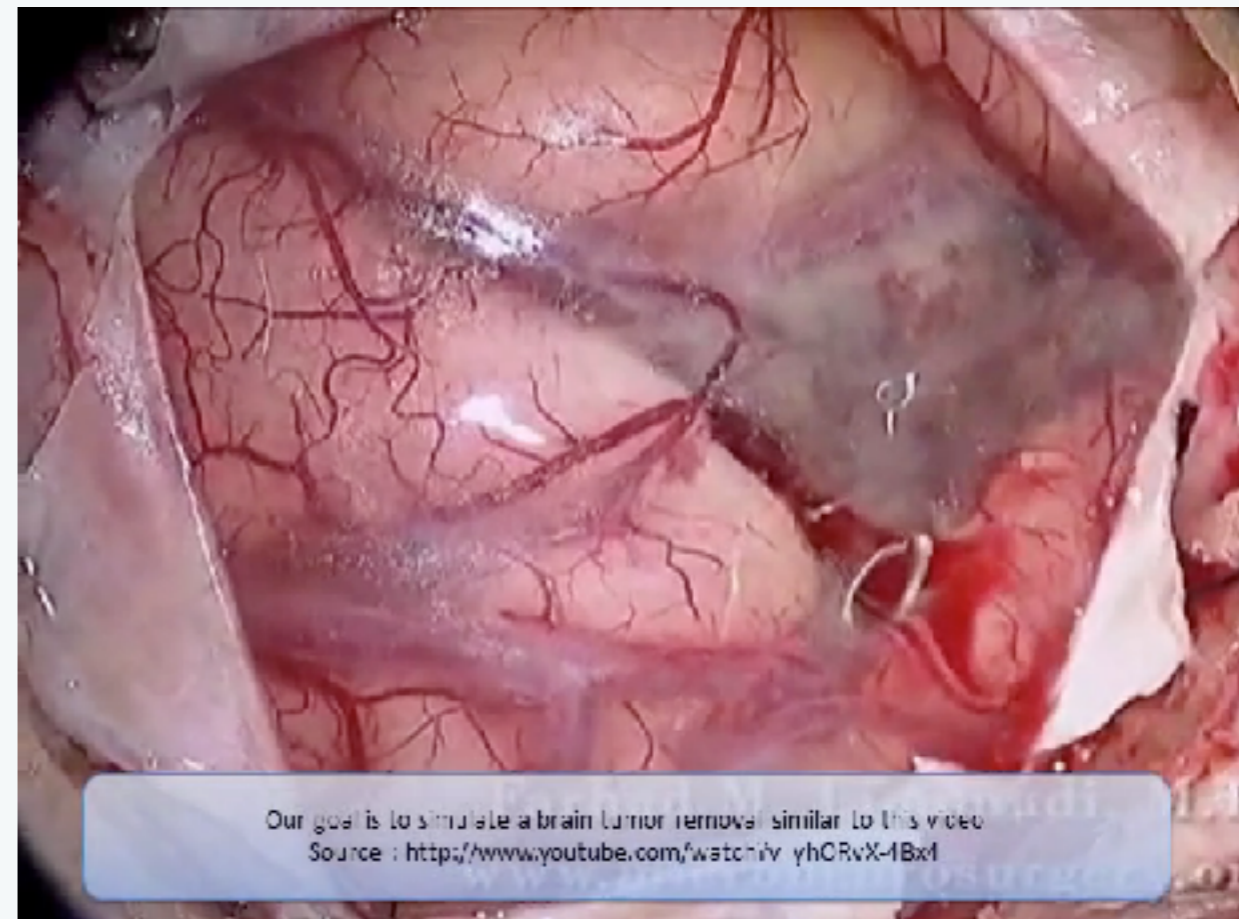
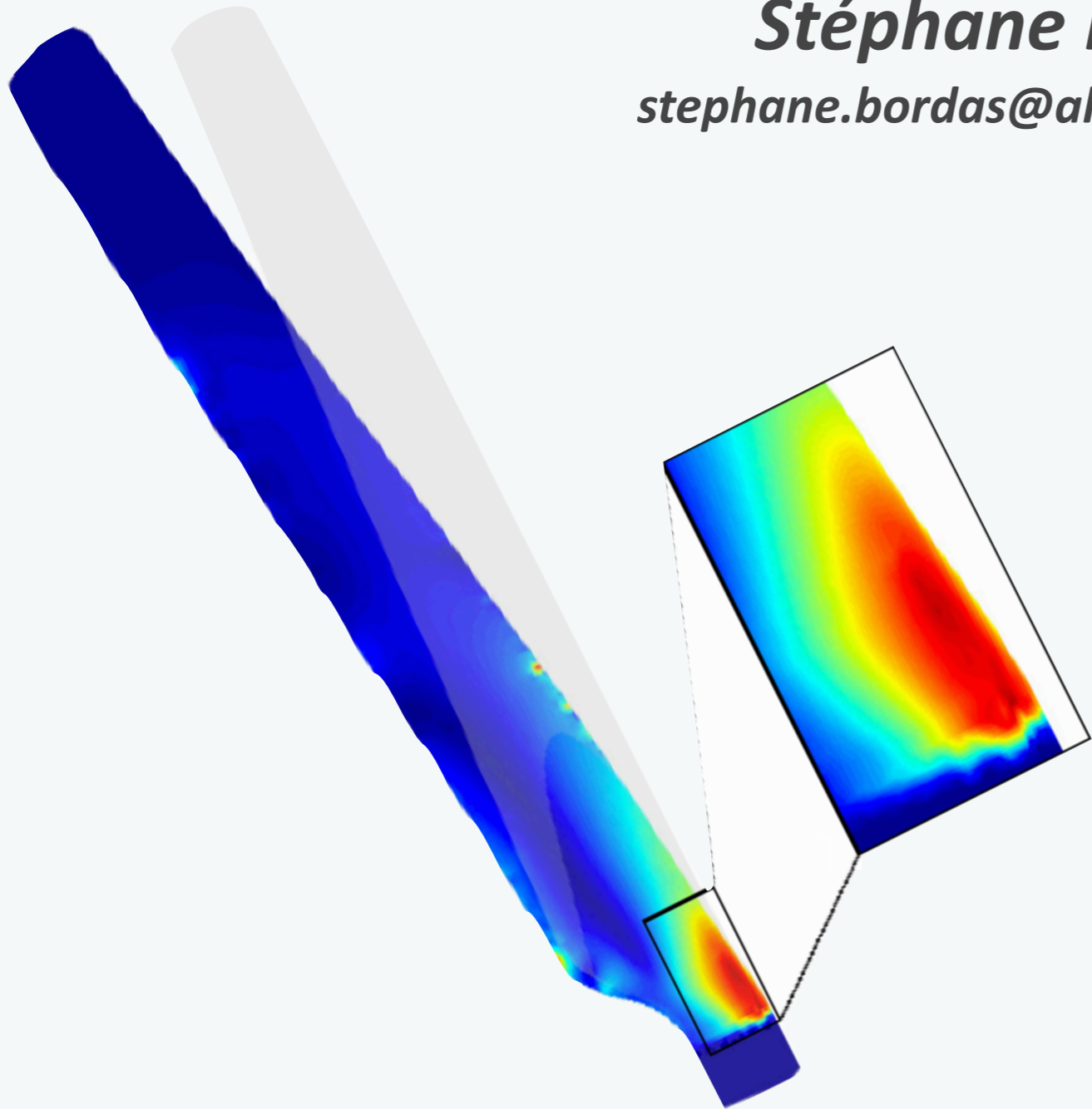


<http://hdl.handle.net/10993/31487>

# Advances in enriched finite element formulations for fracture and cutting: *engineering and surgical simulation applications*

**Stéphane P.A. Bordas**

*stephane.bordas@alum.northwestern.edu*



# Motivation: fracture mechanics

Shuttle crash, 2003



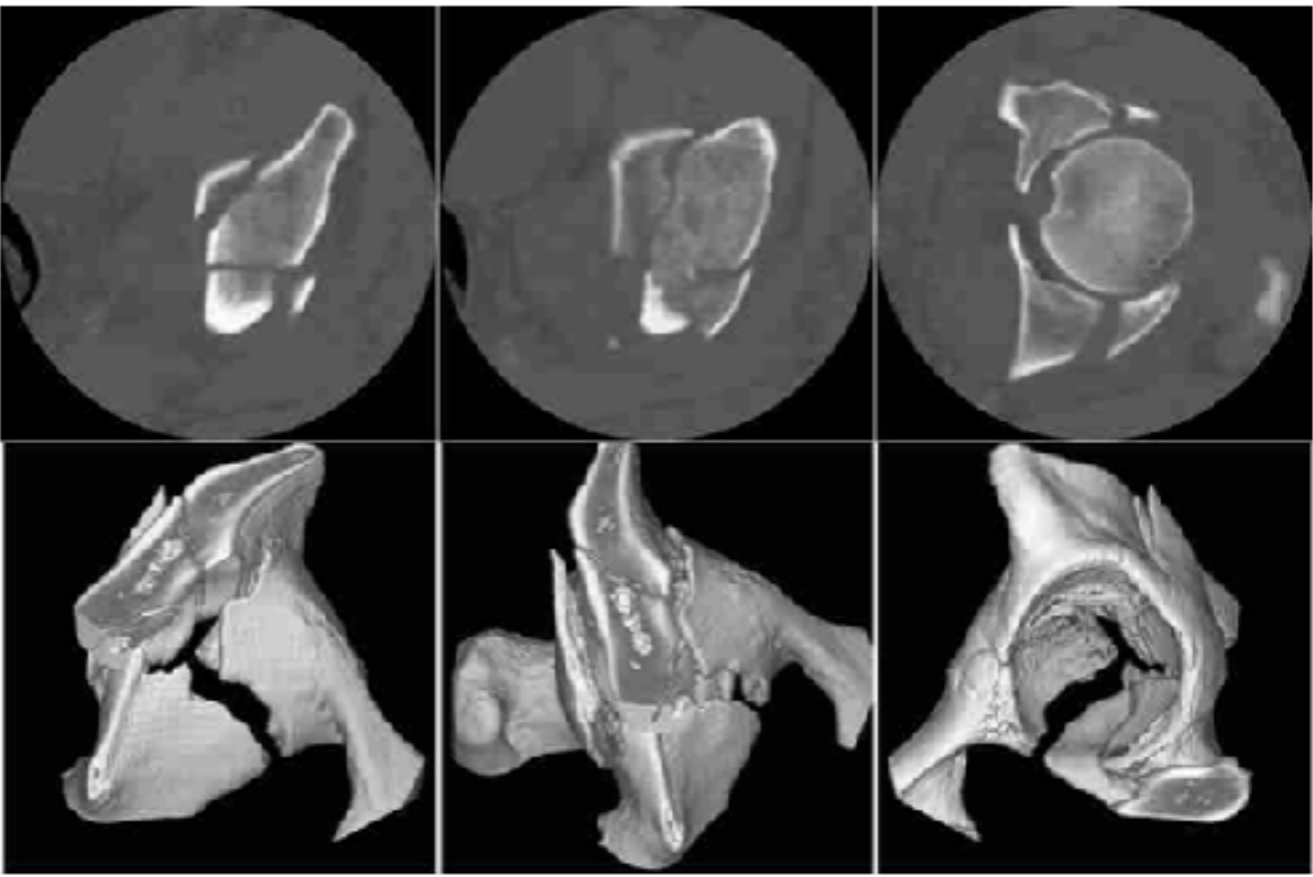
Landslide, Colorado

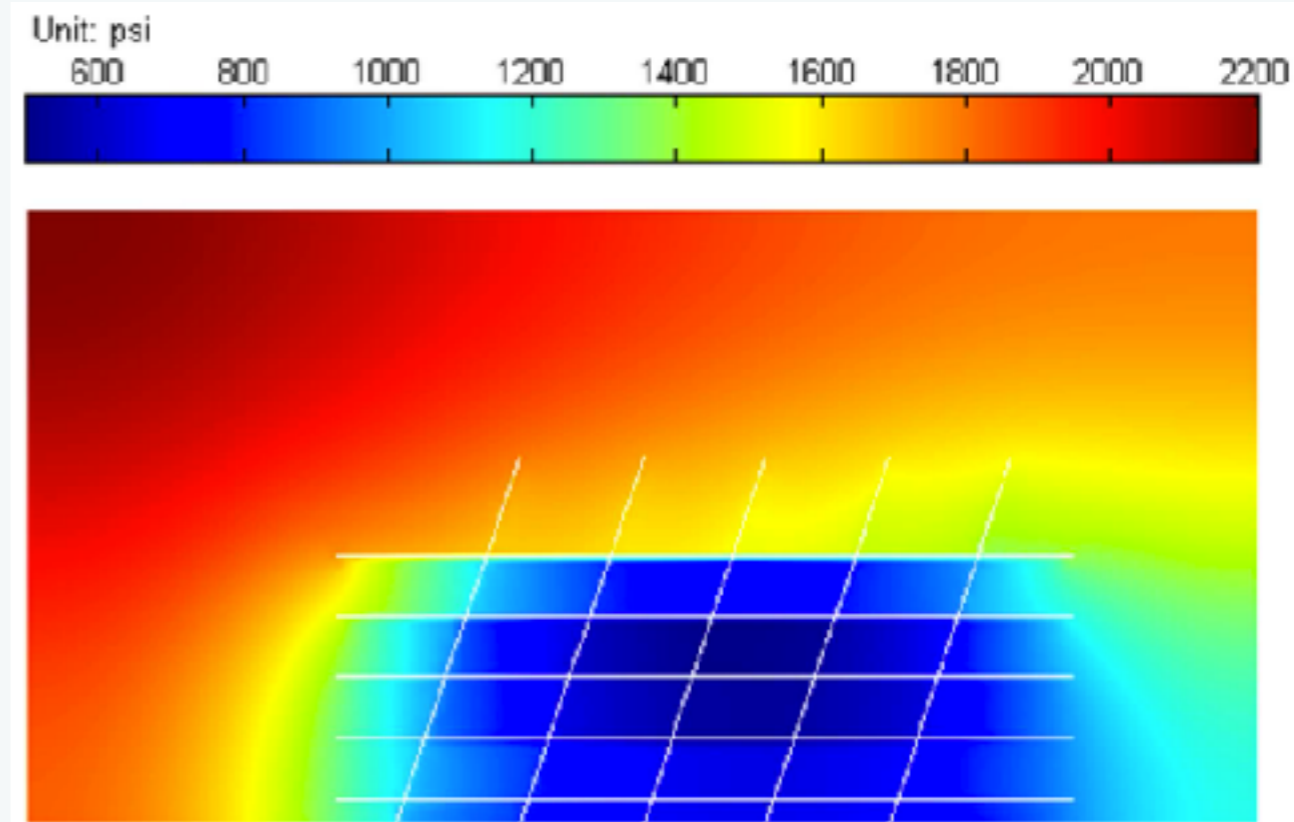
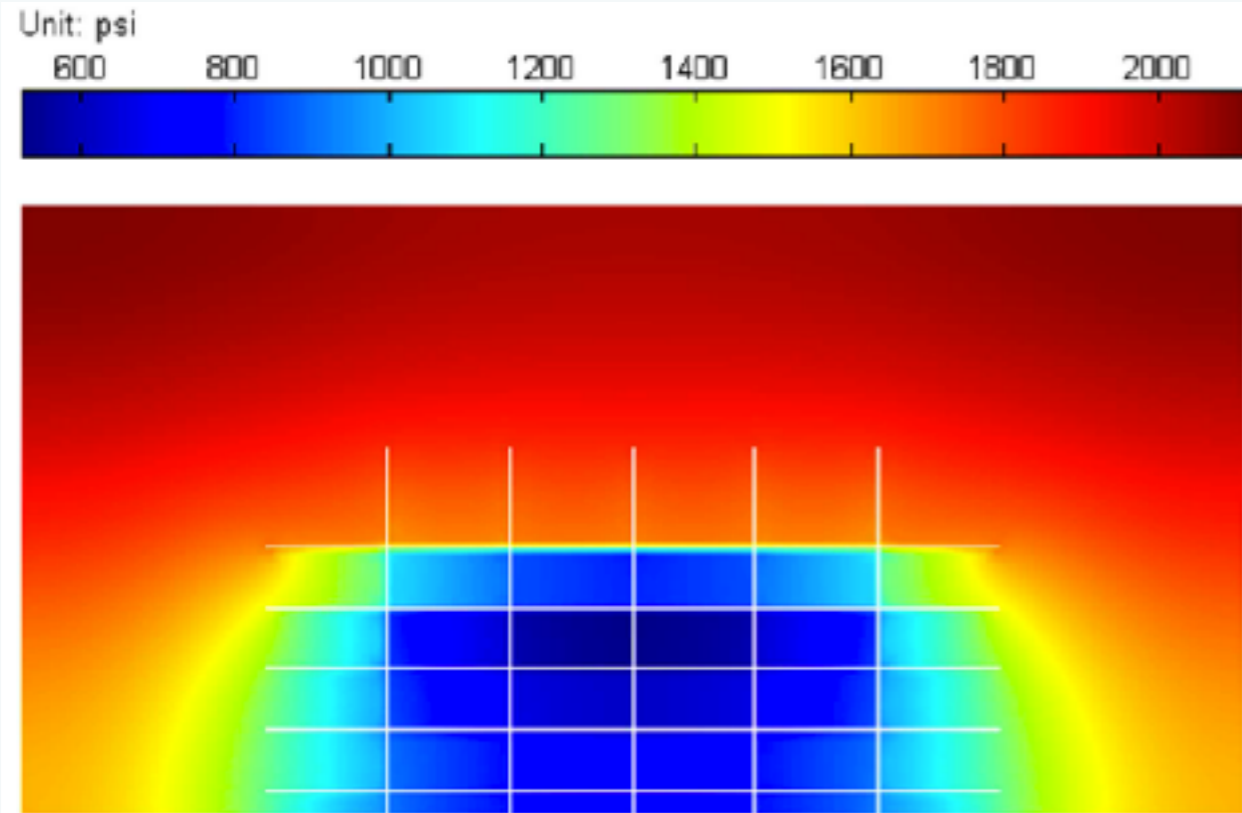
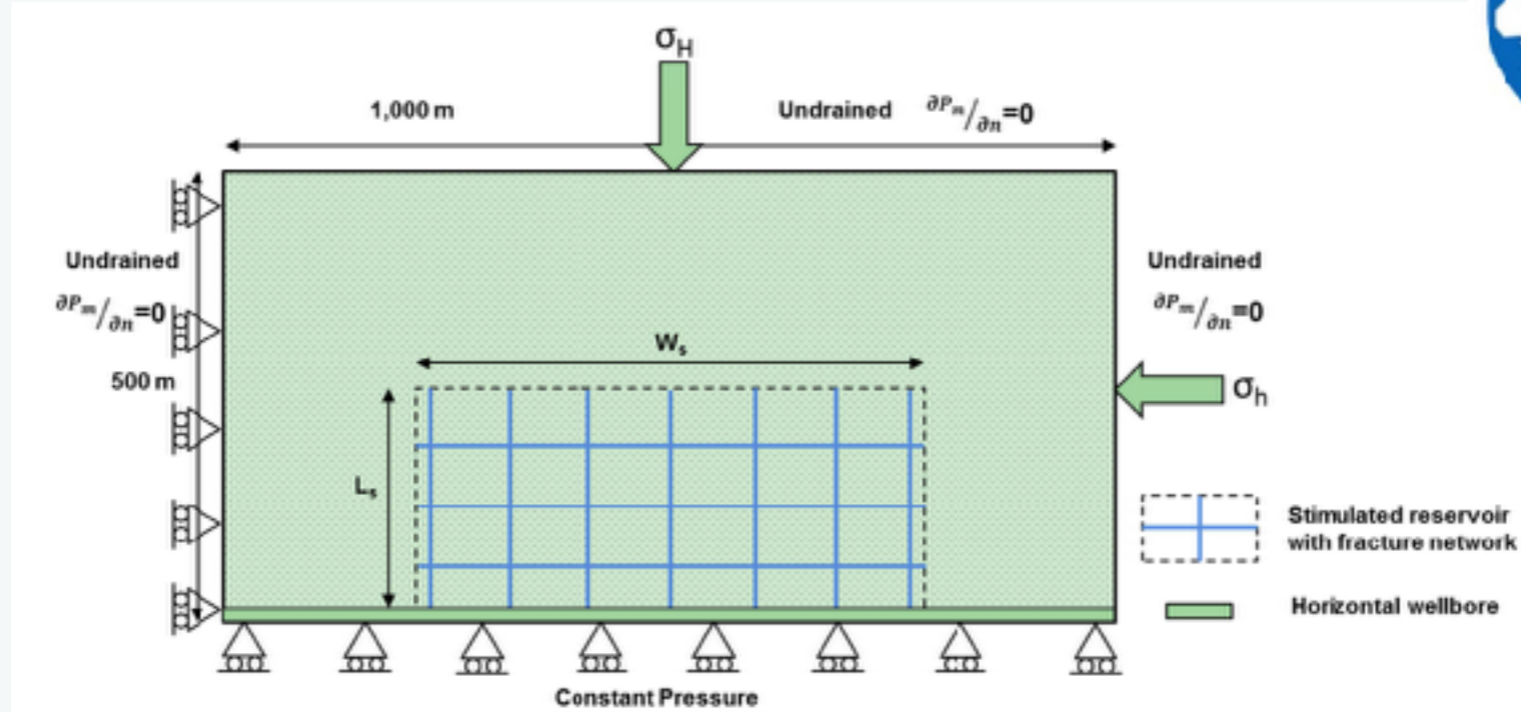


Taiwan earthquake, 2003



Fragmentation of concrete





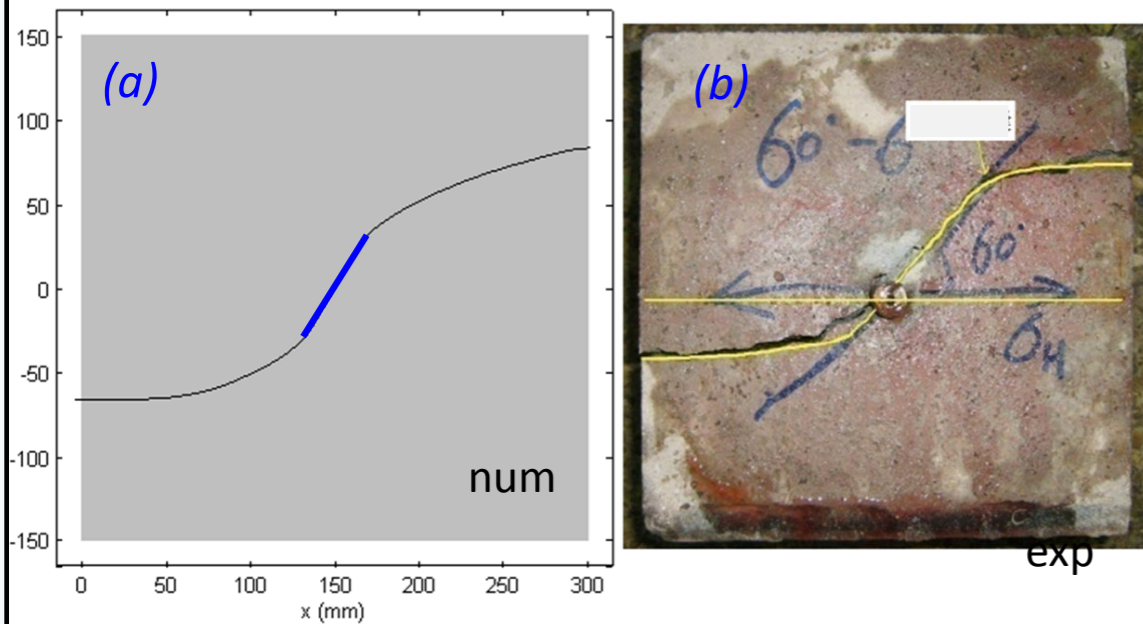
# Motivation: fracture of engineering structures and materials

## ► Limerick: unidirectional composites

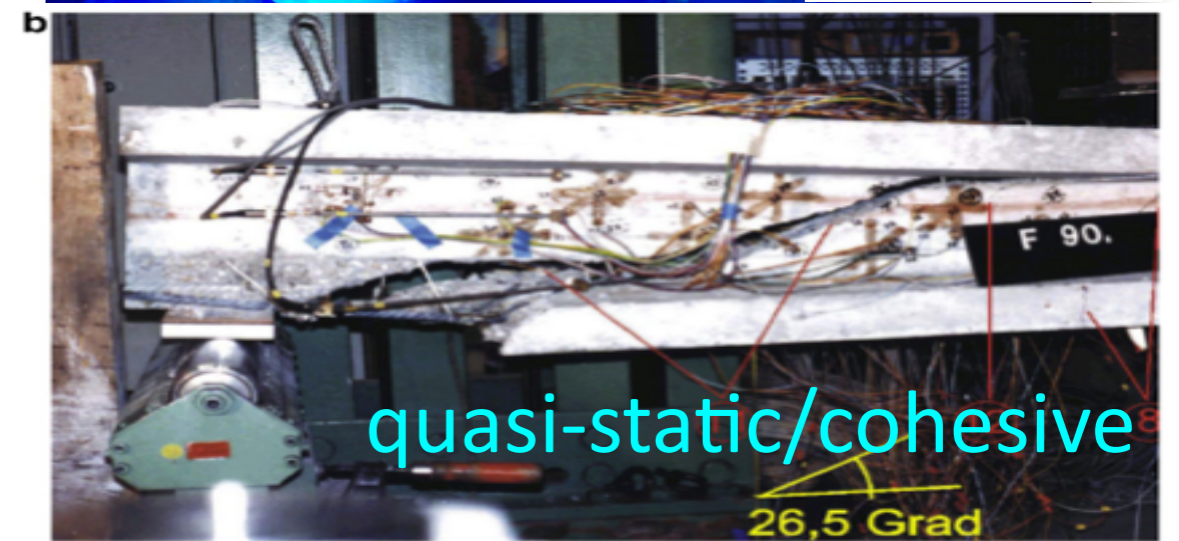
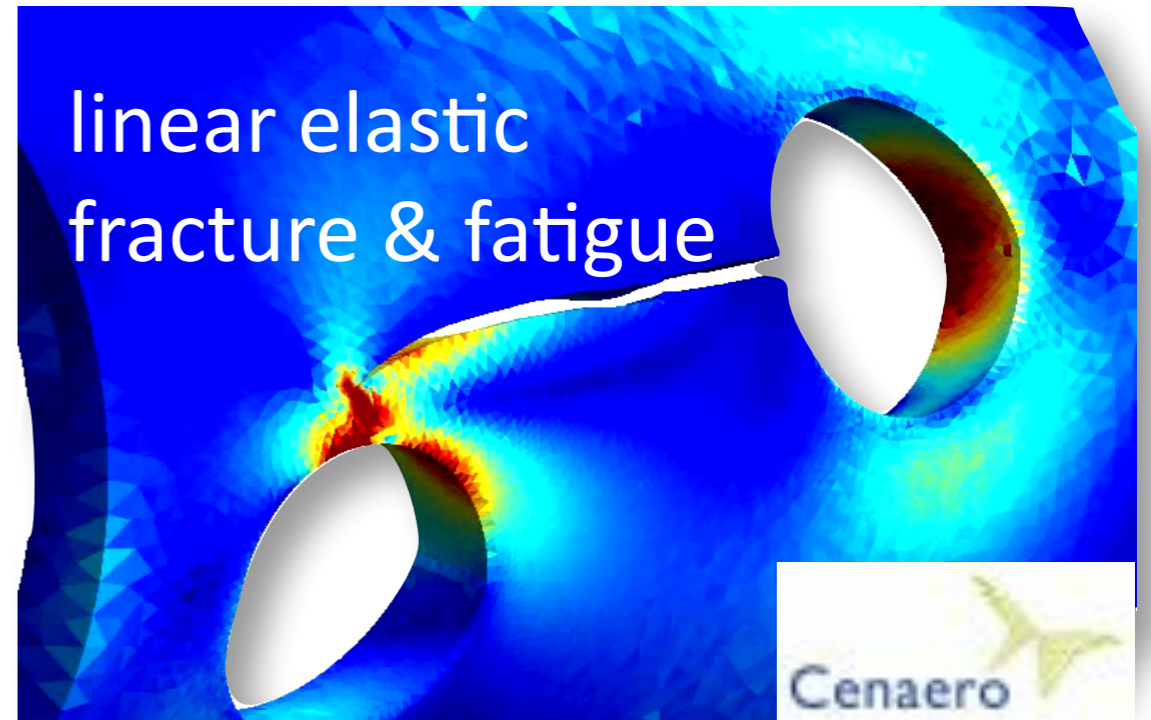


thesis L. Cahill, 2014

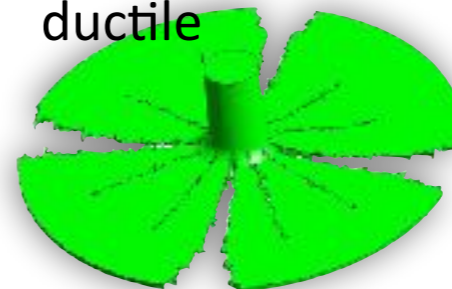
## ► China/USA: hydraulic fracturing (shale gas)



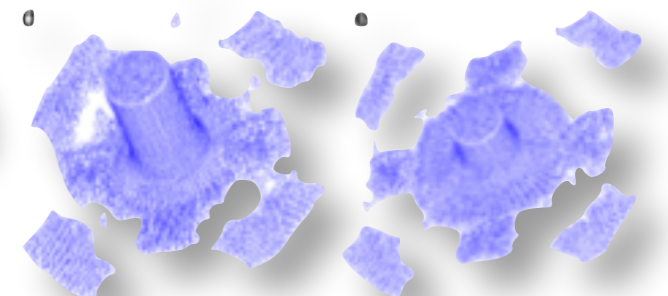
thesis M. Sheng, USA, China, 2016



dynamics  
ductile



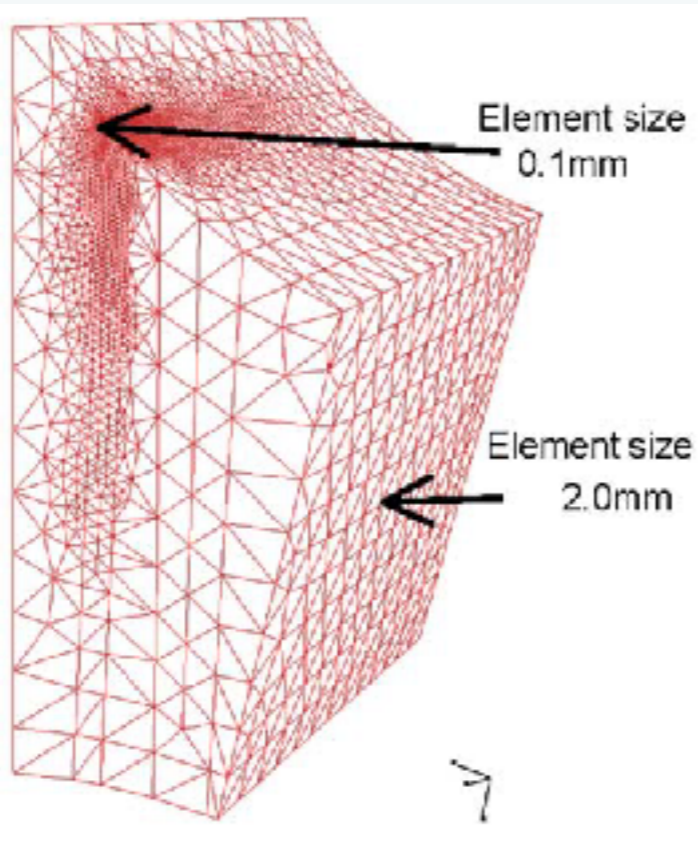
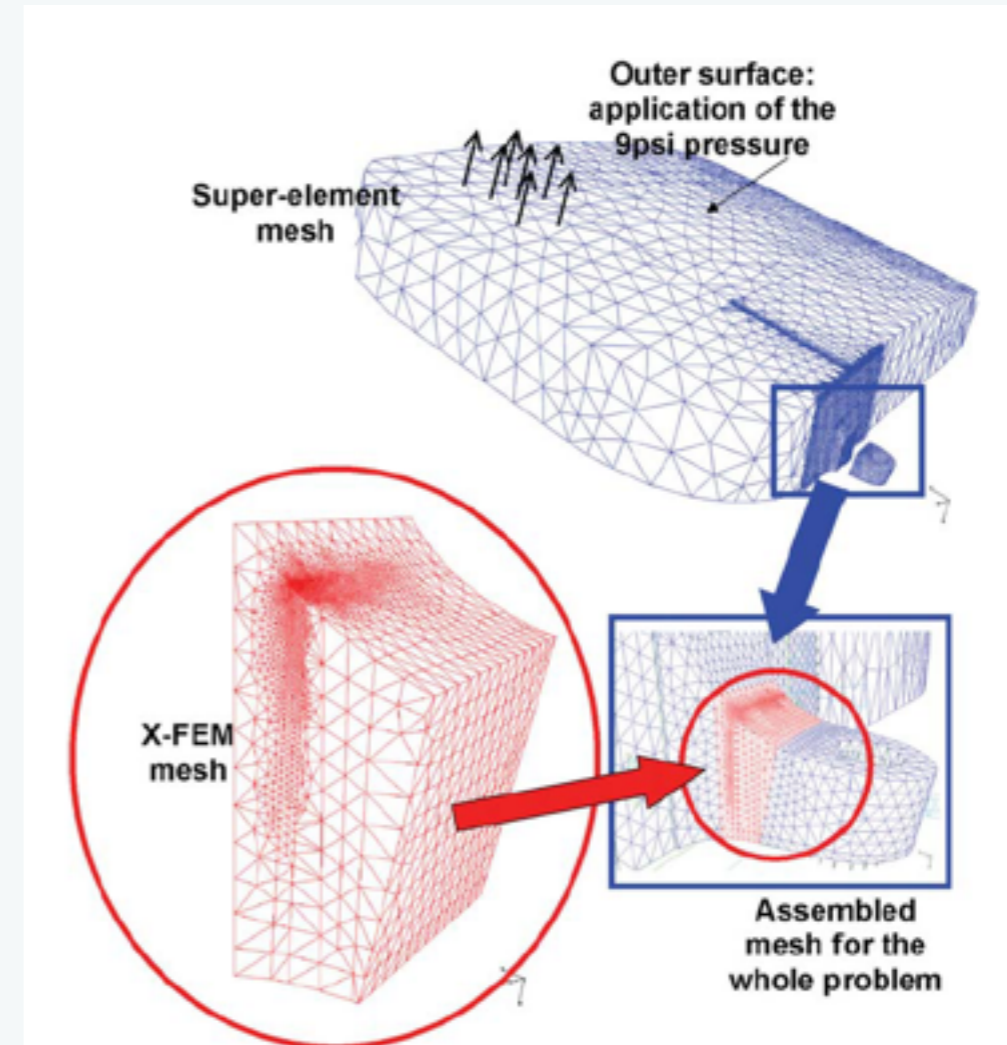
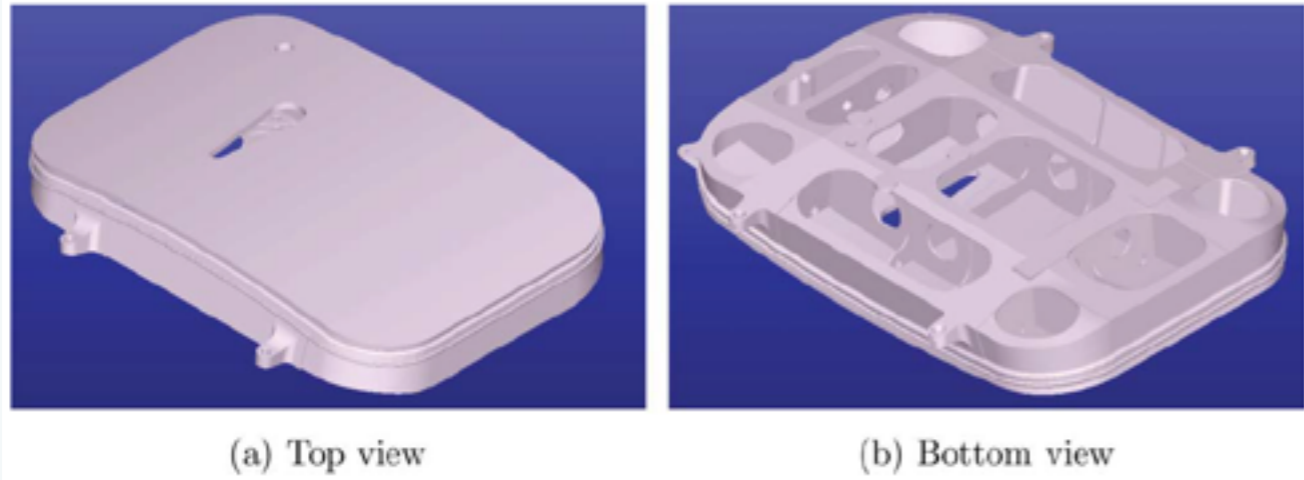
dynamics/brittle





# Fracture of 'homogeneous' materials

**Question: when should a structure be inspected for flaws?**



**ad hoc mesh refinement**

SPAB and B. Moran, Engineering Fracture Mechanics, 2006  
 V.P. Nguyen et al. XFEM C++ Library IJNME, 2007  
**Industrial applications of extended finite element methods**  
 See also E. Wyart et al, EFM, IJNME, 2008

*Choice of the Model*

*Choice of the Discretisation Scheme*

*Small scale yielding? Linear elastic fracture?*

*Elastic-Plastic fracture mechanics?*

*Damage models (local? non-local? gradient?)*

*Multi-scale? (concurrent? semi-concurrent?)*

*Finite element method (remeshing?)*

*Boundary element method (non-linearities?)*

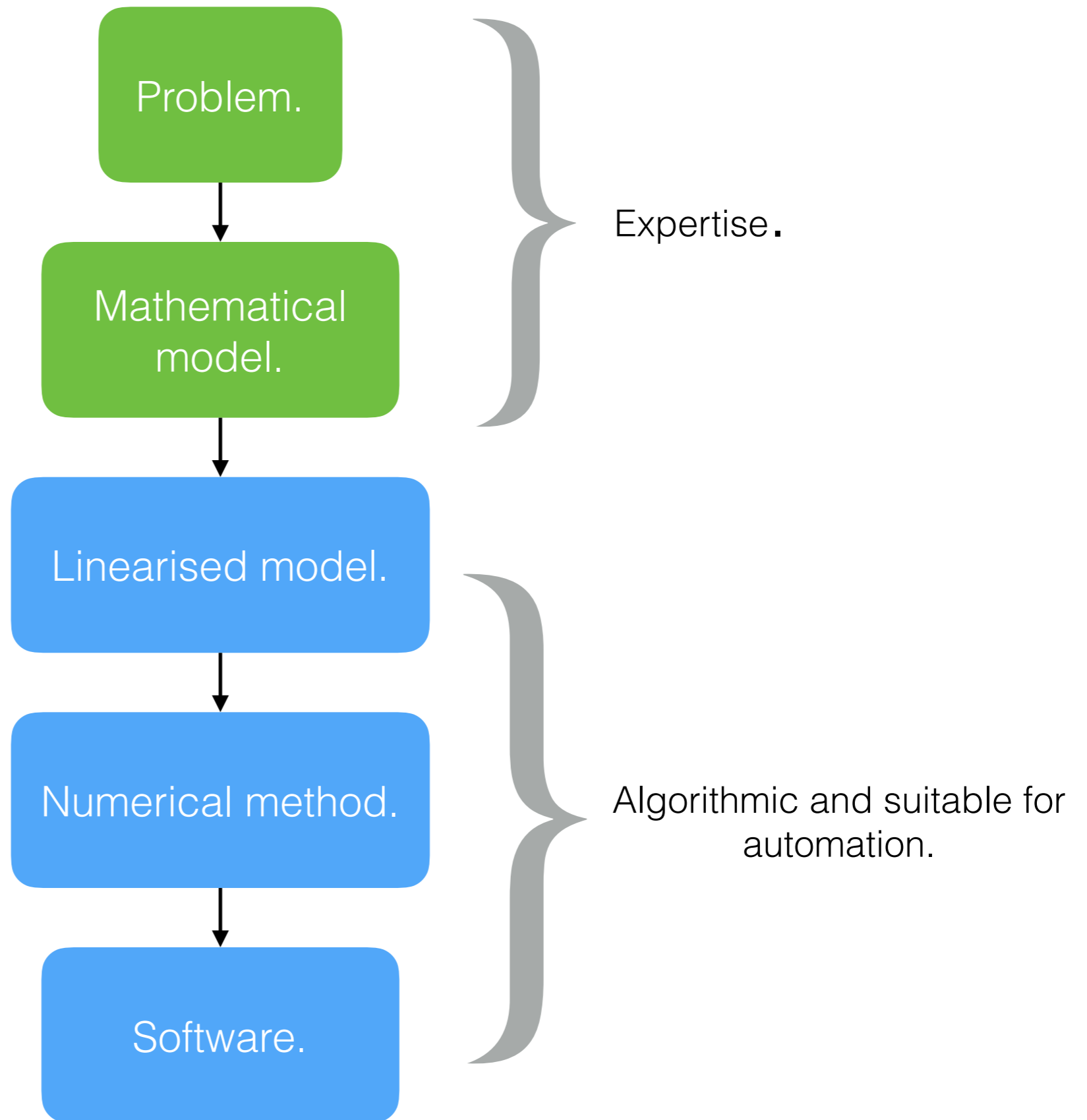
*Extended finite element methods (multi-crack?)*

*Meshfree methods (cost? stability? robustness?)*



Steering council: Alnaes, Bletcha, **Hale**, Logg, Richardson, Ring, Rognes and Wells.  
Contributors: Too many to name!

- Key idea: implement high-level description of finite element models in the Unified Form Language.
- Let algorithms take over the tedious/difficult work of linearisation and transforming maths into lower-level languages.
- Not a toy; scales to huge problems with billions of unknowns on Top 100 supercomputers.

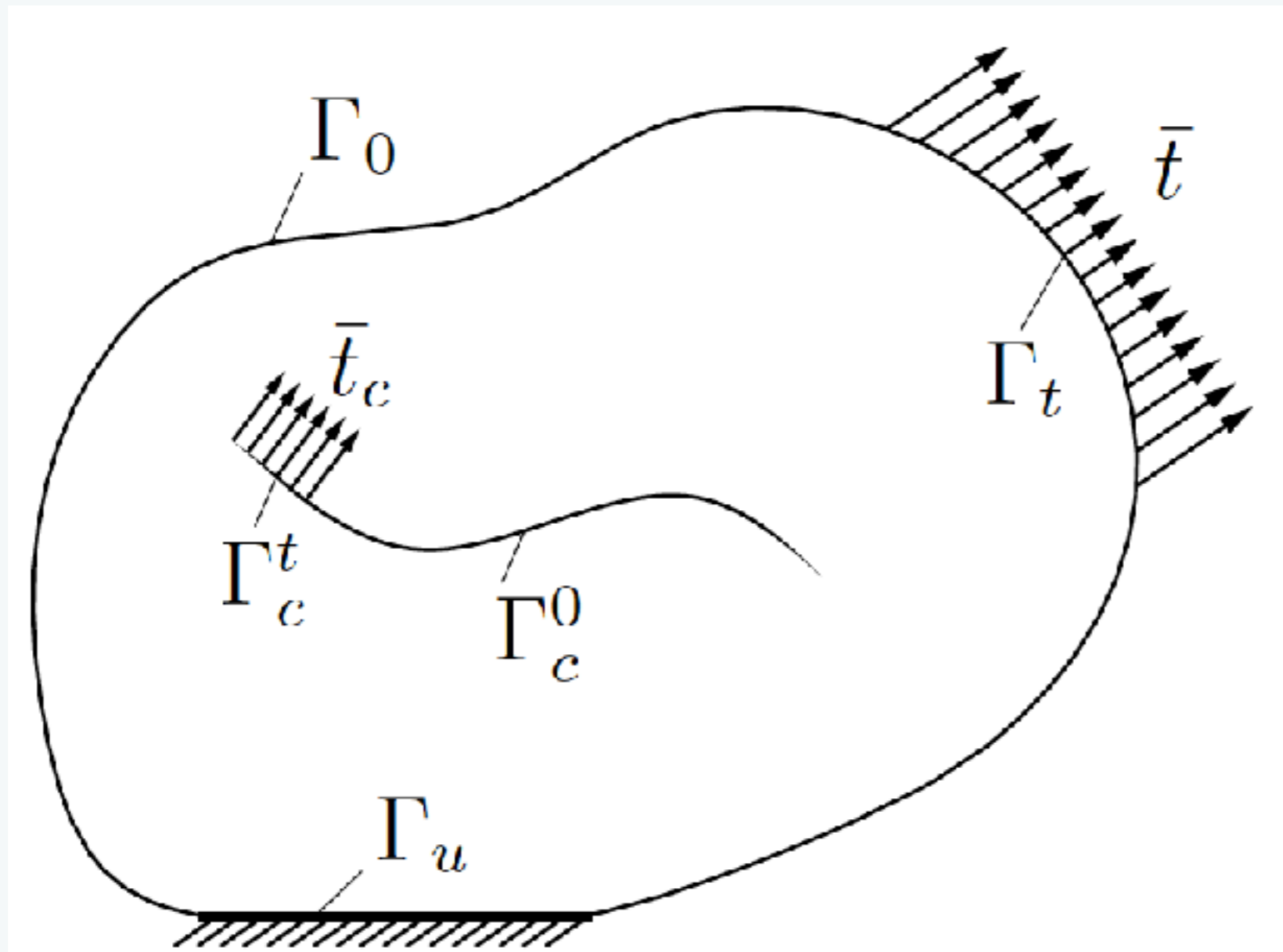


*Linear elastic fracture mechanics (LEFM)*  
*(Extended/Enriched) Finite element methods*  
*(Extended/Enriched) Isogeometric Boundary  
Element Methods*

# What is a crack?

*a 1D line in 2D space*

*a 2D surface in 3D space*

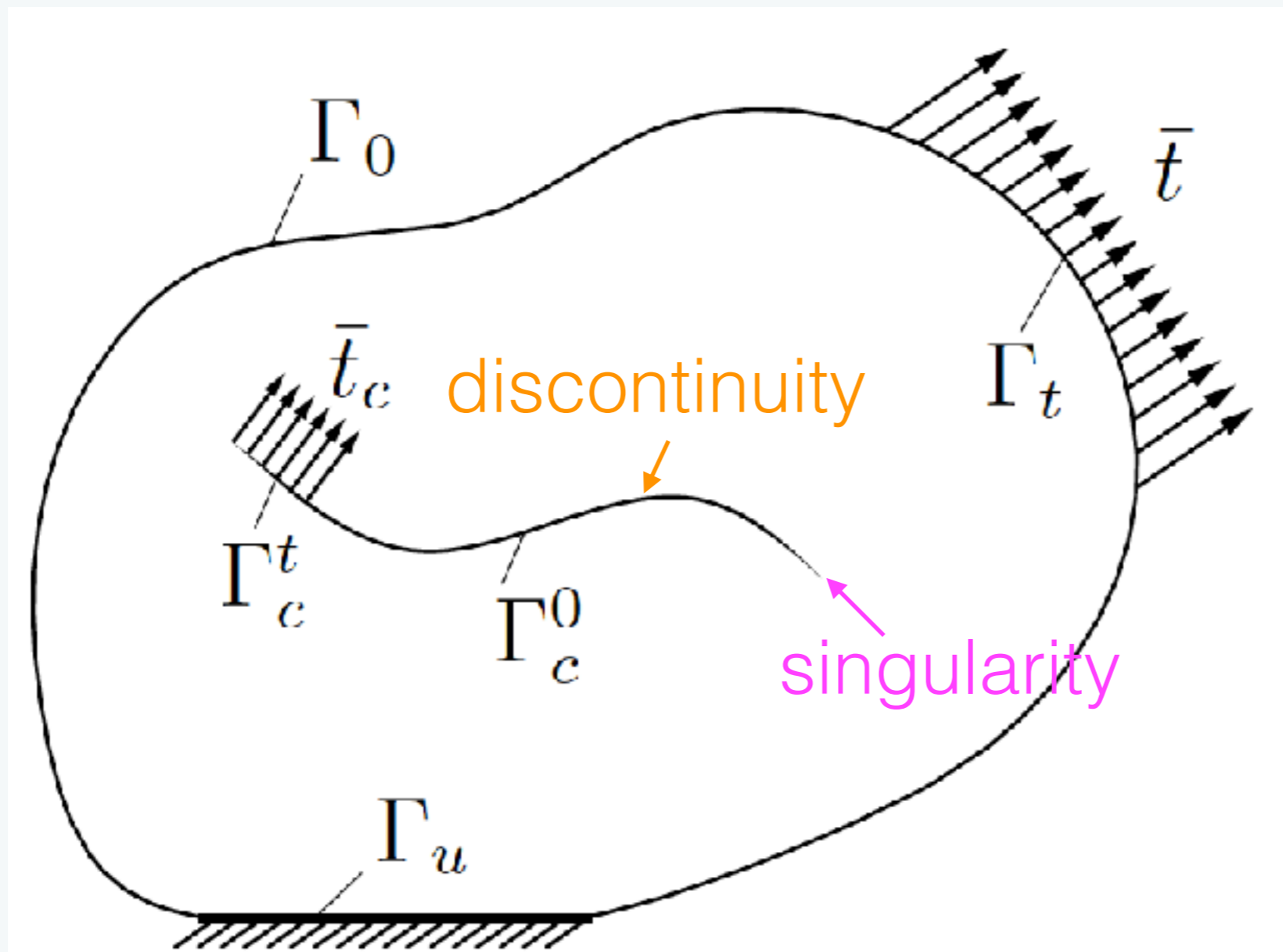




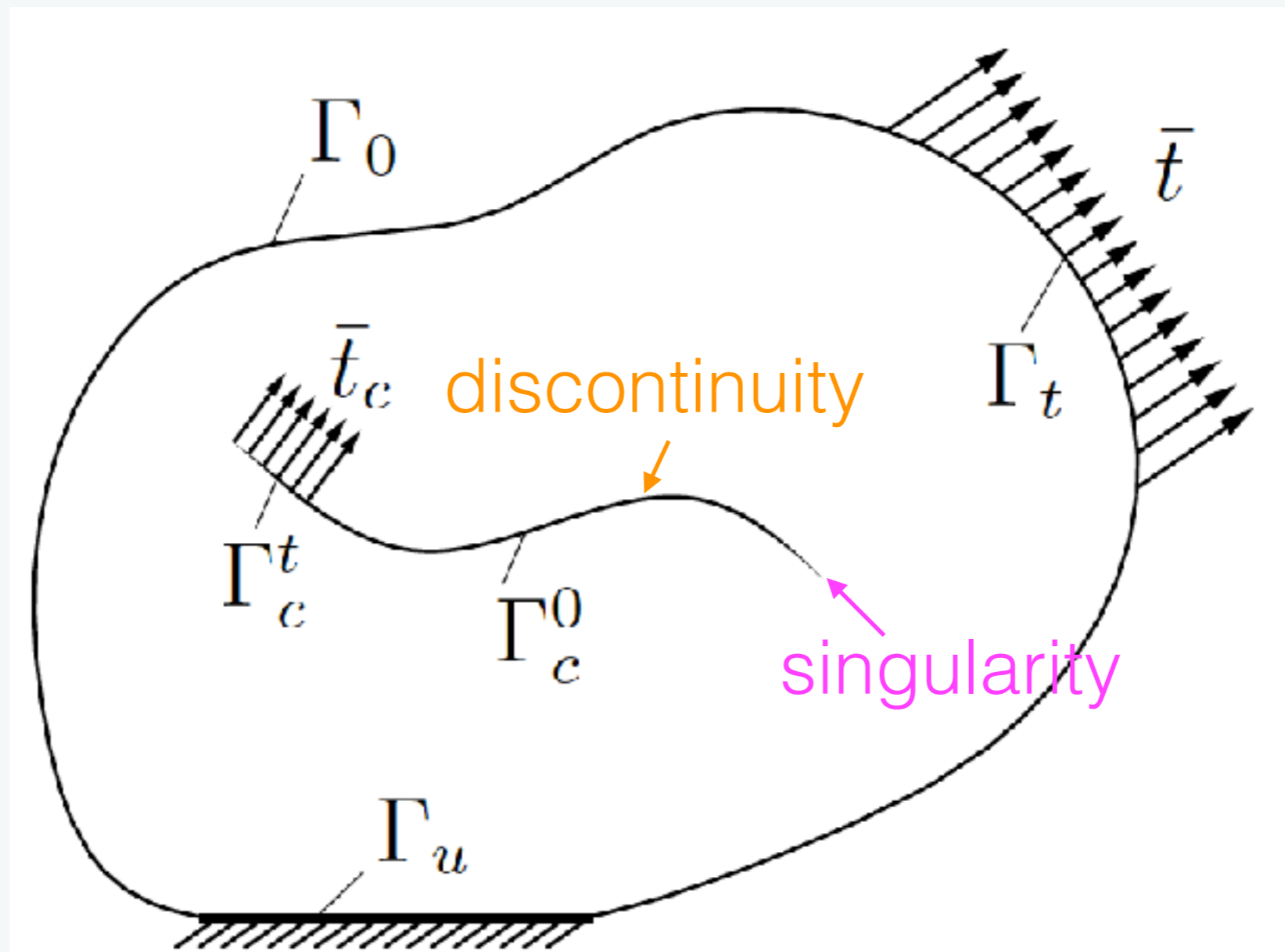
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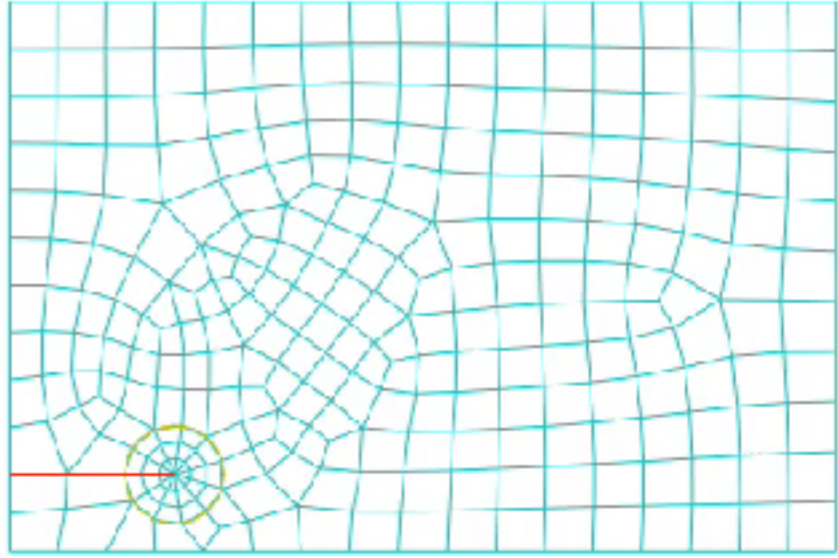
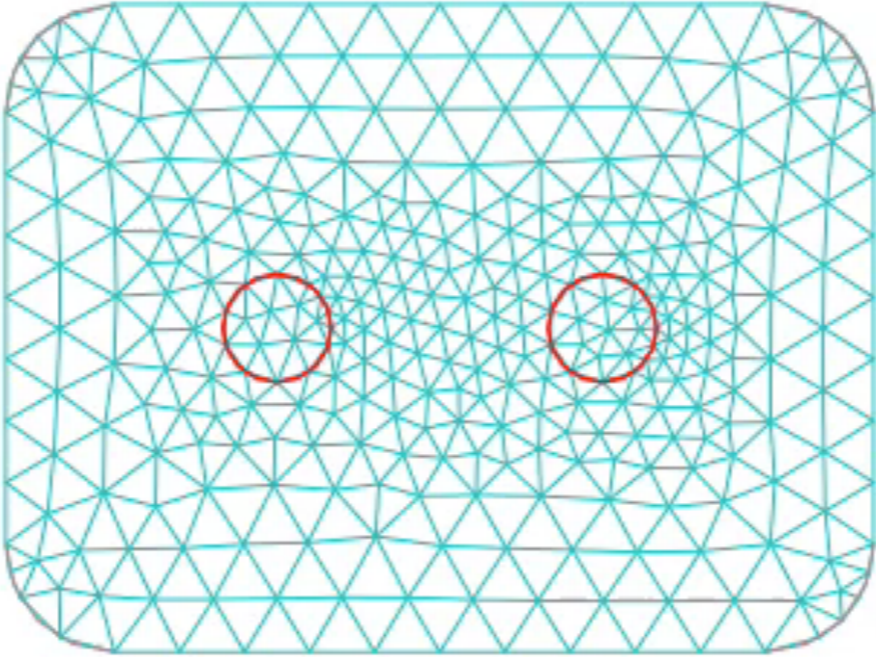
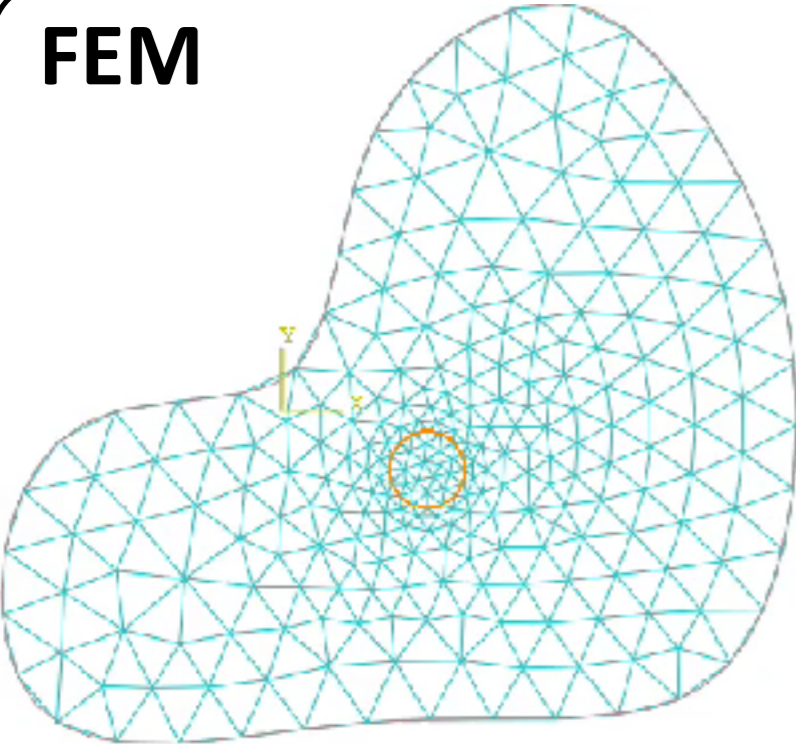


# Finite elements for evolving **discontinuities** & **singularities**

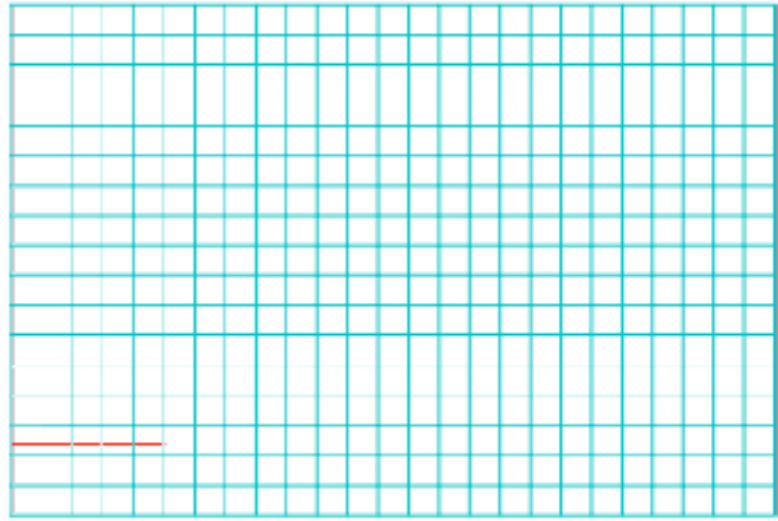
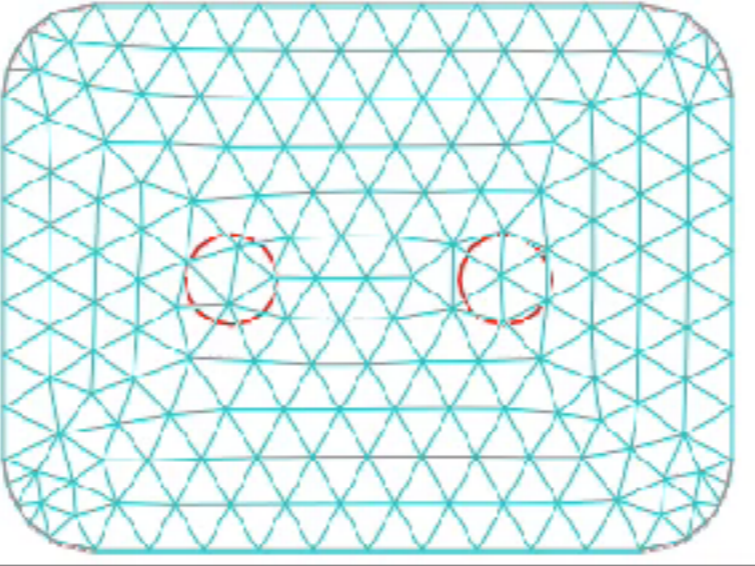
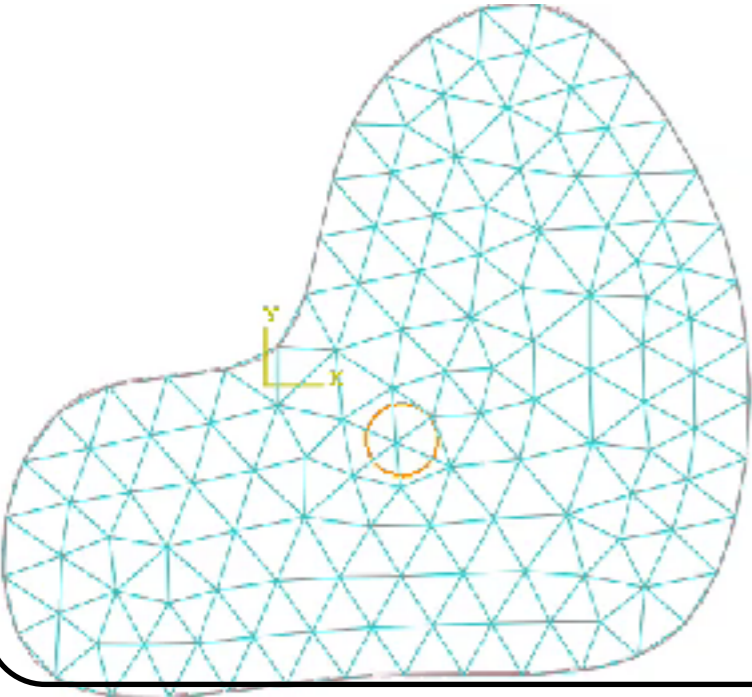




## FEM



## XFEM



One can show . if  $v_h = I_h u$  Lagrange approximation of  $u$ . ⑥  
 Assume  $u \in H^2(\Omega)$  twice weakly differentiable

$$\underbrace{\|u - u_h\|}_{\ell_h} H^1(\Omega) \leq \underbrace{\frac{1}{c}}_{\text{Cea's Constant}} \underbrace{\|v - I_h u\|}_{v_h} H^1(\Omega)$$

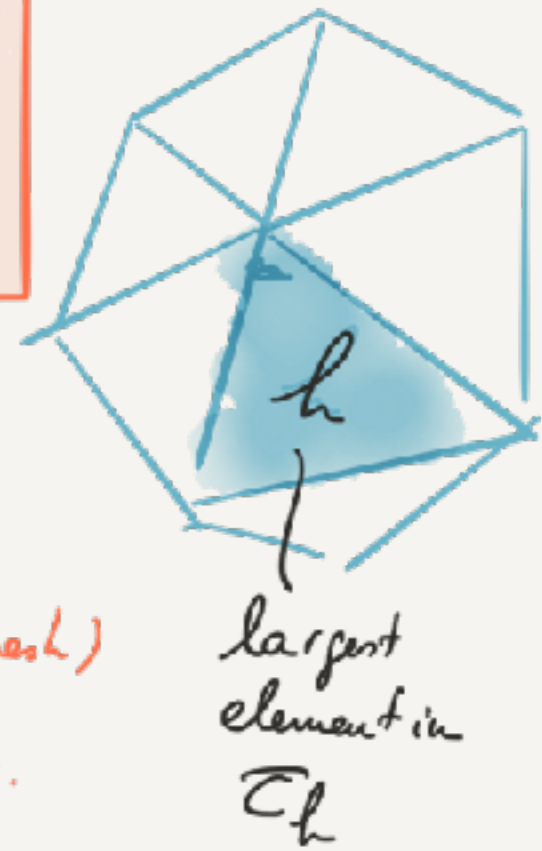
$$\| \text{error} \|_{H^1(\Omega)} \leq C h \|u\|_{H^2(\Omega)}$$

error of FE

approx. in  $H^1(\Omega)$   $\|\cdot\|$ .

Depends on

- Physical Constants in  $\Omega$
- Geometry of  $\Omega$
- Quality of elements in  $\mathcal{T}_h$  (mesh)
- Degree of polynomial approx.



•  $V_h$ : is as good as the best approximant in  $V_h$ :

Babuška, 1994. Partition of Unity.  
 1995.

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error of FE approx. in  $H^1(\Omega)$  ||.||.

- Dependence .
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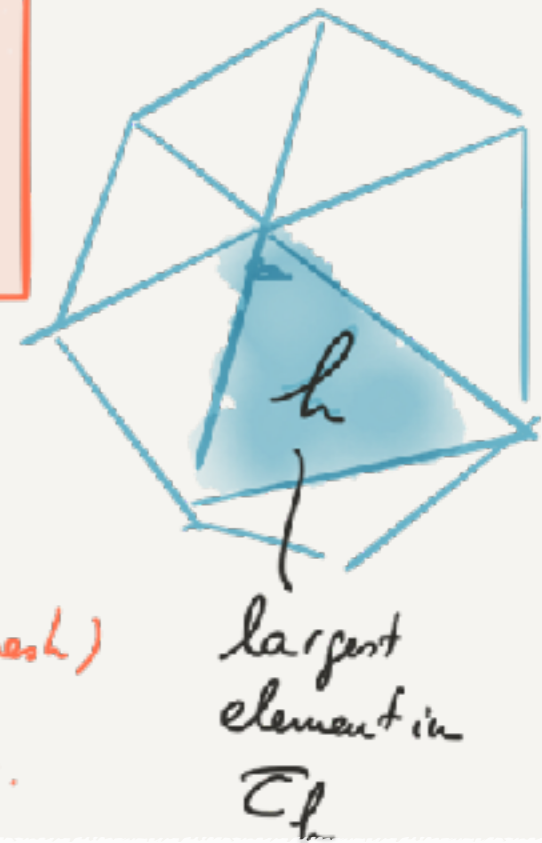
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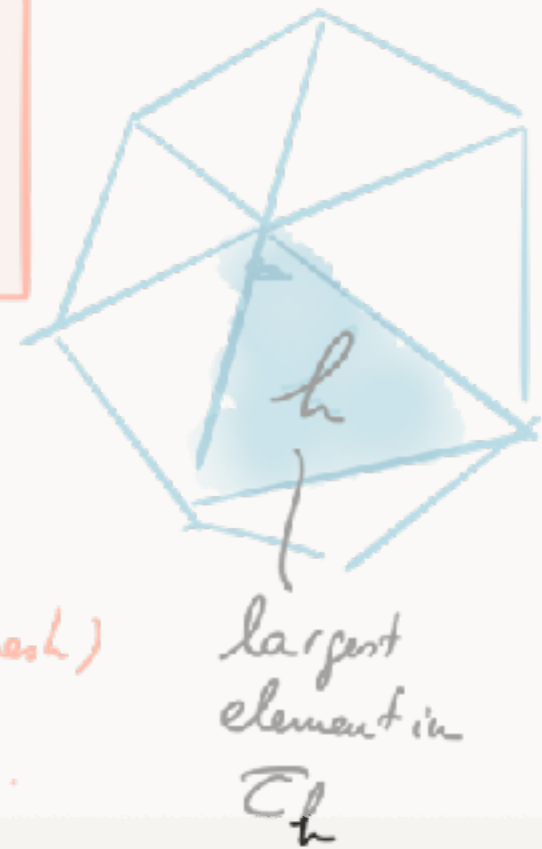
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error of FE approx. in  $H_1(\Omega)$   $\|\cdot\|$ .

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Why PUM?

Babuska 1994 → 1996 ...

A priori error estimate:

$$\|e_h\|_m \leq C h^{\min(p+1-m, r-m)} \|u\|_{H^r(\Omega)}$$

$\underbrace{\|e_h\|_m}_{H^m(\Omega)}$     
 $\downarrow$     
 $\downarrow$     
 $\min(p+1-m, r-m)$     
 $\|u\|_{H^r(\Omega)}$   
 see 6    
 polynomial order

measure of the error

r: smoothness of u

Elasticity  
Fracture

m = 1  
r: small

only a "few" ∂. of u are smooth  
u "not so smooth"

$$\|e_h\|_1 \leq C h^{\min(p, r-1)} \|u\|_{H^r(\Omega)}$$

$\underbrace{\|e_h\|_1}$     
 $\underbrace{\min(p, r-1)}_{\text{"small"}}$     
 $\|u\|_{H^r(\Omega)}$   
 mesh refinement    
 LARGE

# Why PUM?

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A priori error estimate:

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$\underbrace{\|e_h\|_m}_{H^m(\Omega)}$     
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  $\downarrow$     
  $\text{see (6)}$

measure of the error

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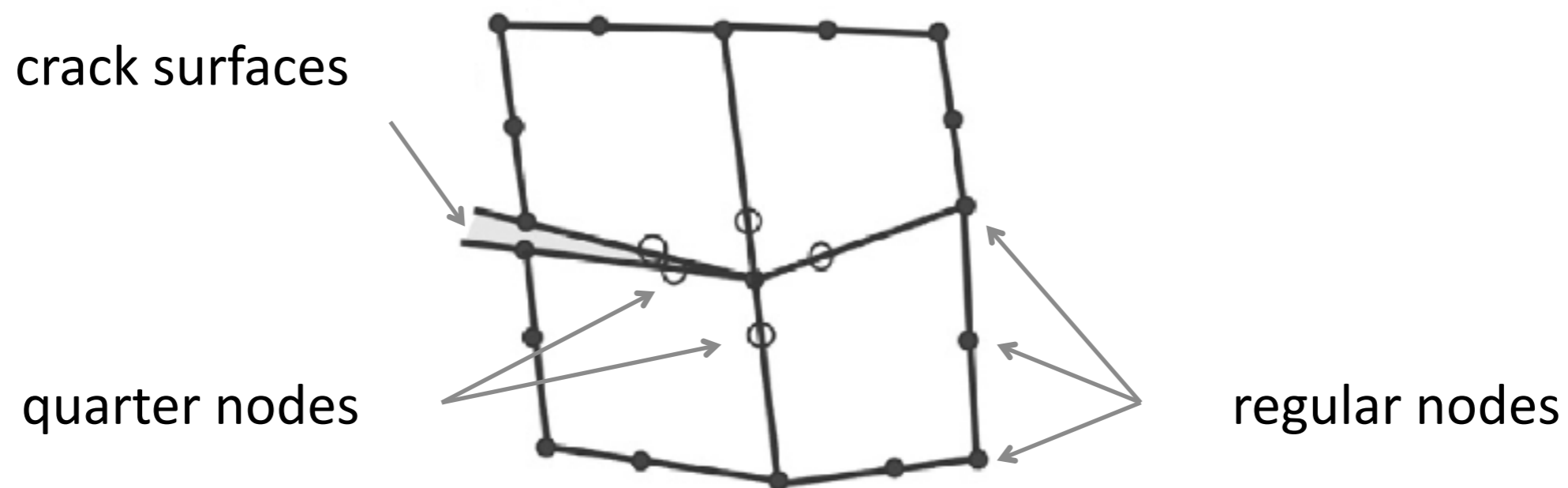
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  $\underbrace{\|u\|_{H^r(\Omega)}}_{\text{LARGE}}$

$\underbrace{C h}_{\text{mesh refinement}}$

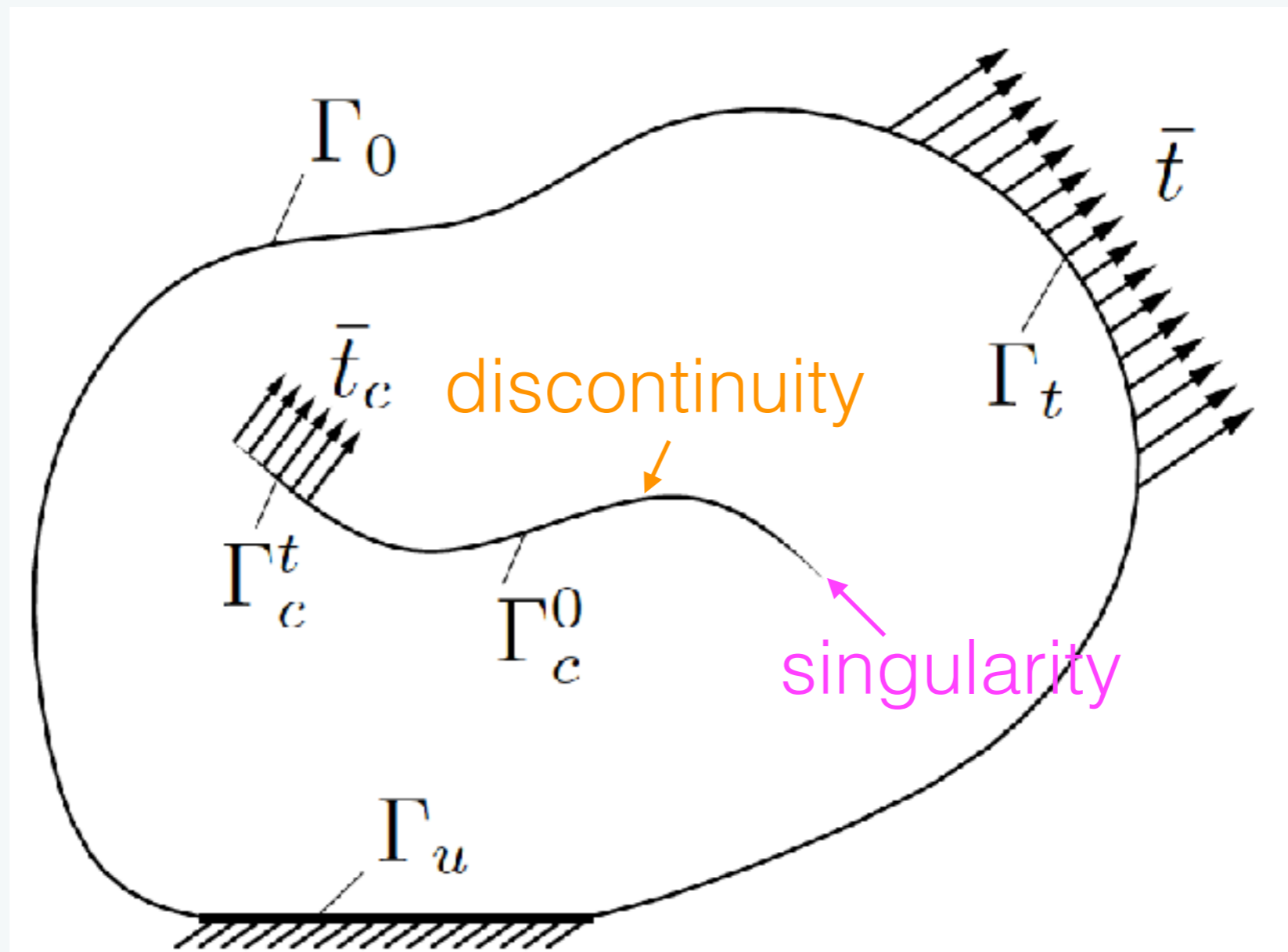
# Singular elements (Barsoum, 1974)

## For simulating the crack tip singular field in LEFM

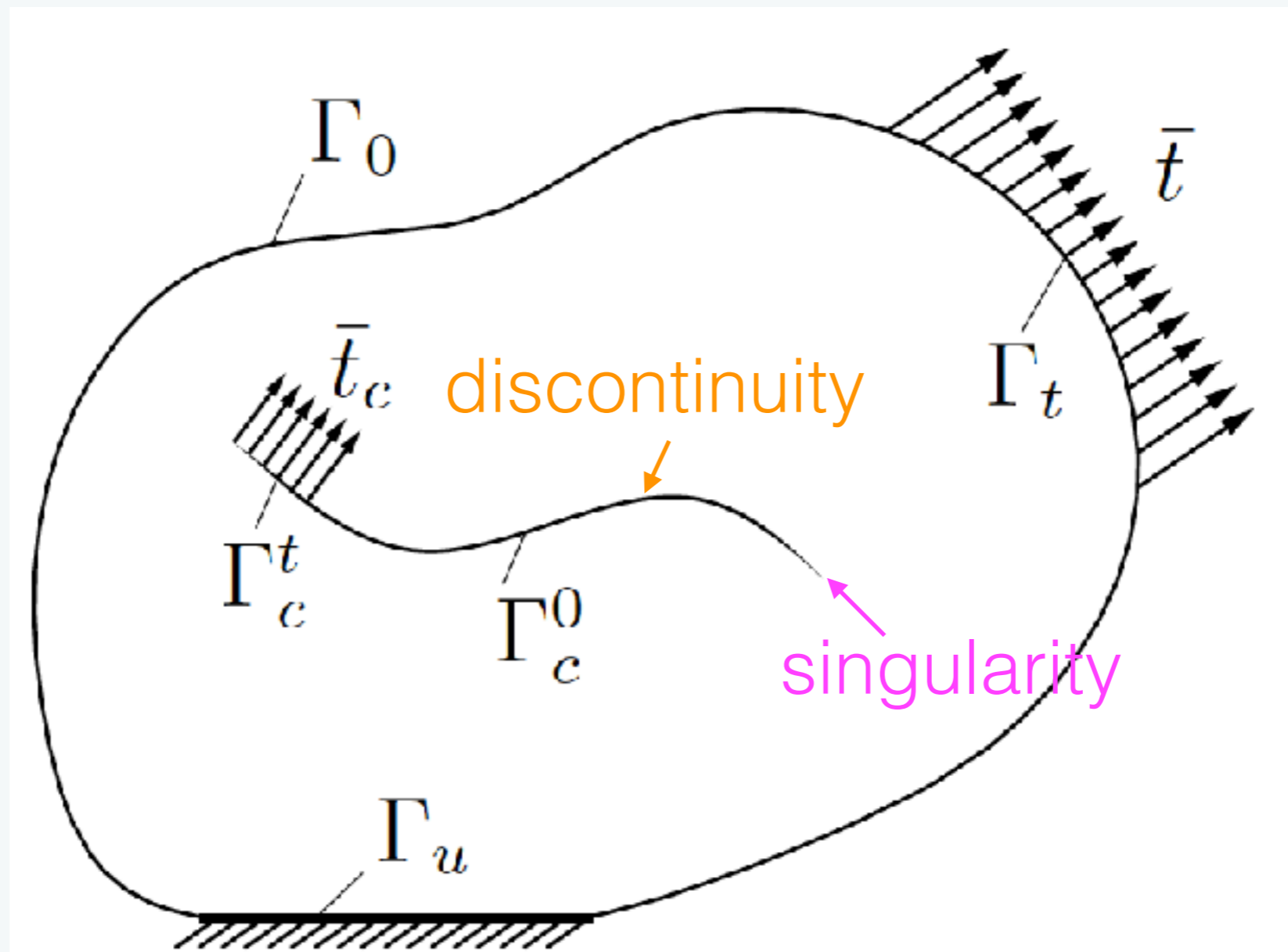
- A simple way how to introduce a singularity of  $1/\sqrt{r}$  in isoperimetric finite elements is by displacing the mid-side nodes of two adjacent edges to one quarter of the element edge length from the node where the singularity is desired.



# Finite elements are intrinsically limited for problems involving **discontinuities** & **singularities** such as cracks



More over, computational fracture (LEFM) requires highly accurate solutions... why?

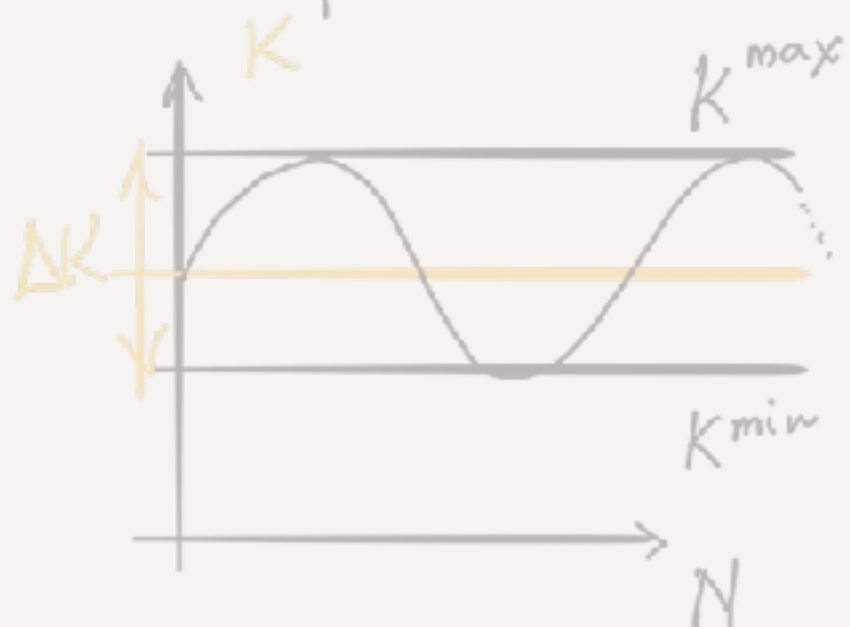


# COMPUTATIONAL FRACTURE

Fracture ①

• Aerospace applications typically assume Linear Elastic Fracture.

• Empirical crack growth laws, e.g. Paris law & generalizations



$$\Delta a = C (\Delta K)^m \Delta N$$

$\Delta a$ : amount of crack growth for  $\Delta N$  cycles  
 $\Delta K$ : Stress Intensity factor amplitude  
 $\Delta N$ : number of cycles

$C, m$  are empirical coefficients  
 $m \in [3, 5]$  typically

SIF: Amount of energy released for a unit increment in crack growth.

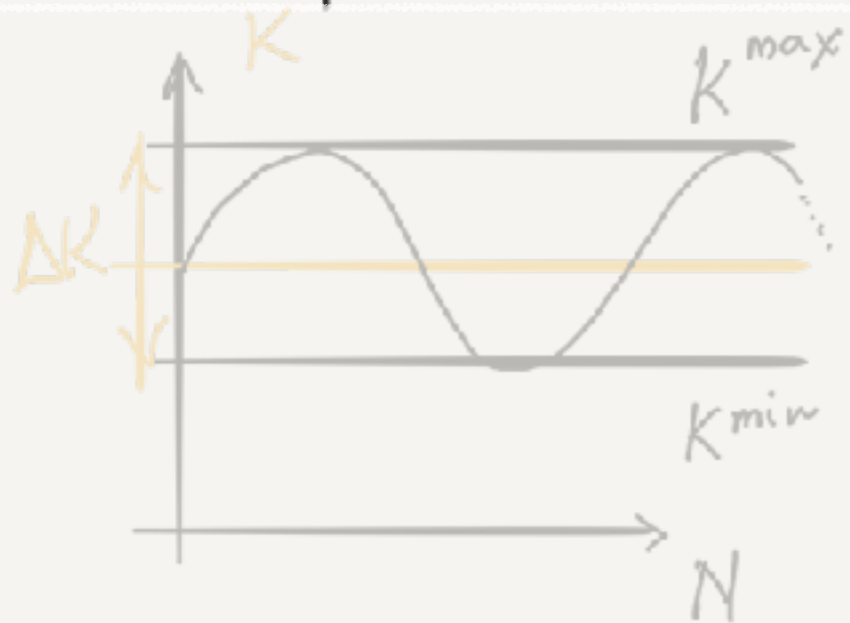
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$$[SIF] = \text{Stress} \sqrt{\text{length}} = \sigma \sqrt{l} = \frac{N}{m^2} \sqrt{m}$$

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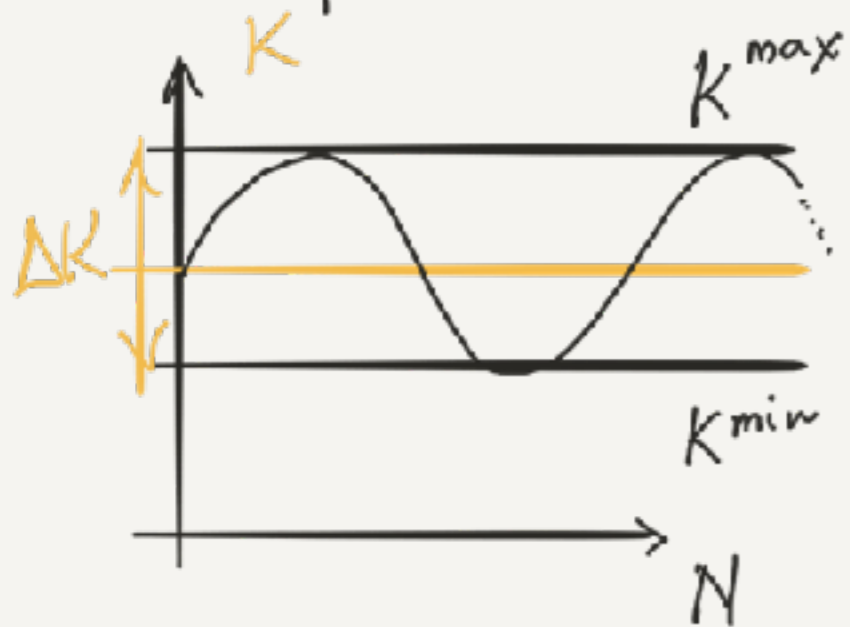
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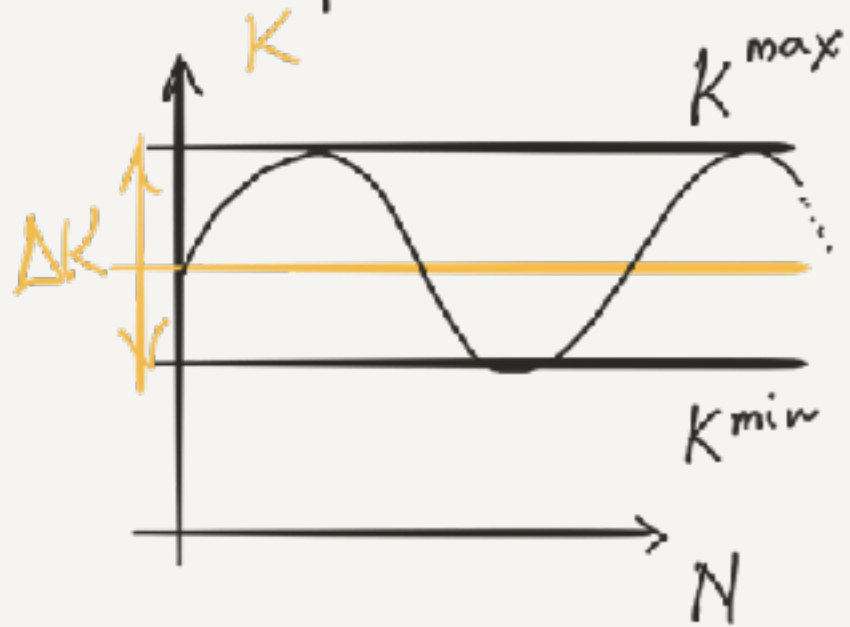
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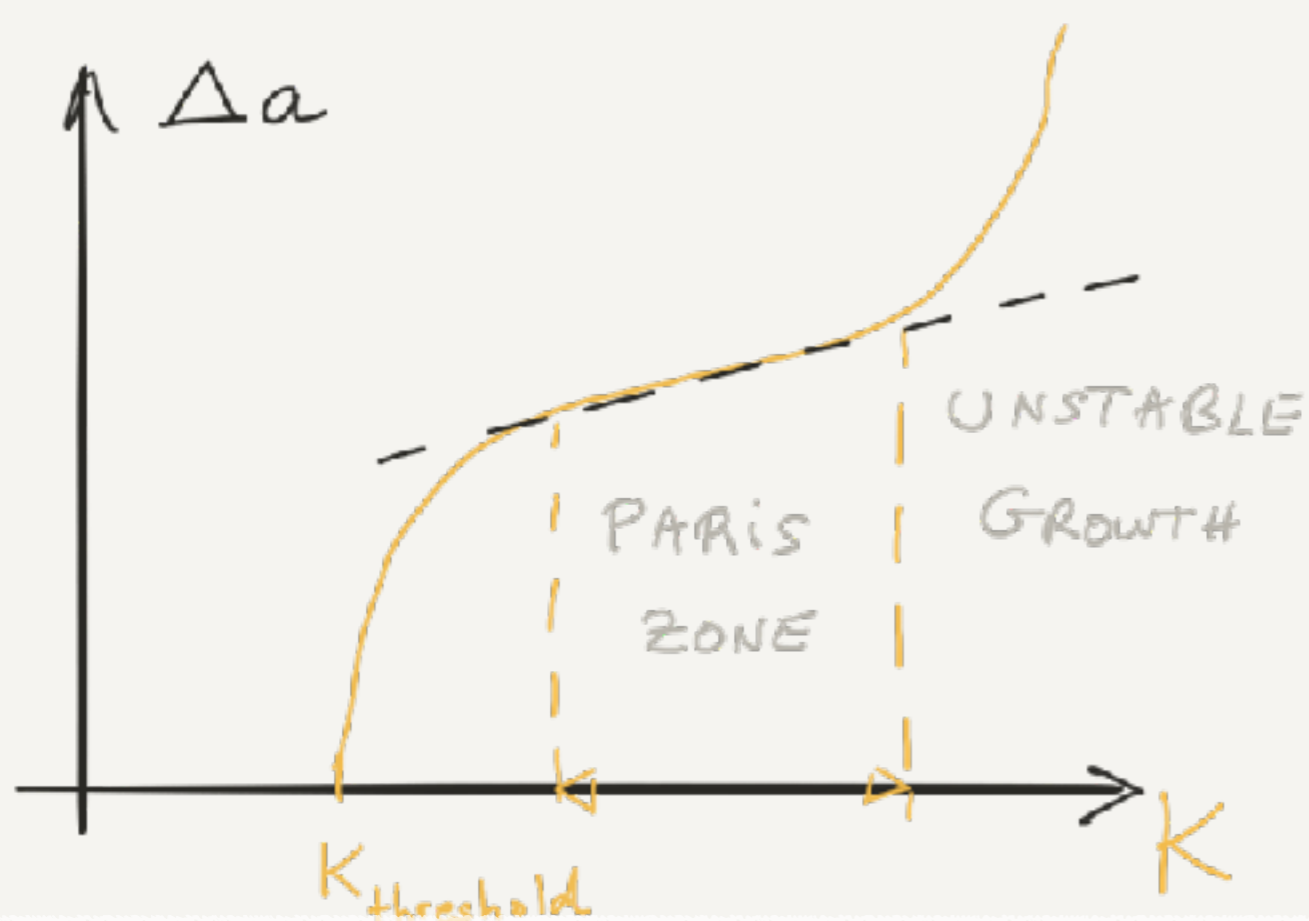
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Numerically Computed  $\text{Fracture } \textcircled{2}$

$$\Delta a = C (K)^m \Delta N$$

$3 \leq m \leq 5$  Paris Exponent

NO GROWTH

Increment in crack advance assuming an error  $\epsilon_K$  is committed

Assume error  $\epsilon_K$  on  $K$

$$\frac{\epsilon_K}{K} \ll 1$$

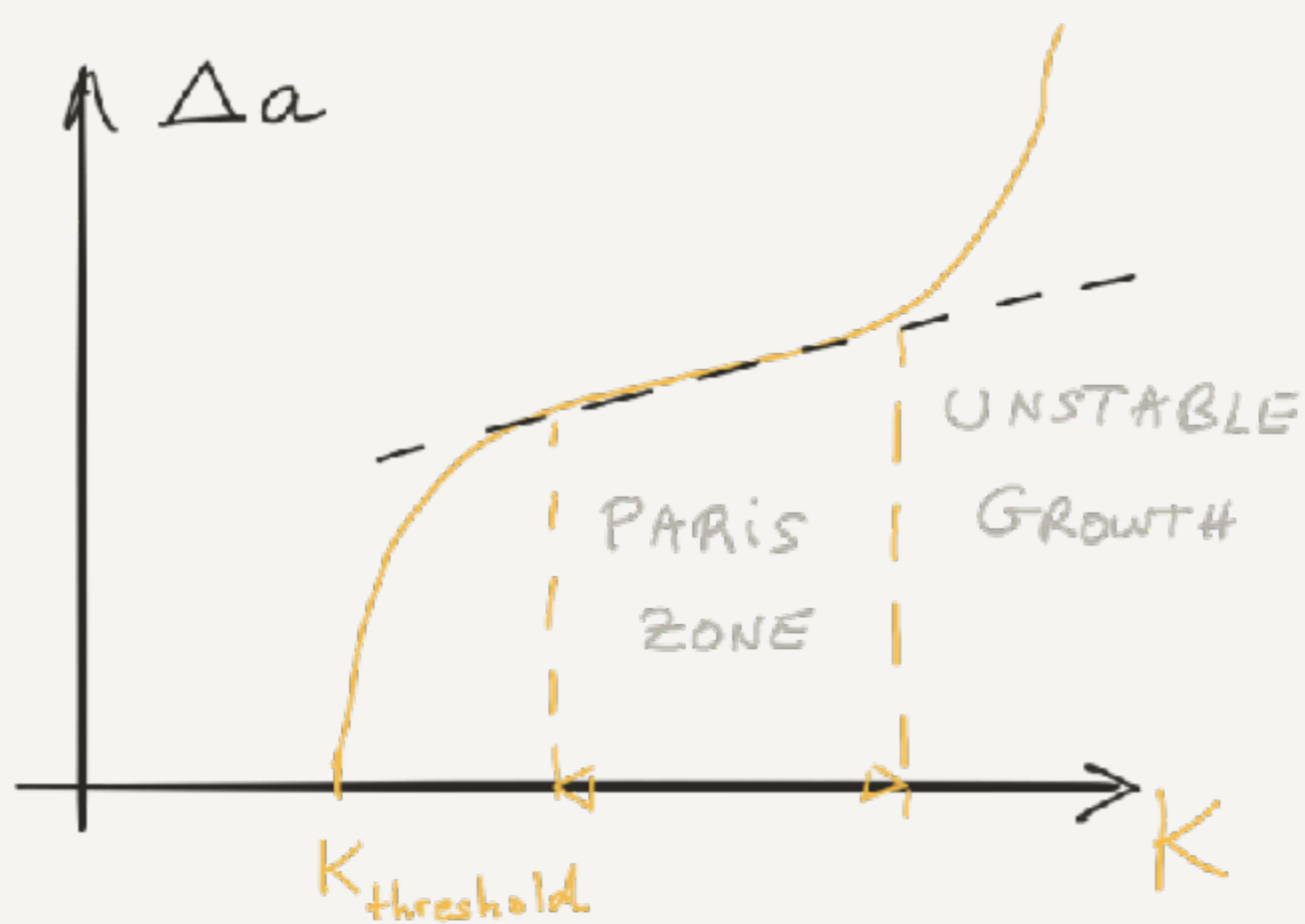
$$\Delta a^\epsilon = C (K + \epsilon_K)^m \Delta N$$

$$\Delta a^\epsilon = C K^m \left(1 + \frac{\epsilon_K}{K}\right)^m \Delta N$$

$$\Delta a^\epsilon \approx C K^m (1 + m \epsilon) \Delta N$$

$$\Delta a^\epsilon \approx \Delta a (1 + m \epsilon)$$

error of  $\epsilon\%$  on  $K$  leads to an error of  $m \epsilon\%$  on  $\Delta a$  !!!



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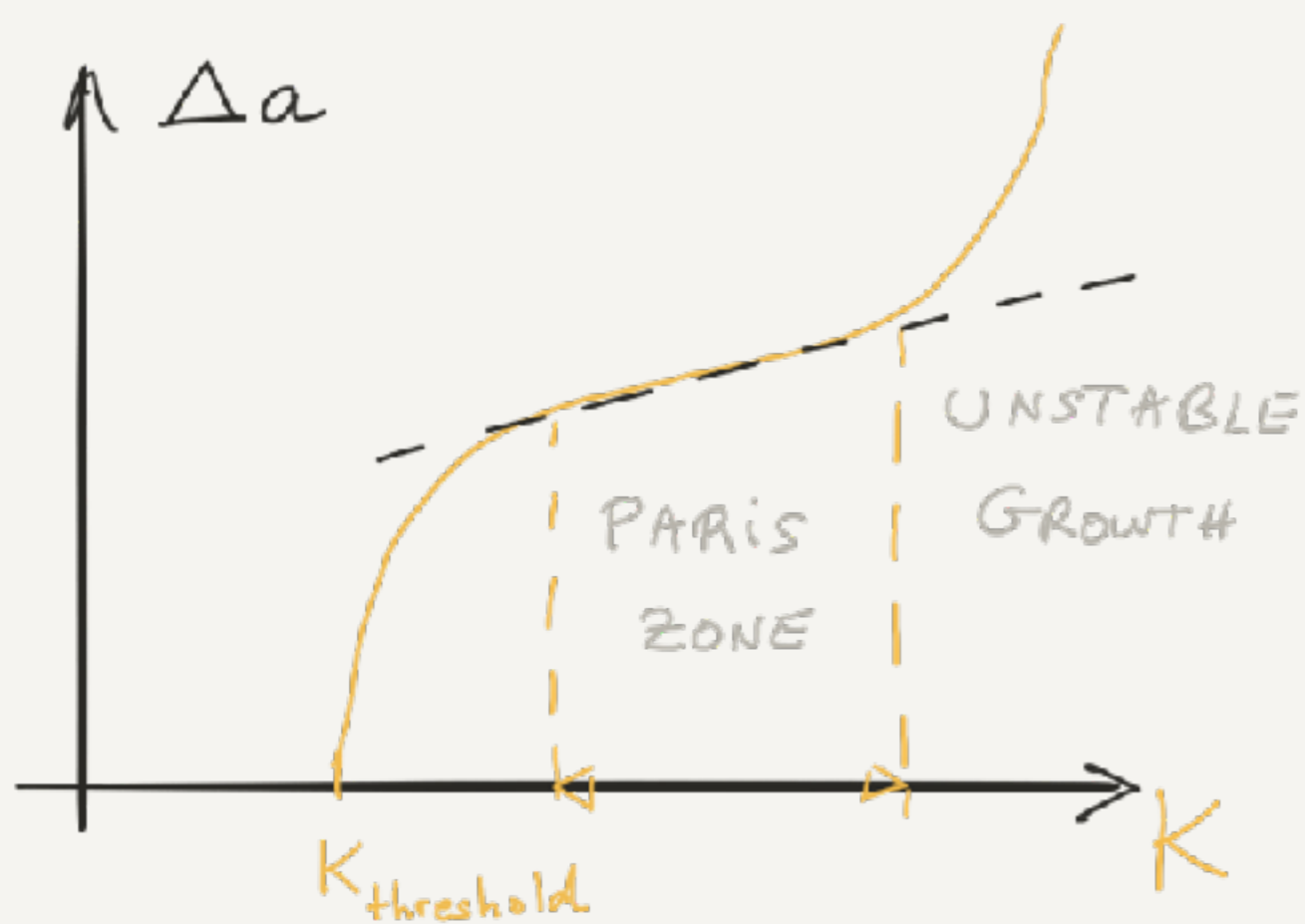
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Conclusion . It is critical to compute SIFs as accurately as possible Fracture ③

①  $\text{error}(\Delta a) = m \text{error}(K)$

$m \in [3, 5]$

② Over 10'000 increments are typically needed to estimate the fatigue life.  $\Rightarrow \text{error}(\text{path}) \approx 10^4 \text{error}(\Delta a)$

$\approx m 10^4 \text{error}(K)$

③ Fracture is history dependent.

Cracks cannot heal.

Error cannot be corrected during growth.

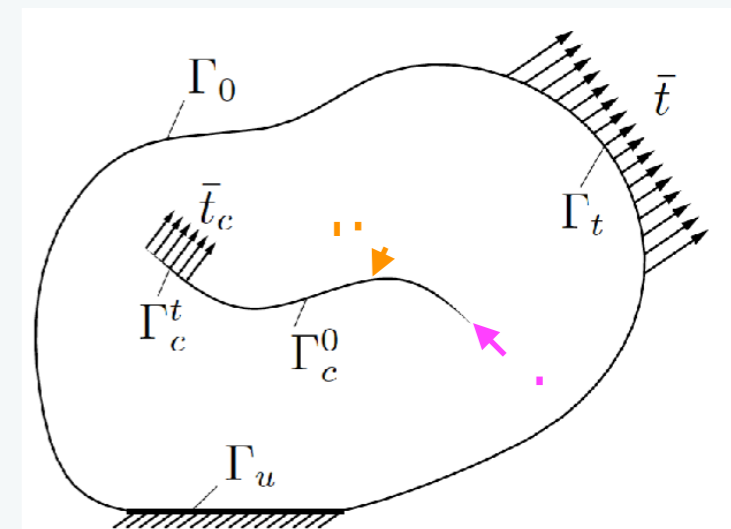
# The idea of Partition of Unity Enrichment (PUFEM, GFEM, XFEM, hp clouds, enriched IGA, enriched meshfree methods, enriched BEM...)

add what you know about the solution to the (finite element) basis

Singularities?

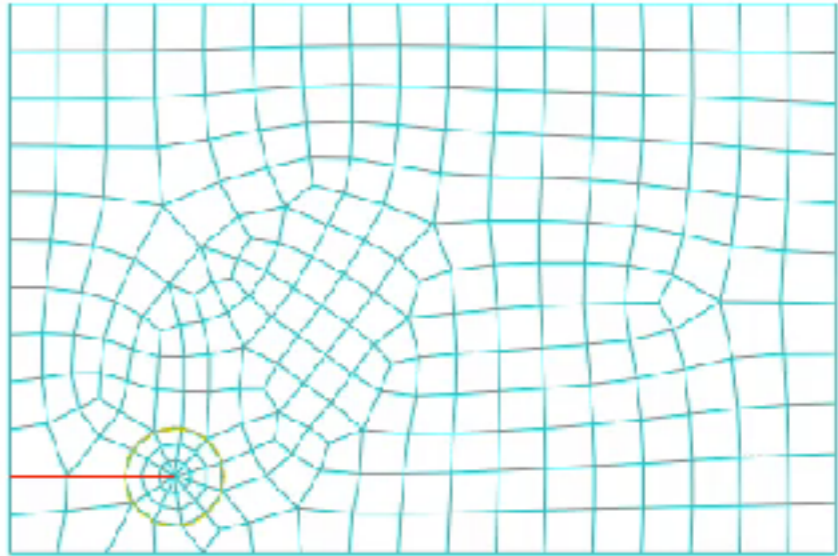
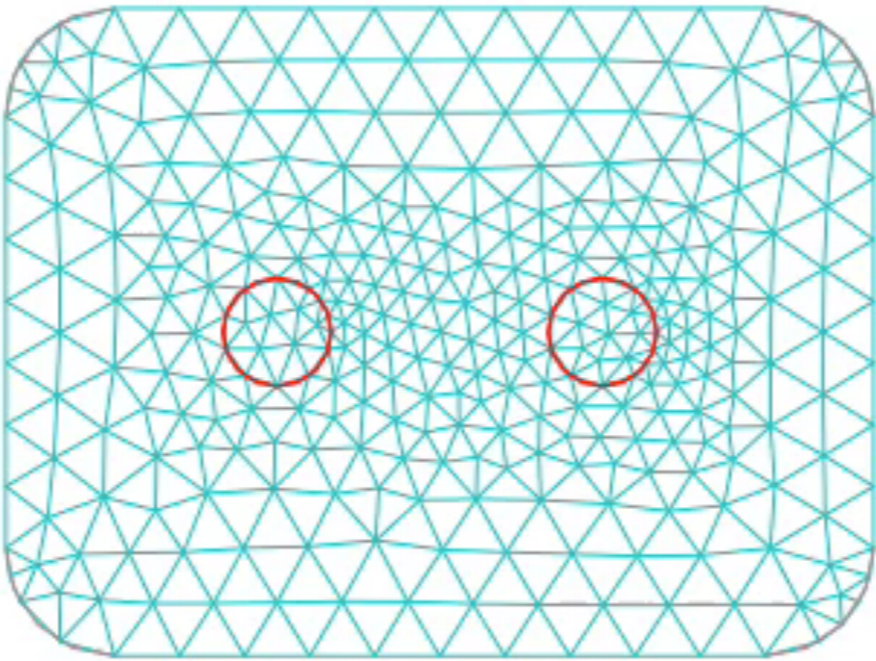
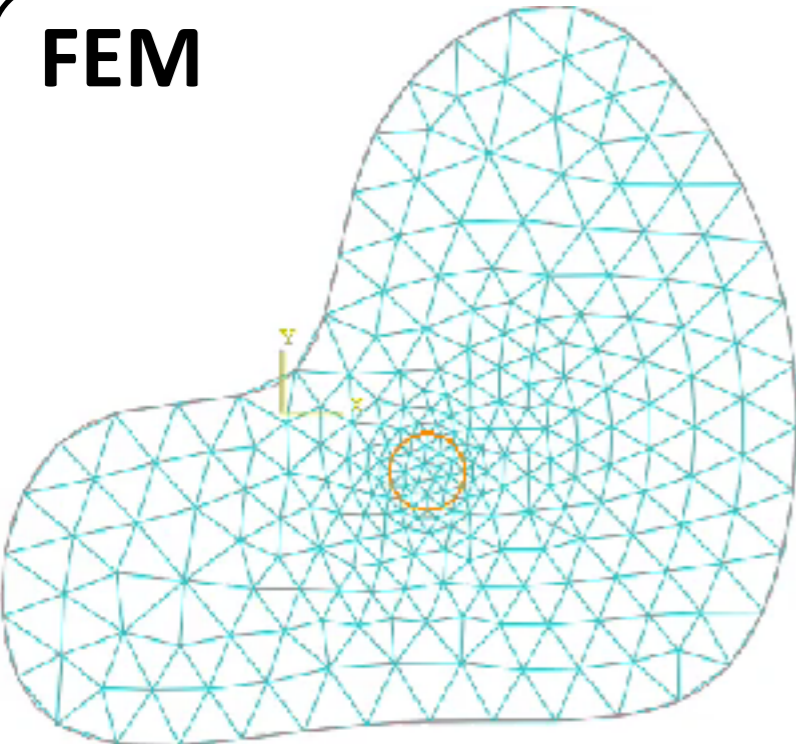
Discontinuities?

Boundary layers?

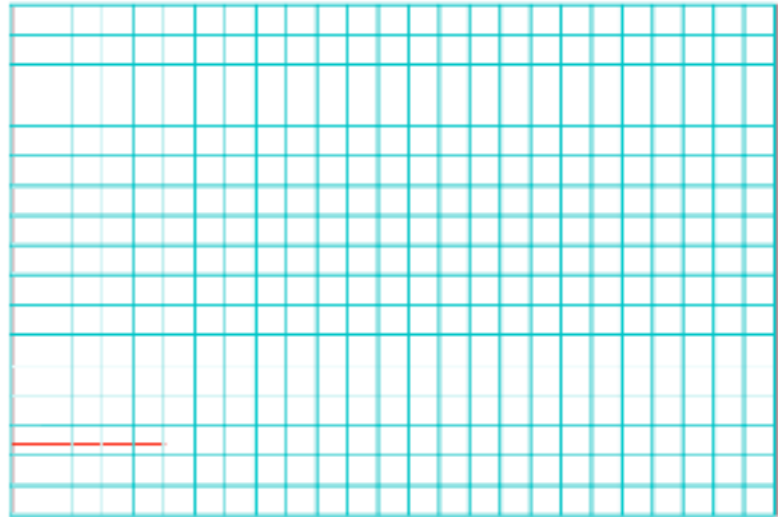
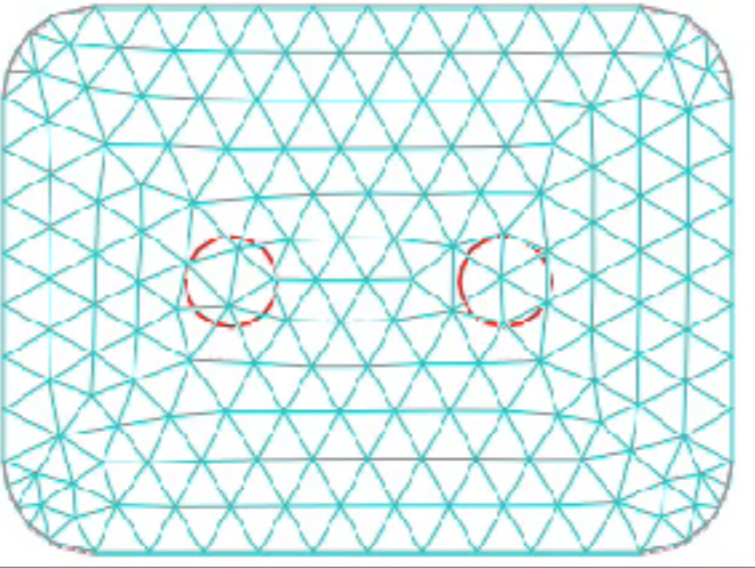
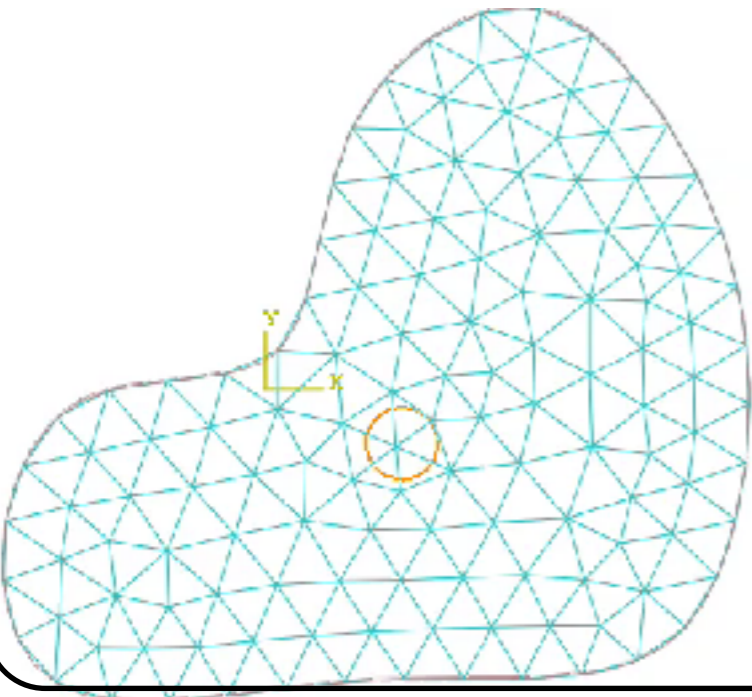




## FEM



## XFEM



# Enrichment

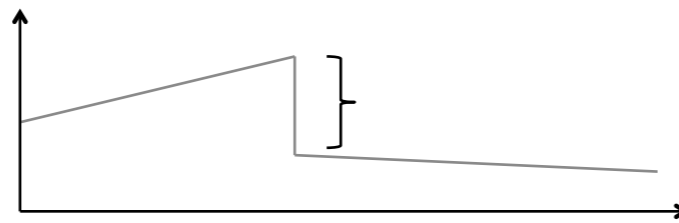
- When the standard finite element method is unable to efficiently reproduce certain features of the sought solution:
  1. Discontinuities - *cracks, material interfaces*
  2. Large gradients - *yield lines, shock waves*
  3. Singularities - *notches, cracks, corners*
  4. Boundary layers - *fluid-fluid, fluid-solid*
  5. Oscillatory behavior - *vibrations, impact*
- The approximation space can be extended by introducing of an *a priori* knowledge about the sought solution, and thereby:
  1. Rendering the mesh independent of any phenomena
  2. reducing error of the approximation locally and globally
  3. improving convergence rates



# Classification of discontinuities

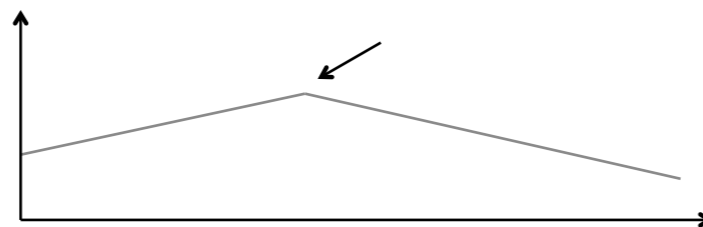
## Strong discontinuities

- The primal field of the solution is discontinuous, e.g. cracks lead to strong discontinuities in the displacement field.



## Weak discontinuities

- The first derivative of the solution is discontinuous, e.g. discontinuities in the strain field through a material interface.



# Classification of enrichments

## Global enrichment

- The enrichment is employed on the global level, over the **entire domain**.
- Useful for problems that can be considered as **globally non-smooth** e.g. high-frequency solutions (Helmholtz equation)

## Local enrichment

- This enrichment scheme is adopted locally, over a **local subdomain**.
- Useful for problems that only involve **locally non-smooth** phenomena, e.g. solutions with discontinuities.

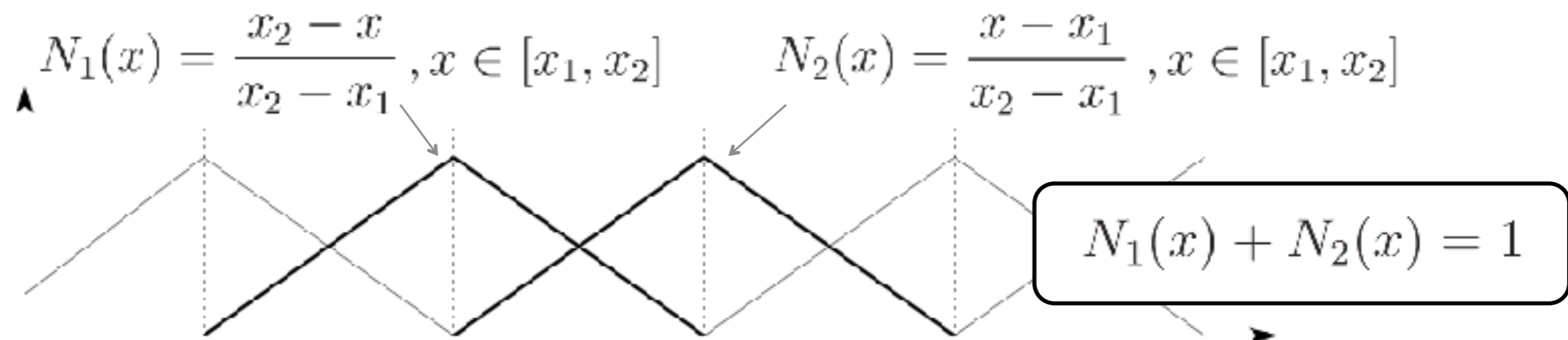
# Partition of unity finite element method (PUFEM)

## Partition of unity (PU)

- A set of functions  $\phi_i$  whose sum at any point  $\mathbf{x}$  inside a domain  $\Omega$  is equal to unity:

$$\forall \mathbf{x} \in \Omega, \mathbf{x} : \sum_{I=1} \phi_I(\mathbf{x}) = 1$$

- Example PU functions are the finite element “hat” functions:



## Reproducibility of PU

- Any function  $p(\mathbf{x})$  can be reproduced by a product of that function and the partition of unity functions:

$$\sum_{I=1} \phi_I(\mathbf{x}) p(\mathbf{x}) = p(\mathbf{x})$$

- The function can be adjusted if the sum is modified by introducing parameters  $q_I$ :

$$\sum_{I=1} \phi_I(\mathbf{x}) p(\mathbf{x}) q_I = \bar{p}(\mathbf{x})$$

- Reproducibility of  $p(\mathbf{x})$  can be controlled and localised to arbitrary regions where  $q_I \neq 0$

# Partition of unity finite element method (PUFEM)

## Formulation of PUFEM (example)

- Find the solution to the following 1D boundary value problem (BVP):

$$\forall x \in [0, l] : \frac{d^2 u}{dx^2} + f = 0$$

$$\text{with BC : } u(0) = 0, u(l) = u_l$$

- If we define two bilinear forms:

$$a(w, u) = \int_0^l \frac{dw}{dx} \frac{du}{dx} dx \quad (w, f) = \int_0^l w f dx$$

- The discrete variational problem can be stated as:

***find  $u^h \in U^h$  satisfying the BC such that for all  $w^h \in W^h$ :***

$$a(w^h, u^h) = (w^h, f)$$

# Partition of unity finite element method (PUFEM)

## Formulation of PUFEM (example)

- The approximation/trial function in PUFEM:

$$u^h(x) = \underbrace{\sum_{I=1} N_I(x)u_I}_{\text{standard FE}} + \underbrace{\sum_{J=1} \phi_J(x)\psi(x)q_J}_{\text{PU enriched}}$$

- By choosing  $w^h = \delta u^h$ , leads to the discrete system of equations:

$$a(\delta u^h, u^h) = (\delta u^h, f)$$

$$\begin{array}{l}
 \mathbf{K}_{ij}^{se} = \int_0^l \frac{dN_i}{dx} \frac{d(\phi_j\psi)}{dx} dx \\
 \mathbf{K}_{ij}^{ss} = \int_0^l \frac{dN_i}{dx} \frac{dN_j}{dx} dx \\
 \mathbf{K}_{ij}^{es} = \int_0^l \frac{d(\phi_i\psi)}{dx} \frac{dN_j}{dx} dx \\
 \mathbf{K}_{ij}^{ee} = \int_0^l \frac{d(\phi_i\psi)}{dx} \frac{d(\phi_j\psi)}{dx} dx
 \end{array}
 \quad \Downarrow \quad
 \begin{array}{l}
 f_i^s = \int_0^l N_i f_x dx \\
 f_i^e = \int_0^l (\phi_i\psi) f_x dx
 \end{array}$$

$$\begin{bmatrix} \mathbf{K}^{ss} & \mathbf{K}^{se} \\ \mathbf{K}^{es} & \mathbf{K}^{ee} \end{bmatrix}
 \begin{Bmatrix} \mathbf{u}^s \\ \mathbf{q}^e \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}^s \\ \mathbf{f}^e \end{Bmatrix}$$

# Partition of unity finite element method (PUFEM)

## Remarks

- Allows to introduce an arbitrary function  $\psi(\mathbf{x})$  in the approximation space by splitting the approximation into a **standard** and **enriched** parts.
- Enrichment can be **localised** to a small region around the features of interest – computationally advantageous.
- Provides a systematic means of introducing multiple enrichments.

## References:

- Melenk and Babuska (1996)
- Duarte and Oden (1996)

# The Generalised Finite Element Method (GFEM)

## GFEM

- Originally associated with global PU enrichment
- Shape functions in the enriched part are usually different from the shape functions in the standard part i.e.  $\phi_I(x) \neq N_I(x)$
- Introduced numerically generated enrichment functions, e.g. a solution in the vicinity of a bifurcated crack as enrichment

## References:

- Melenk (1995)
- Melenk and Babuška (1996)
- Strouboulis et al. (2000)



# The Extended Finite Element Method (XFEM)

## XFEM

- Associated with local discontinuous PU enrichment e.g.:
  - a. propagation of cracks
  - b. evolution of dislocations
  - c. phase boundaries
- Both GFEM and XFEM are essentially identical in their application, i.e. extrinsic PU enrichment

## References:

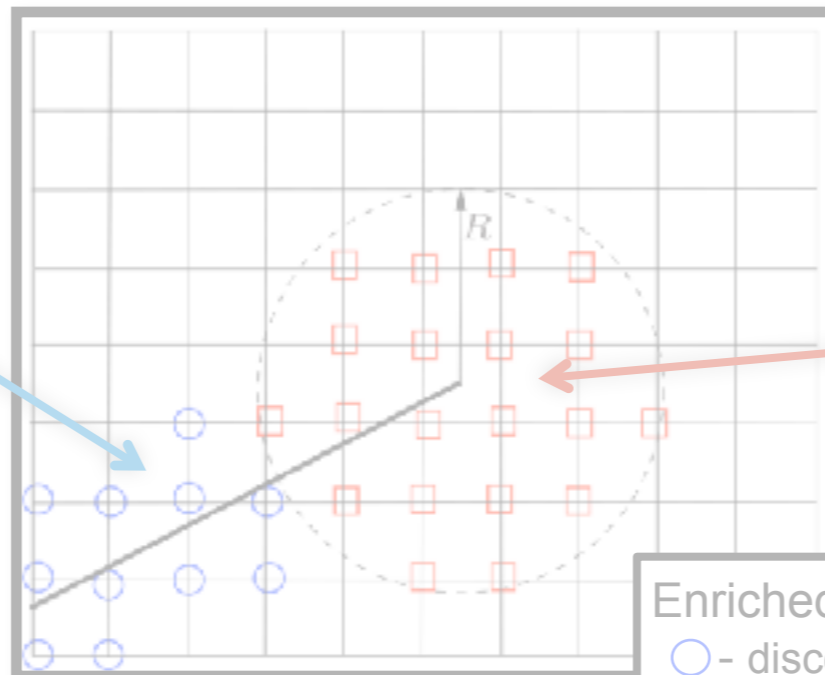
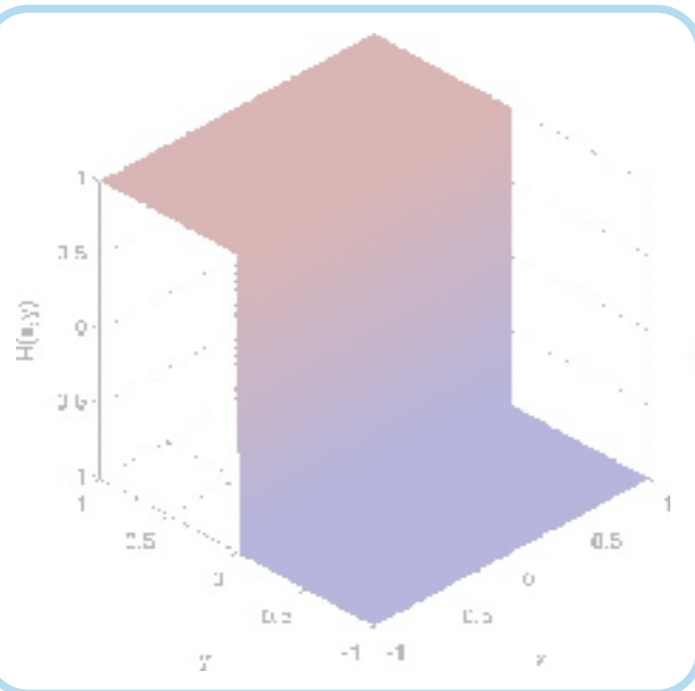
- Belytschko and Black (1999)
- Moës et. al. (1999)
- Dolbow (1999)

## Formulation for crack growth:

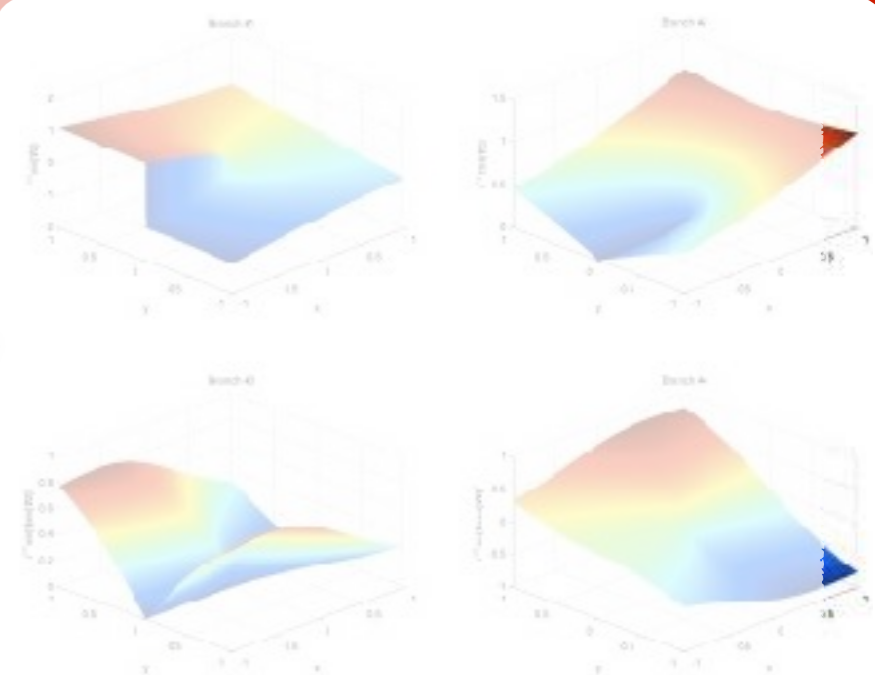
$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) \mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K \in \mathcal{N}_K} N_K(\mathbf{x}) \sum_{\alpha=1}^4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

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

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



Enriched nodes  
 ○ - discontinuous  
 □ - singular

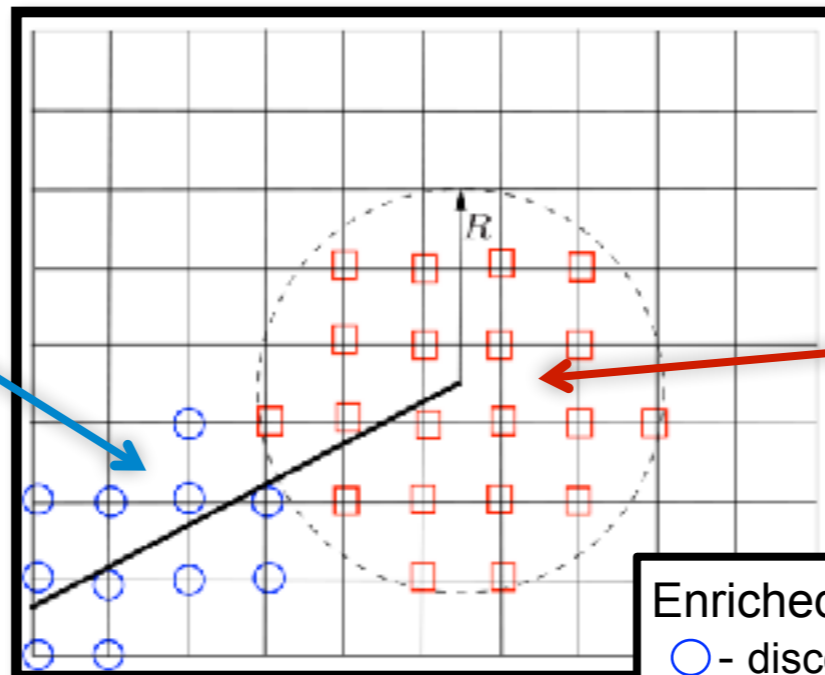
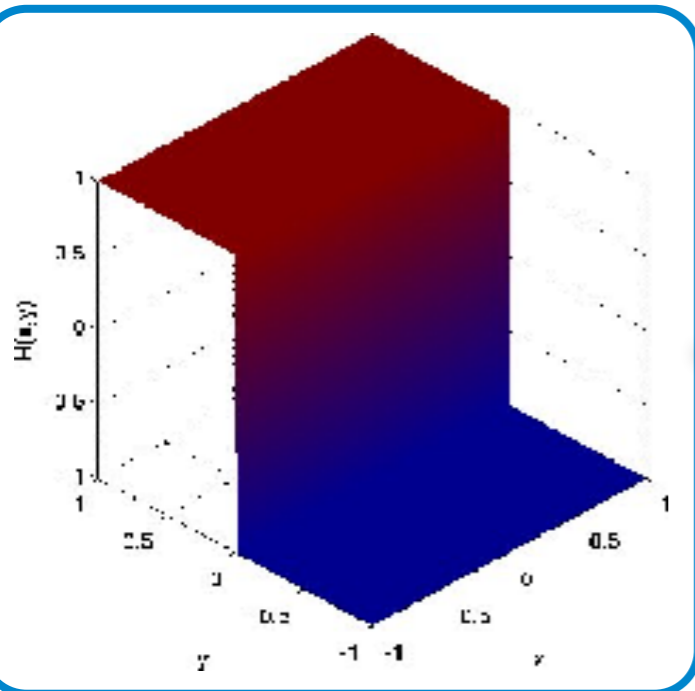


## Formulation for crack growth:

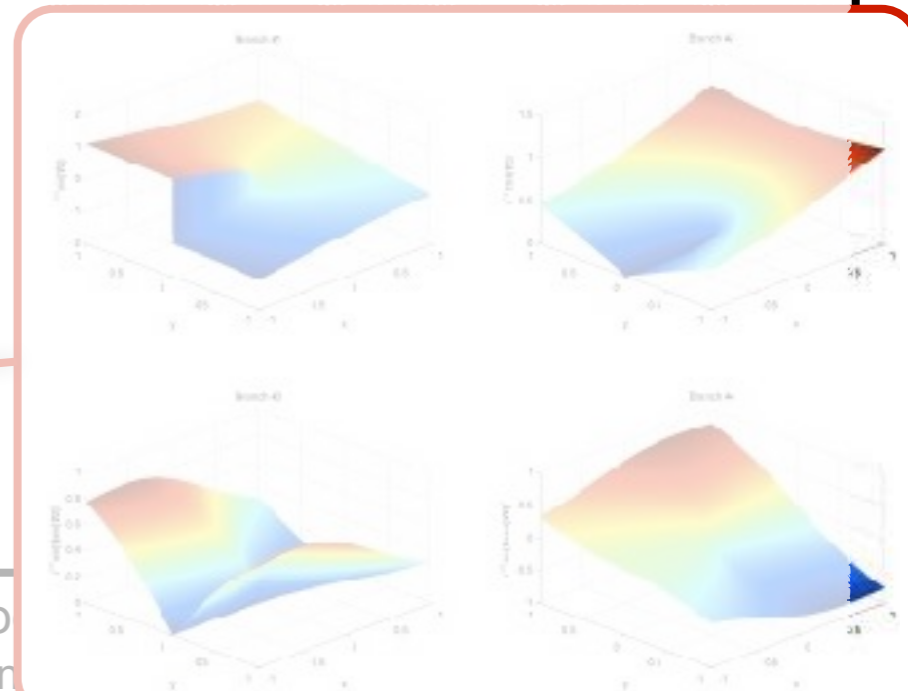
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Enriched nodes  
 ○ - discontinuous  
 □ - singular

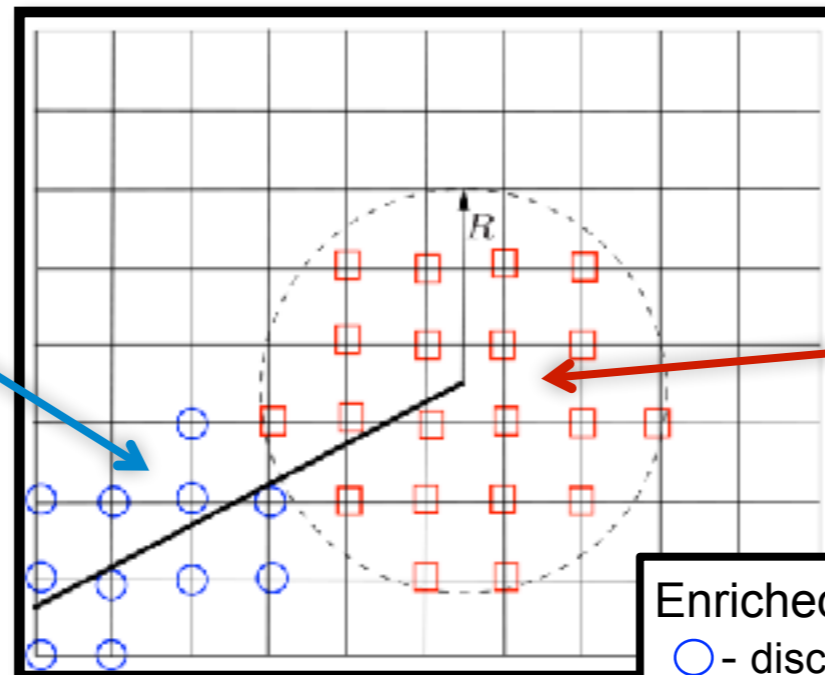
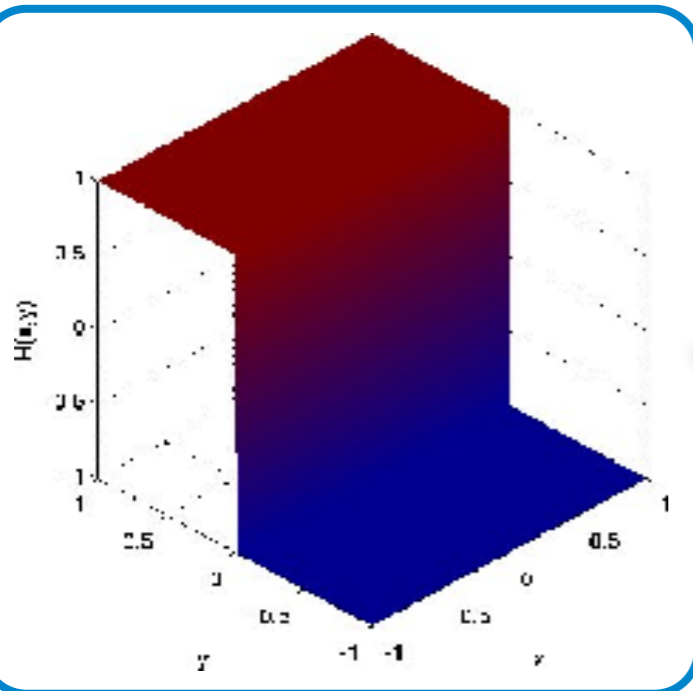


## Formulation for crack growth:

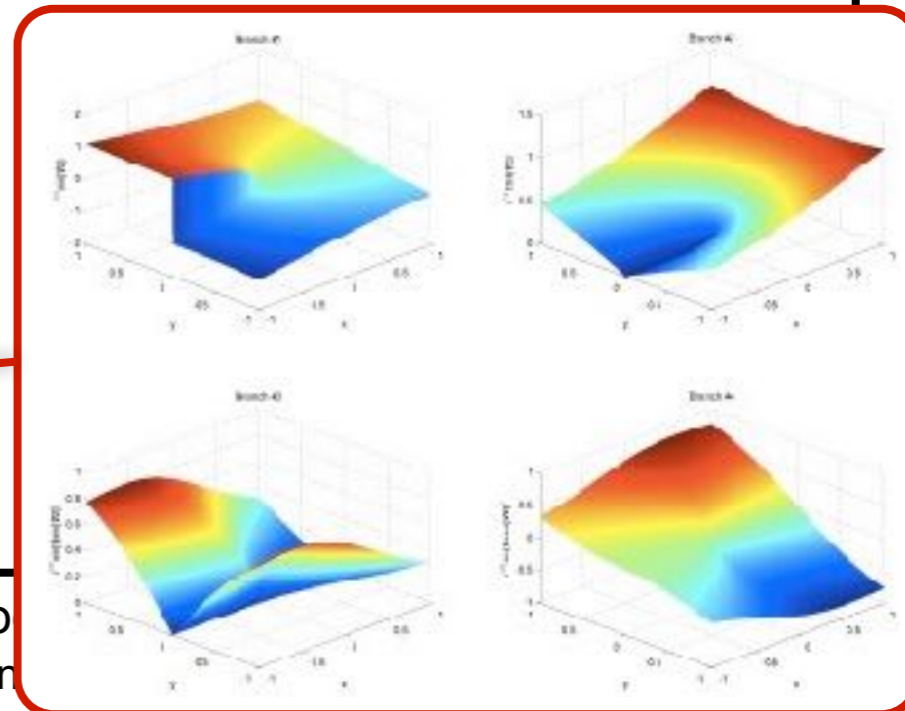
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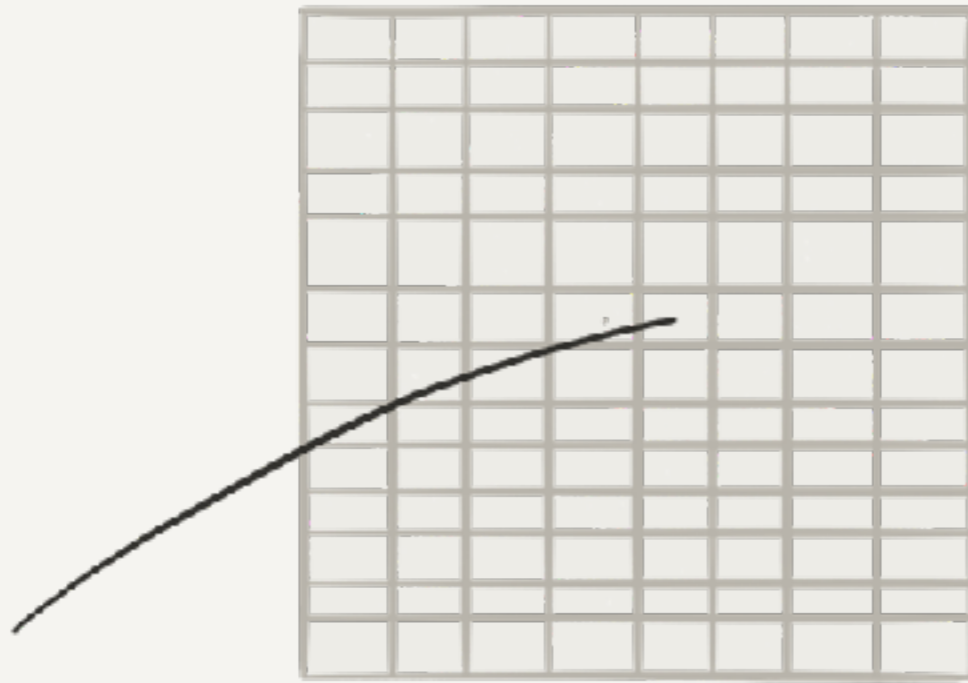
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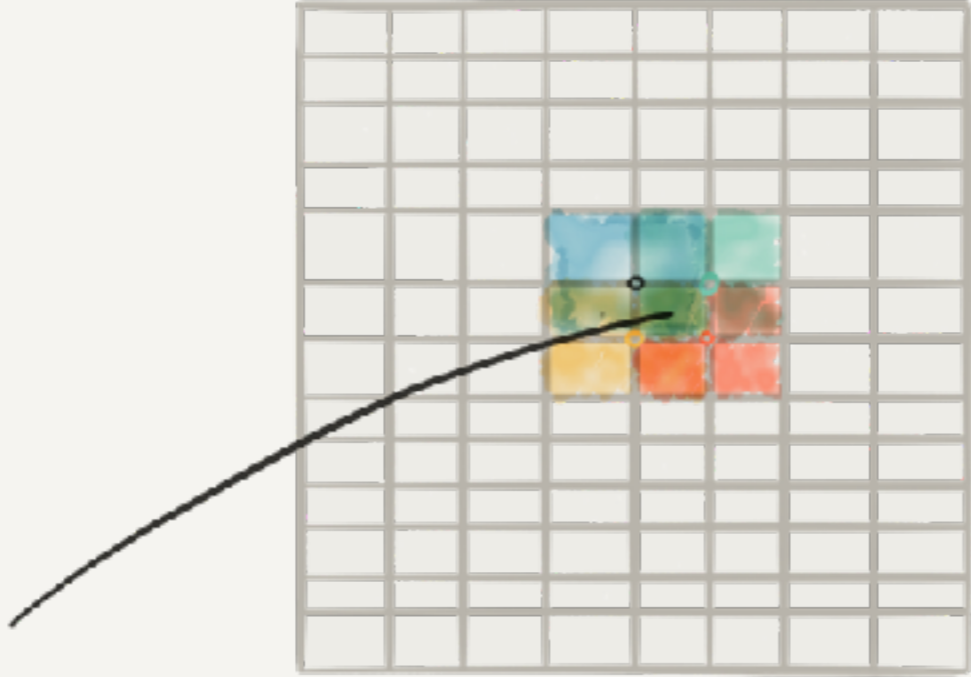
Enriched nodes  
 ○ - discontinuous  
 □ - singular





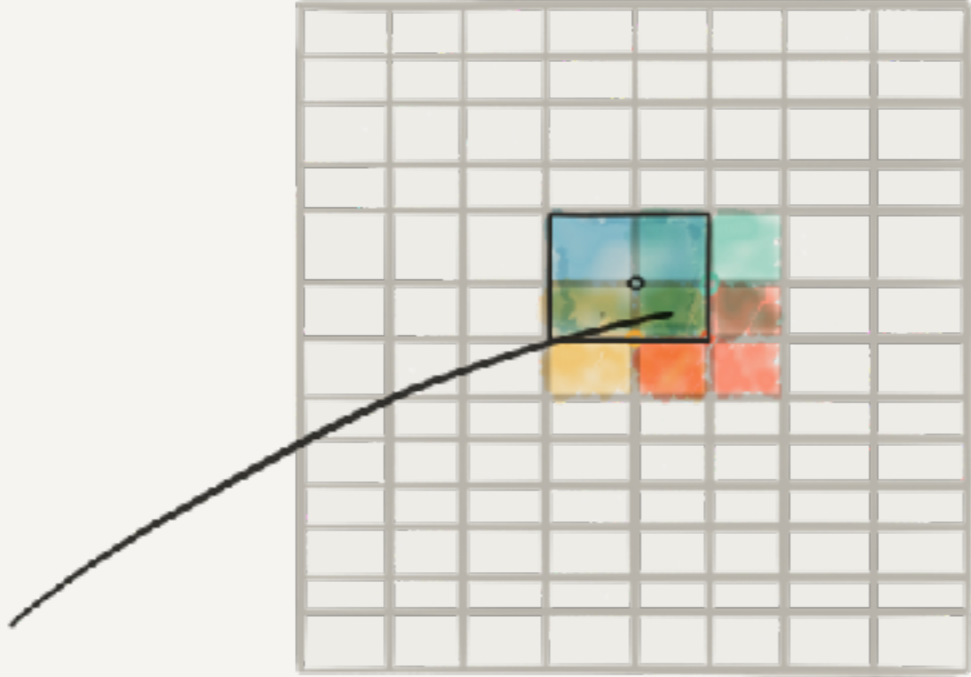


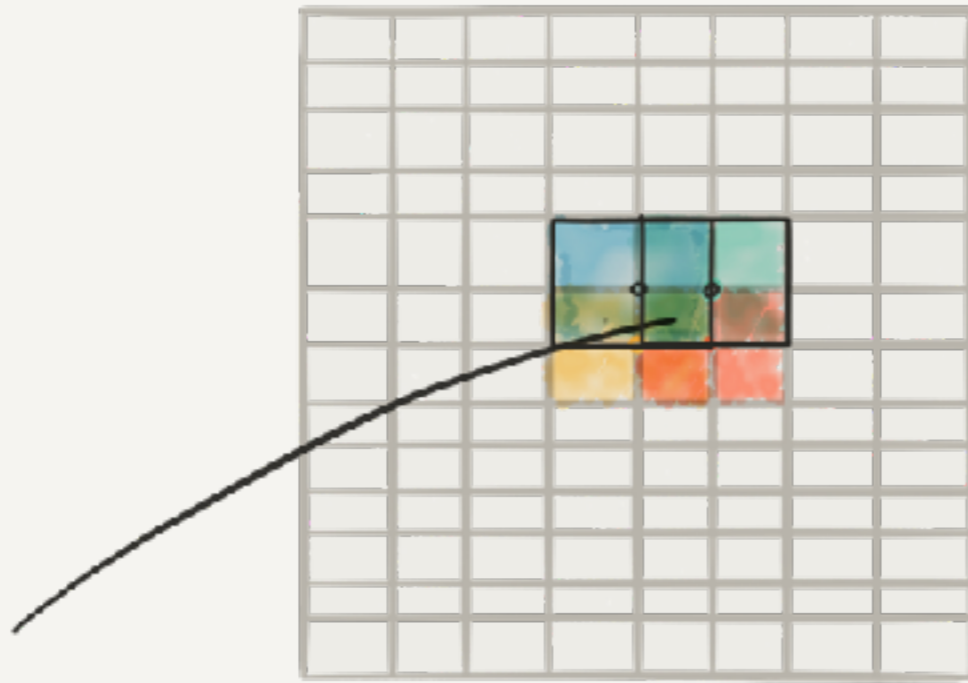


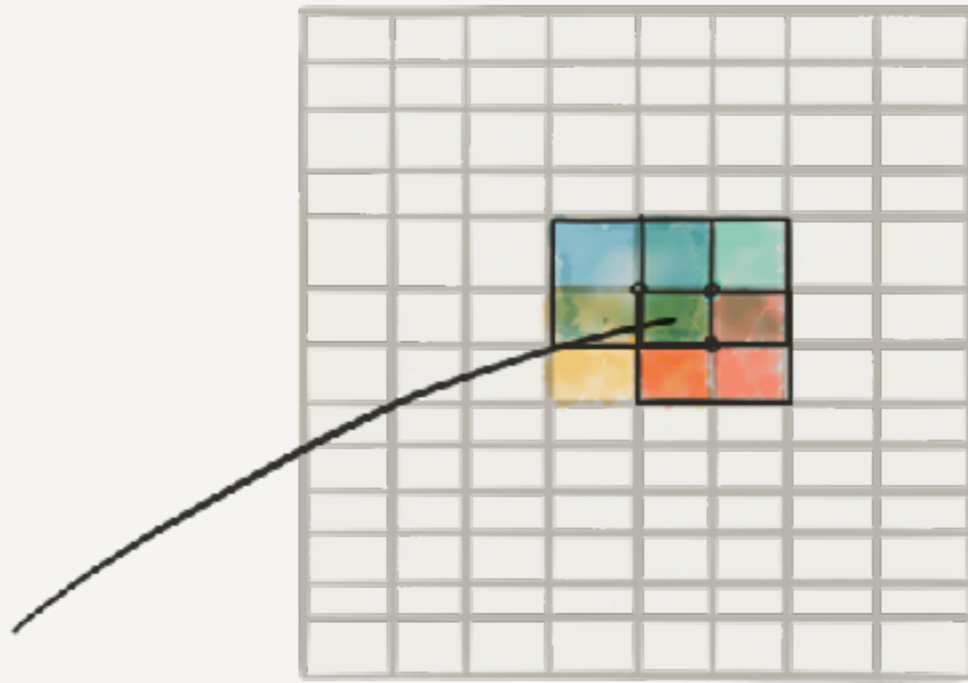


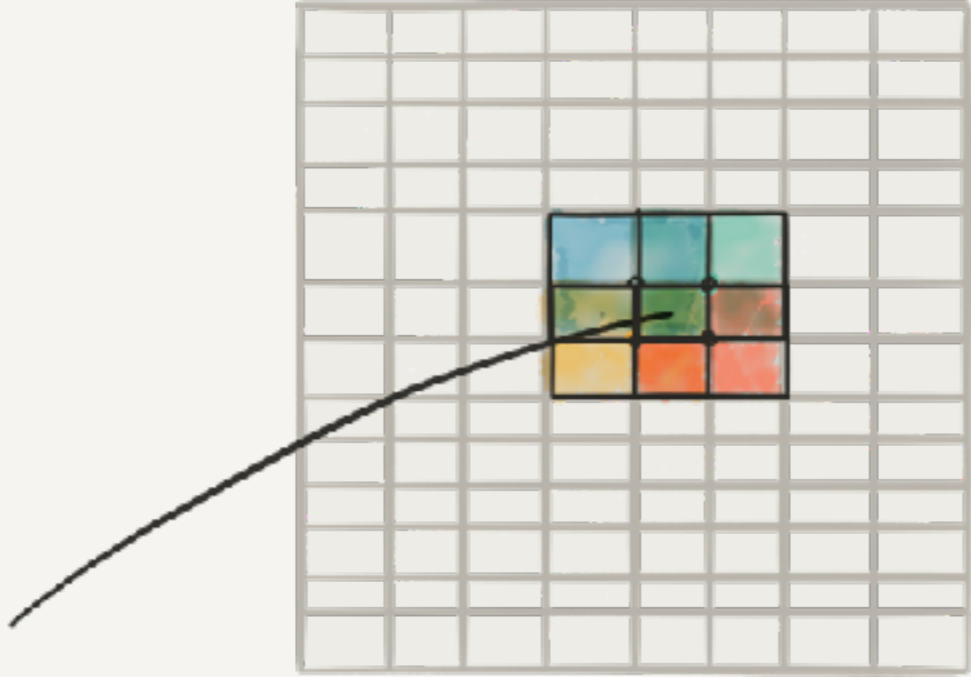
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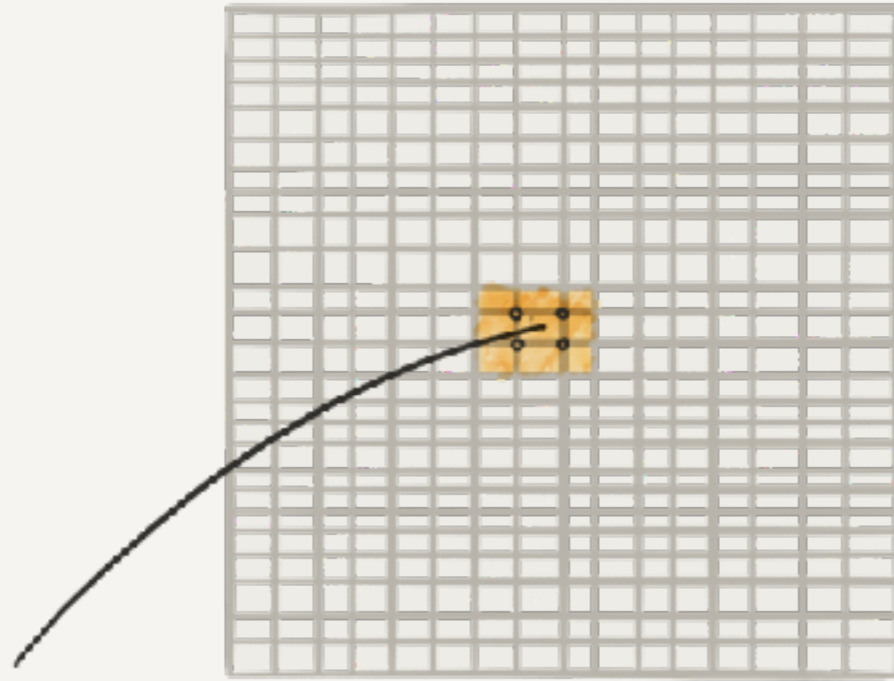


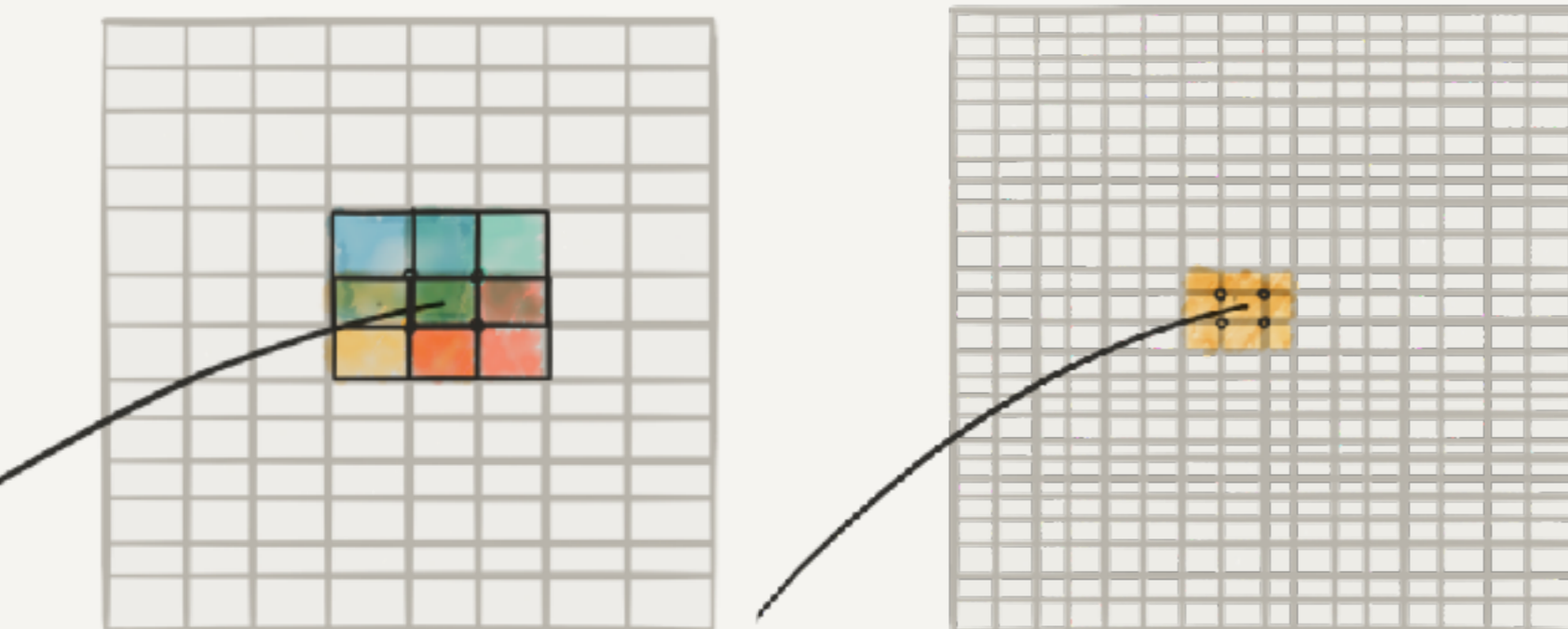






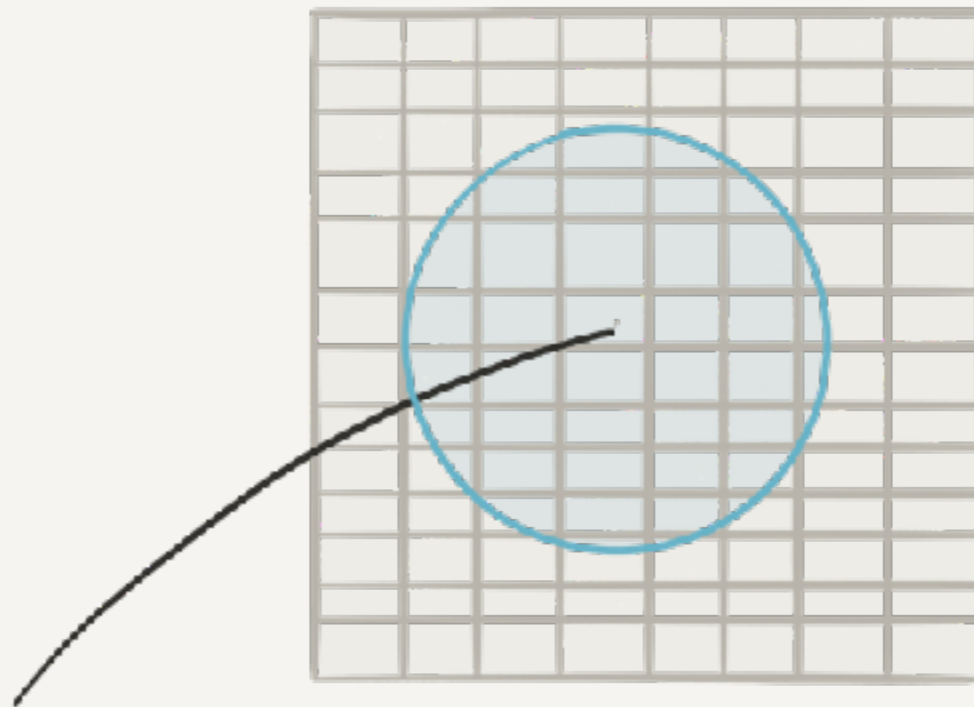




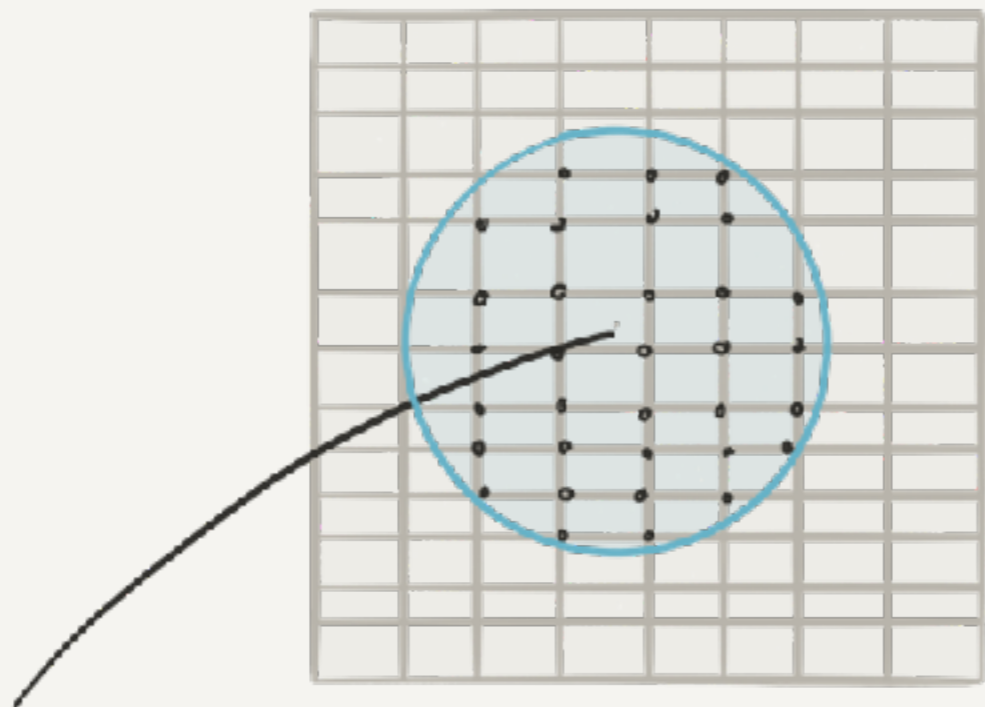


**By refining the mesh, the influence of the enrichment zone on the convergence of the method tends to zero**

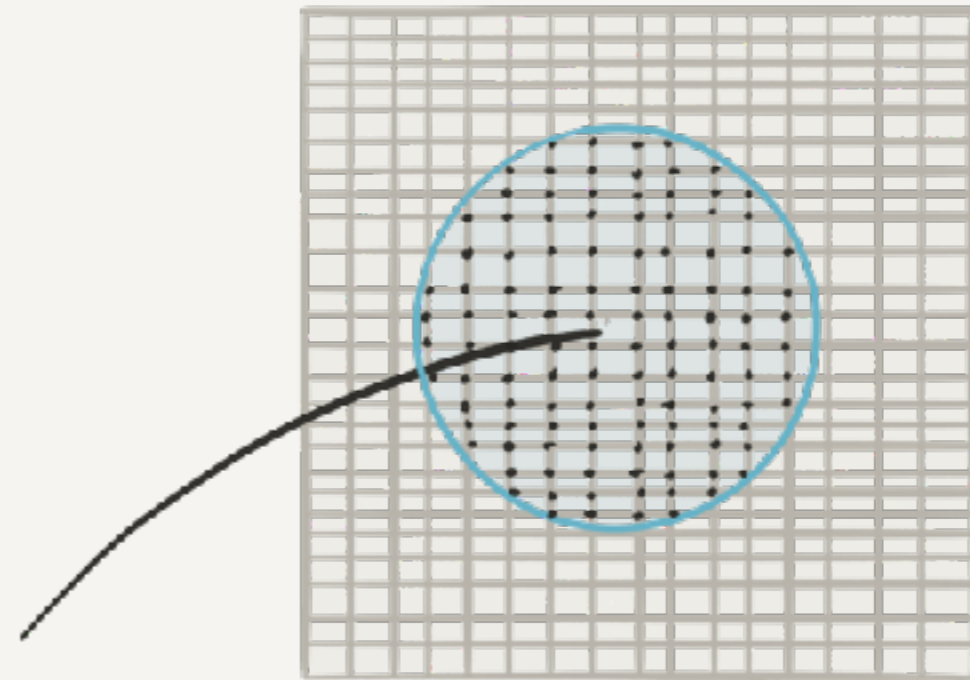
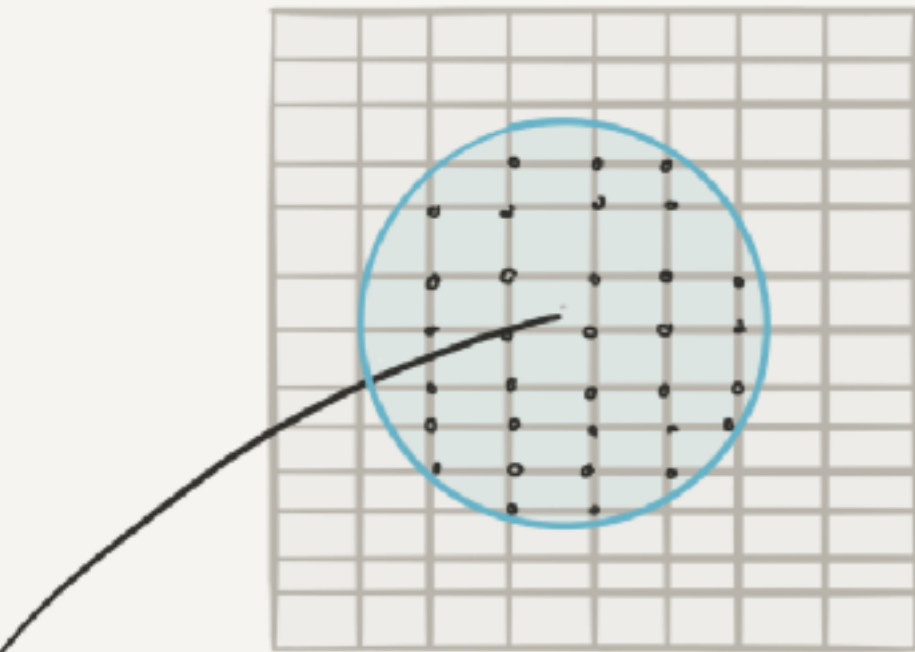
**We lose the benefit of enrichment**



**Enriching an area independent of the mesh size**



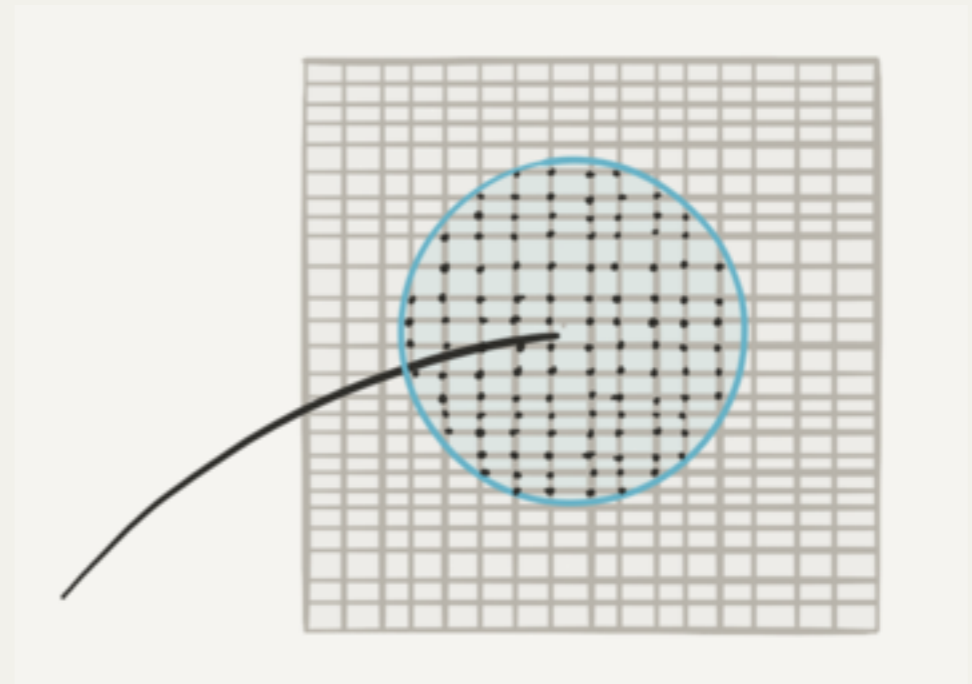
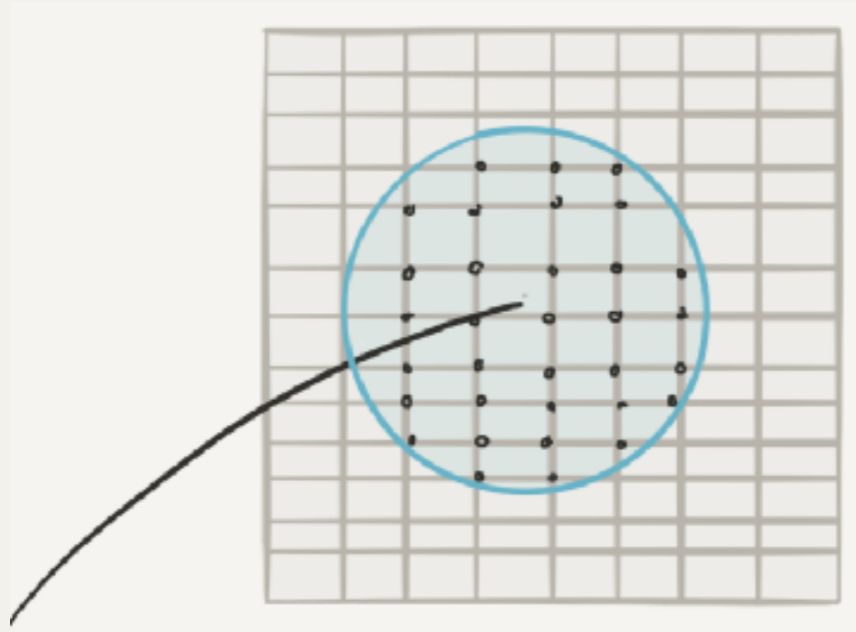




**ensures that as the mesh is refined, more and more nodes become enriched**

**the optimal convergence rate is preserved**

# Conditioning issues can be so severe that the set of equations is unsolvable



- Large enrichment zones (see stable GFEM, Banerjee, Babuška + Agathos)
- For arbitrary enrichment schemes
  - T-stress - 2nd order terms in Westergaard expansion
  - Multiple enrichments due to multiple cracks

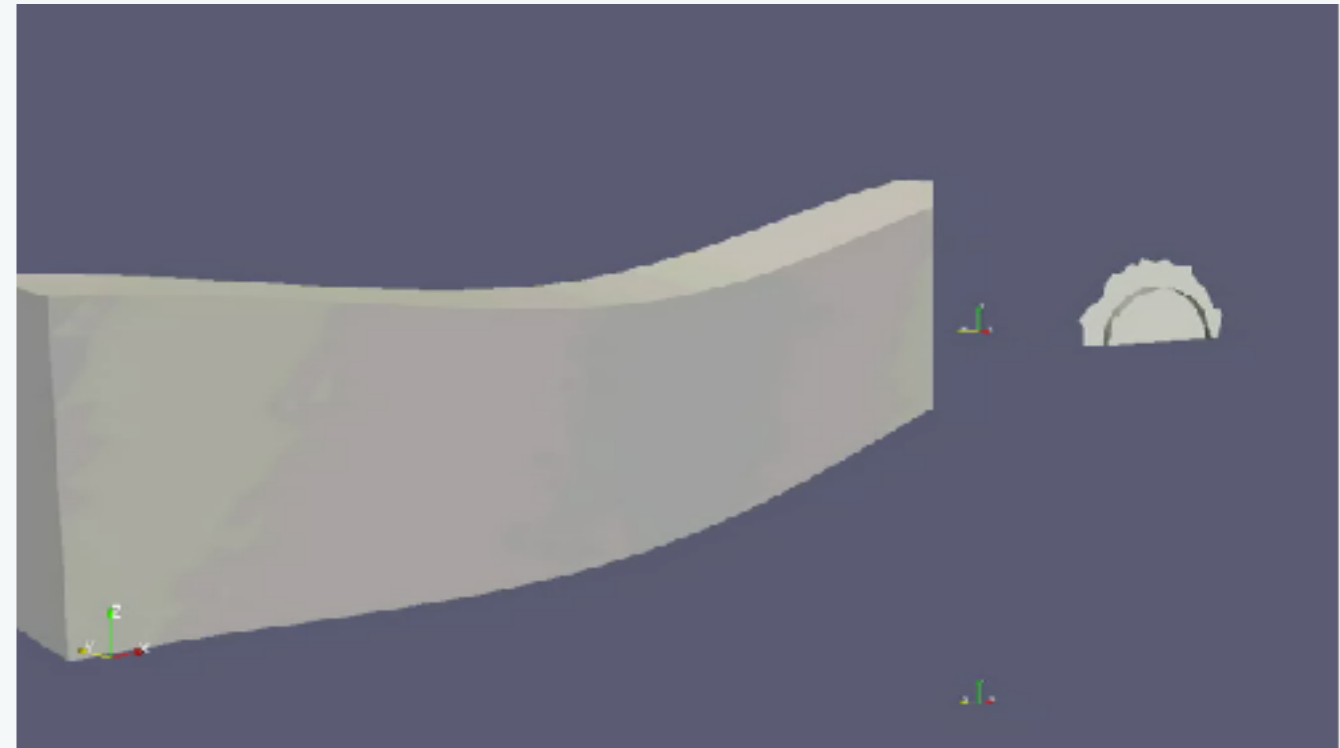
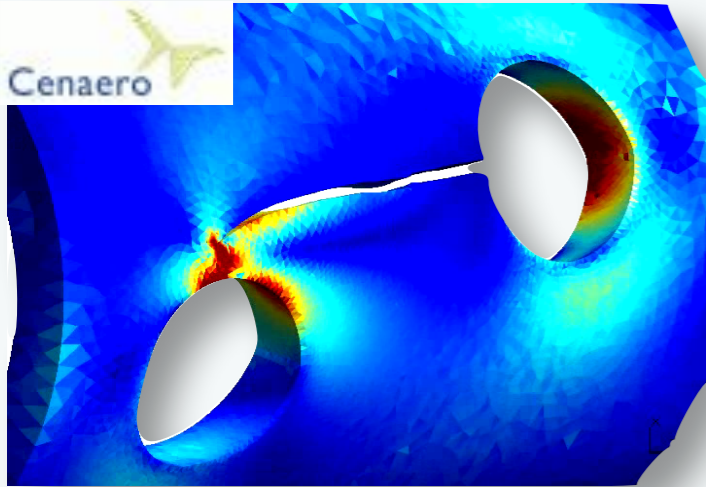
**Conclusion: difficult to set up robust and automatic enrichment schemes without specific tricks (preconditioner, e.g. Béchet or Menk)**

## *Fracture of homogeneous materials*

**Question: How to control accuracy and simplify/avoid meshing?**

- ▶ Partition of Unity - eXtended/Generalized Finite Element Methods
  - Discretisation error governed by the worst approximant
  - Local enrichment of approximations
  - Requires enrichment volumes independent of the mesh
  - Conditioning issues for large enrichment zones or arbitrary enrichment (see stable GFEM, Banerjee, Babuška + Agathos)
  
- ▶ 3D fracture requires **accurate** stress intensity factors (SIFs)
  - Error at each step  $\sim (\text{Error on SIF})^4$
  - Standard enrichment  $\Rightarrow$  oscillations along the front

## Question: How to control accuracy and simplify/avoid meshing?



K. Agathos et al. IJNME 2016, CMAME 2016, IJNME 2017, CMAME 2017 with Eleni Chatzi and Giulio Ventura

**How can we use large enrichment radii?**

**How can we control conditioning in large-scale enriched FEM?**

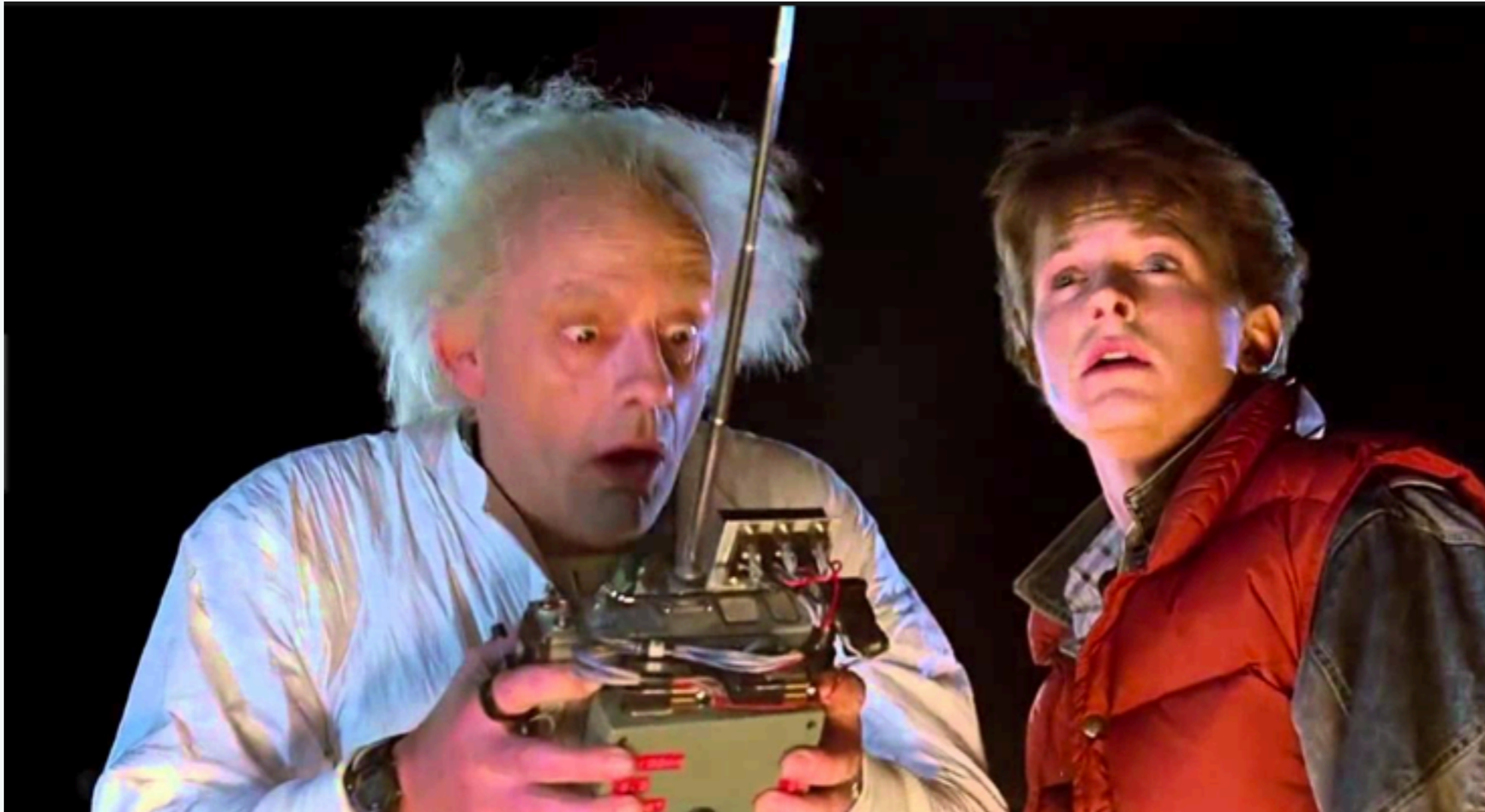
**How can we use higher order terms in the expansion?**



X. Peng et al. IJNME 2016, CMAME 2017  
Enriched Isogeometric Boundary Elements

**How to avoid meshing completely for crack propagation simulations?**

# Don't worry...



# You can get a gradual introduction to the method in the following papers

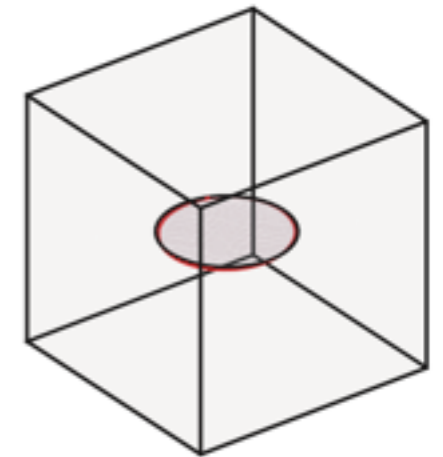
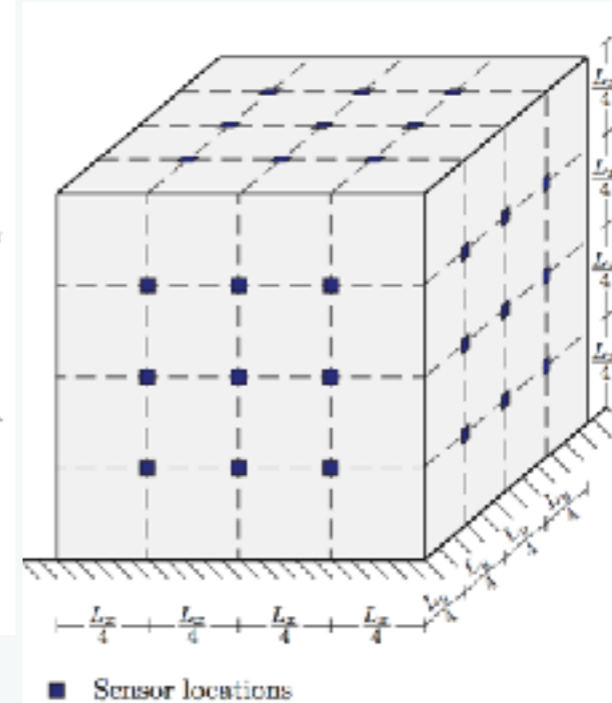
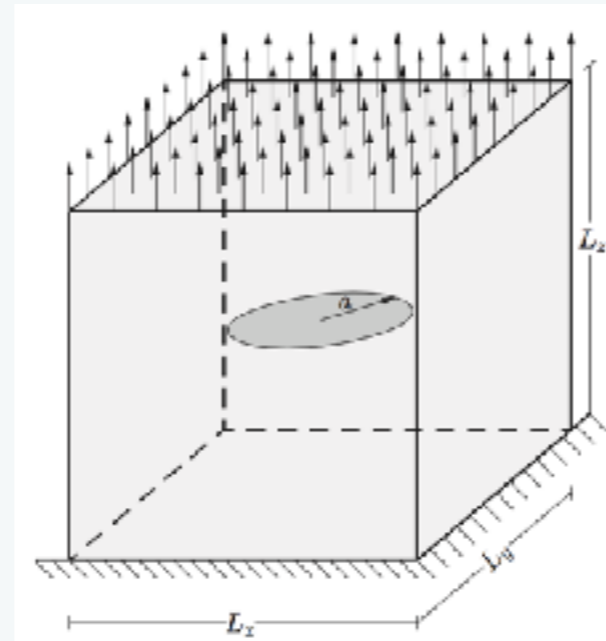
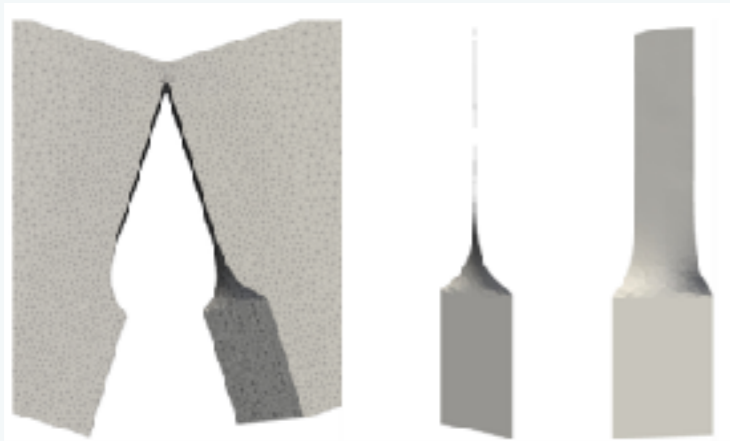
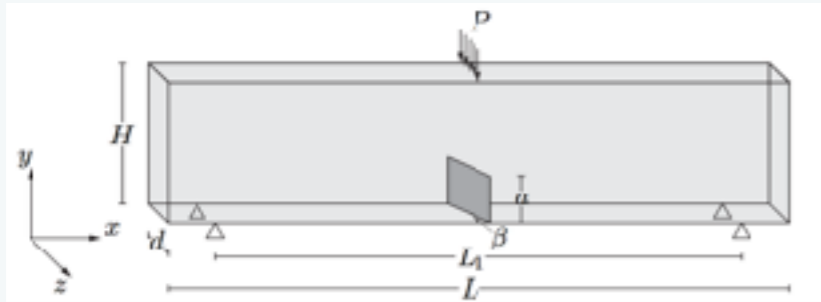
Agathos K, Ventura G, Chatzi E, Bordas S. Stable 3D XFEM/vector-level sets for non-planar 3D crack propagation and comparison of enrichment schemes. *International Journal for Numerical Methods in Engineering. Computational Mechanics*, 2017.

Agathos K, Chatzi E, Bordas S, Talaslidis D. A well-conditioned and optimally convergent XFEM for 3D linear elastic fracture. *International Journal for Numerical Methods in Engineering*. 2016 Mar 2;105(9):643-77.

Agathos, K., E. Chatzi, and SPA Bordas. "Stable 3D extended finite elements with higher order enrichment for accurate non planar fracture." *Computer Methods in Applied Mechanics and Engineering* 306 (2016): 19-46.

<https://orbilu.uni.lu/bitstream/10993/22331/2/paper.pdf>

<http://orbilu.uni.lu/bitstream/10993/22420/1/presentation.pdf>



2000 evaluations

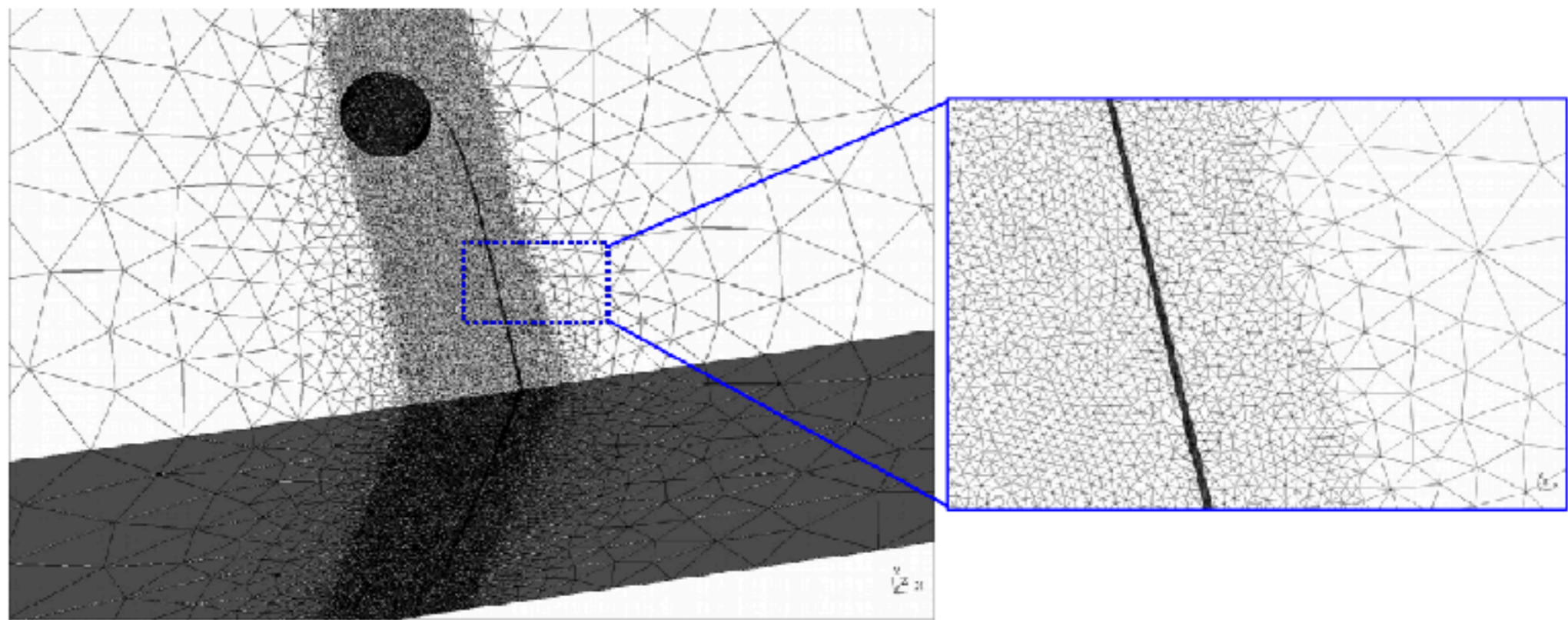
- ✓ Introduces a novel form of enrichment.
- ✓ Provides improved conditioning.
- ✓ Enables the use of geometrical enrichment.
- ✓ Enables the use of higher order terms in fracture mechanics
- ✓ Was combined to vector level sets to solve crack propagation problems.
- ✓ Was applied to inverse problems.
- ✓ Provides high accuracy and optimal convergence.

**Conclusion: we can now add arbitrary numbers of enrichments and enrich over 'large' volumes of the domain.**

**What if you can't add new functions or  
you don't want to increase the  
enrichment radius?**



*(Goal oriented) adaptive computational fracture  
use h-refinement*



**Before: mesh “finely” in the region where the crack is “expected” to propagate**

Y. Jin, O. Pierard, et al. *Comput. Methods Appl. Mech. Engrg.* 318 (2017) 319–348

O.A. González-Estrada et al. *Computers and Structures* 152 (2015) 1–10

O.A. González-Estrada et al. *Comput Mech* (2014) 53:957–976

C. Prange et al. *IJNME* 91.13 (2012): 1459-1474.

M. Duflot, SPAB, *IJNME* 2007, *CNME* 2007, *IJNME* 2008.

J-J. Ródenas Garcia, *IJNME* 2007

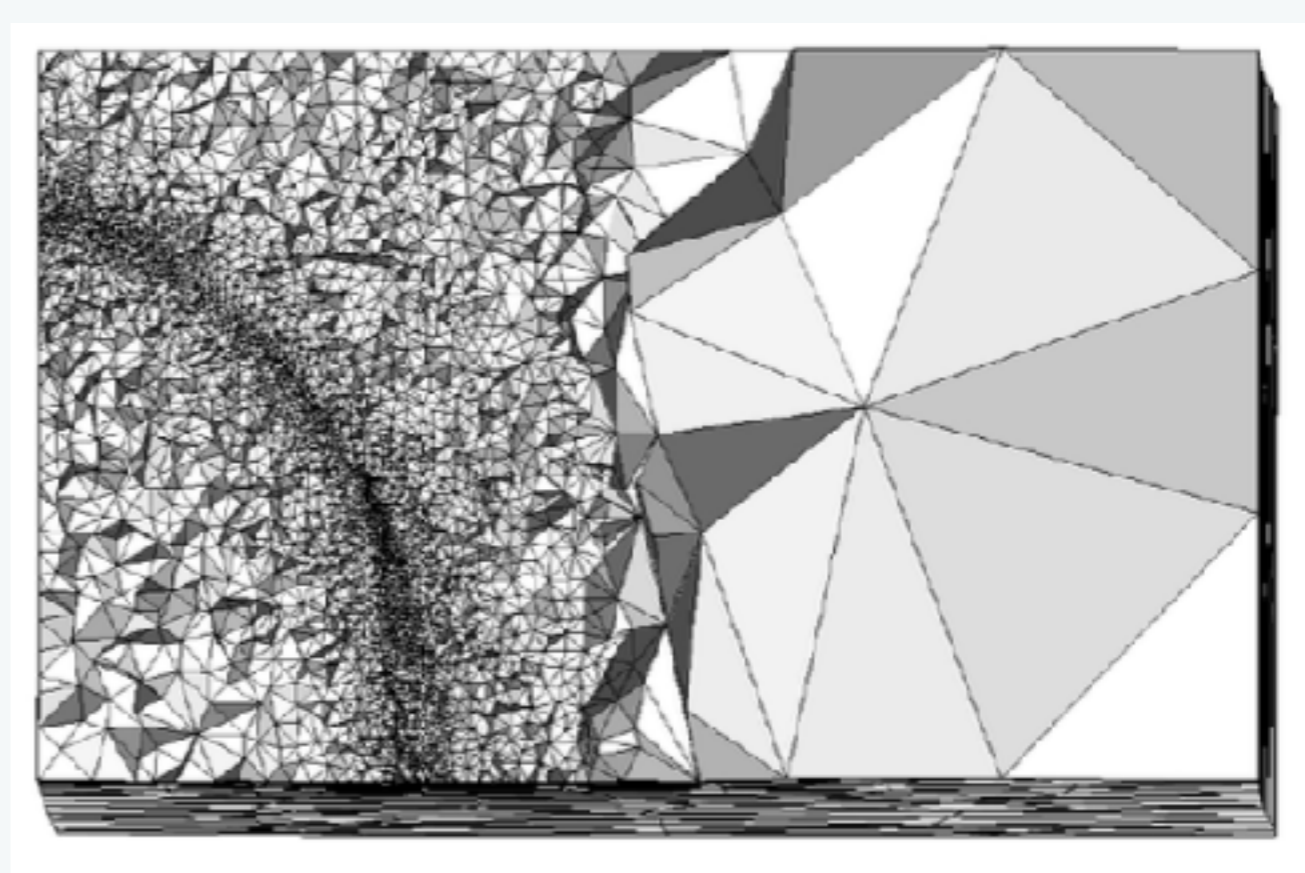
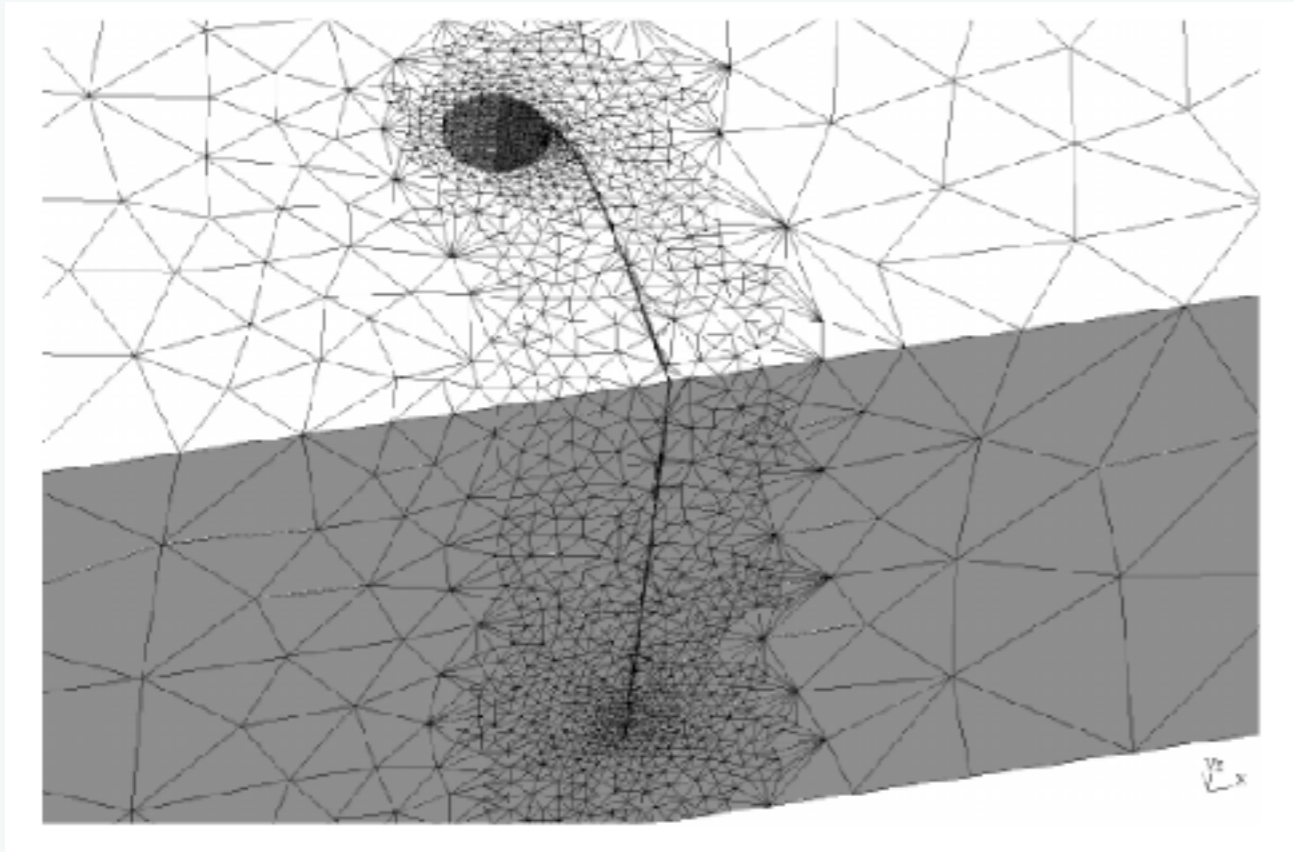
F.B. Barros, et al *IJNME* 60.14 (2004): 2373-2398.

M. Rüter *CMECH* (2013) 1;52(2):361-76.

J. Panetier *IJNME* 81.6 (2010): 671-700.

P. Hild, *CMECH* (2010): 1-28.

## *Fracture of homogeneous materials: error estimation and adaptivity*



**After: determine mesh refinement adaptively using a (goal-oriented) error estimate**

Y. Jin, O. Pierard, et al. Error-controlled adaptive extended finite element method for 3D linear elastic crack propagation *Comput. Methods Appl. Mech. Engrg.* 318 (2017) 319–348

M. Duflot, SPAB, IJNME 2007, CNME 2007, IJNME 2008.

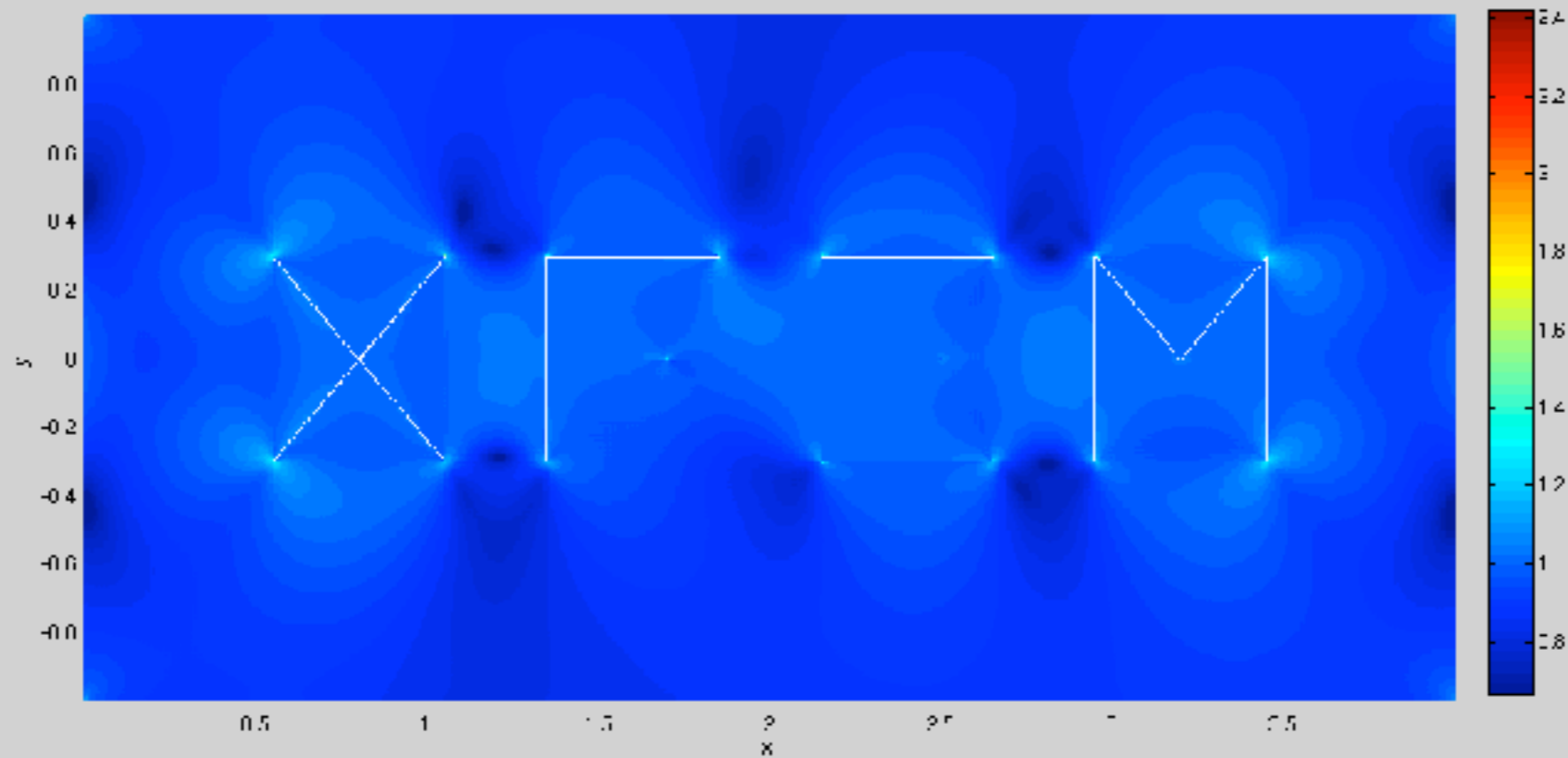
# Partial Conclusions

- ◆ FEM has intrinsic difficulties with singularities and discontinuities
- ◆ Enrichment helps to decrease but not eliminate remeshing
- ◆ This remeshing can be driven by error estimates
- ◆ Arbitrary enrichment functions can be chosen
- ◆ (almost) arbitrary enrichment zones
- ◆ **Question:** what are the limitations of these enrichment approaches?

# What if we have to deal with more cracks...

## Extended Finite Element Method (XFEM)

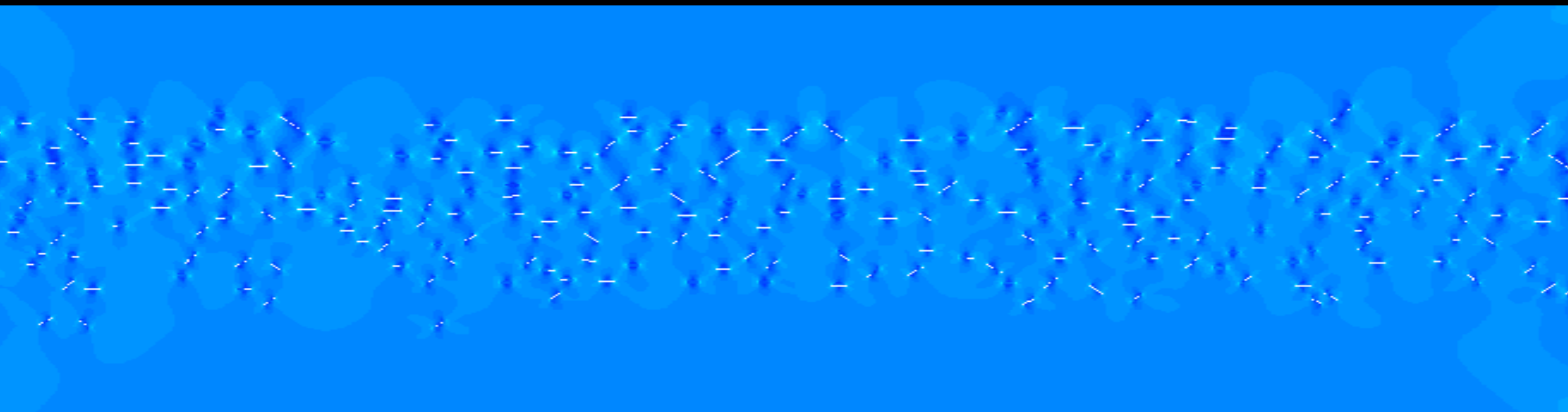
Fracture of “XFEM” using XFEM



# Case study II. Plate with 300 cracks vertical extension BCs



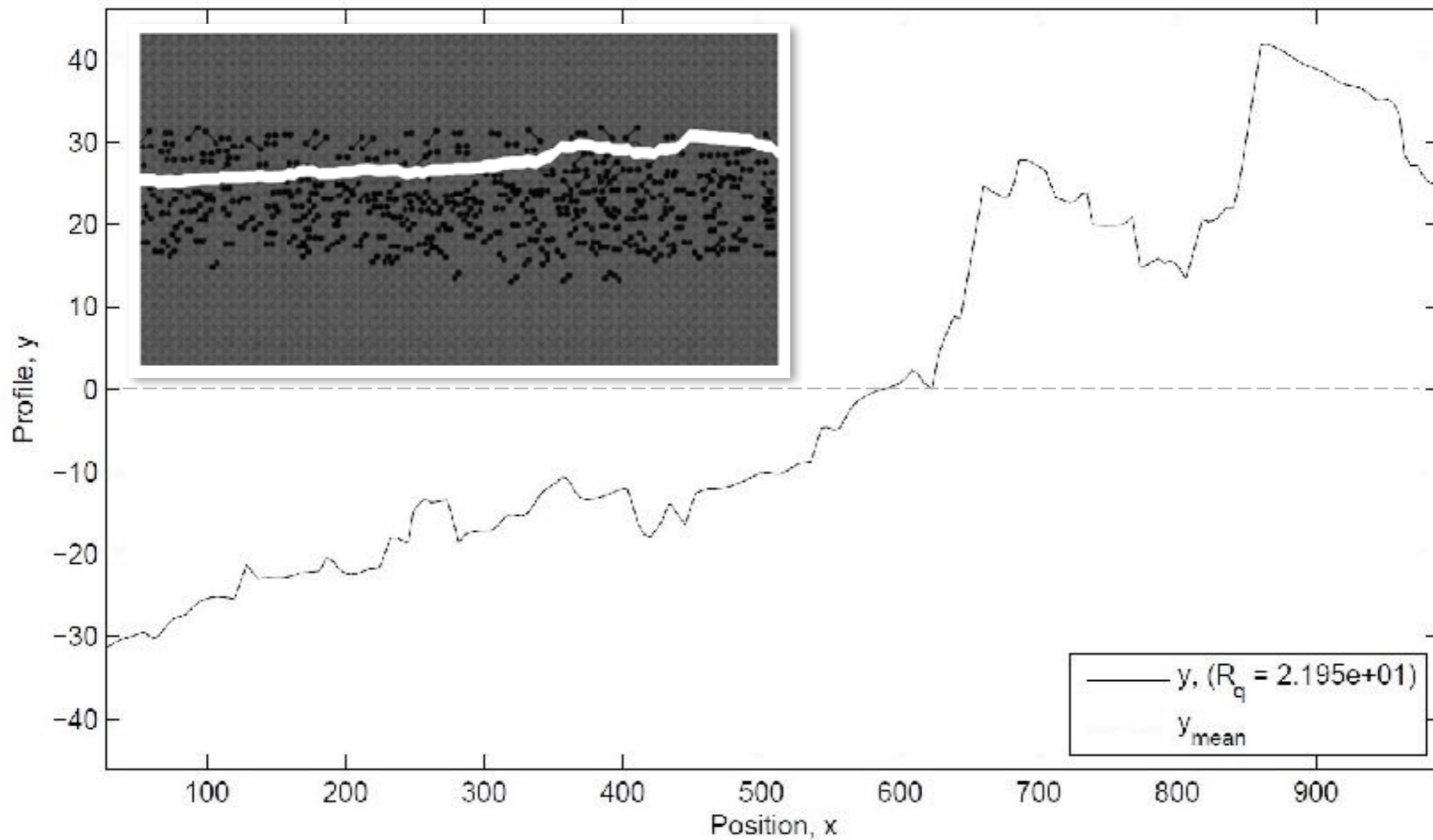
## Energy-minimal crack growth using XFEM



Sutula et al. Preprint of three part EFM paper at  
<http://hdl.handle.net/10993/29414>

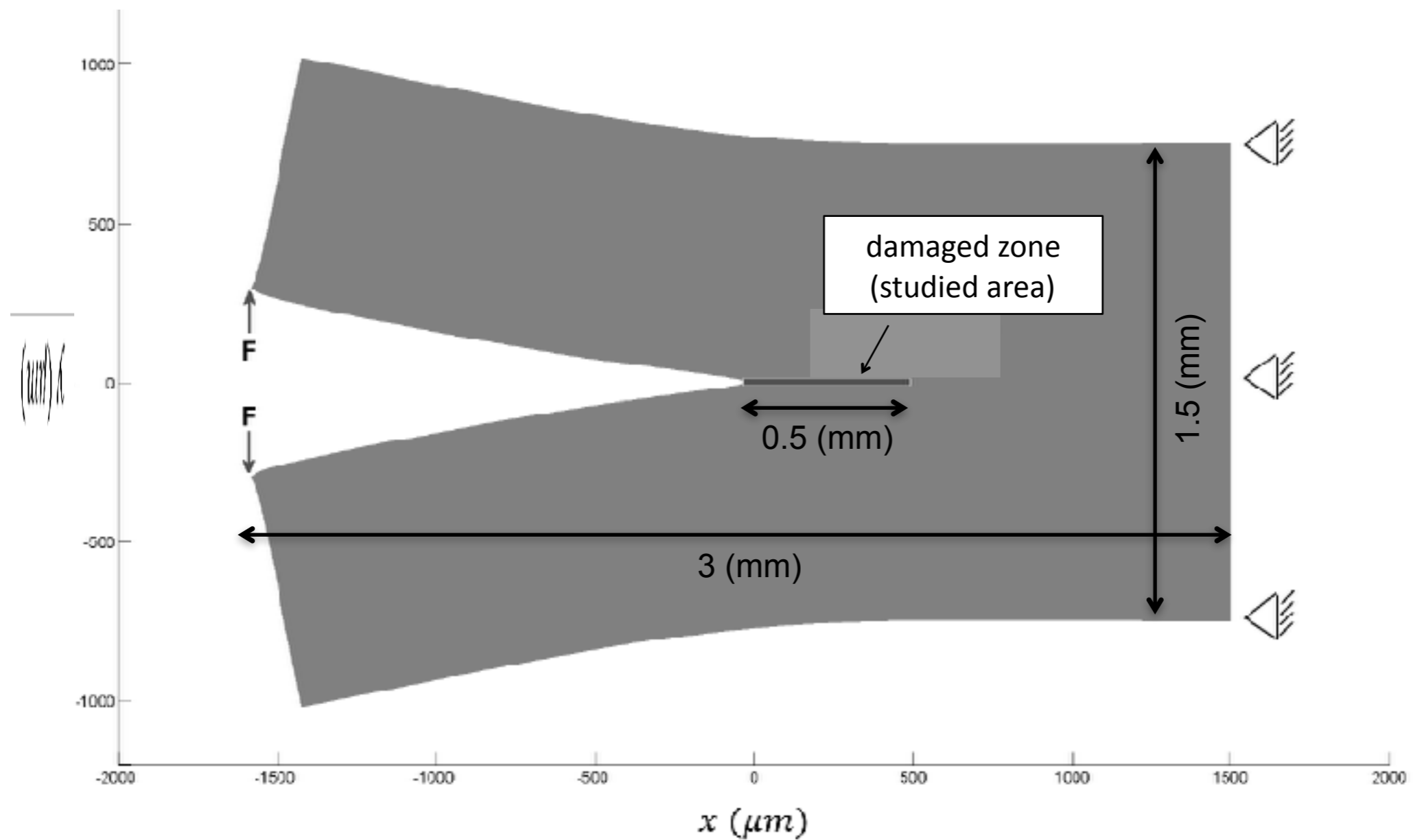
## Vertical extension of a plate with 300 cracks

Post-split roughness



## Mechanical splitting of a wafer sample

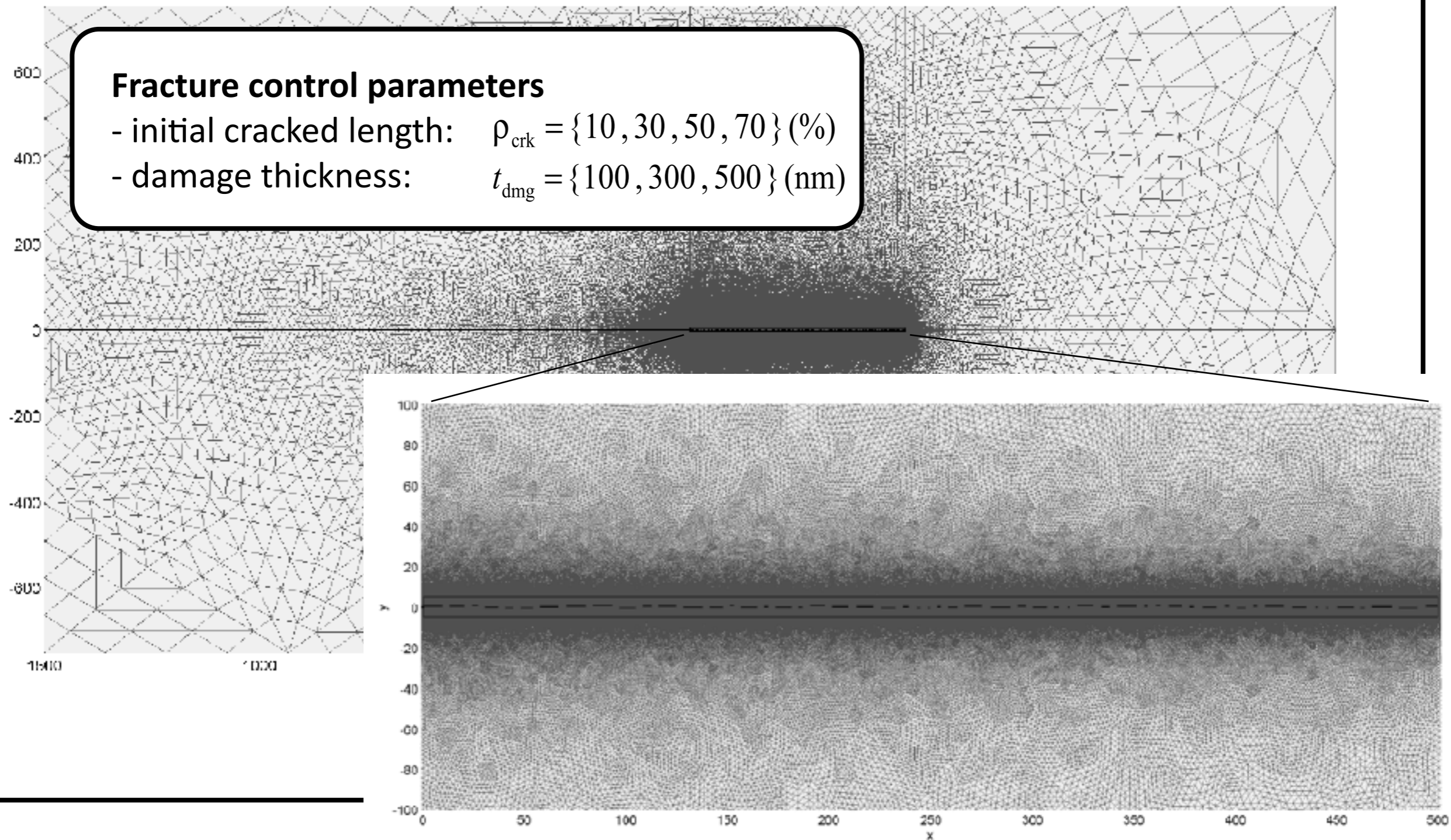
- Post-split roughness as a function of micro crack distribution





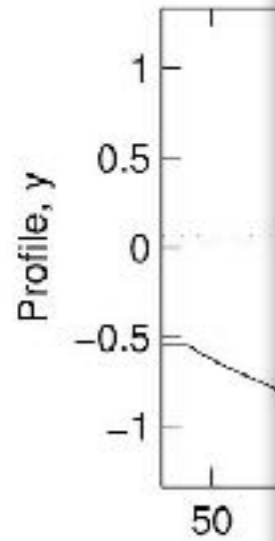
## Mechanical splitting of a wafer sample

- Discretisation ( $\approx 1$  mln. DOF,  $h_e = 150$  nm)

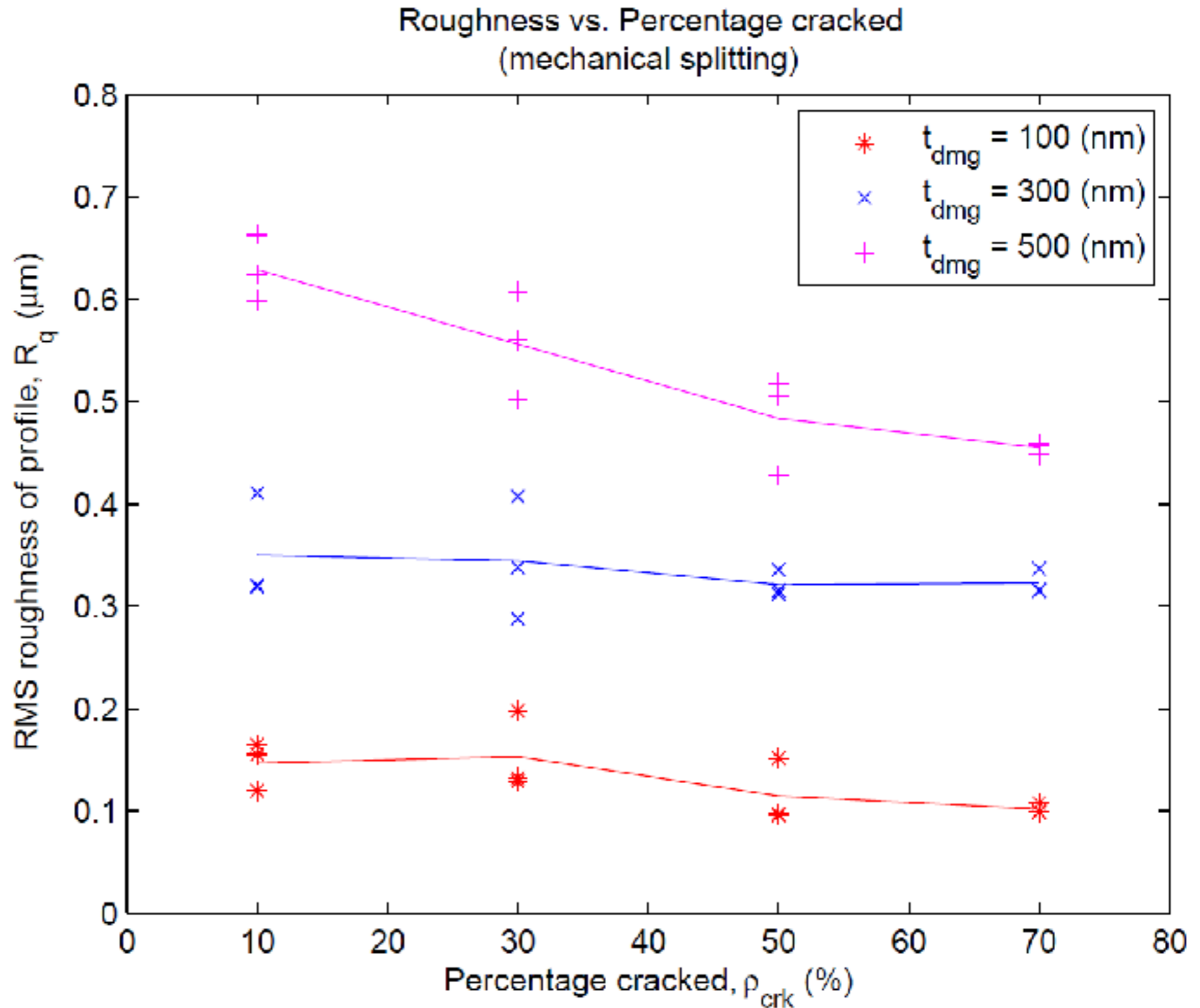
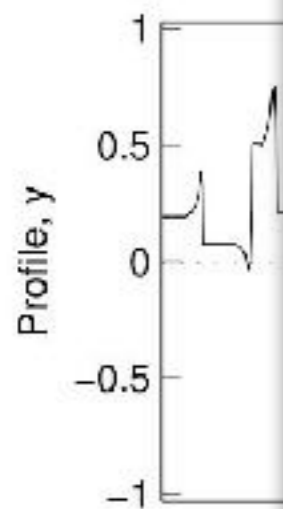


## Fracture ro

- Case exa



- Case exa



## **LEFM model**

- Assuming mechanical interactions dominate during micro crack growth

## **Crack growth**

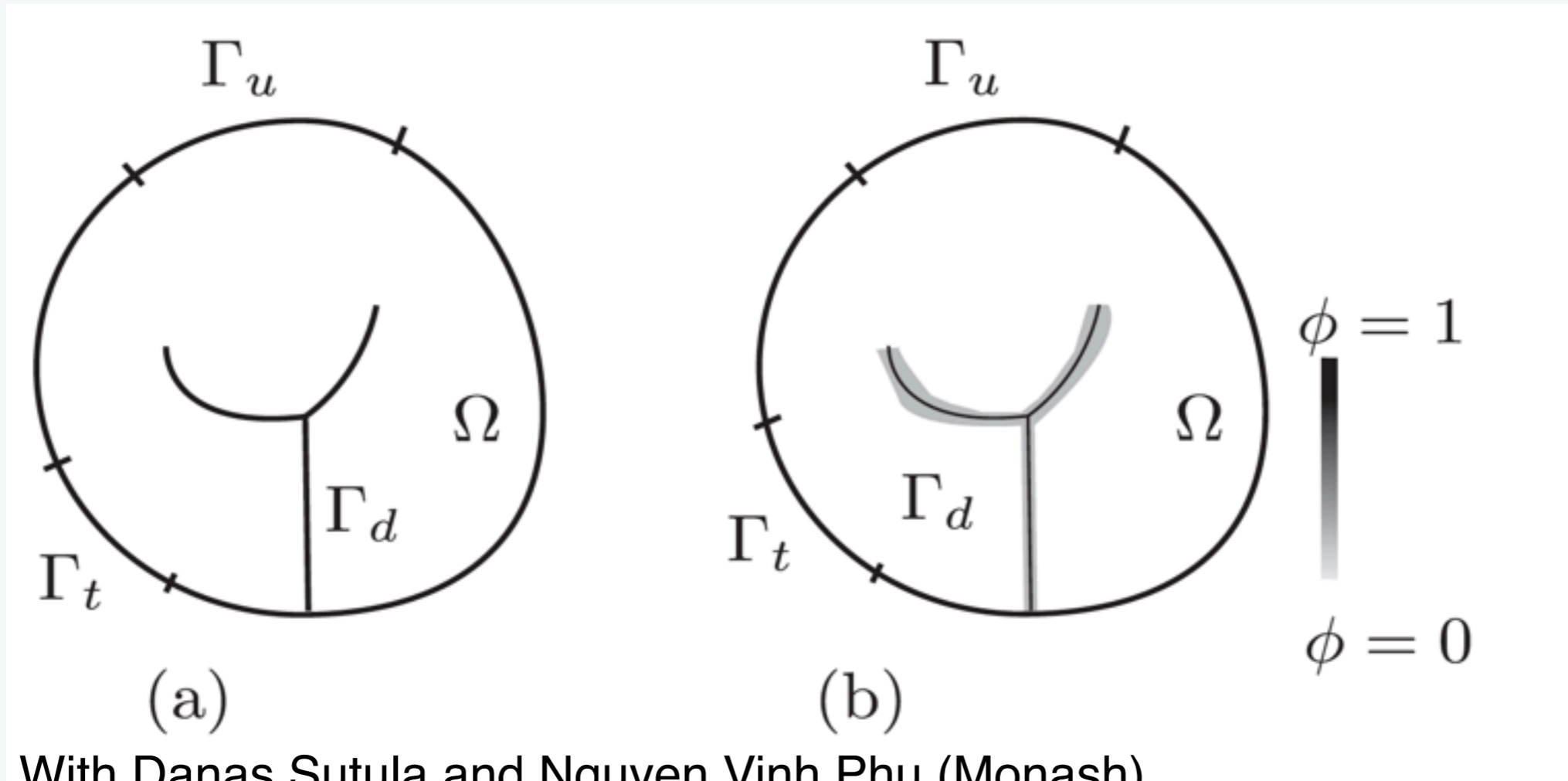
- crack tip with max SIF in direction of max hoop stress

## **Discretization**

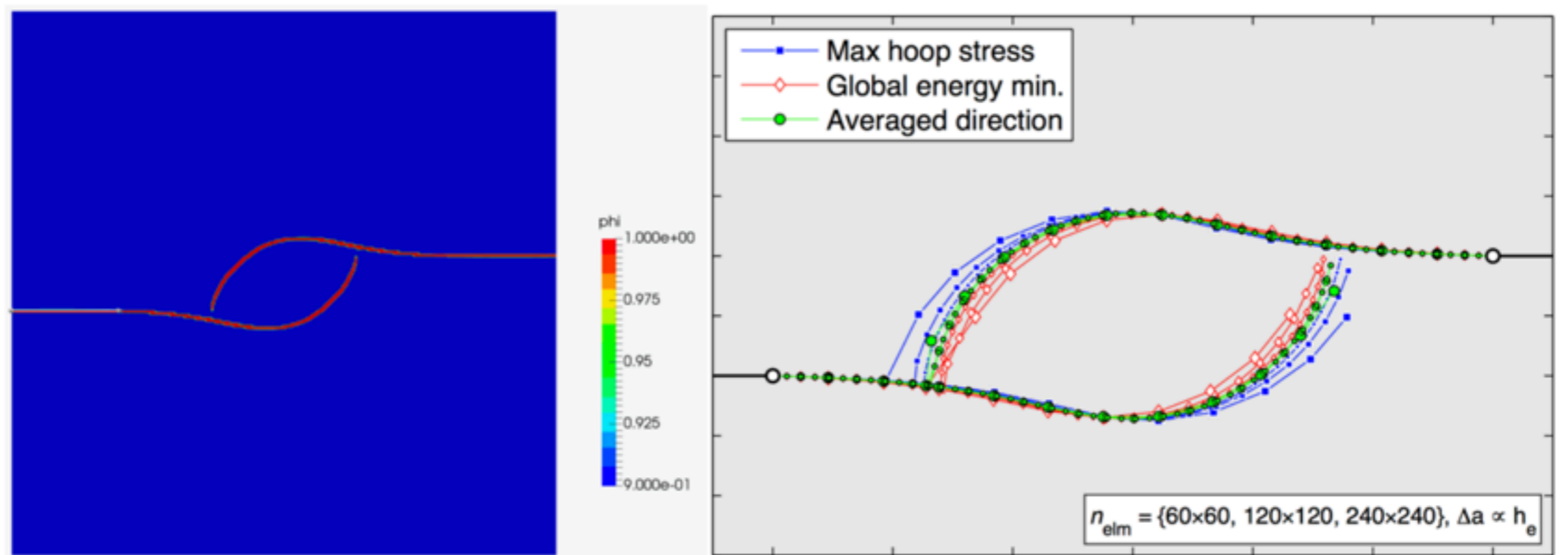
- XFEM for efficient multiple fracture modeling

# More cracks?... 3D? ...

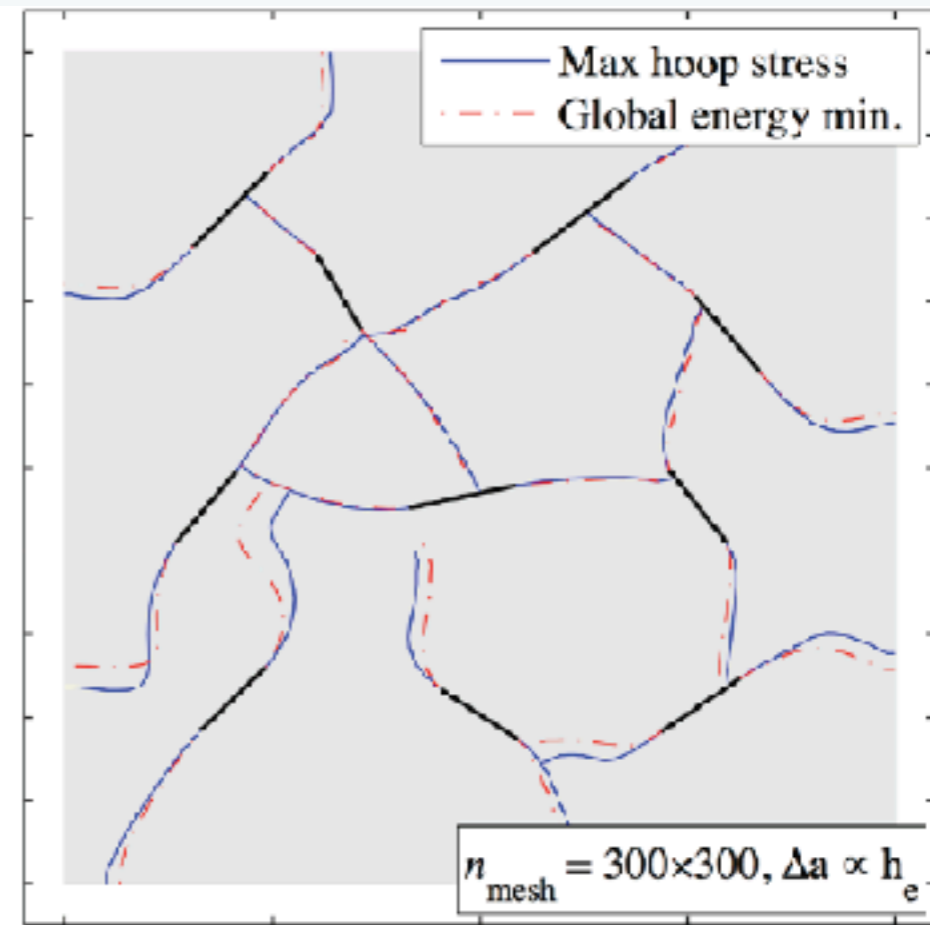
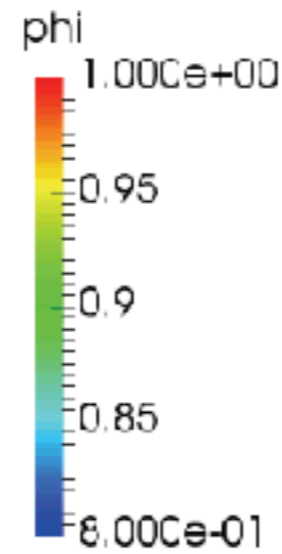
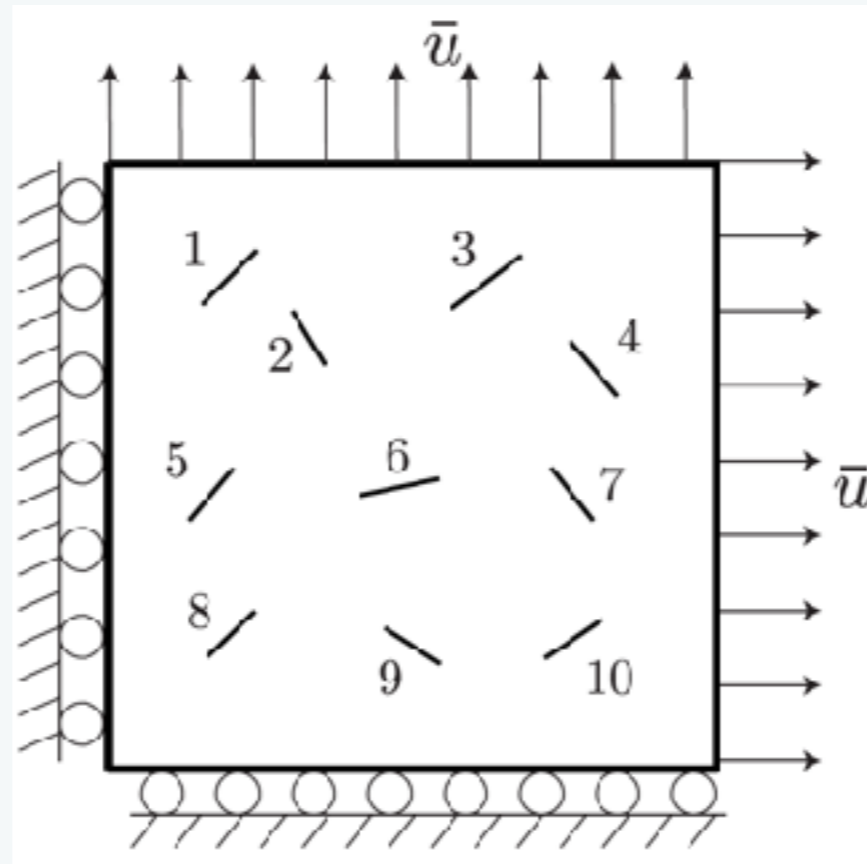
## *Phase field/thick level sets*

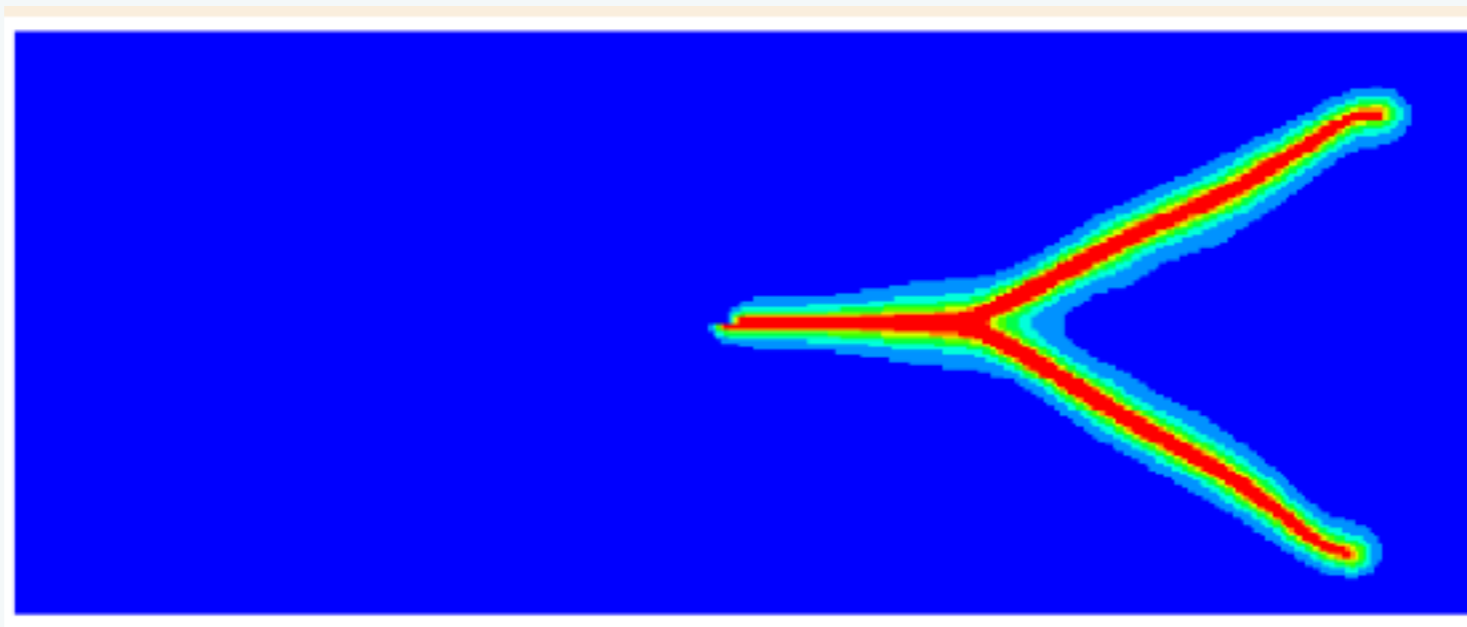
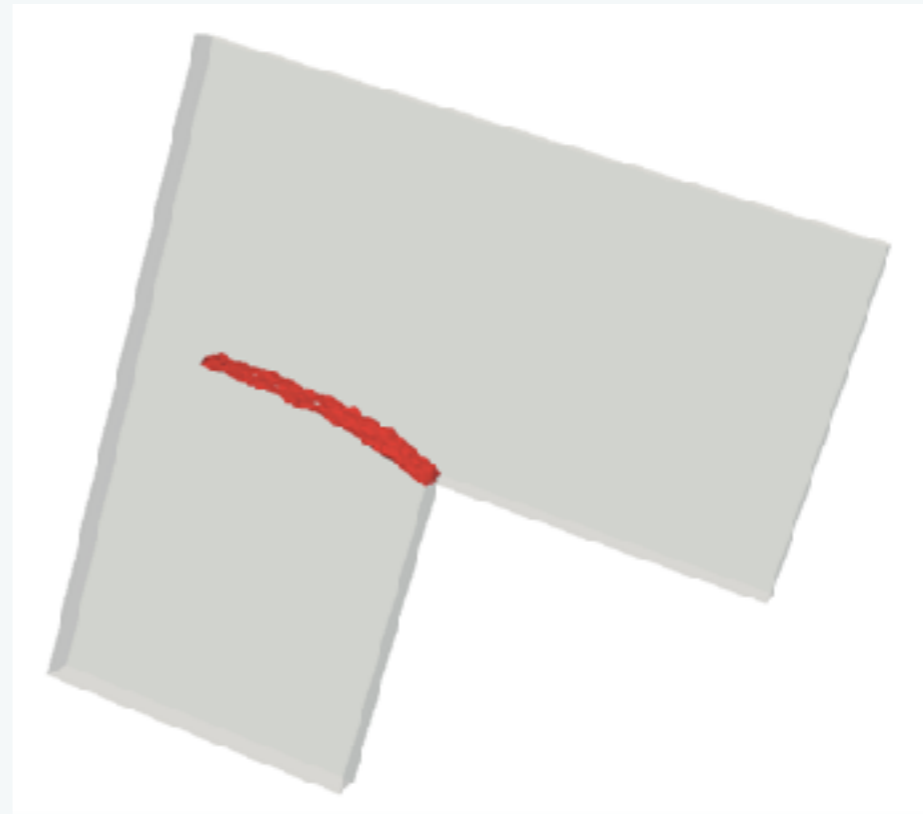
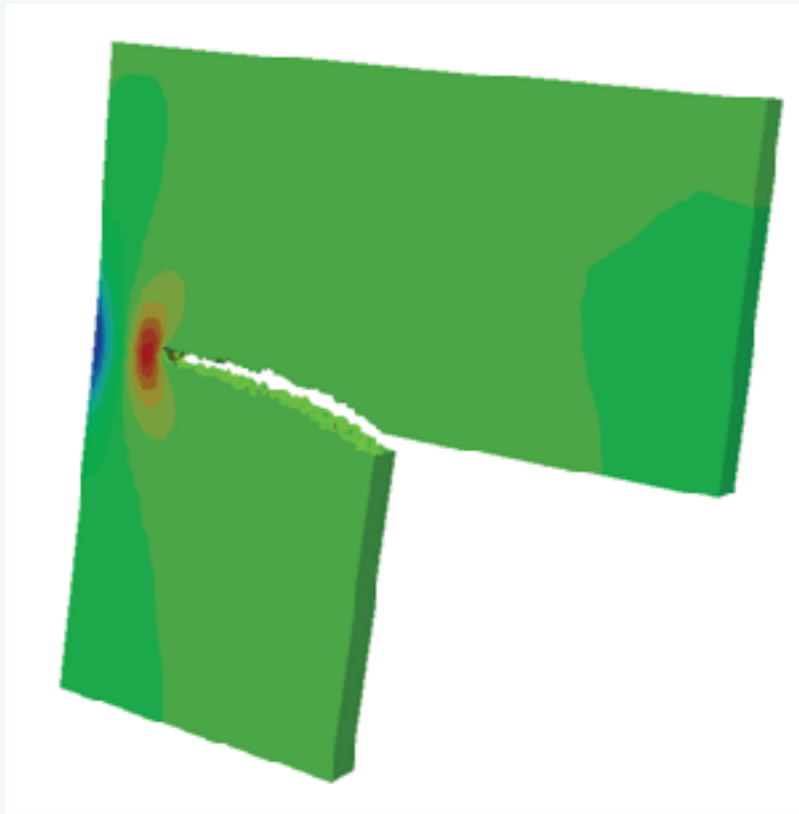


With Danas Sutula and Nguyen Vinh Phu (Monash)  
9TH Australasian Congress on Applied Mechanics (ACAM9)  
27 - 29 November 2017  
[phu.nguyen@monash.edu](mailto:phu.nguyen@monash.edu)



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# Partial conclusions on fracture of homogeneous materials using enriched FEM

- More than a few cracks in 3D may warrant using phase fields models as opposed to discrete cracks
- Meshfree methods are possible alternatives  
(See the work of Rabczuk, Belytschko, Zi, SPAB)

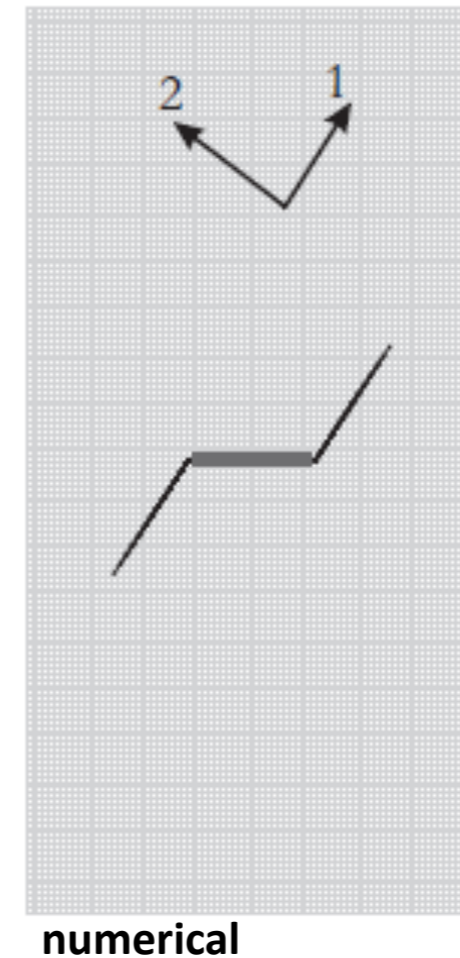
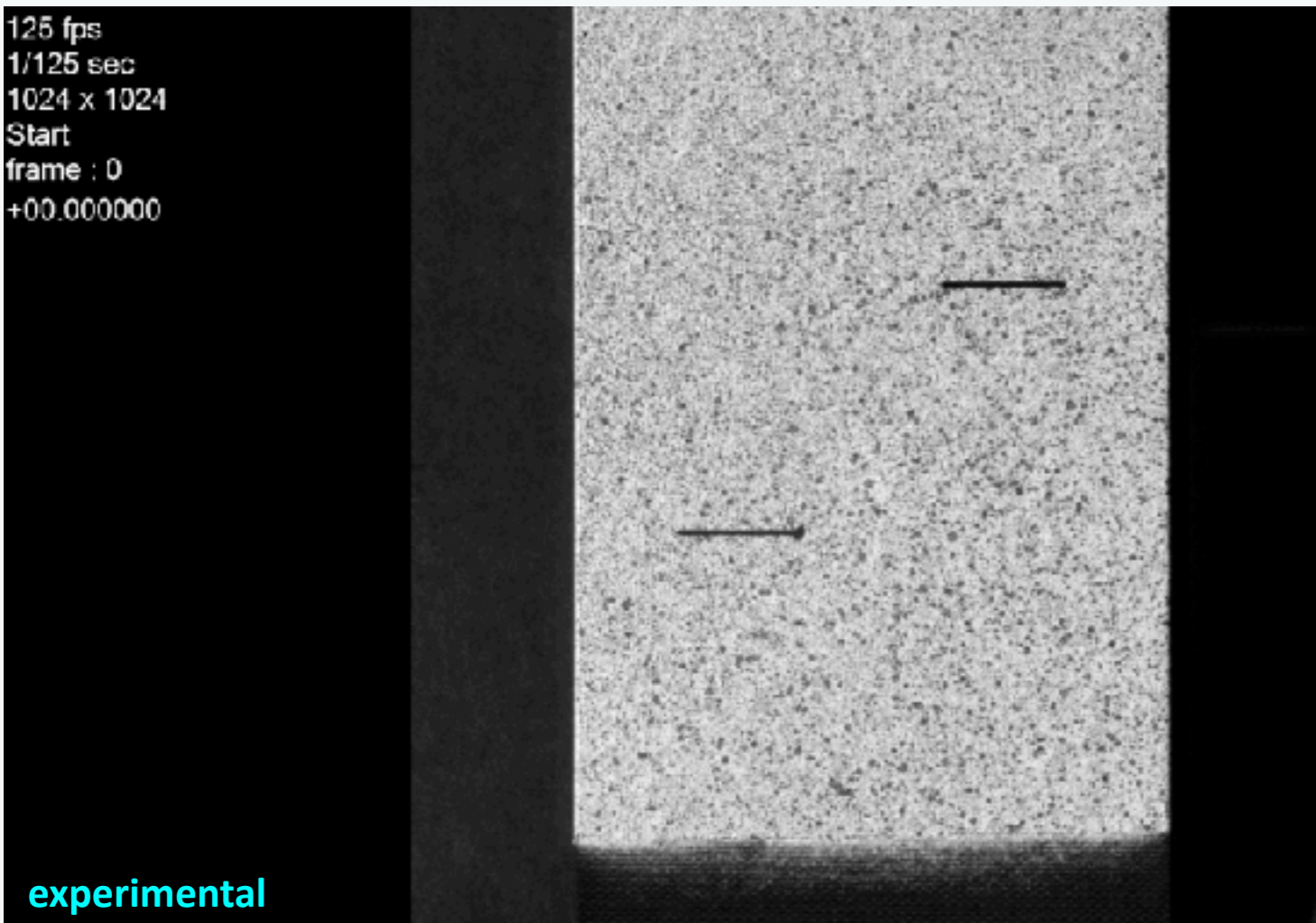


# Question: how to handle heterogeneities over the scales in computational fracture ?

## Case study III: Fracture of heterogeneous materials

# Mild heterogeneities/anisotropy Homogenized models are sufficient

**Question: what main factors govern crack growth in composite laminates?**



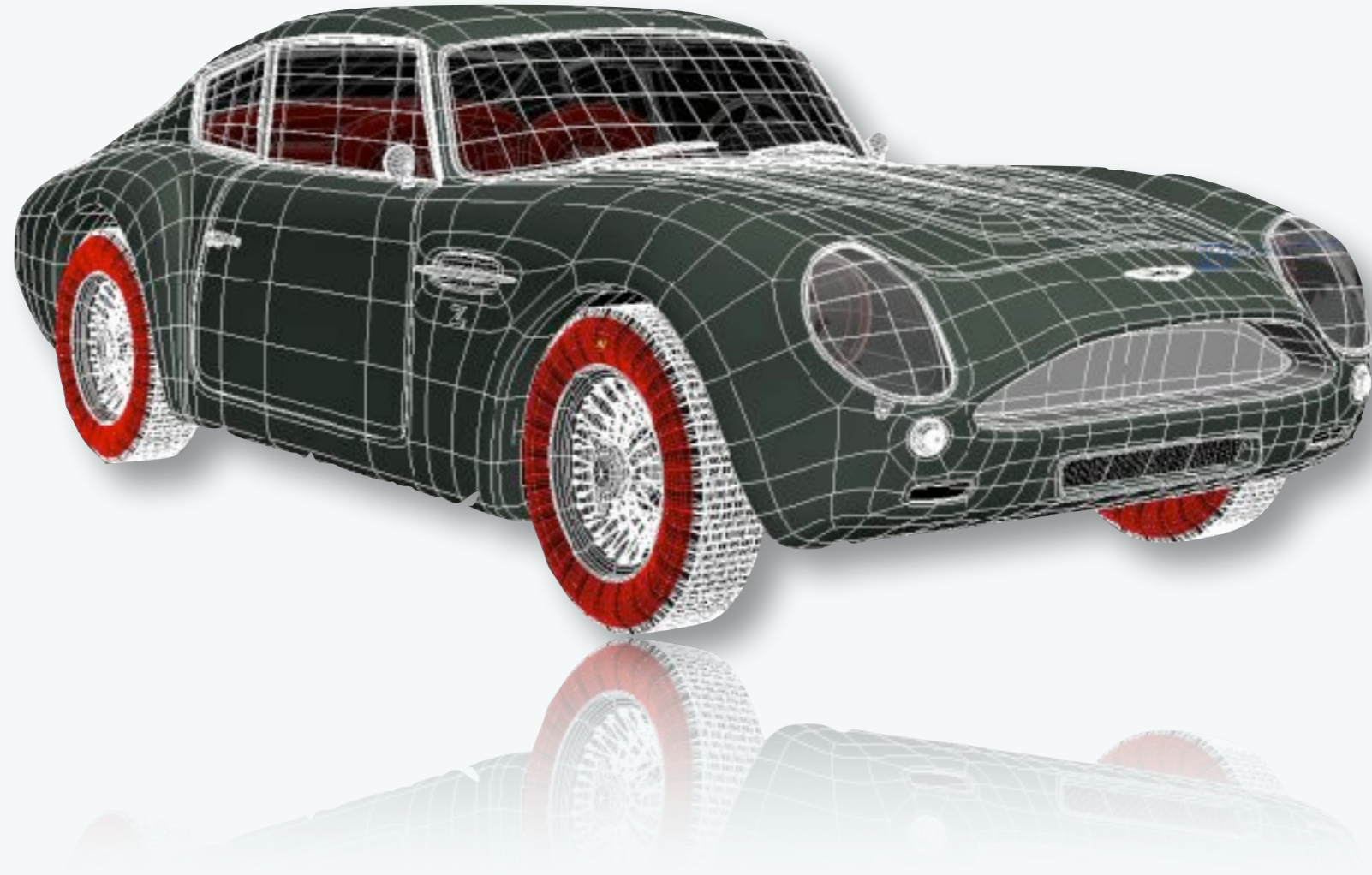
L. Cahill et al. Composite Structures, 2014

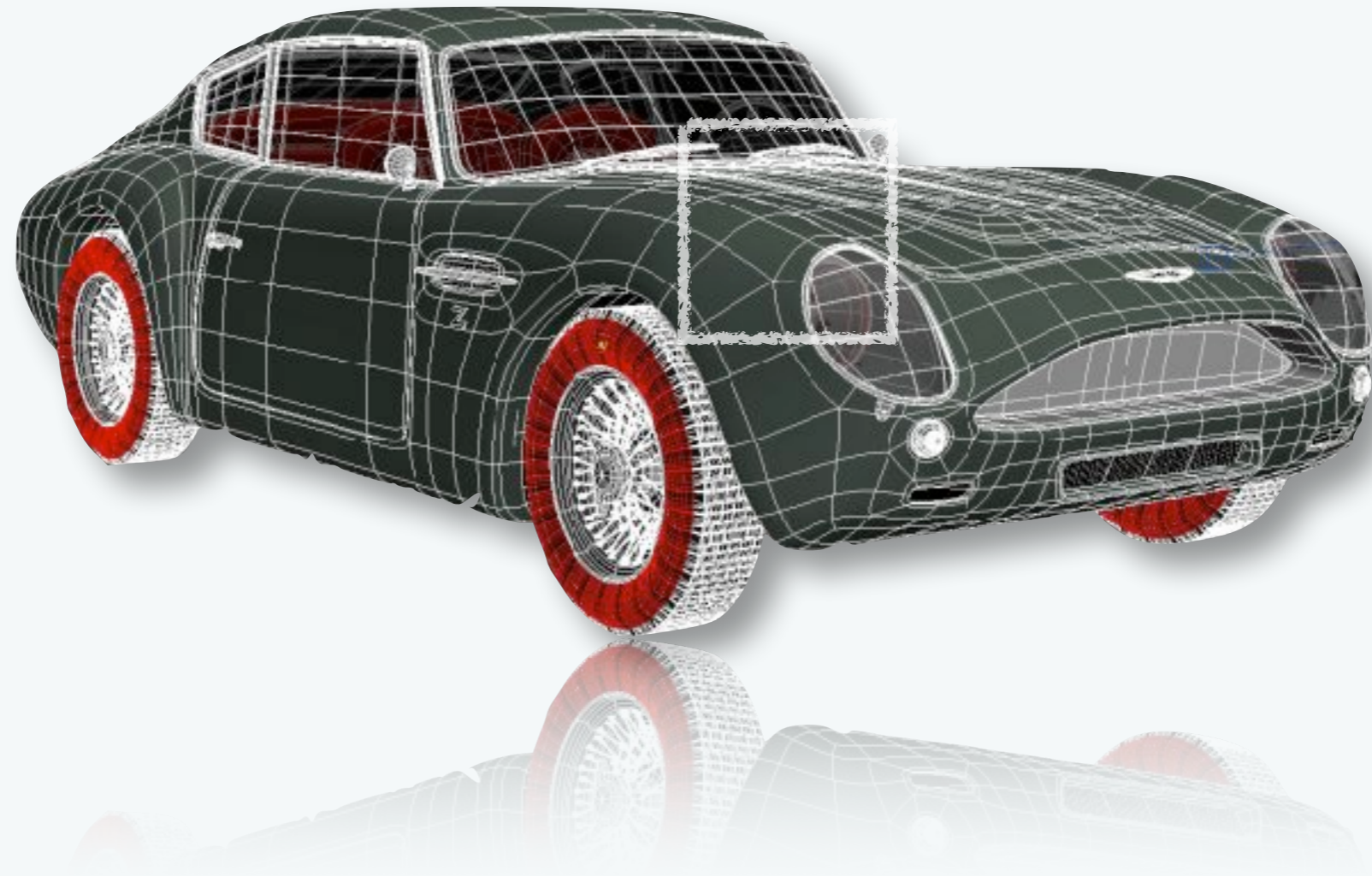
*Experimental/Numerical approach to determining the driving force for fracture in composites*

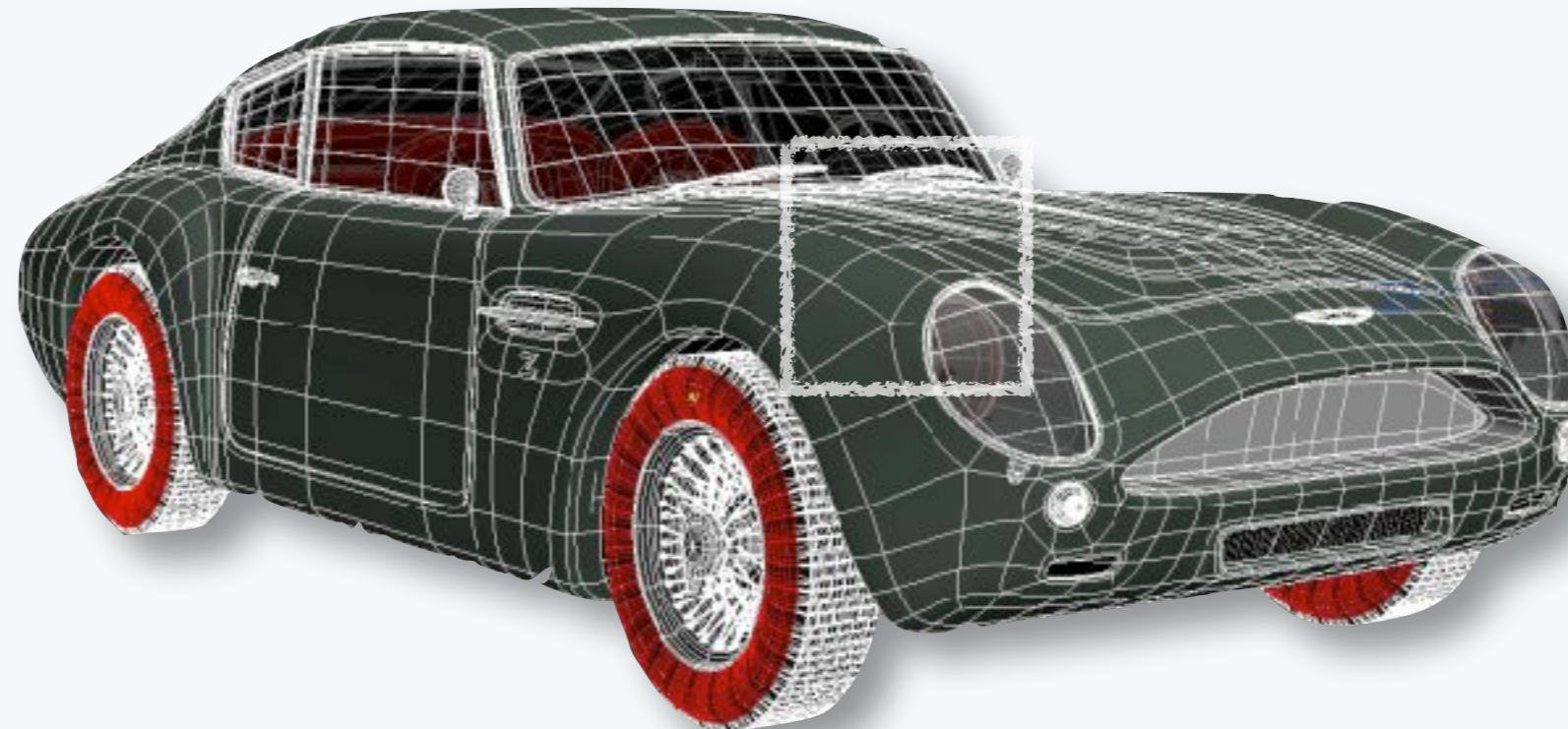
## XFEM can effectively deal with orthotropic fracture

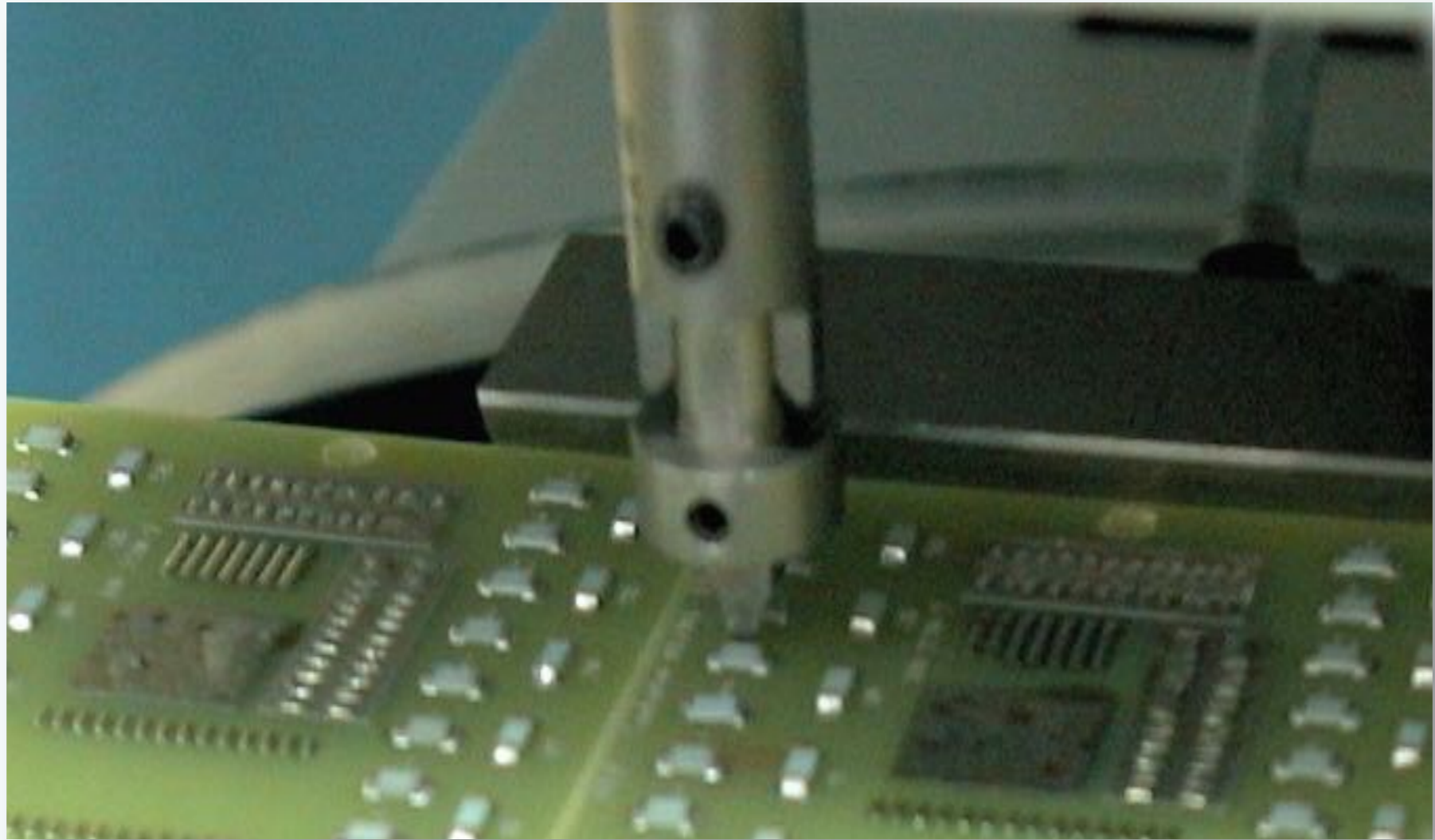
# *Strong heterogeneities*

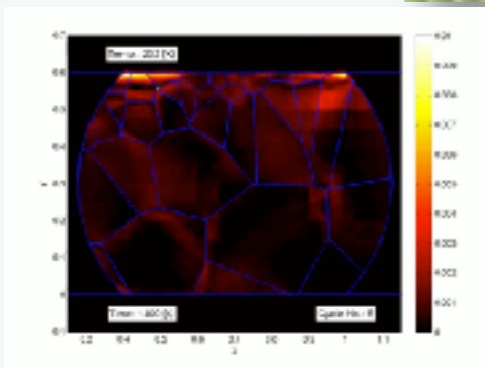
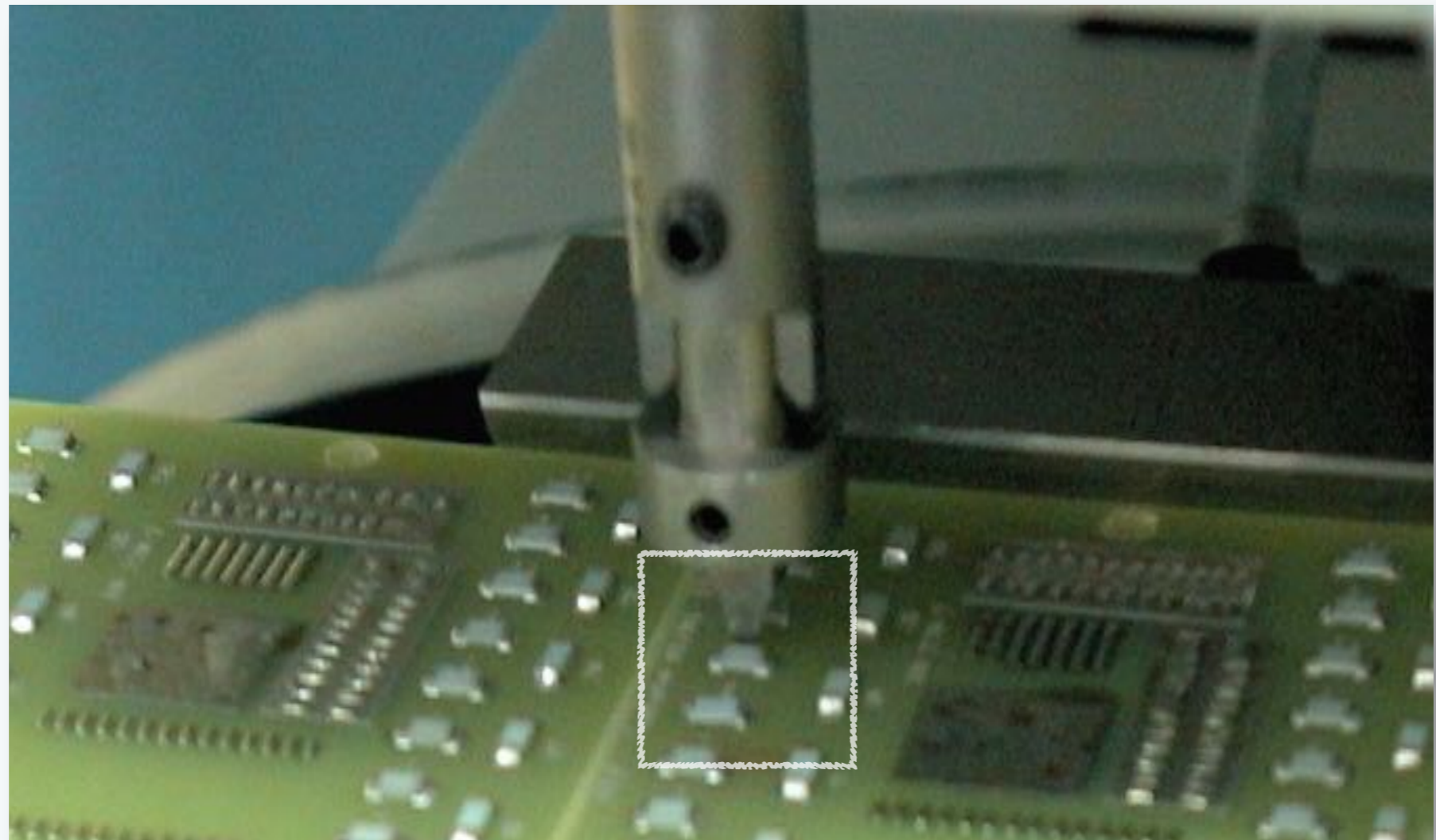
## *Homogenized models are insufficient*

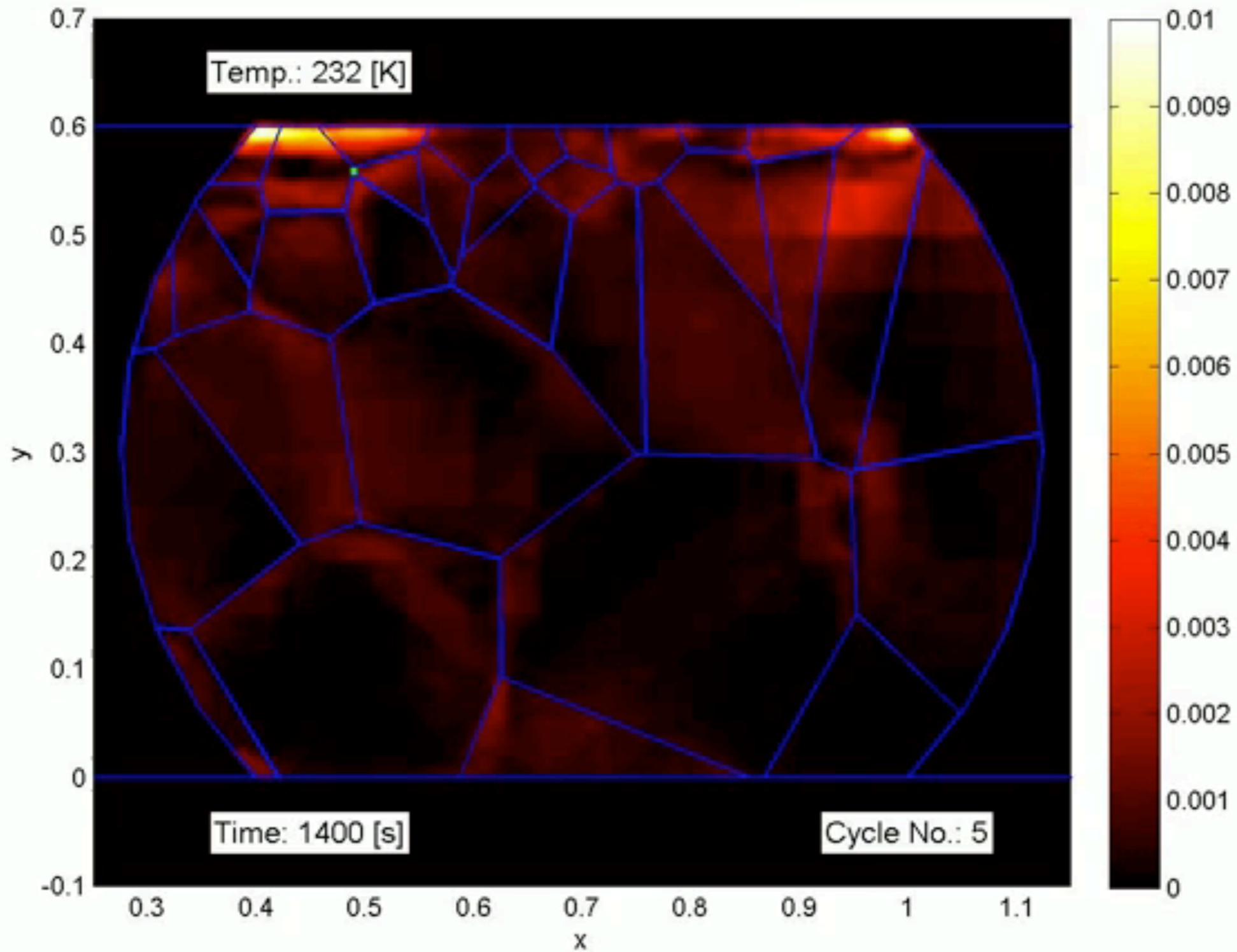






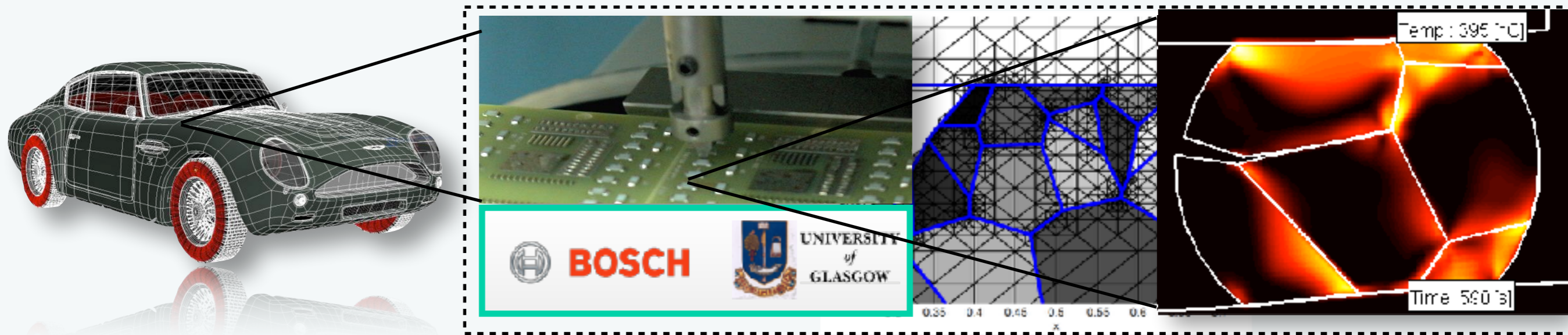








## Solder joint durability (microelectronics), Bosch GmbH



**Question: what is the role of Pb in thermo-mechanical reliability of solder joints?**

A. Menk and SPAB, IJNME 2011, Comp. Mat. Sci. 2012

XFEM Preconditioning and application to polycrystalline fracture

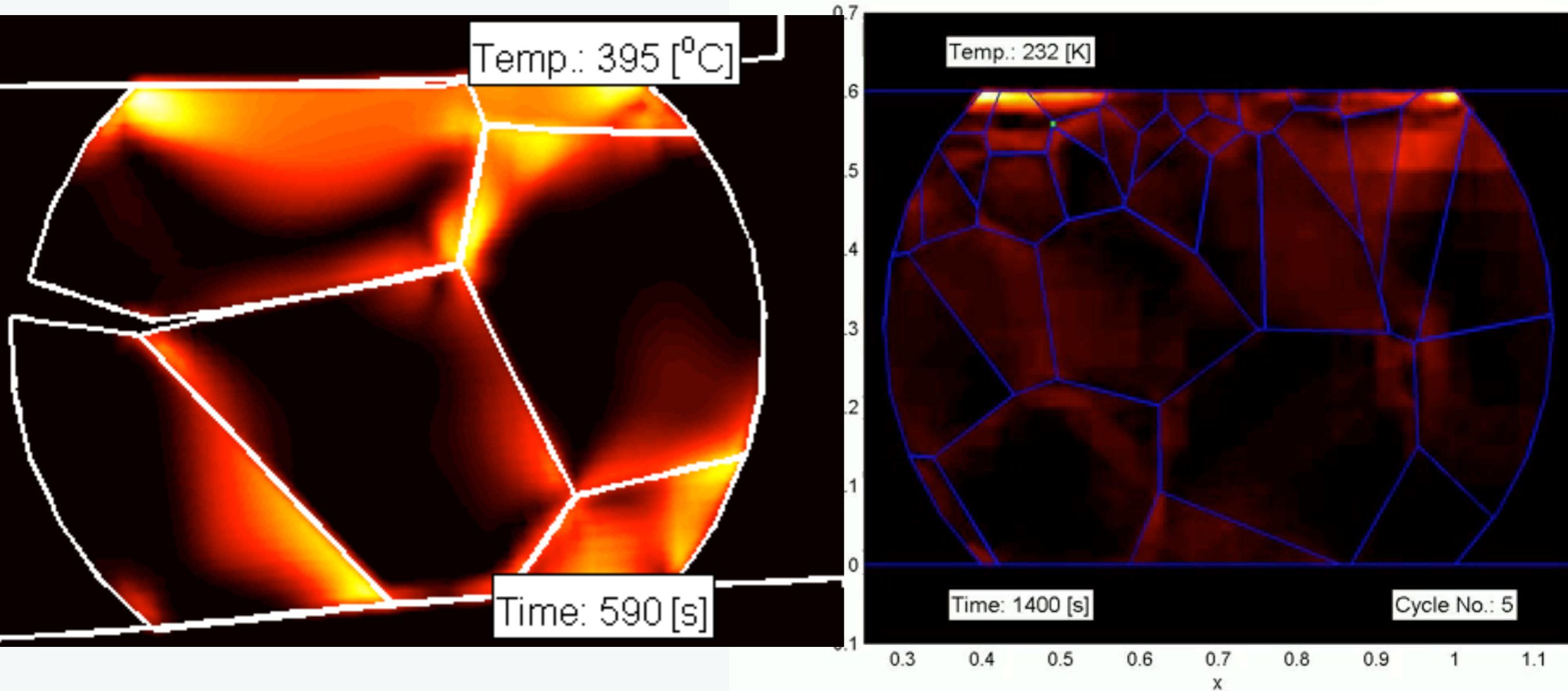
D. A. Paladim et al. Int. J. Numer. Meth. Engng 2017; 110:103–132

P. Kerfriden et al. Int. J. Numer. Meth. Engng 2014; 97:395–422

P. Kerfriden et al. Int. J. Numer. Meth. Engng 2012; 89:154–179

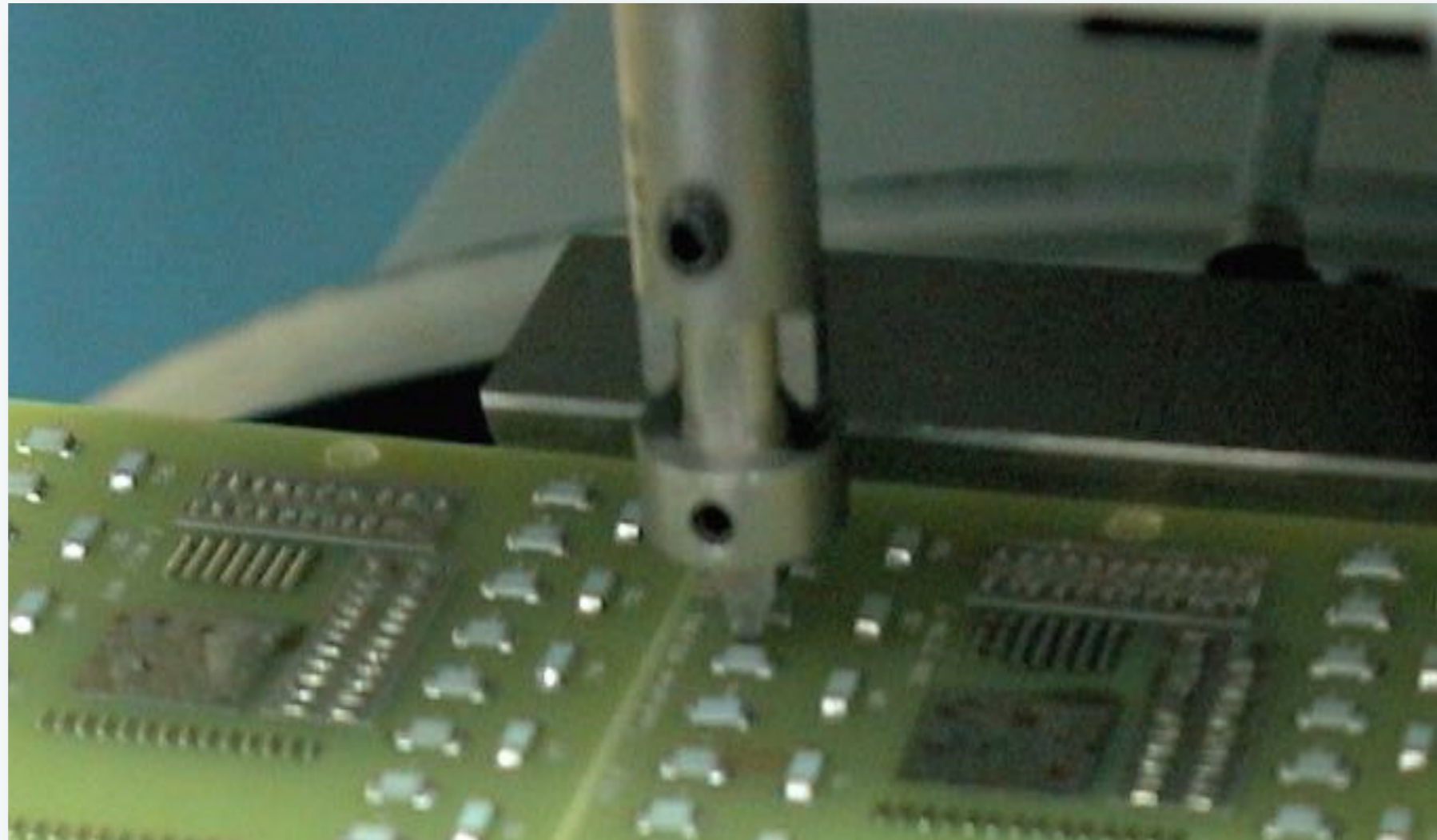
P. Kerfriden et al. Comput. Methods Appl. Mech. Engrg. 200 (2011) 850–866

K. C. Hoang et al. Num Meth PDEs DOI 10.1002/num.21932

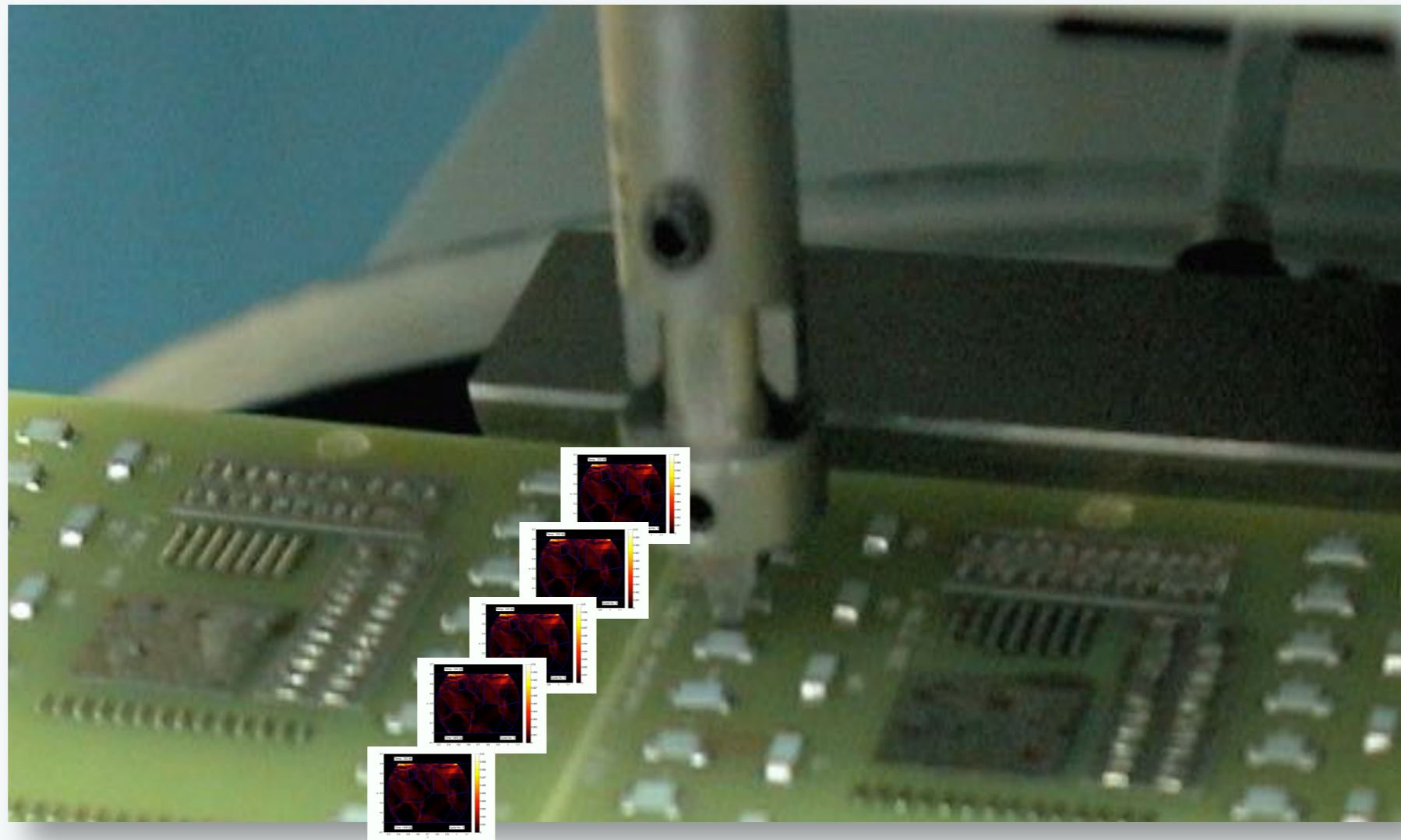


**Microstructure plays a major role in thermomechanical durability in Pb-free solders**

# Microstructures have a critical effect on the durability of structures at the engineering scale

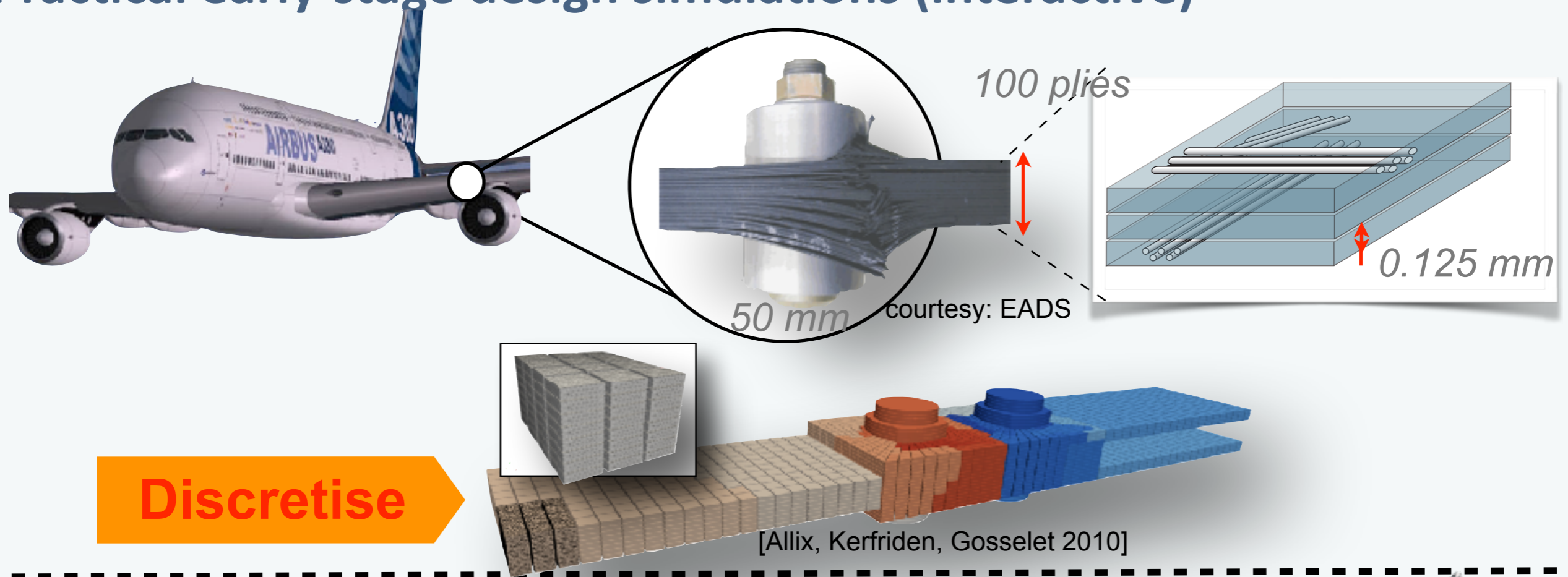


# What can be done to account for microstructures for structures of engineering relevance?

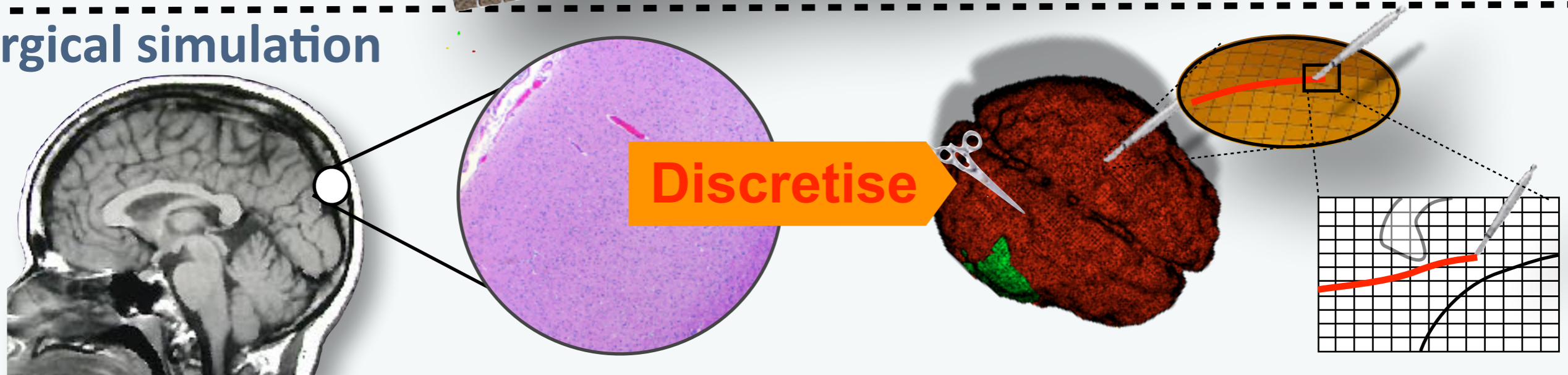


**All is fine as long as the microstructures simulations are localised or few in number**

## Practical early-stage design simulations (interactive)

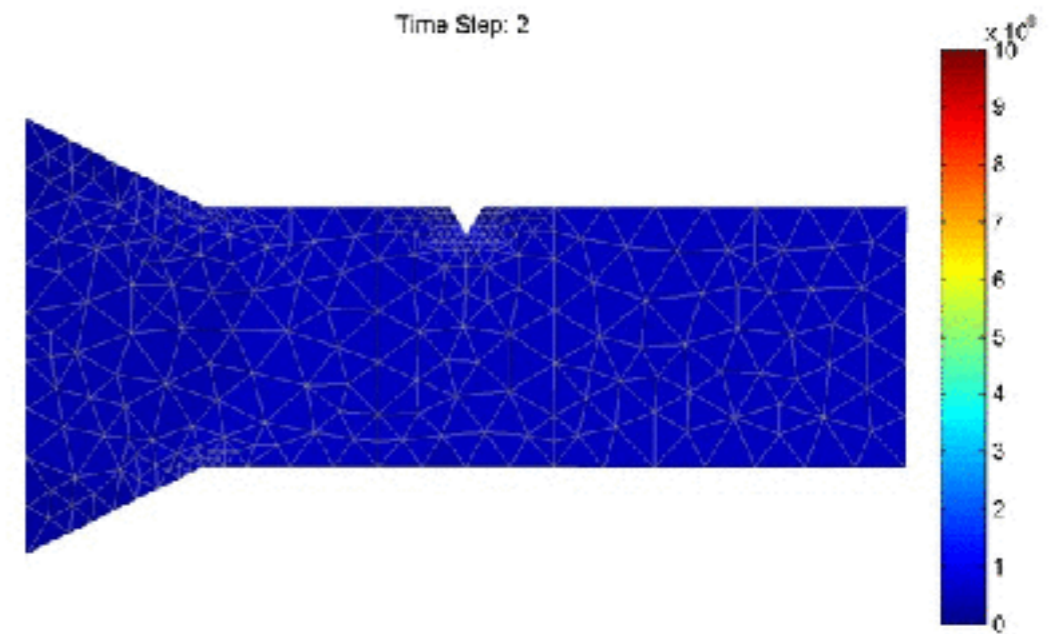
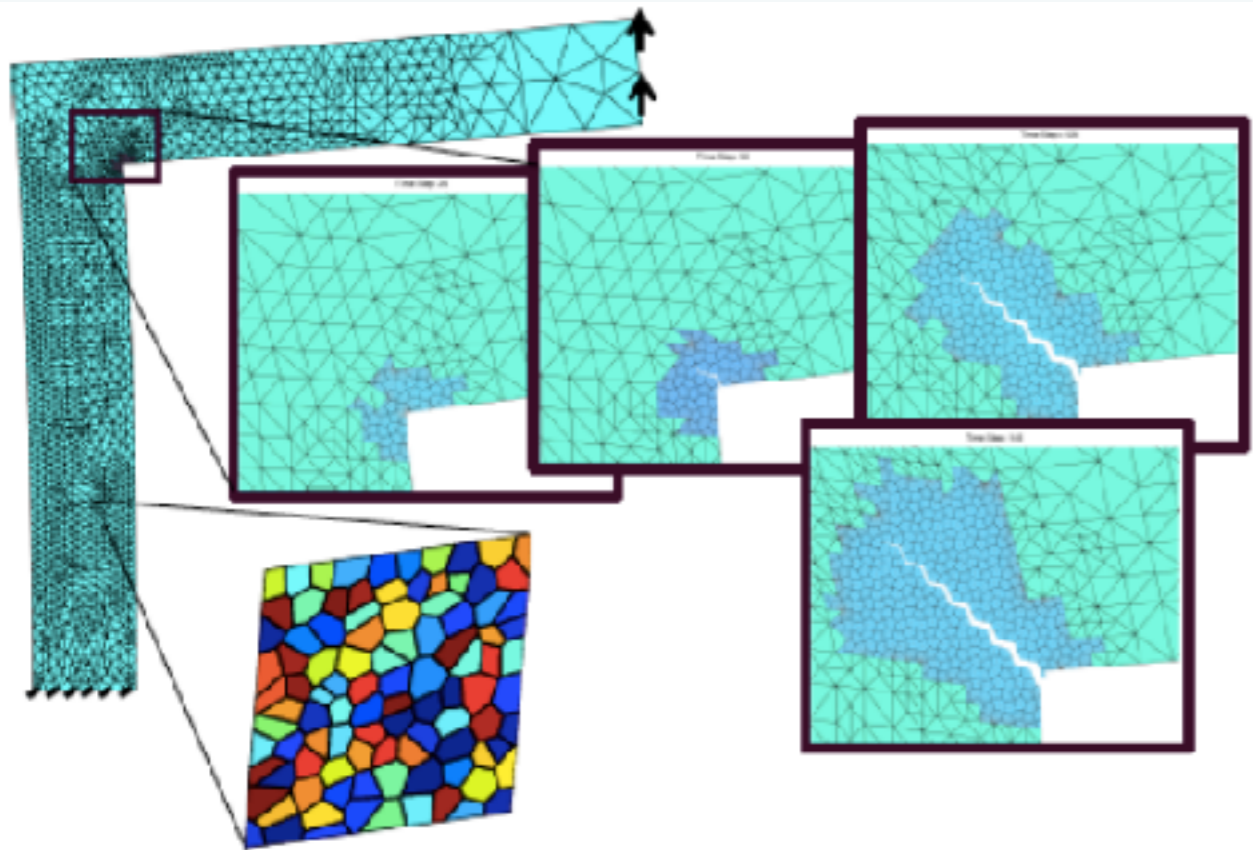


## Surgical simulation



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

# Fracture over the scales, adaptivity model reduction and selection

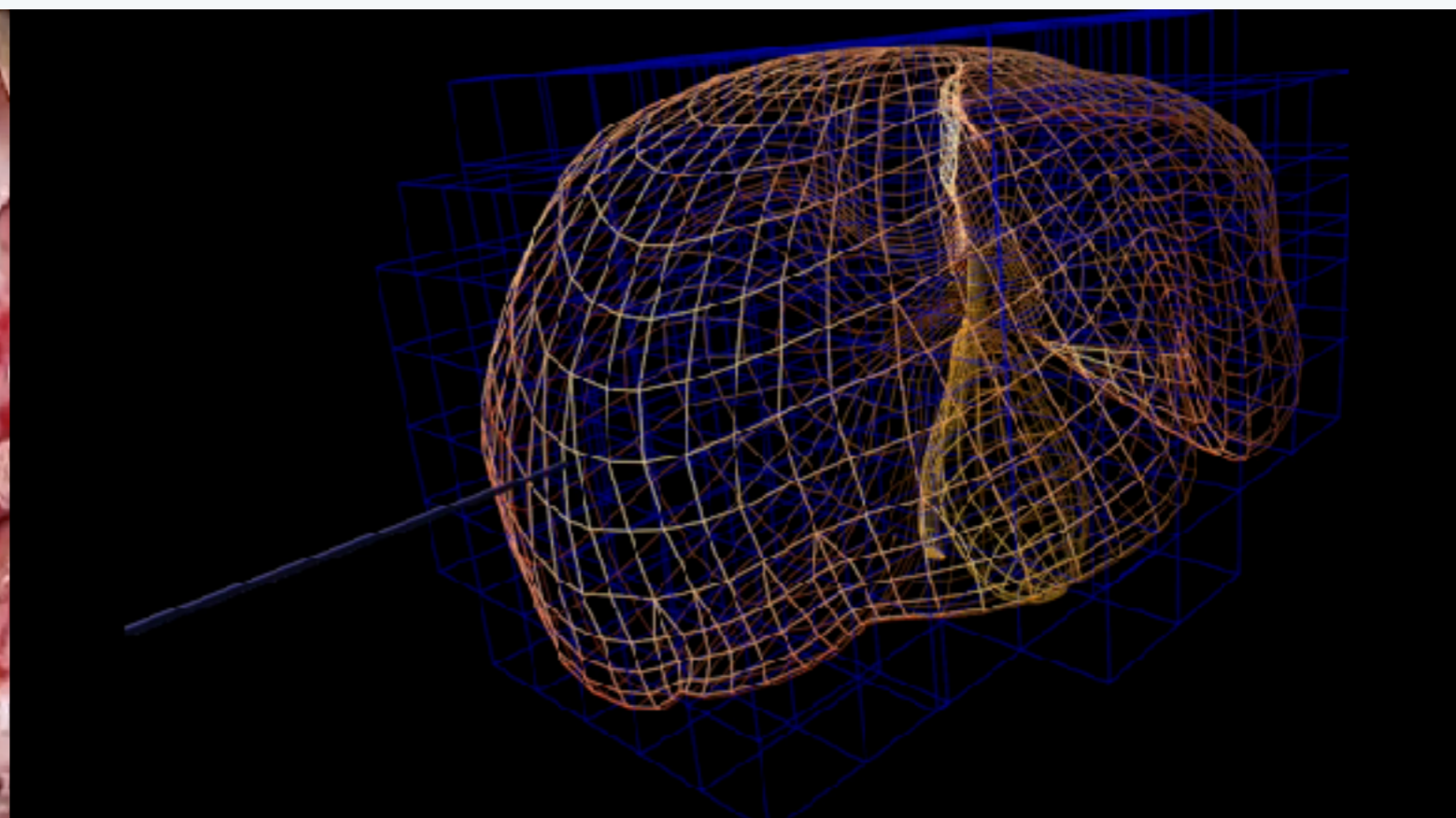
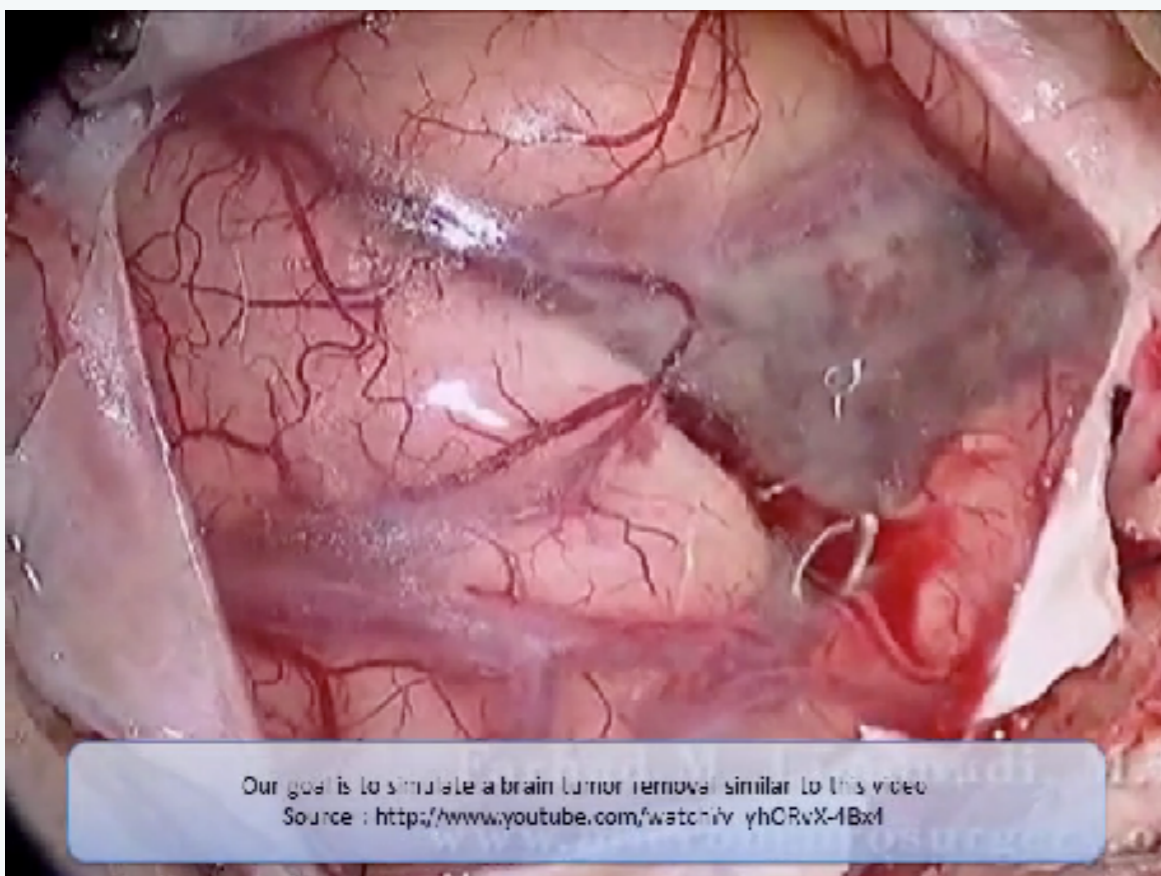


**Question: how can we account for microstructures in a computationally tractable way?**

- O. Goury, P. Kerfriden et al. CMAME, 2016, CMECH (2017) DOI 10.1007/s00466-016-1290-2 - Model reduction for fracture
- C. Hoang et al. Comput. Methods Appl. Mech. Engrg. 298 (2016) 121–158 - Model reduction for elastodynamics
- A. Akbari, P. Kerfriden and SPAB, Philosophical Magazine, (2015) <http://dx.doi.org/10.1080/14786435.2015.1061716>
- P. Kerfriden et al. Comput. Methods Appl. Mech. Engrg. 256 (2013) 169–188 - Model reduction methods for fracture

- Model + mesh adaptivity for adaptive fracture mechanics simulations: expensive + implementation must be done carefully
- Model order reduction, e.g. POD, PGD are ineffective for problems lacking separation of scales (see Kerfriden, Gouy and others)
  - Domain-wise model selection
  - Adaptive model selection
  - Machine learning...

## Cutting and Needle Insertion



H. Courtecuisse et al. Medical Image Analysis, 2014

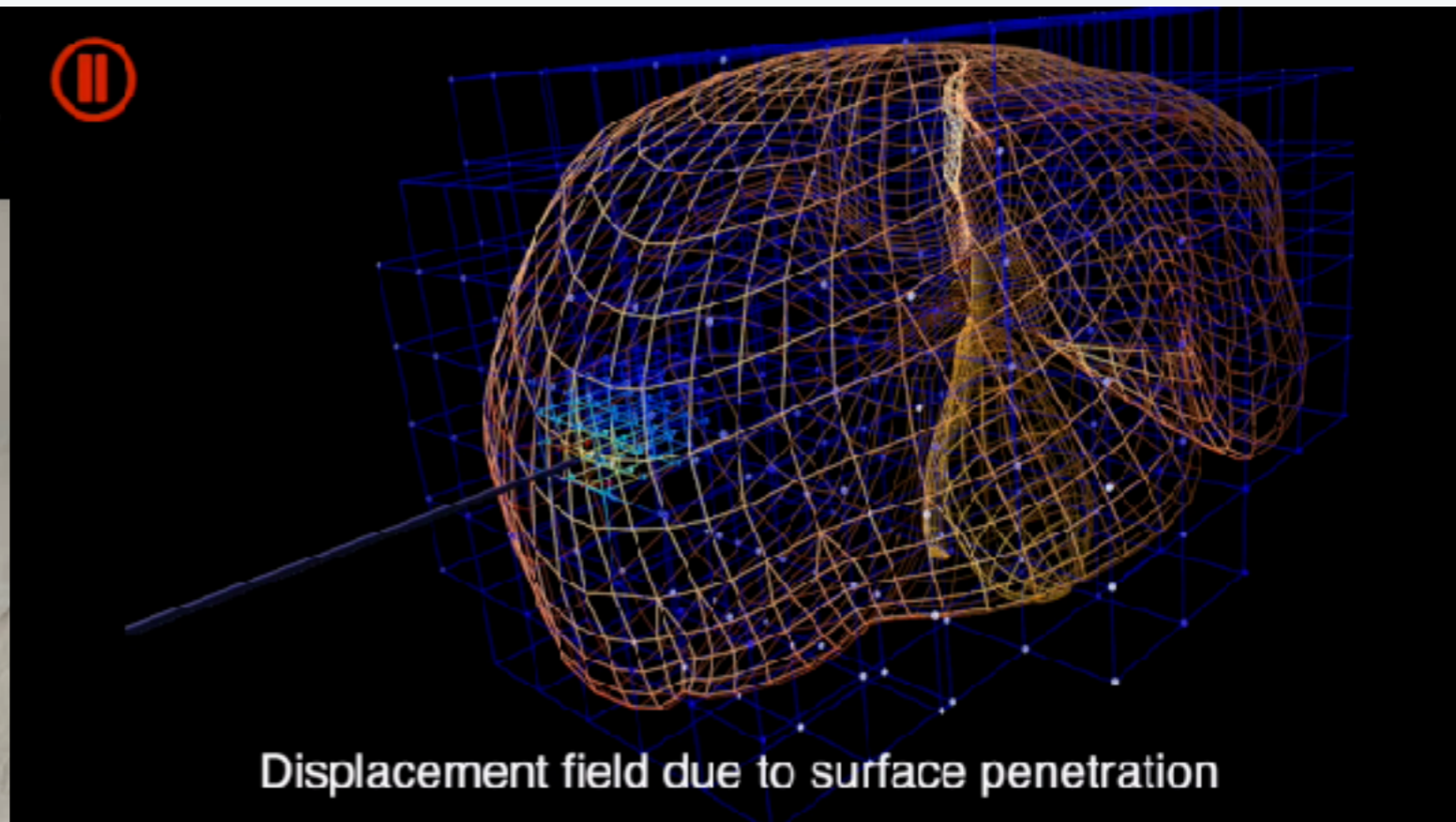
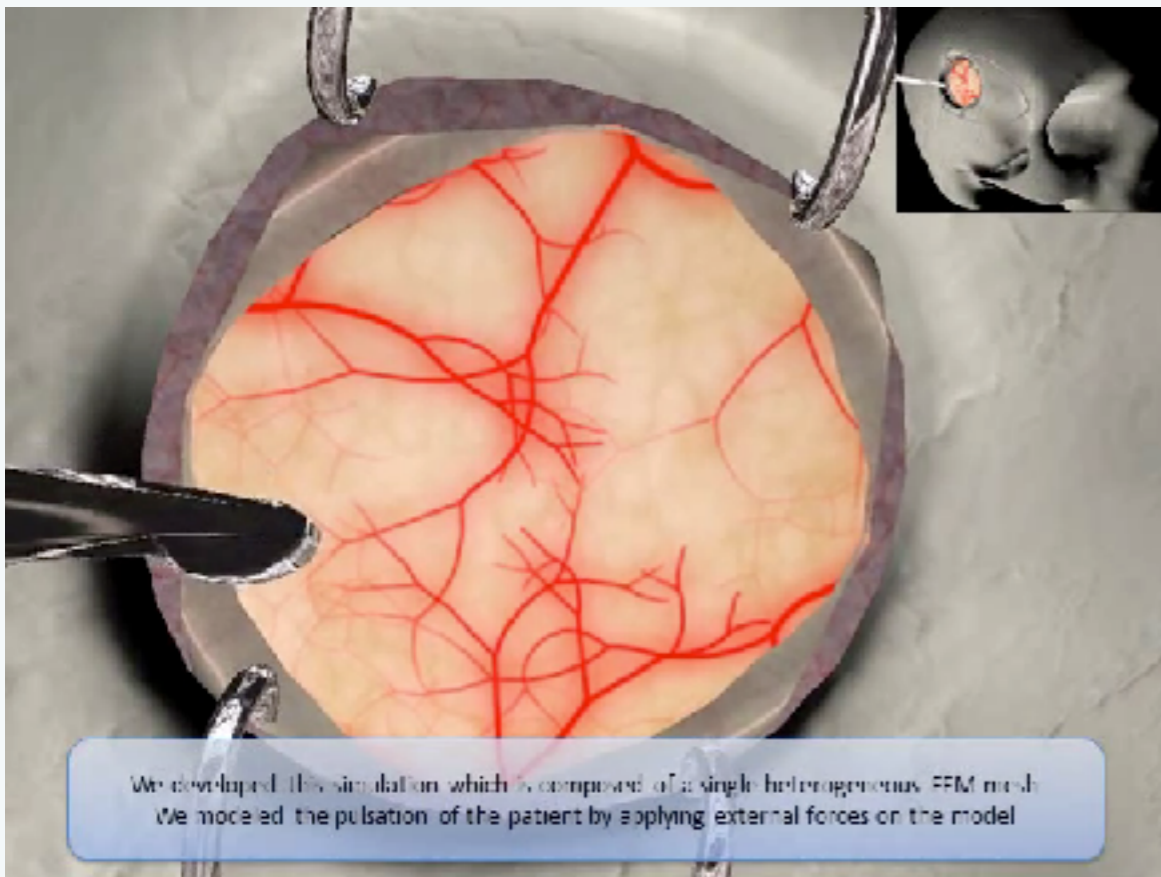
P.H. Bui et al. IEEE T. Biomed Eng. 2017 & Frontiers in Surgery, 2017

<http://orbidu.uni.lu/handle/10993/30937>

<http://orbidu.uni.lu/handle/10993/29846>



## Cutting and Needle Insertion

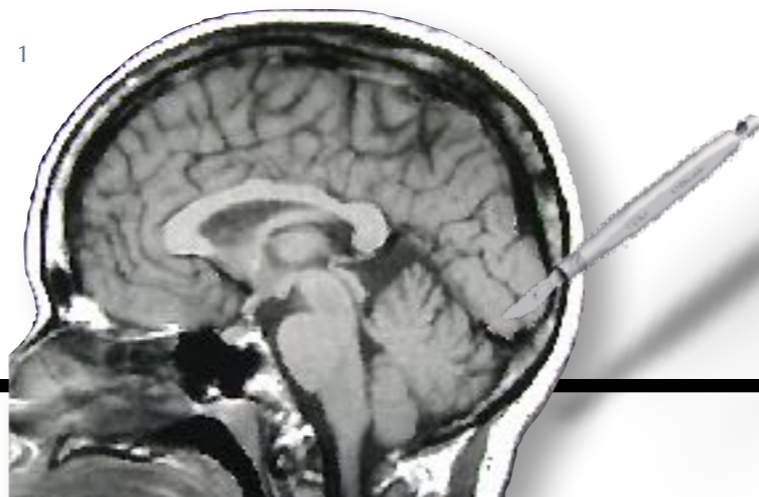


H. Courtecuisse et al. Medical Image Analysis, 2014  
**Question: how can we simulate cutting/fracture in real time using implicit time stepping?**

P.H. Bui et al. IEEE T. Biomed Eng. 2017 & Frontiers in Surgery, 2017  
**Question: how can we adapt the mesh in real time using a posteriori error estimates?**

<http://orbilu.uni.lu/handle/10993/30937> <http://orbilu.uni.lu/handle/10993/29846>

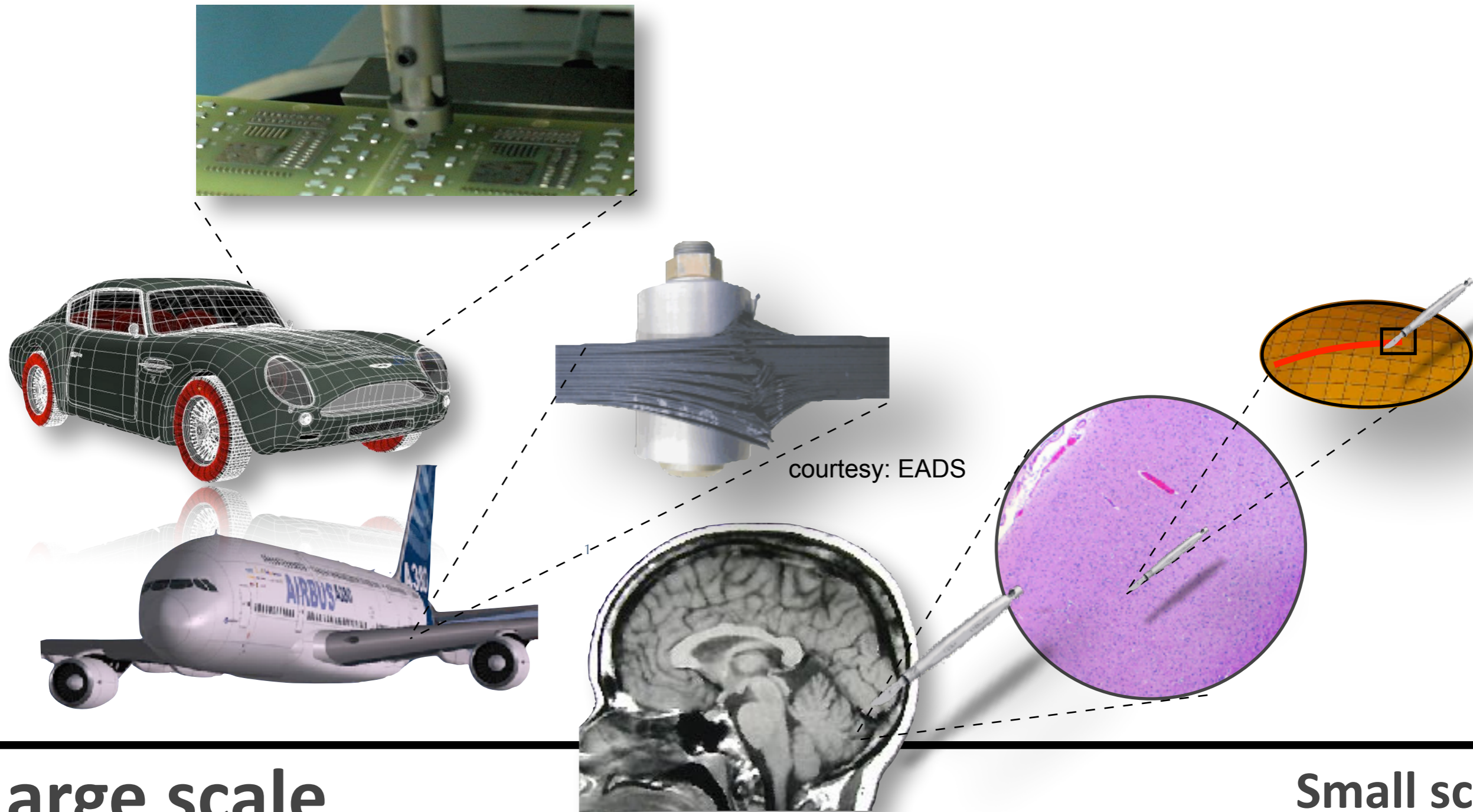
# Discontinuities



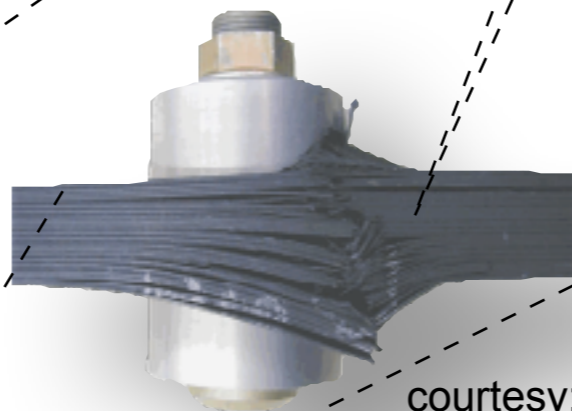
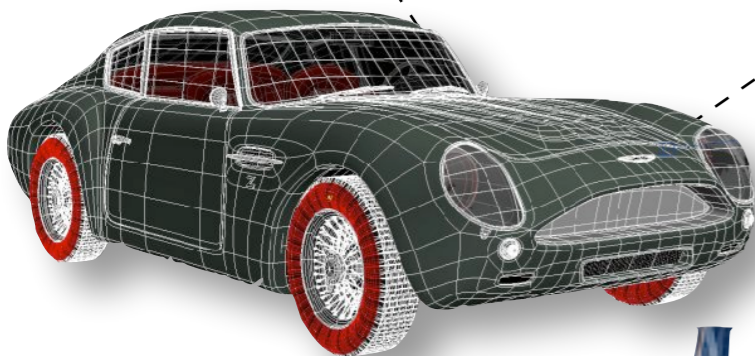
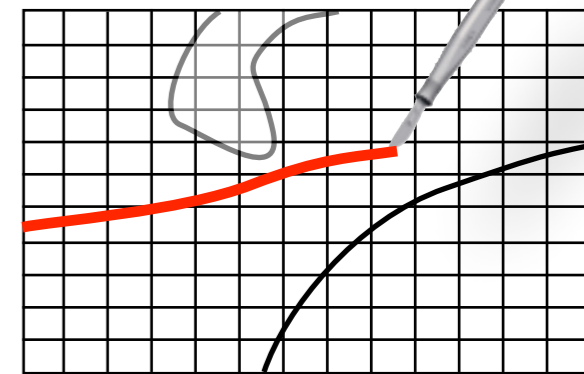
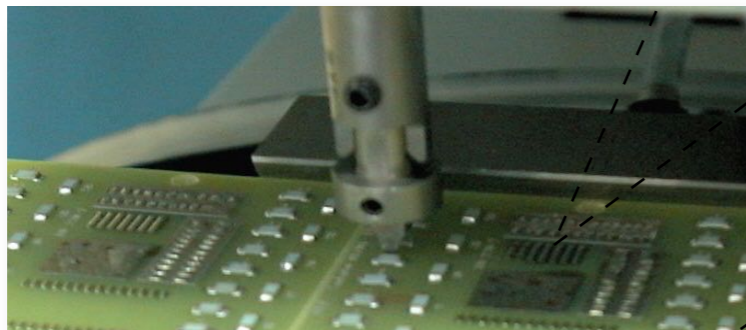
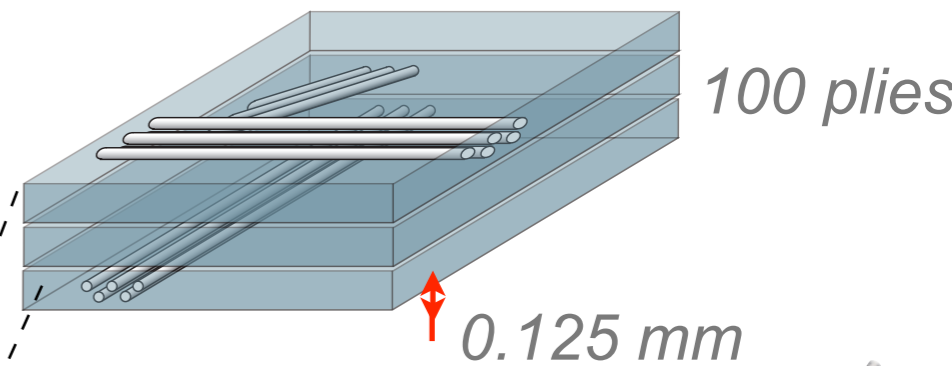
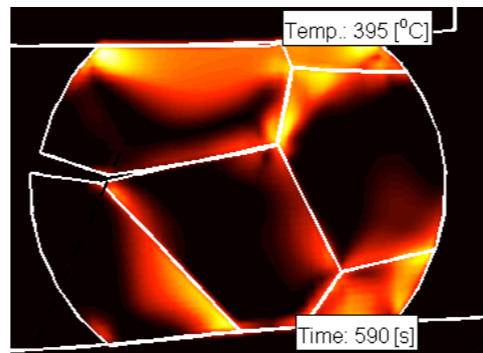
Large scale

Small scale

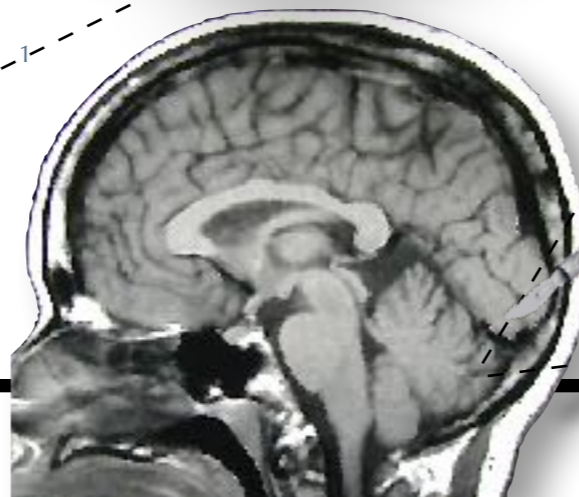
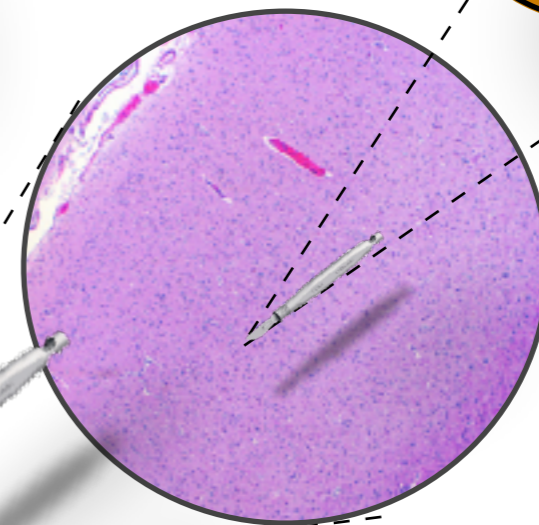
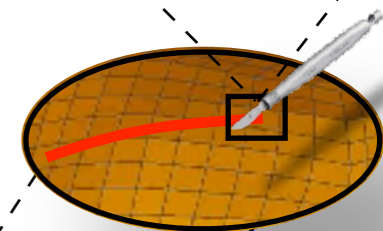
# Discontinuities



# Discontinuities



courtesy: EADS



Large scale

Small scale

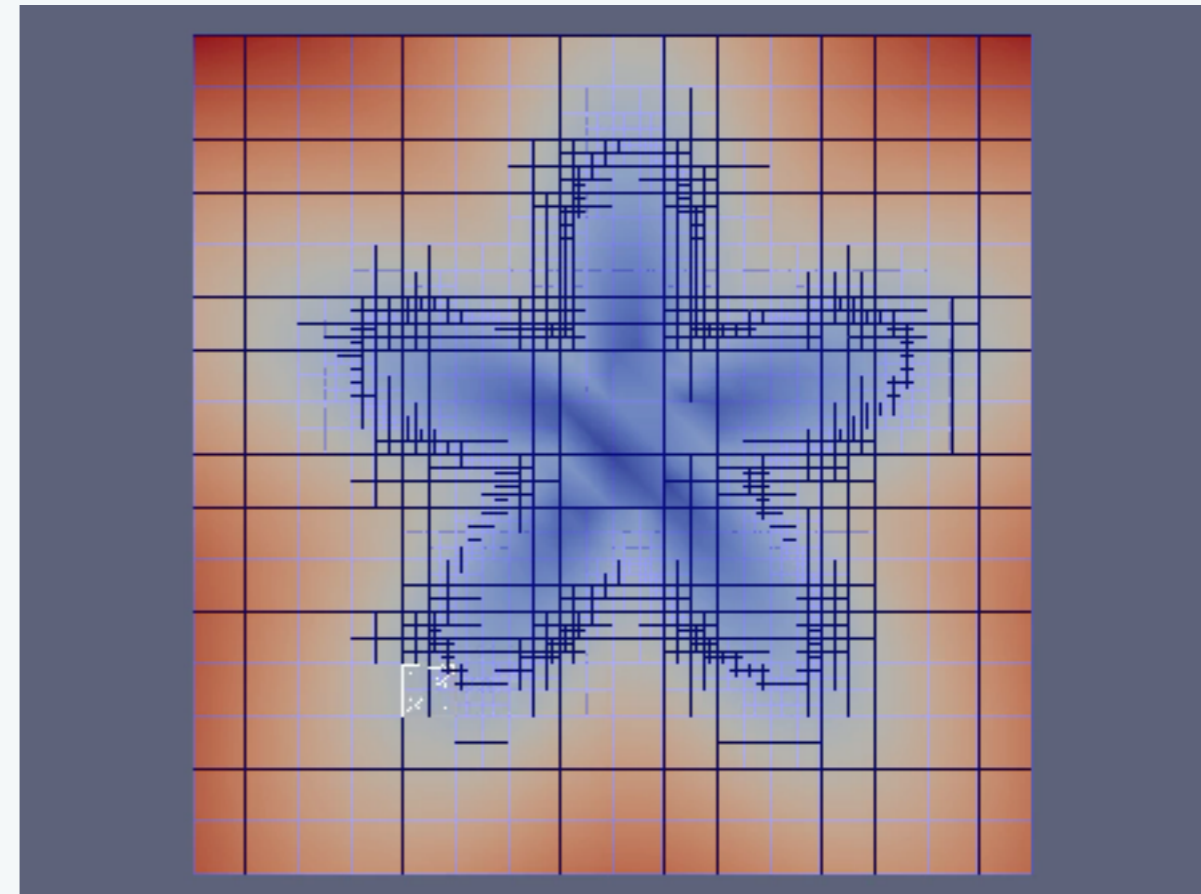
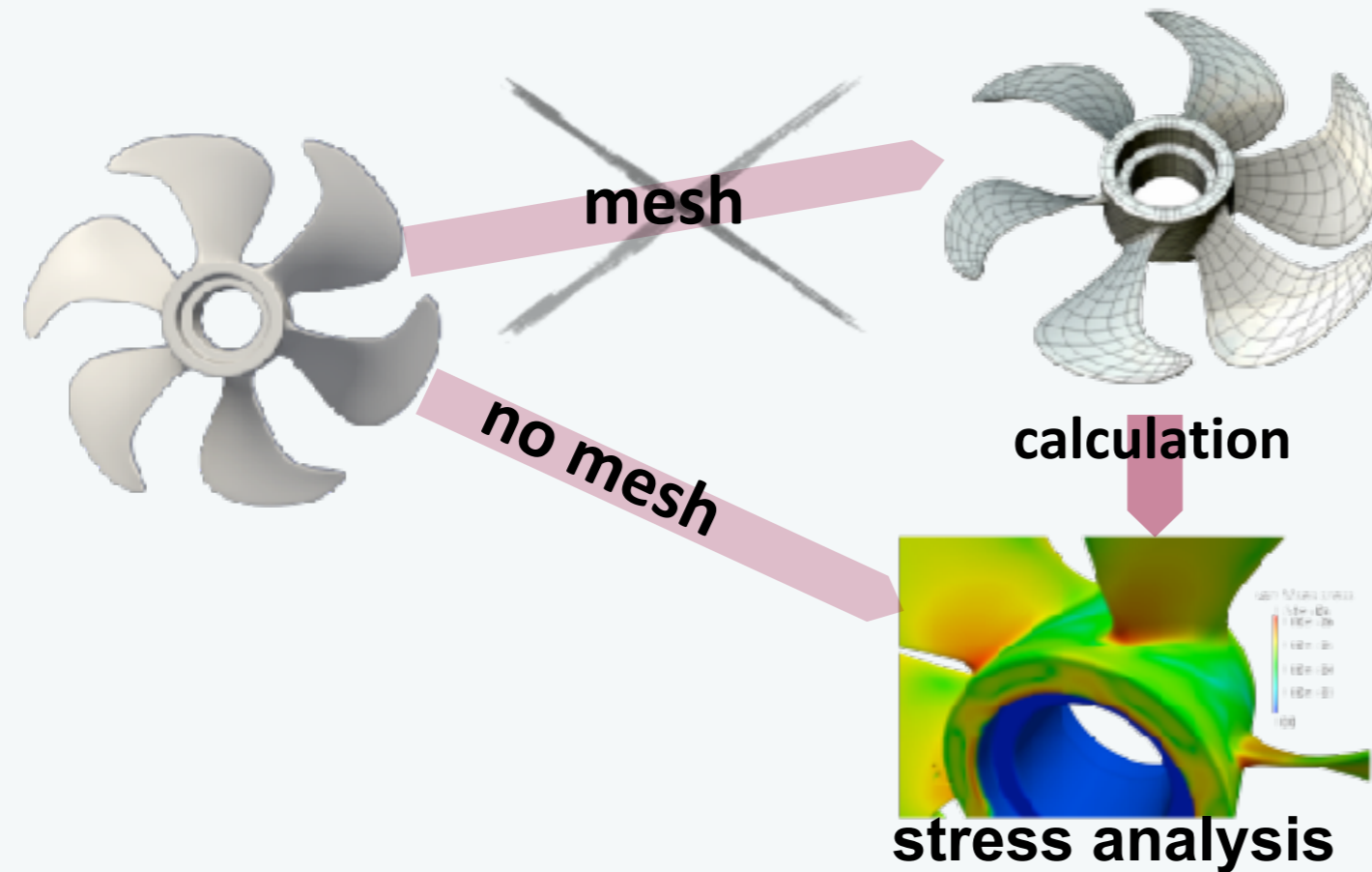
## Partial conclusions

- Zooming into materials/structures reveals discontinuities with complex shapes
- Geometries of domains are complex, even at the continuum level

**Next: a few methods to deal with this complexity**

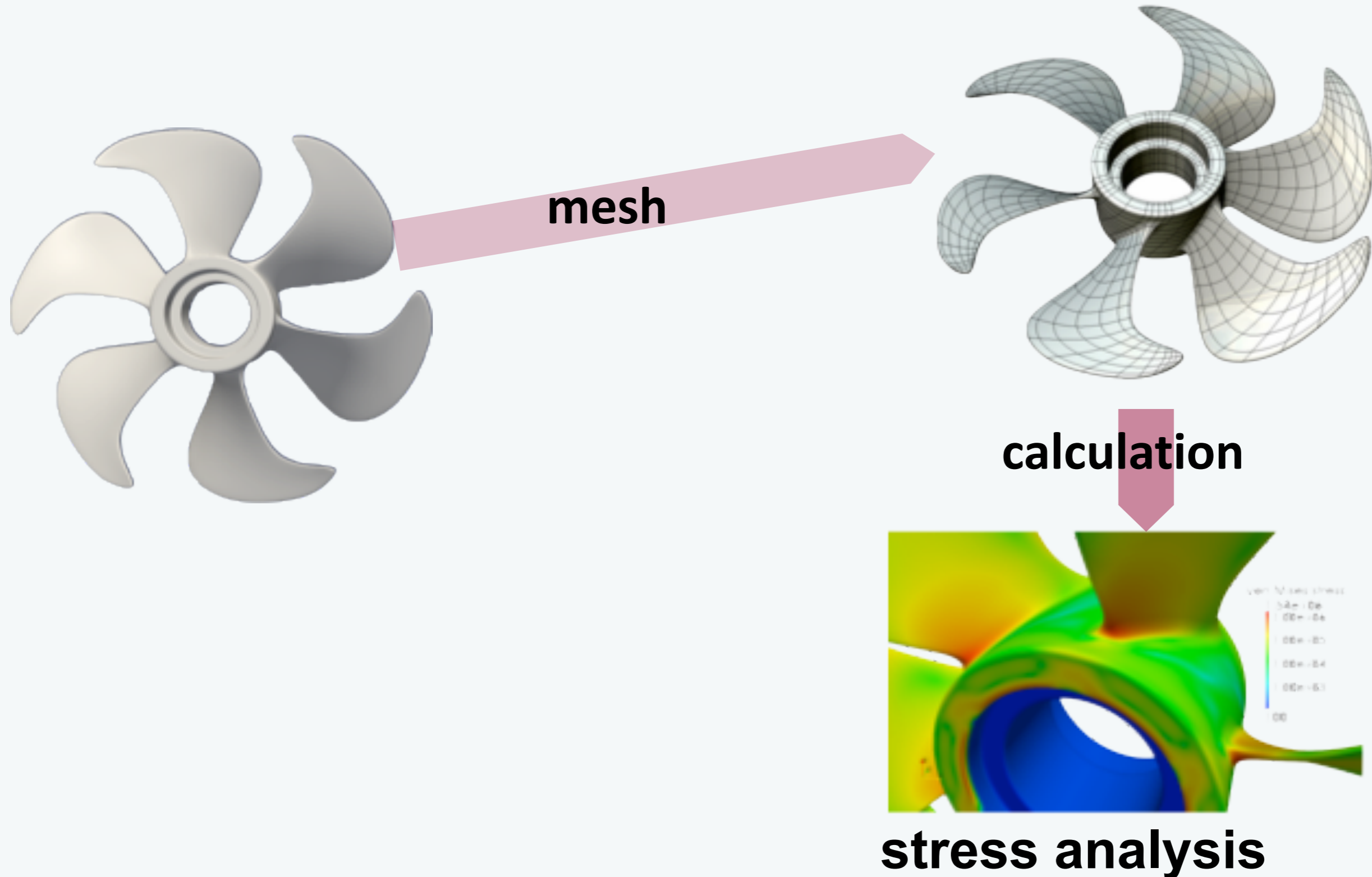
# Handling (complex) interfaces numerically

*Coupling, or decoupling?*

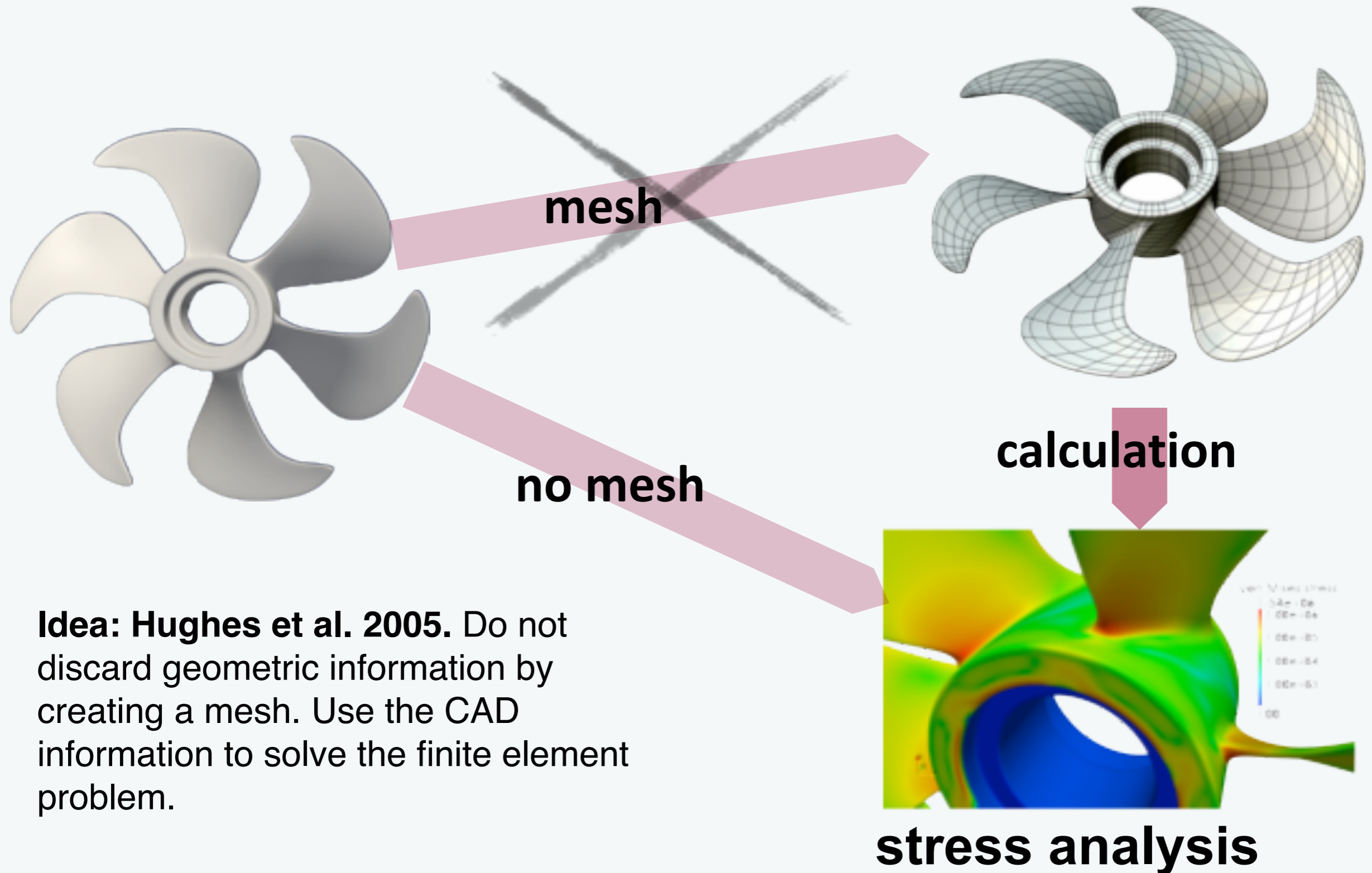


**Question: When are we better off coupling/decoupling the geometry from the field approximation?**

# Isogeometric analysis

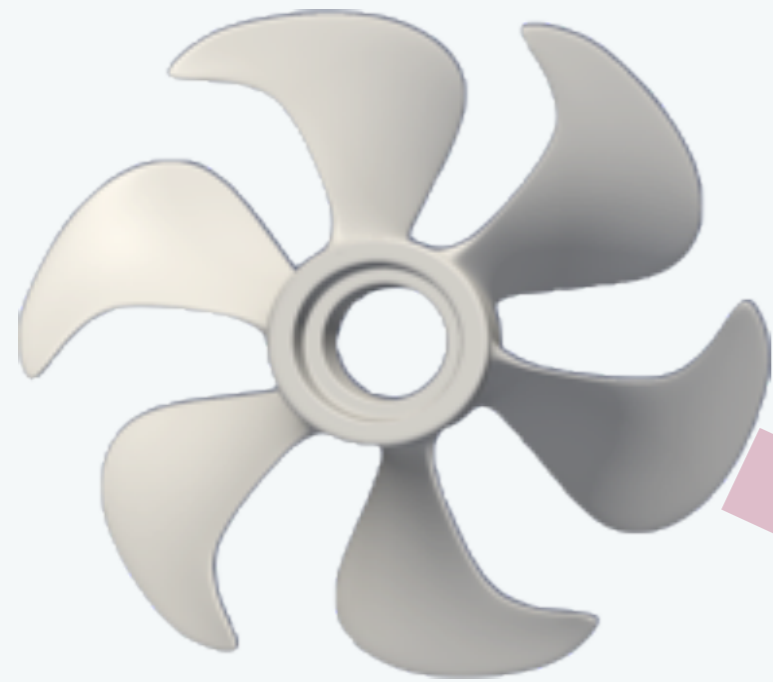


# Isogeometric analysis



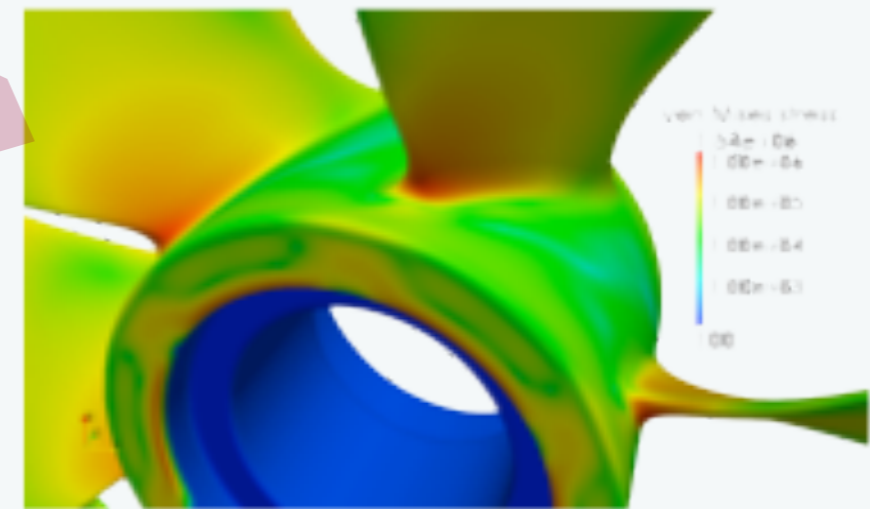
**Idea: Hughes et al. 2005.** Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.





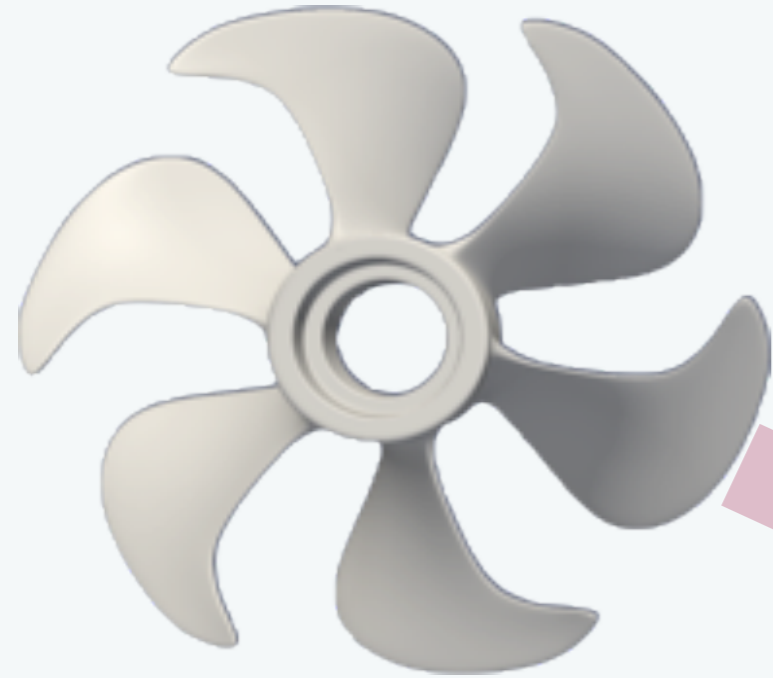
**direct calculation**

**Idea: Hughes et al. 2005.** Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.



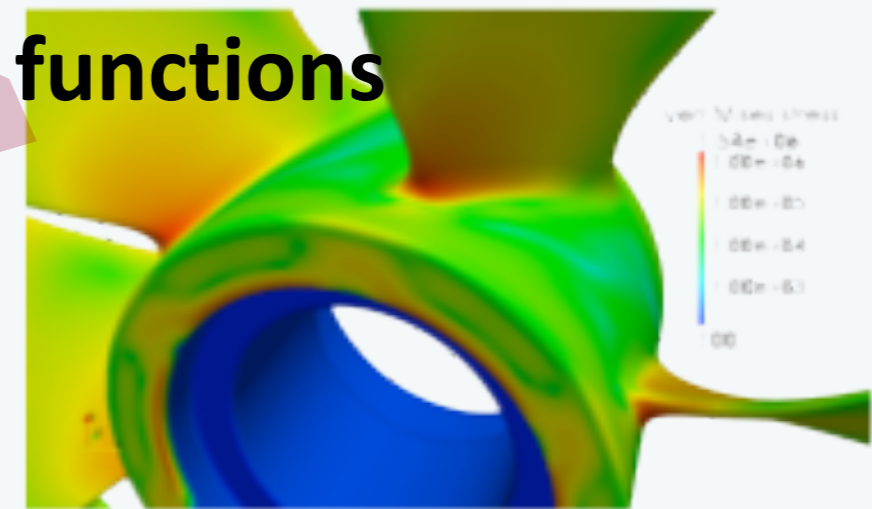
**stress analysis**

## CAD: described by NURBS



**Idea: Hughes et al. 2005.** Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.

**Use NURBS as FE basis functions**



**stress analysis**

## Geometry

- For shell-like domains
- For volumes (needs volume parameterisation)
- Coupling between multiple patches (Nitsche, Mortar...)

## Adaptivity

- Global refinement - cannot refine field without refining geo...
- Local refinement (not with NURBS)... (PH)T-splines...
- Geometry independent refinement for the field variables?

# Handling (complex) interfaces numerically

## *Coupling geo and field: Isogeometric Analysis*

### Question:

***What is the performance of Isogeometric Analysis in Reducing the Mesh Burden?***

## Isogeometric Finite Element Analysis

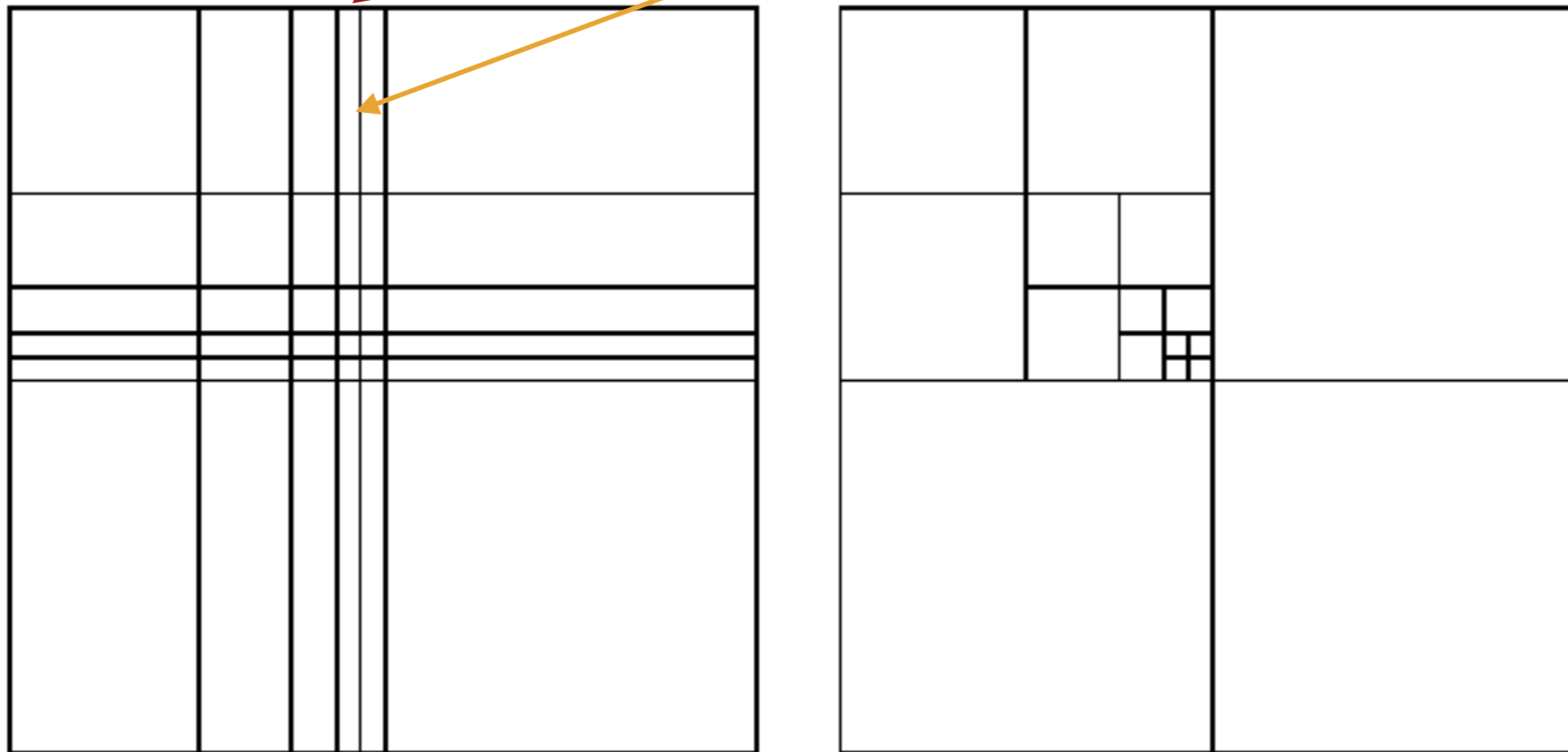
- For shell-like domains
- For volumes (needs volume parameterisation)
- Coupling between multiple patches (Nitsche, Mortar...)

## Adaptivity

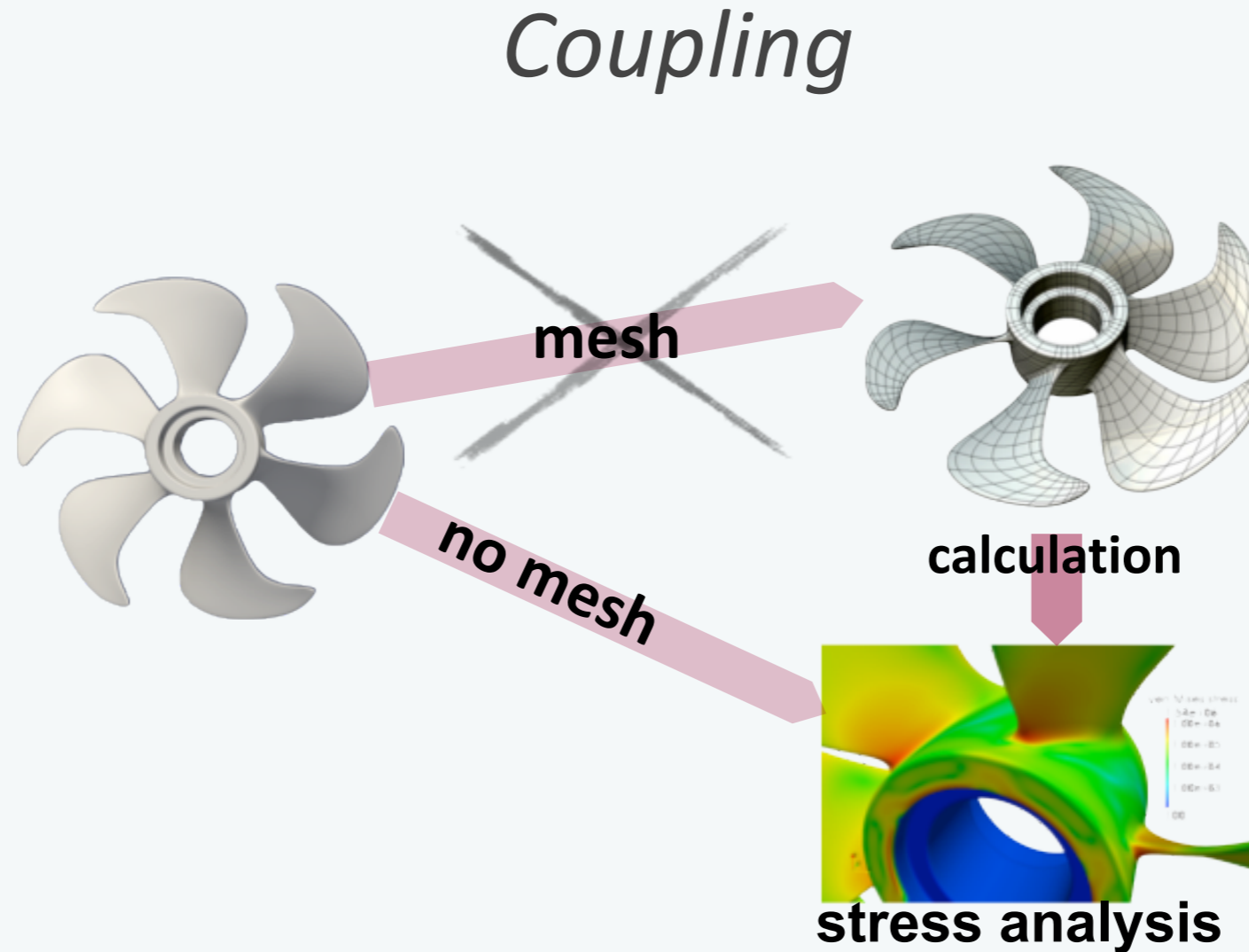
- Global refinement - cannot refine field without refining geo...
- Local refinement (not with NURBS)... (PH)T-splines...
- Geometry independent refinement for the field variables?

Using NURBS,

**Refinement in one direction** forces refinement in the other



Global refinement (tensor-product mesh) vs local refinement (T-mesh)



**Question: How can we fully benefit from the “IGA” concept?**

- Refine the field independently from the geometry
- Suppress the mesh generation and regeneration completely

# Handling (complex) interfaces numerically

## *Coupling geometry and field approximation*

**Question: How can we fully benefit from the “IGA” concept?**

Refine the field independently from the geometry

### Isogeometric Finite Elements

For shell-like domains

For volumes (needs volume parameterisation)

### Geometry Independent Field approximation (GIFT)

Super/Sub-geometric

[REF] Weakening the tight coupling between geometry and simulation in isogeometric analysis: from sub- and super-geometric analysis to Geometry Independent Field approximation (GIFT), IJNME, 2017, submitted [preprint available on arXiv]

**Permalink:** <http://hdl.handle.net/10993/31469>

# Handling (complex) interfaces numerically

## *Coupling geometry and field approximation*

**Question: How can we fully benefit from the “IGA” concept?**

Refine the field independently from the geometry

[REF] Weakening the tight coupling between geometry and simulation in isogeometric analysis: from sub- and super-geometric analysis to Geometry Independent Field approximation (GIFT), IJNME, 2017, submitted [preprint available on arXiv]

**Permalink:** <http://hdl.handle.net/10993/31469>



Together with the given (exact) geometry parametrization at the coarsest level, the convergence rate is entirely defined by the solution basis, and does not depend on the further refinement of the geometry parametrization:

- For a given geometry parameterization, the degree of the solution basis can be increased or decreased without changing the degree of the geometry (from iso-geometric to super-geometric and sub-geometric elements)
- For solution approximation, using same degree B-Splines or NURBS yields almost identical results

# Geometry Independent Field approximation (GIFT)

## *Conclusions*

- ☑ Tight link between CAD and analysis
- ☑ The same basis functions, which are used in CAD to represent the geometry, are used in the IGA as shape functions to approximate the unknown solution
- ☑ Geometry is exact at any stage of the solution refinement process
- ☑ Better accuracy per DOF in comparison with standard FEM but higher computational cost (bandwidth...)

# Geometry Independent Field approximation (GIFT) Conclusions

- ✓ Retain the advantages of IGA but decouple the geometry and the field approximation
- ✓ Standard patch tests may not always pass, yet the convergence rates are optimal as long as the geometry is exactly represented by the geometry basis
- ✓ With geometry exactly represented by NURBS, using same degree B-splines or NURBS for the approximation of the solution field yields almost identical results
- ✓ With geometry exactly represented by NURBS, using PHT splines for the approximation of the solution gives additional advantage of local adaptive refinement
- ✓ Any other approximation field can be used for the field variables

## *Coupling*

**Question: How can we fully benefit from the “IGA” concept?**

Suppress the mesh generation and regeneration completely

## Isogeometric Finite Elements

- For shell-like domains
- For volumes (needs volume parameterisation)

## Isogeometric Boundary Element Analysis

- For shell-like domains
- For volumes

### **Stress analysis and shape optimisation directly from CAD**

H. Lian et al. (2017). *CMAME*: 317 (2017): 1-41.

H. Lian et al. (2015). *IJNME*

H. Lian et al. (2013). *EACM*:166(2):88-99.

M. Scott et al. (2013) *CMAME* 254: 197-221.

R. N. Simpson et al. (2013) *CAS* 118: 2-12.

R. N. Simpson et al. (2012) *CMAME* Feb 1;209:87-100.

### **Fracture mechanics directly from CAD**

X. Peng, et al. (2017). *IJF*, 204(1), 55–78.

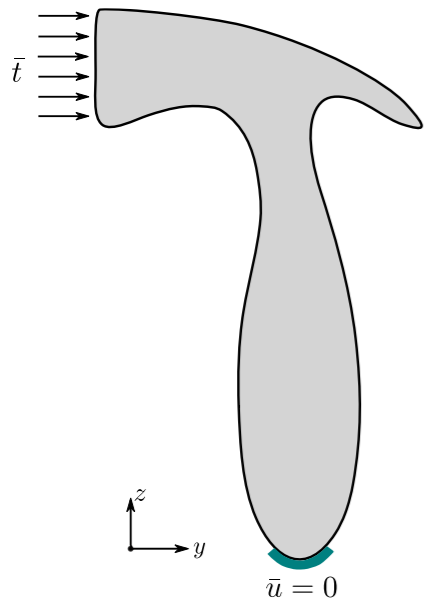
X. Peng, et al. (2017). *CMAME*, 316, 151–185.

# Handling (complex) interfaces numerically

*Example applications*

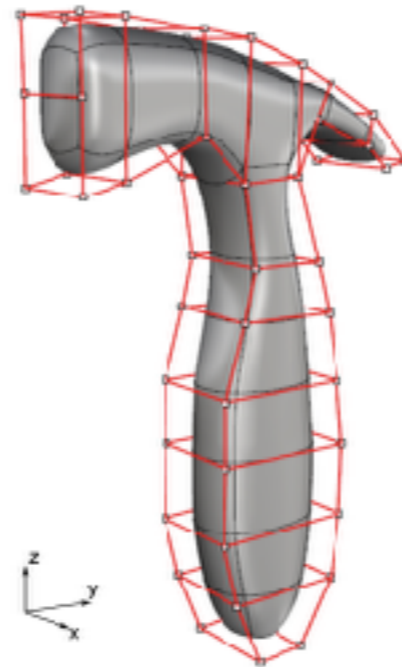
*Isogeometric Boundary Element Analysis  
(IGABEM)*

# Shape optimisation



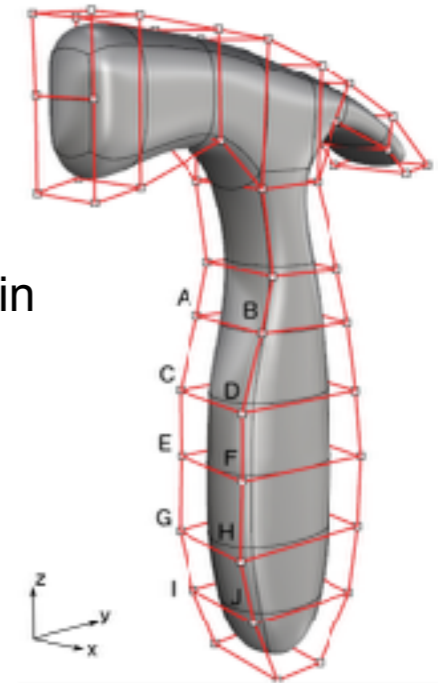
Problem definition

Model construction with CAD



Control points

Design points selection in control points



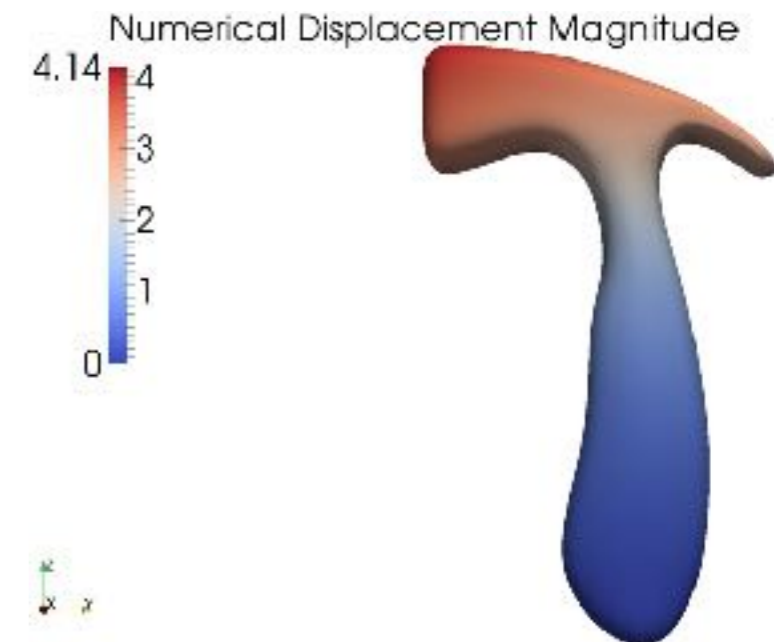
Design points

Objective function:  $\int_S t_i u_i dS$

Volume constraint:  $V - V_0 \leq 1$

Side constraints:

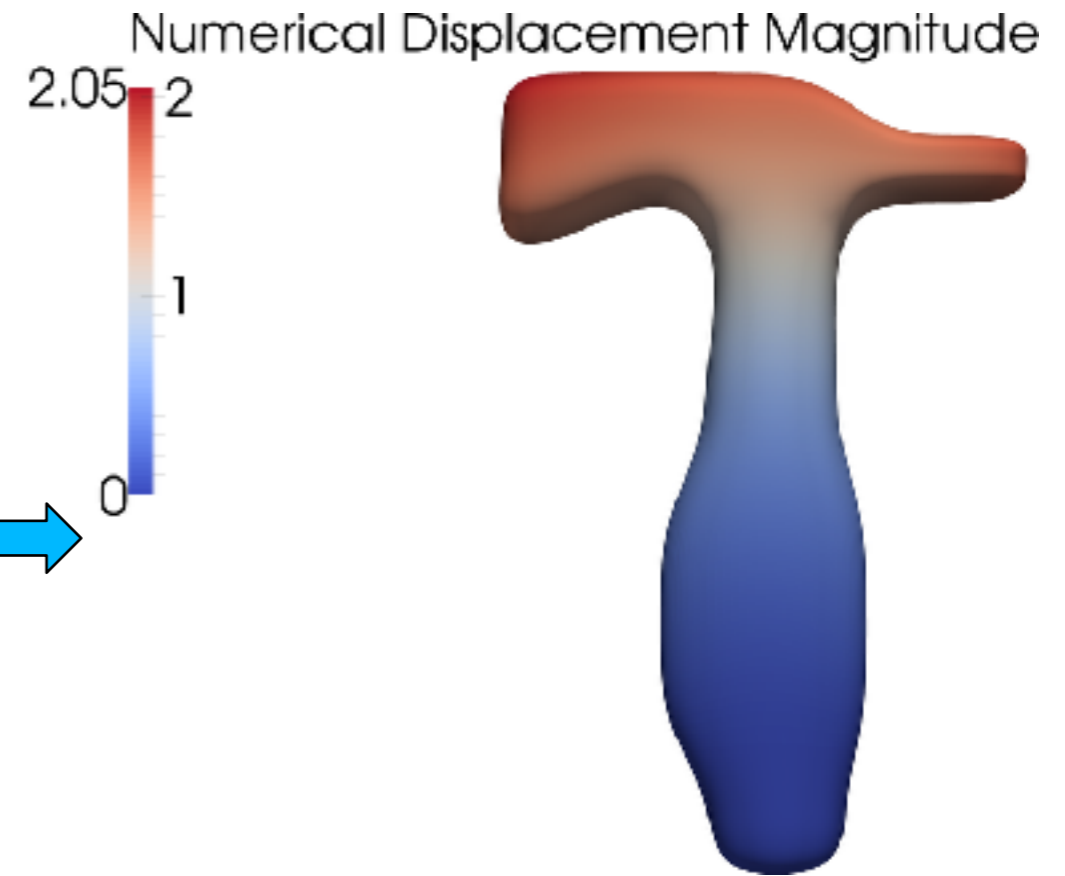
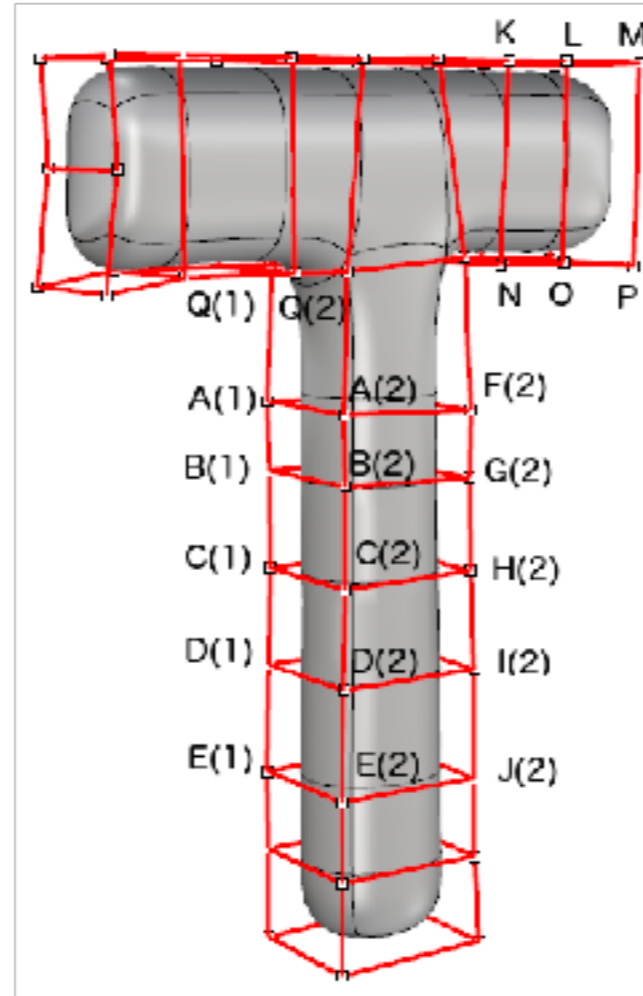
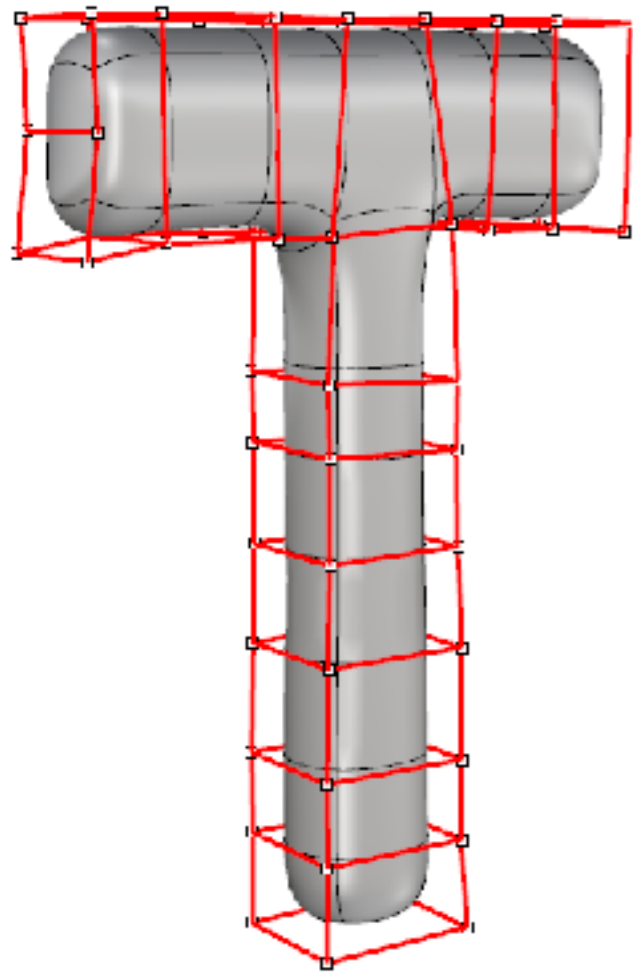
Structural analysis;  
Sensitivity analysis;  
gradient-based optimizer



Optimized solution

Design variable	Lower bound	Upper bound	Initial value
$t_1$	0	4	2.45
$t_2$	0	4	1.25
$t_3$	0	4	1.33
$t_4$	0	4	1.28
$t_5$	0	4	2.30

# Shape optimisation



Construct the geometric model

Choose design points from the control points

Conduct sensitivity analysis to converge to the optimized solution

## Stress analysis and shape optimisation directly from CAD

H. Lian et al. (2017). CMAME: 317 (2017): 1-41.

H. Lian et al. (2015). IJNME

H. Lian et al. (2013). EACM:166(2):88-99.

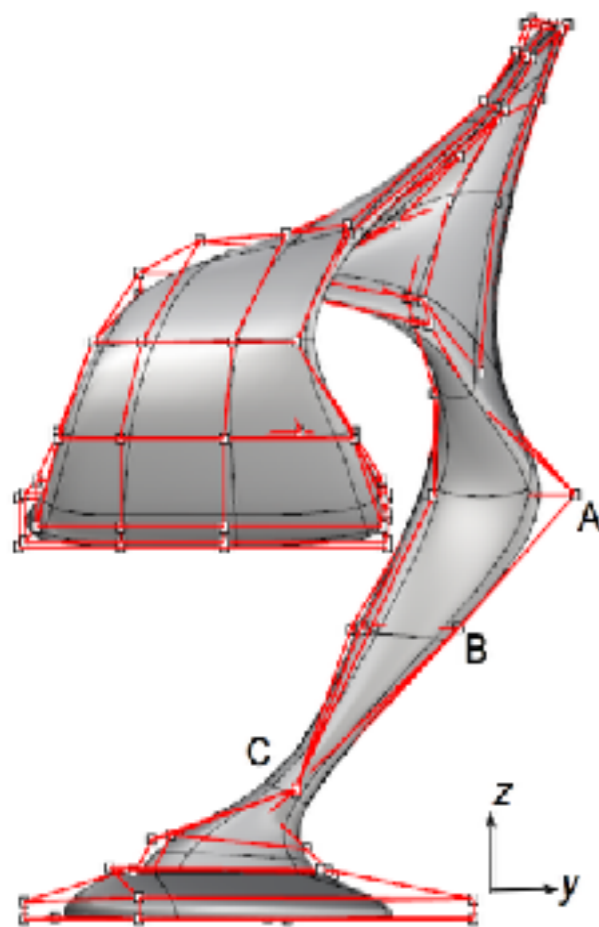
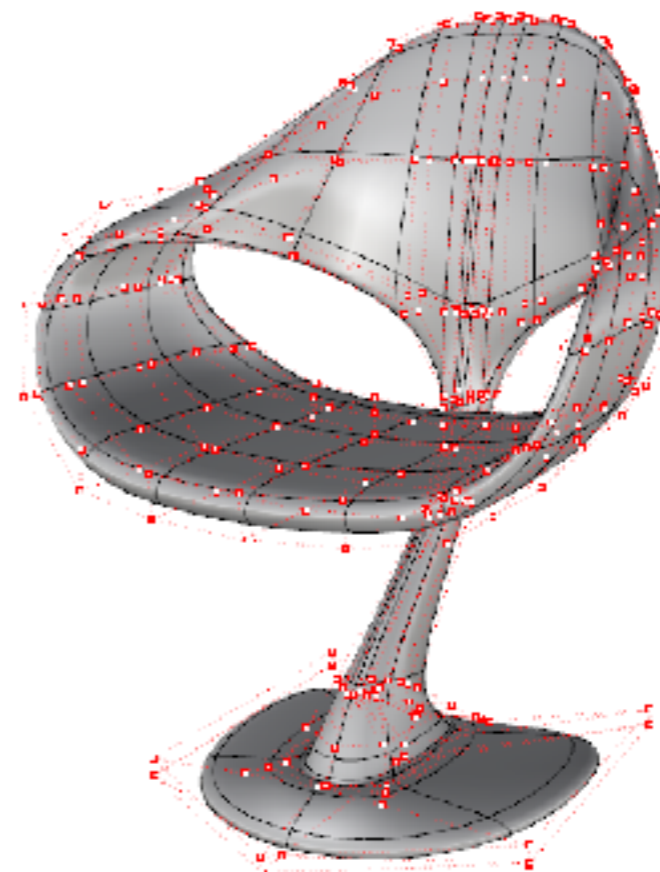
M. Scott et al. (2013) CMAME 254: 197-221.

R. N. Simpson et al. (2013) CAS 118: 2-12.

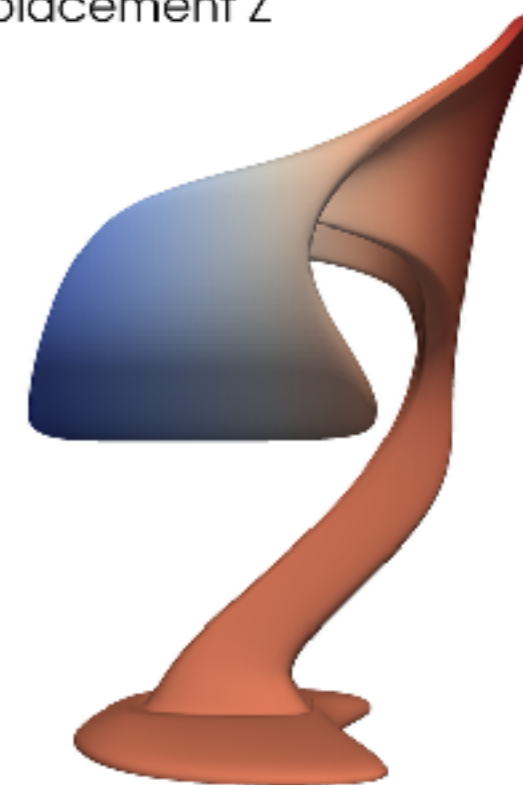
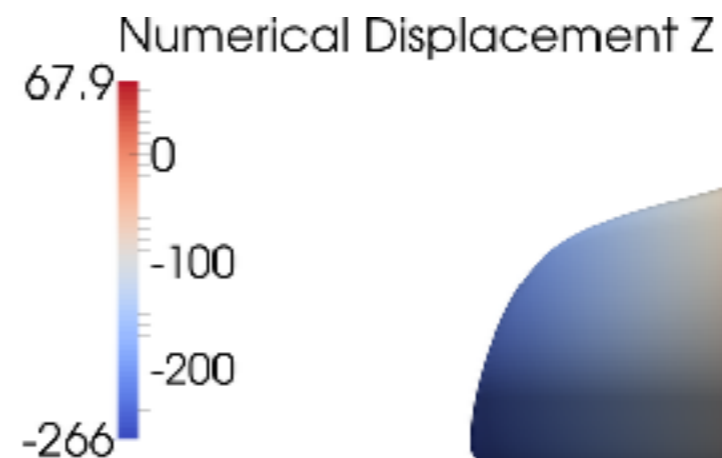
R. N. Simpson et al. (2012) CMAME Feb 1;209:87-100.

# Shape optimisation

Construct the geometric model  
(imported from Rhino)



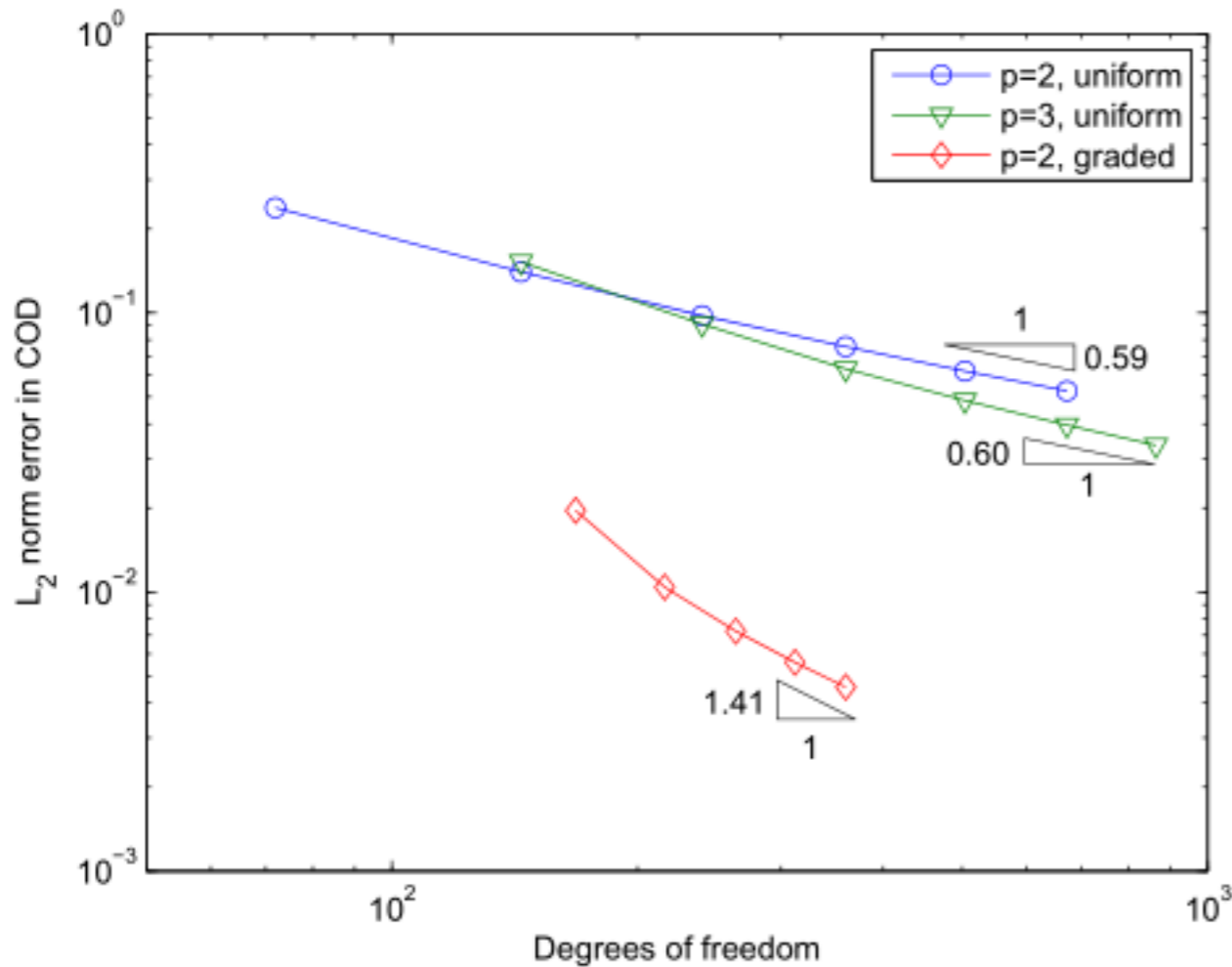
Select design points from control points



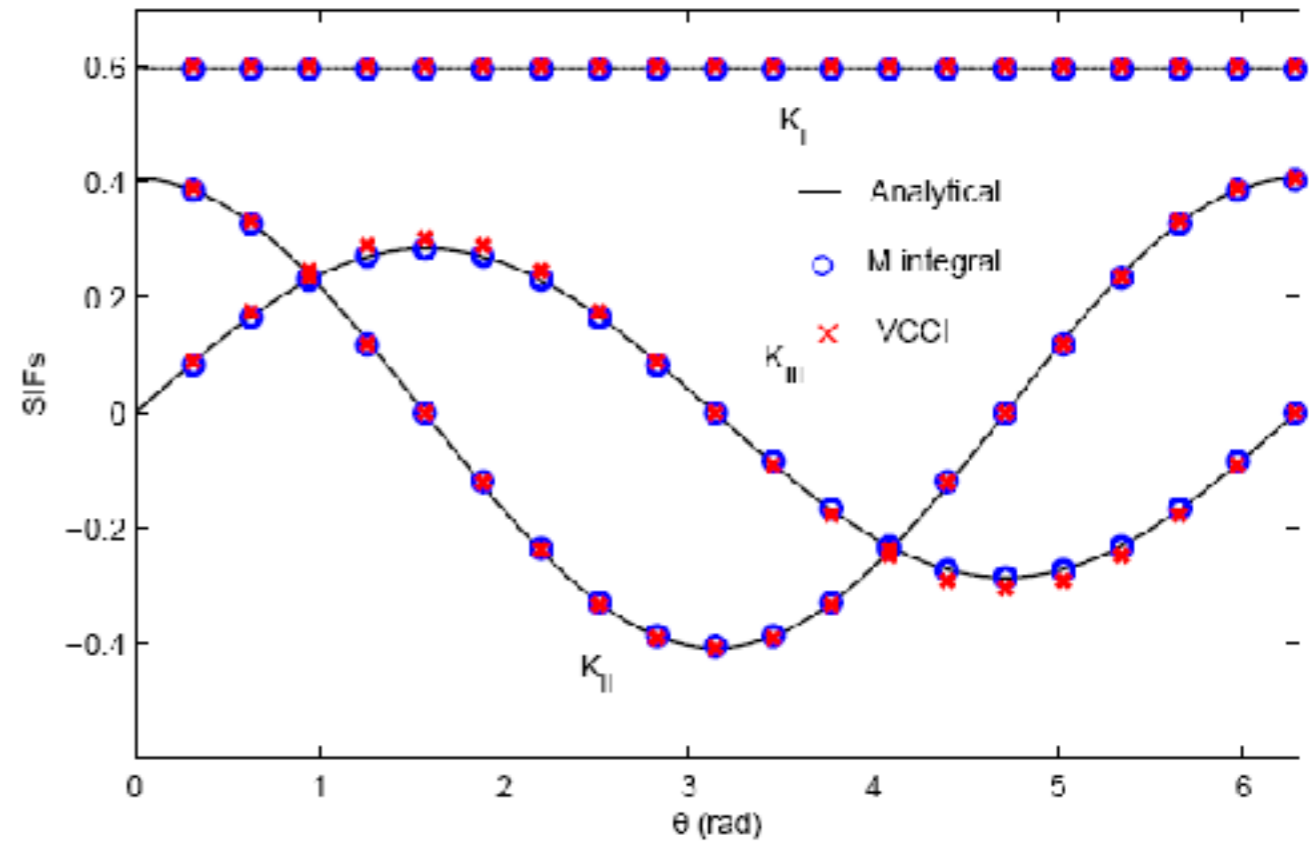
Find optimized solution



# Penny-shaped crack under remote tension



$L_2$  norm error of COD for penny-shaped crack



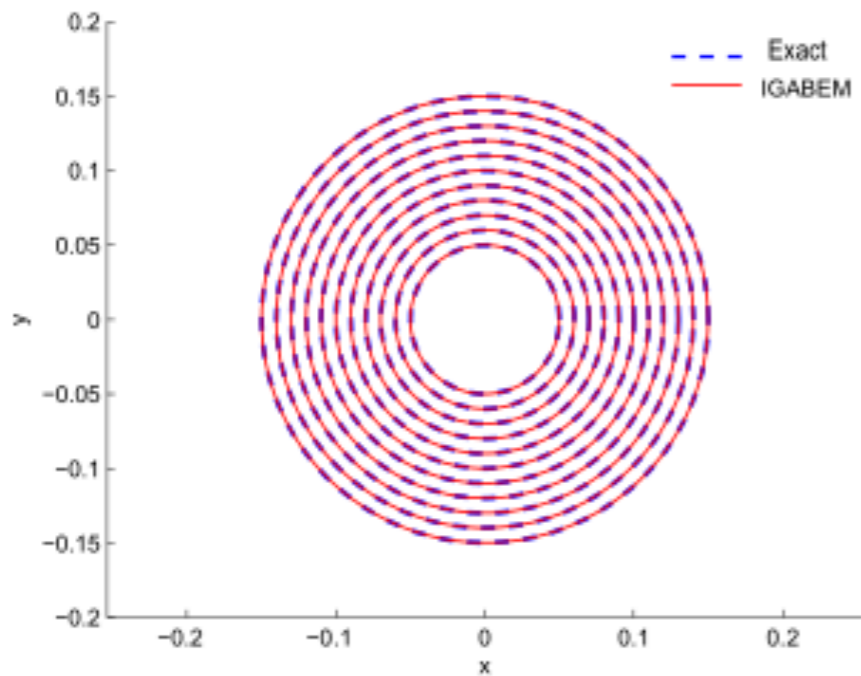
stress intensity factors for penny crack  
with  $\varphi = \pi/6$

## Fracture mechanics directly from CAD

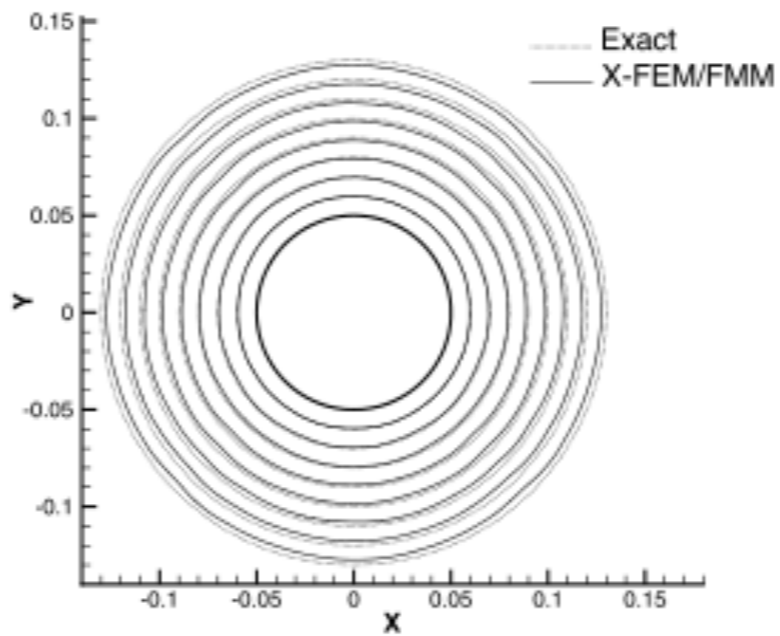
X. Peng, et al. (2017). *IJF*, 204(1), 55–78.

X. Peng, et al. (2017). *CMAME*, 316, 151–185.

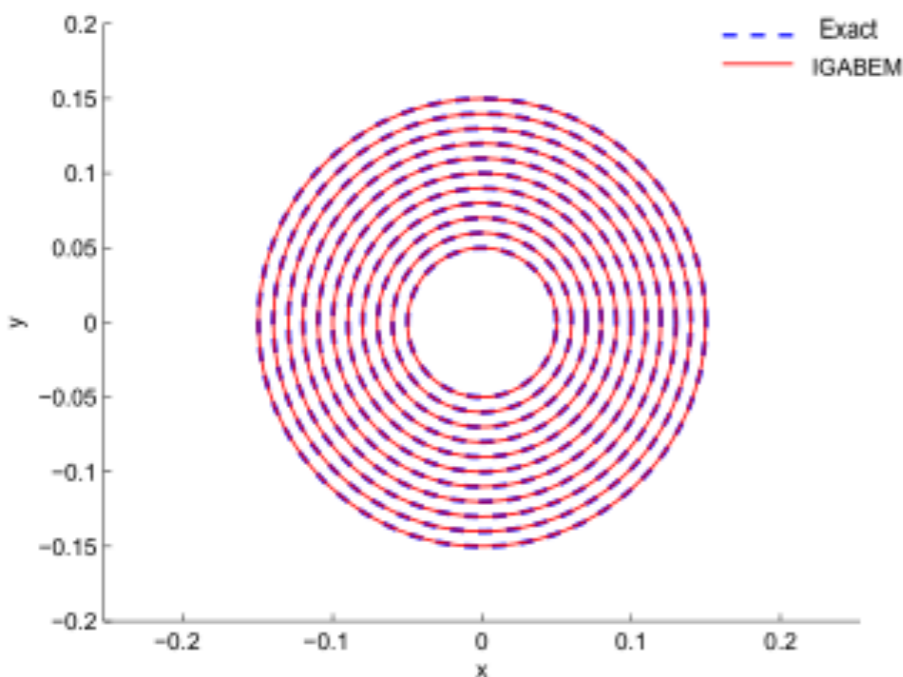
# Numerical example of horizontal penny crack growth (first 10 steps)



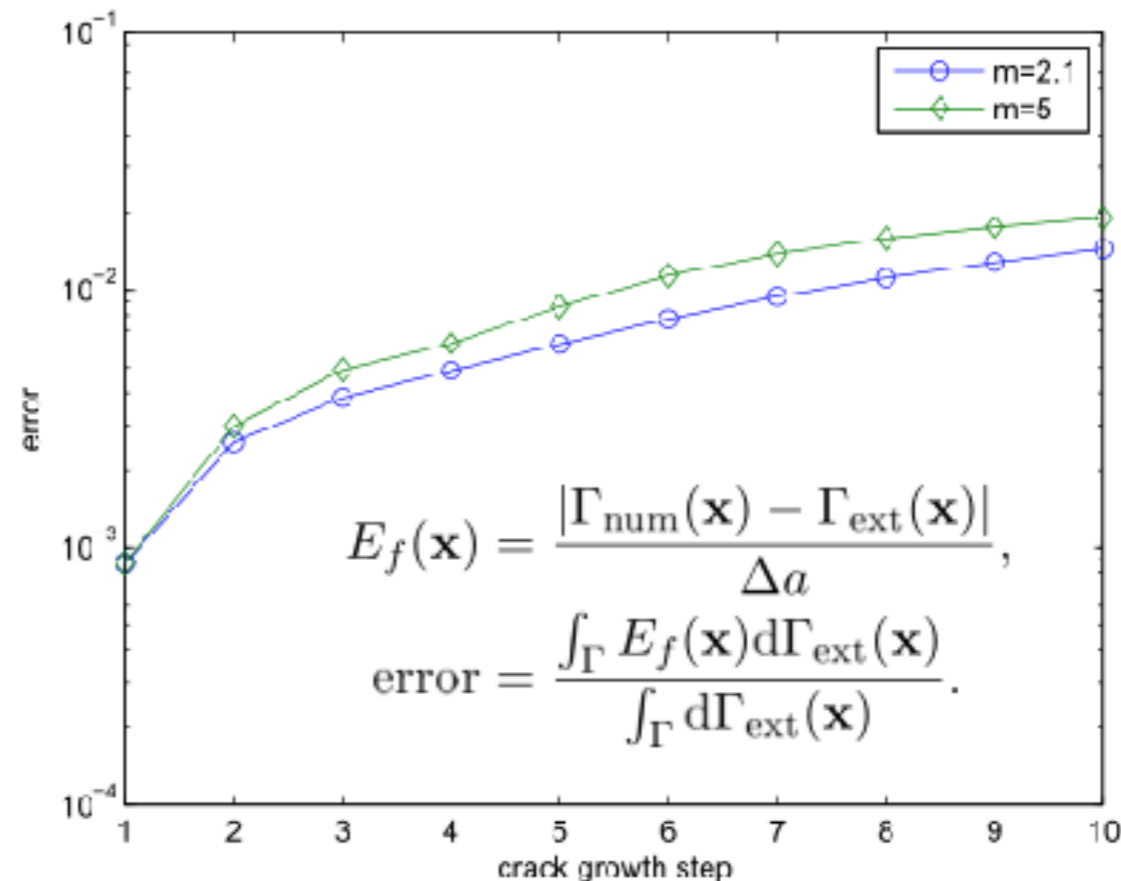
(a) IGABEM,  $m = 2.1$



(b) XFEM/FMM,  $m = 2.1$ , Sukumar *et al* 2003

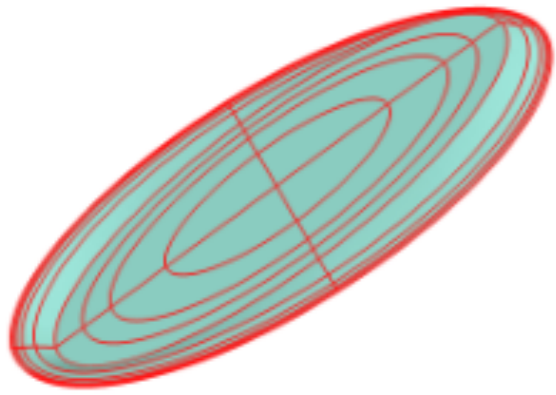


(c) IGABEM,  $m = 5$

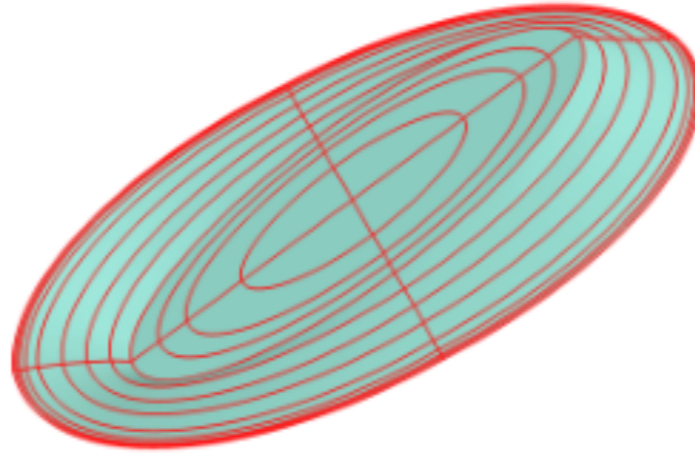


Relative error of the crack front for in each crack growth step by IGABEM

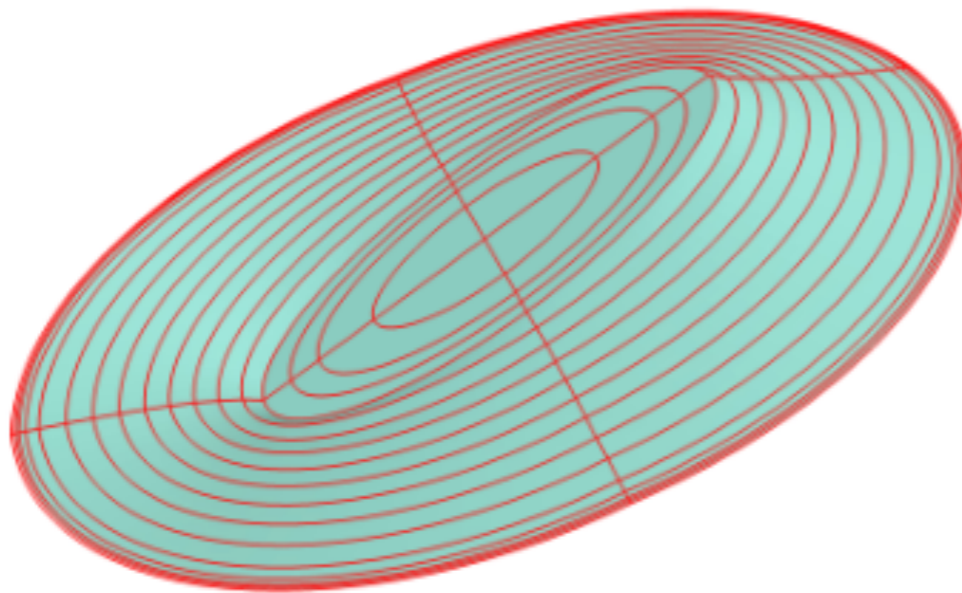
# Numerical example of inclined elliptical crack growth (first 10 steps)



(a) Step 2

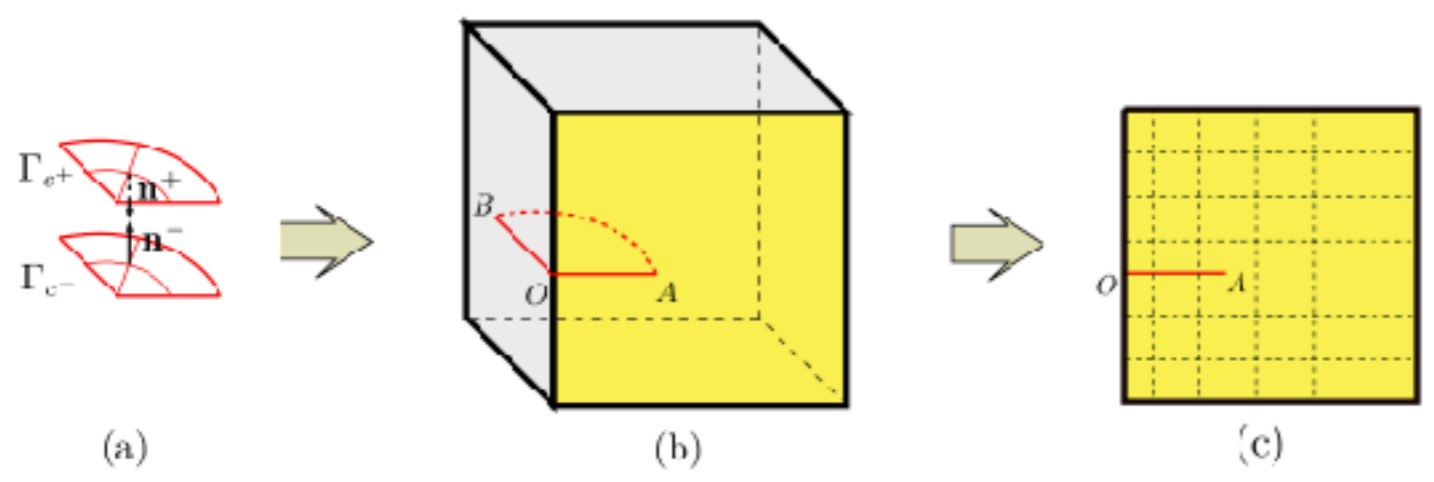


(b) Step 5

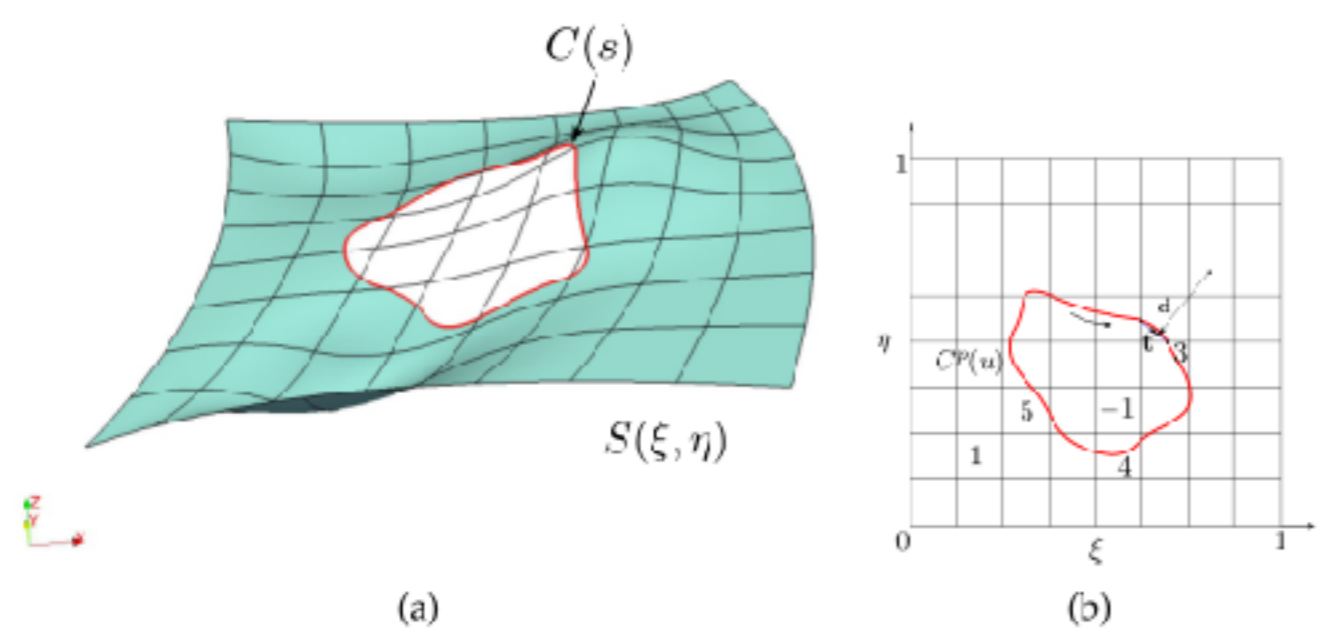


(c) Step 10

# Modeling techniques for surface cracks? Trimmed curves...



Surface discontinuity is introduced

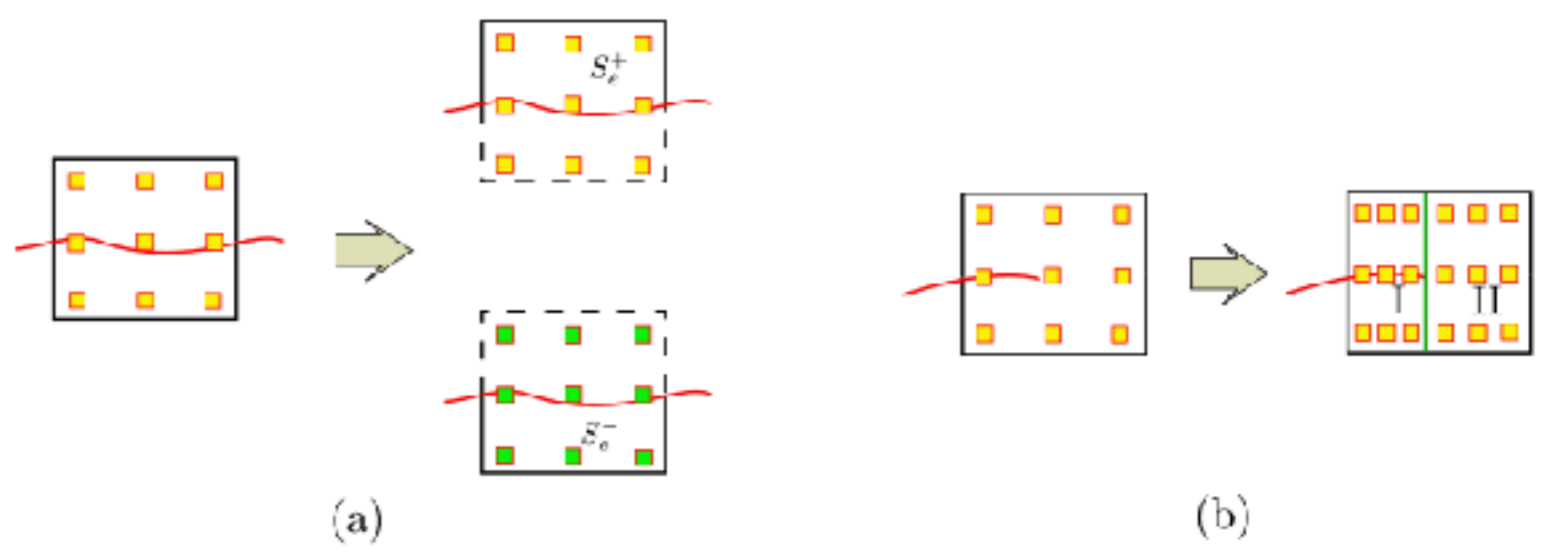


Trimmed NURBS technique

Crack = trimming curve  
Phantom node method

$$\mathbf{u}^+(\mathbf{x}) = \sum_j^{N^e} \mathbf{R}_j(\mathbf{x}) \mathbf{d}_j, \quad \mathbf{x} \in S_e^+$$

$$\mathbf{u}^-(\mathbf{x}) = \sum_k^{N^e} \mathbf{R}_k(\mathbf{x}) \mathbf{d}_k, \quad \mathbf{x} \in S_e^-$$



## References

- Peng, X., Atroshchenko, E., Kerfriden, P., & Bordas, S. P. A. (2017). Linear elastic fracture simulation directly from CAD: 2D NURBS-based implementation and role of tip enrichment. *International Journal of Fracture*, 204(1), 55–78.
- Peng, X., Atroshchenko, E., Kerfriden, P., & Bordas, S. P. A. (2017). Isogeometric boundary element methods for three dimensional static fracture and fatigue crack growth. *Computer Methods in Applied Mechanics and Engineering*, 316, 151–185.
- Simpson, R. N., Bordas, S. P. A., Trevelyan, J., & Rabczuk, T. (2012). A two-dimensional Isogeometric Boundary Element Method for elastostatic analysis. *Computer Methods in Applied Mechanics and Engineering*, 209–212(0), 87–100.
- Guiggiani, M., Krishnasamy, G., Rudolphi, T. J., & Rizzo, F. J. (1992). A General Algorithm for the Numerical Solution of Hypersingular Boundary Integral Equations. *Journal of Applied Mechanics*, 59(3), 604–614.
- Rong, J., Wen, L., & Xiao, J. (2014). Efficiency improvement of the polar coordinate transformation for evaluating BEM singular integrals on curved elements. *Engineering Analysis With Boundary Elements*, 38, 83–93.
- Mi, Y., & Aliabadi, M. H. (1992). Dual boundary element method for three-dimensional fracture mechanics analysis. *Engineering Analysis with Boundary Elements*, 10(2), 161–171.
- Becker, A. (1992). The Boundary Element Methods in Engineering. *McGraw-Hill Book Company*.

## Partial conclusions on methods coupling geometry and field approximations

- ◆ There are numerous alternatives (subdivision surfaces, IGA, NEFEM, NIGFEM)
- ◆ IGA can offer simulations directly from CAD when used with boundary elements
- ◆ GIFT generalizes this approach by decoupling geometry and field approximations

**Next: methods which decouple geometry and field approximation**

# Conclusions and future work

Used the same basis functions in CAD to discretize Boundary Integral Equations (BIE)

1. 2D geometry construction using NURBS, and 3D geometry using T-splines.

2. No meshing in all the optimization iterative steps.

3. Implicit differentiation method is suitable for a small number of design variable and a large number of constraints.

## Future work

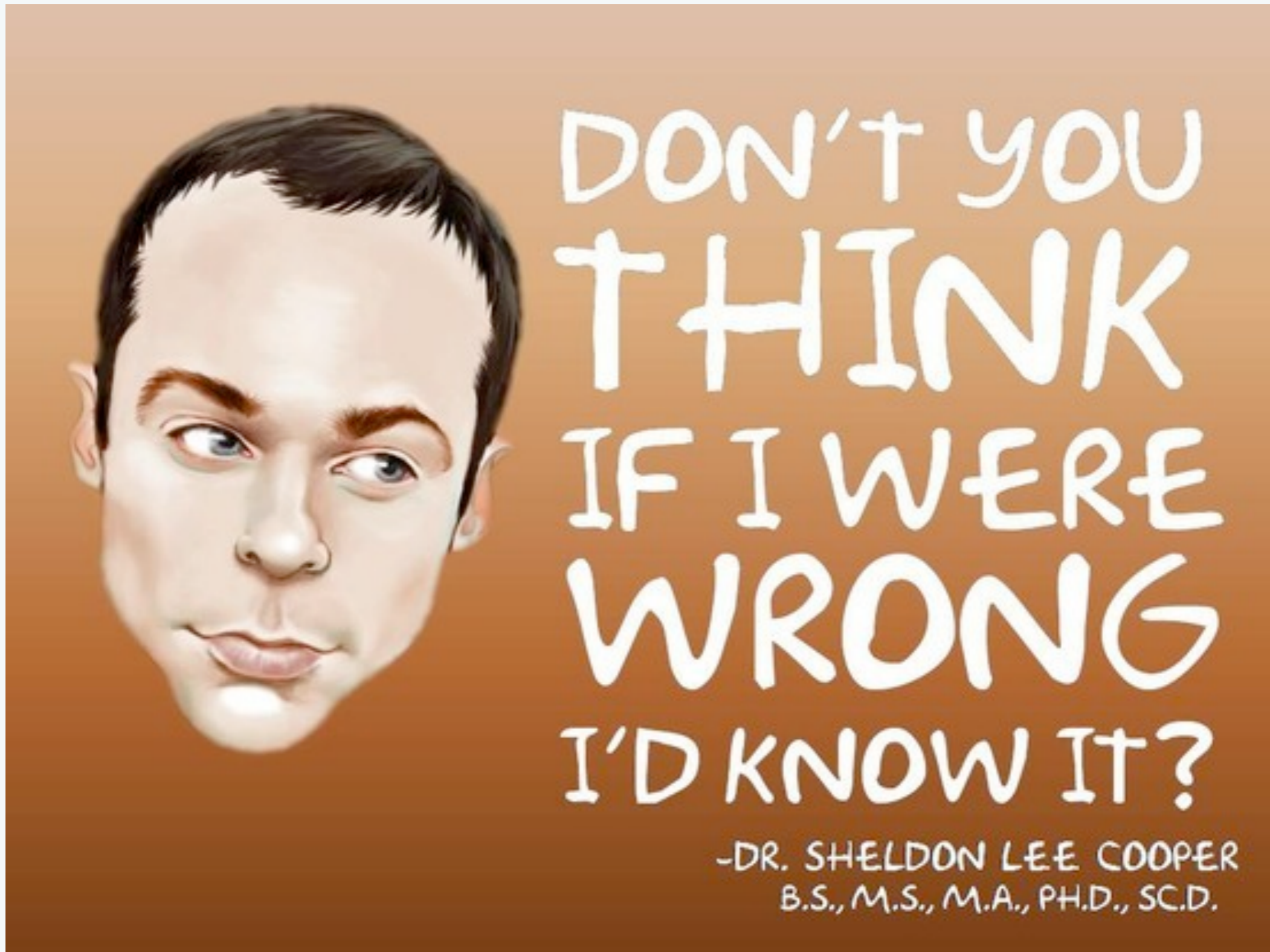
1. Adjoint methods for a large number of design variables and a small number of constraints.

2. A robust algorithm is needed for moving control points in a large scale without distorting the control mesh.

3. Combined with the gradient-less solver.

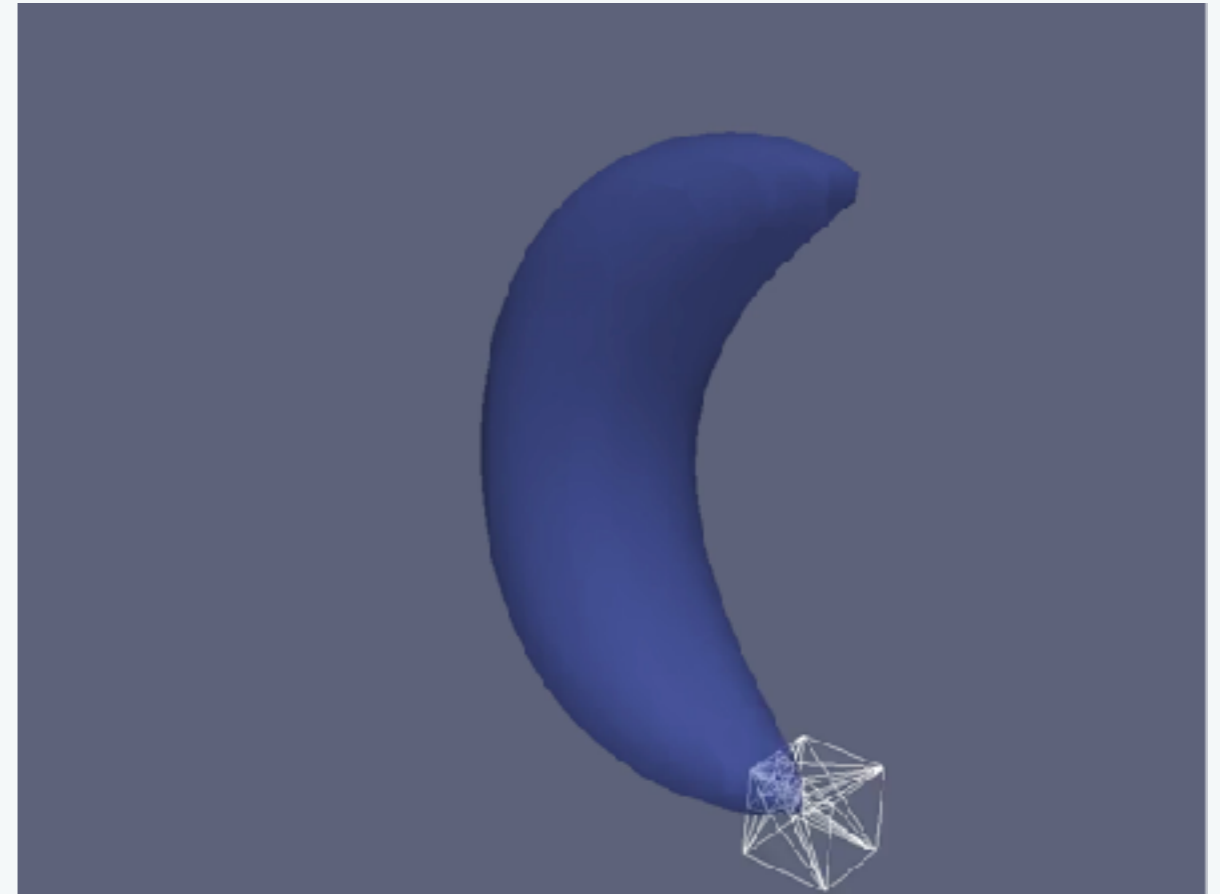
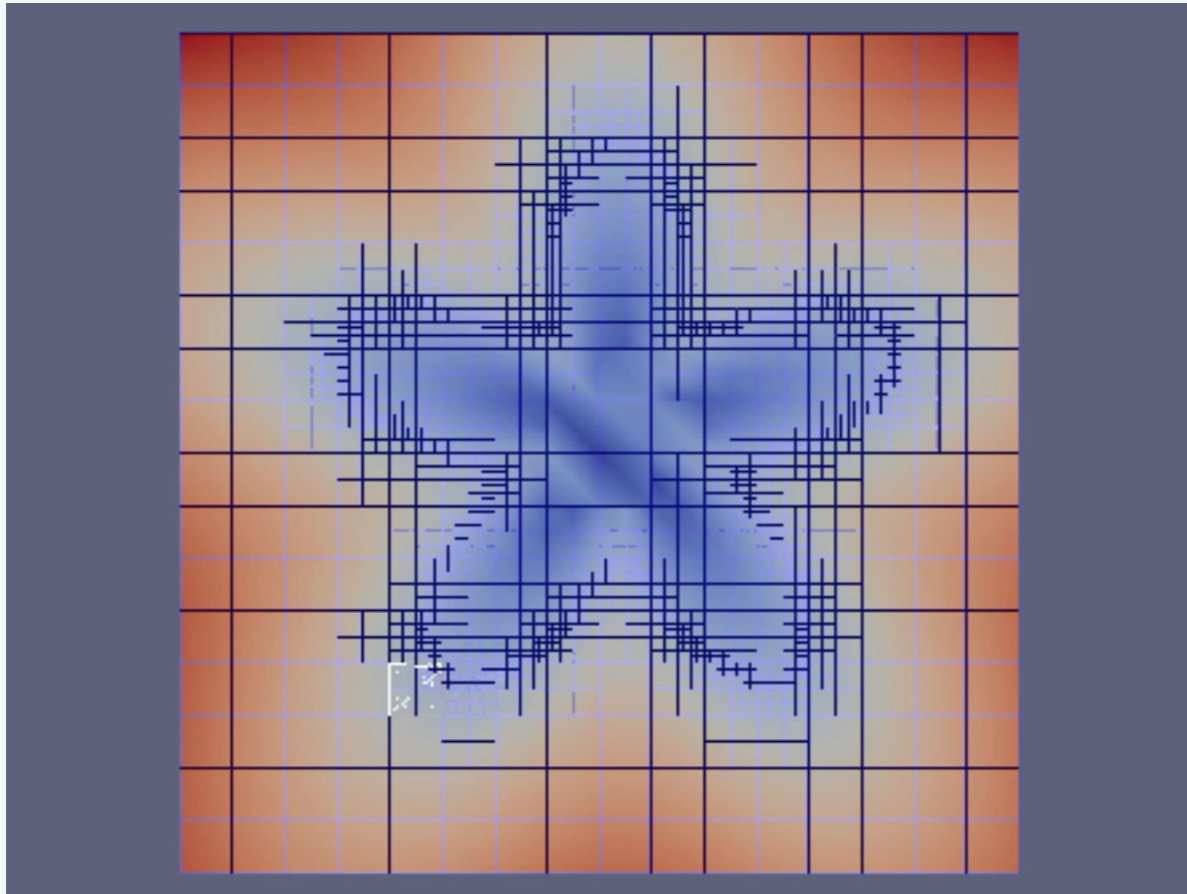
4. Using PHT-splines.

5. GIFT-IGABEM optimization.





## *Decoupling - Unfitted FEM?*



**Question: for which problems are we better off coupling/decoupling the geometry from the field approximation?**

### **Implicit surfaces**

T. Rüberg (2016) *Advanced Modeling and Simulation in Engineering Sciences* 3 (1), 22

M. Moumnassi (2011) *CMAME* 200(5): 774-796. (CSG and multiple level sets)

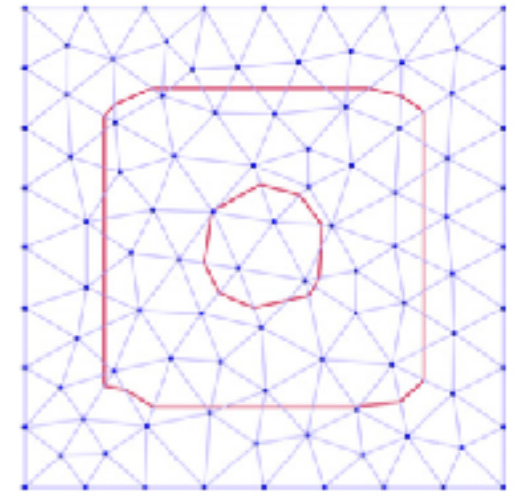
N. Moës (2003) *CMAME* 192.28 (2003): 3163-3177. (Single level set)

T. Belytschko *IJNME* 56.4 (2003): 609-635. (Structured XFEM)

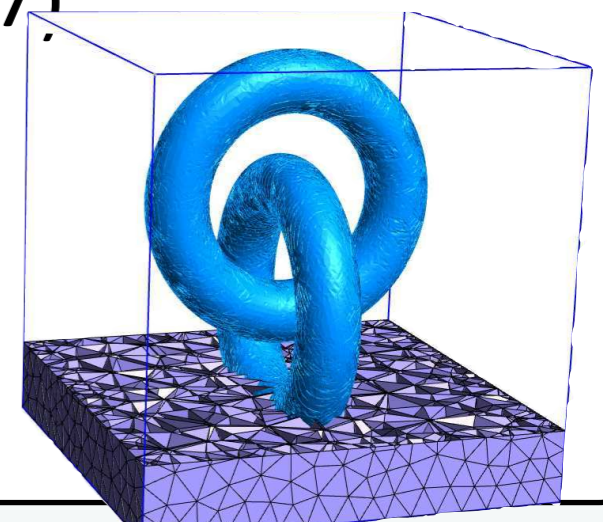
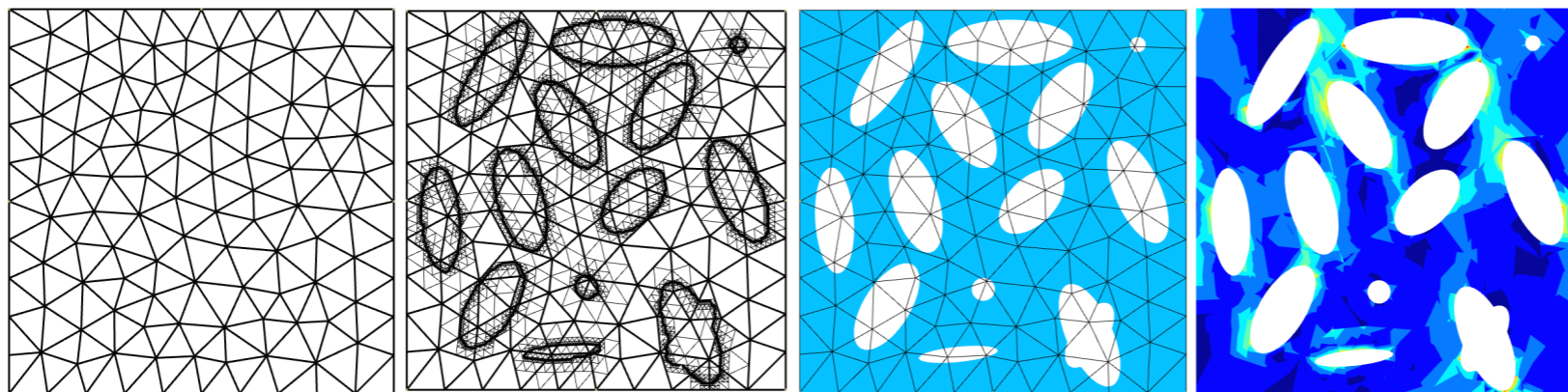
...

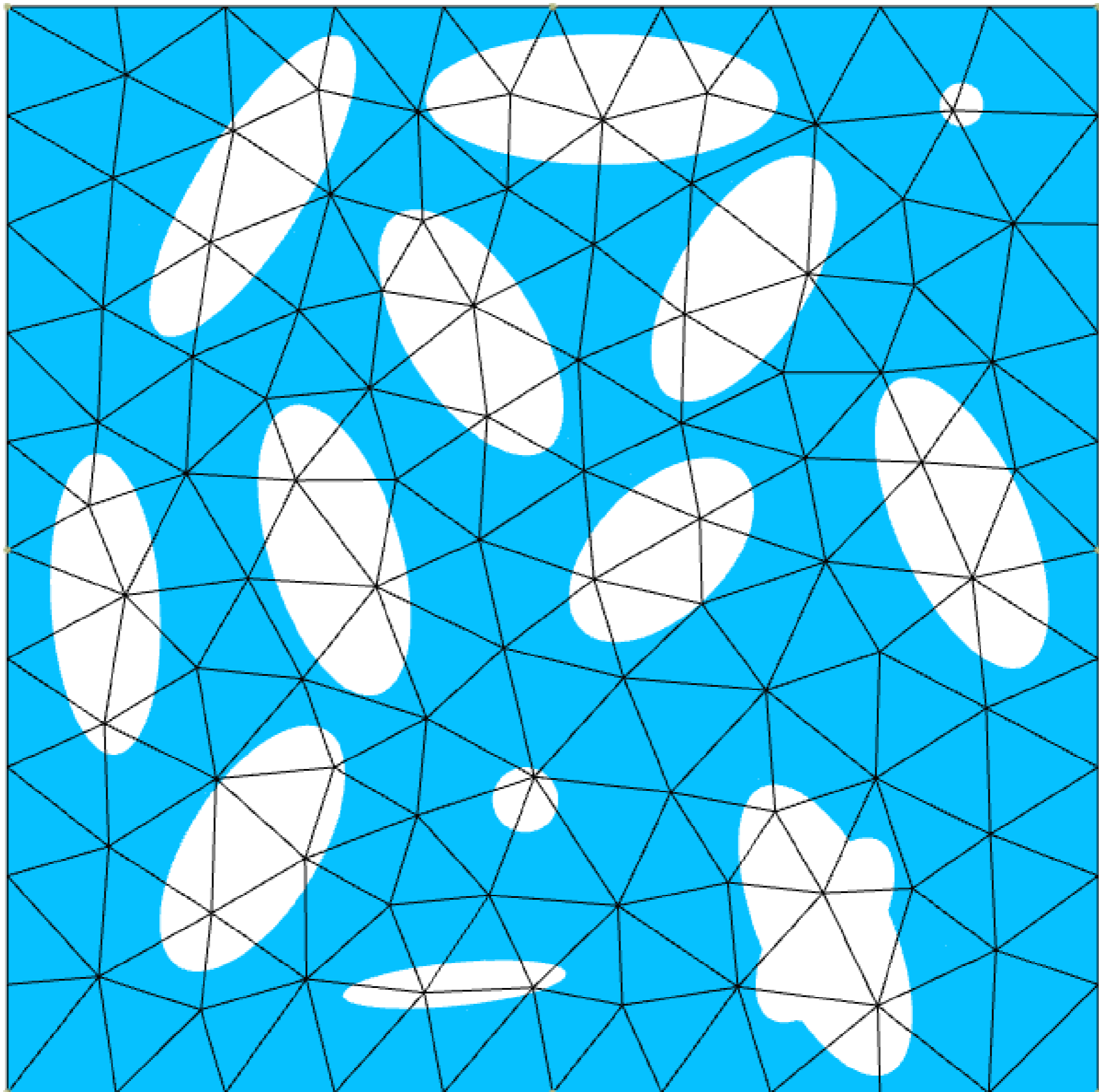
# Separate field and boundary discretisation

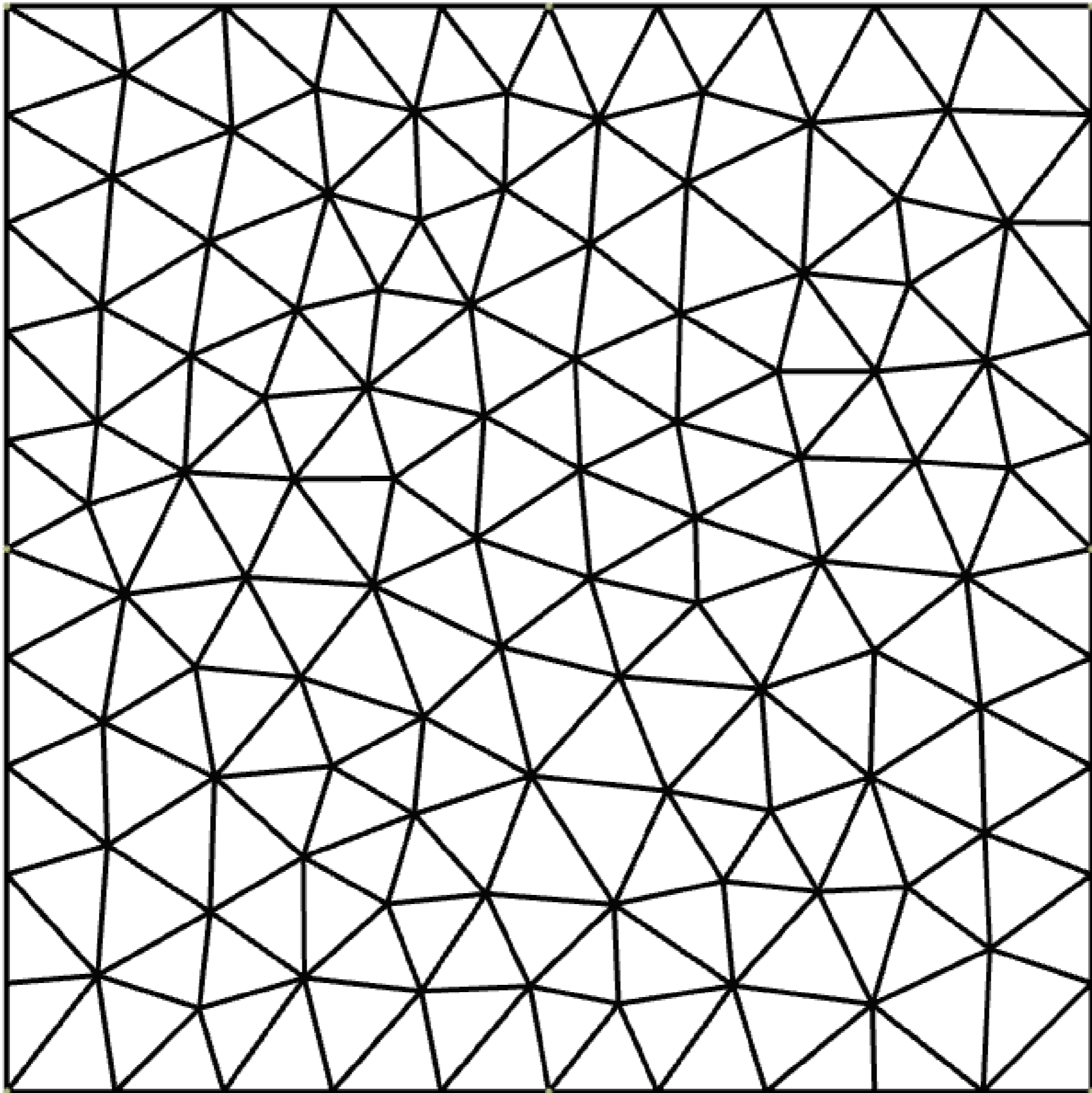
- Immersed boundary method (Mittal, *et al.* 2005)
- Fictitious domain (Glowinski, *et al.* 1994)
- Embedded boundary method (Johansen, *et al.* 1998)
- Virtual boundary method (Saiki, *et al.* 1996)
- Cartesian grid method (Ye, *et al.* 1999, Nadal, 2013)

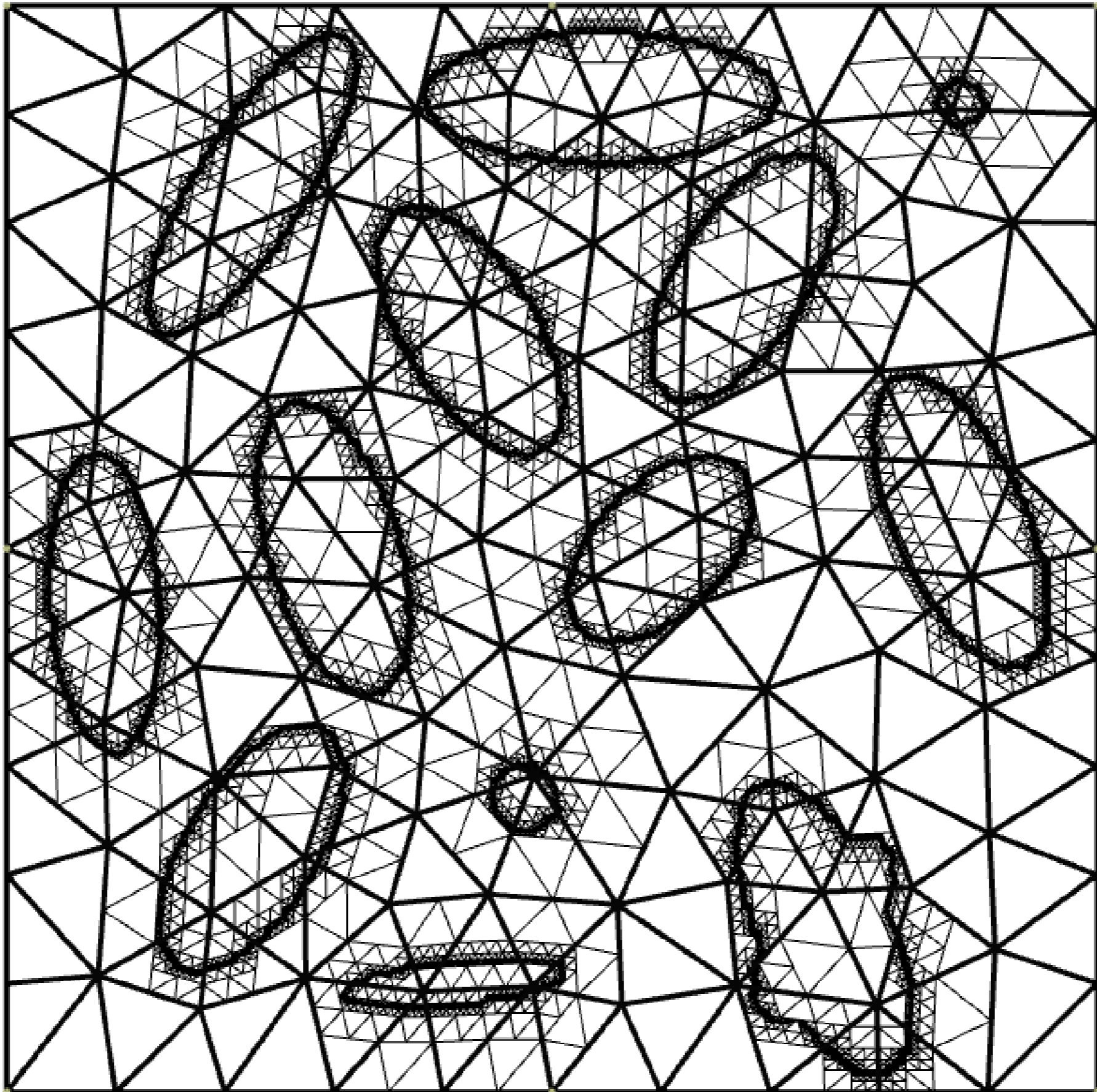


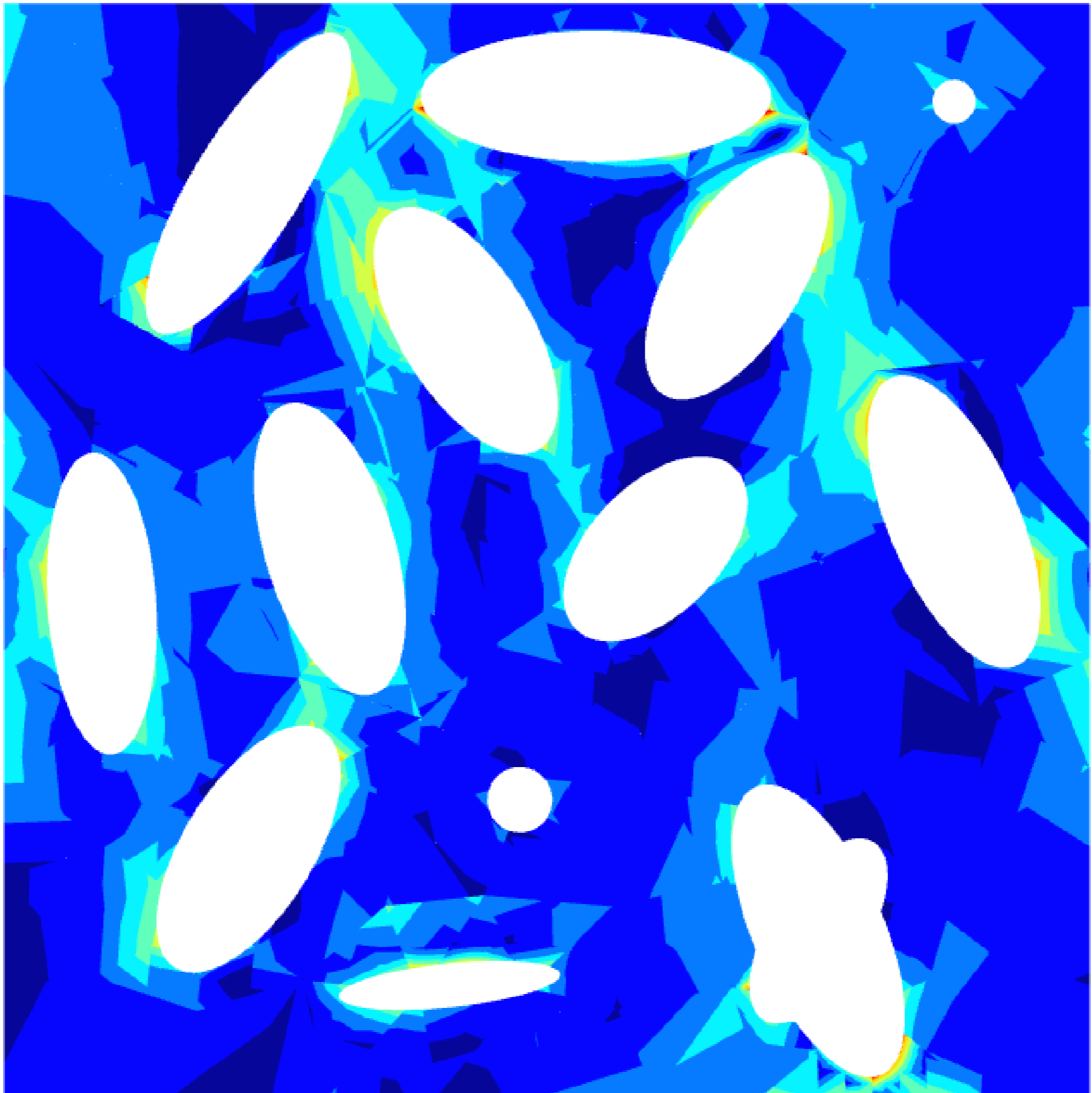
- ✓ Easy adaptive refinement + error estimation (Nadal, 2013)
- ✓ Flexibility of choosing basis functions
- Accuracy for complicated geometries? BCs on implicit surfaces?
- ➔ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi 2011; Ródenas Garcia 2016; Fries 2017)

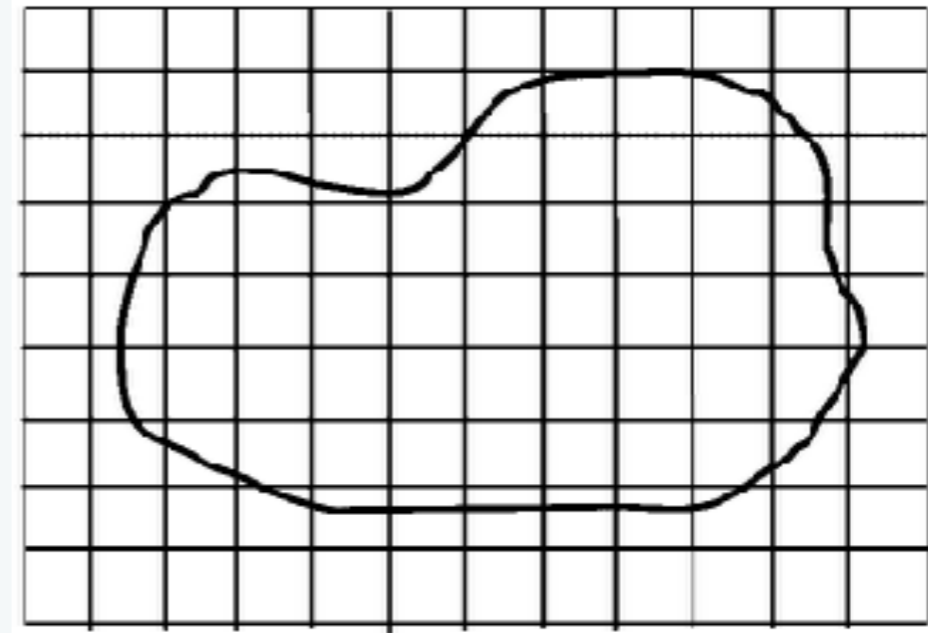
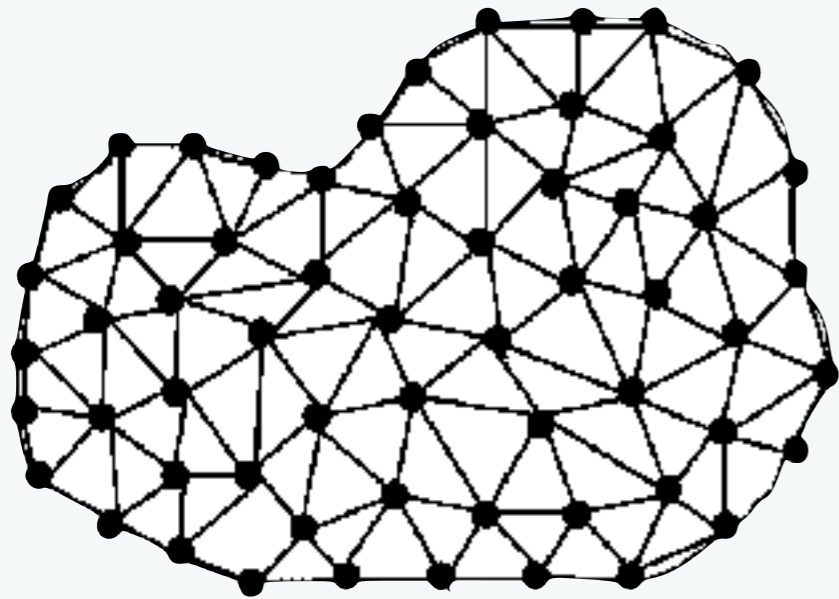




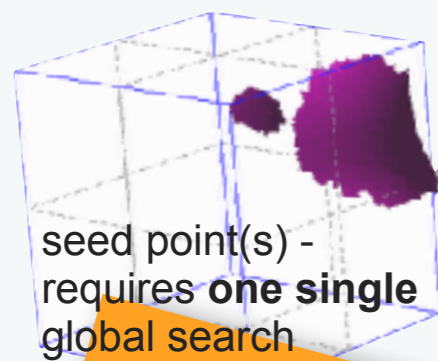




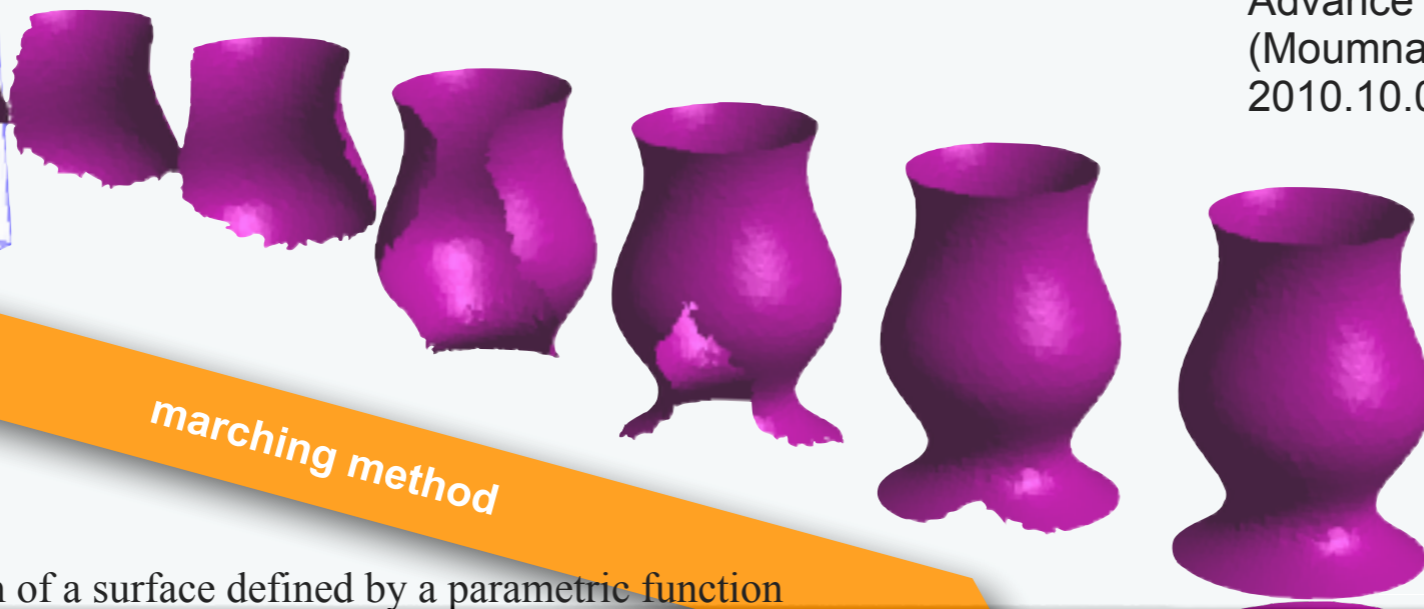




**Question: How can we generate level set functions from CAD descriptions (including corners/vertices)?**



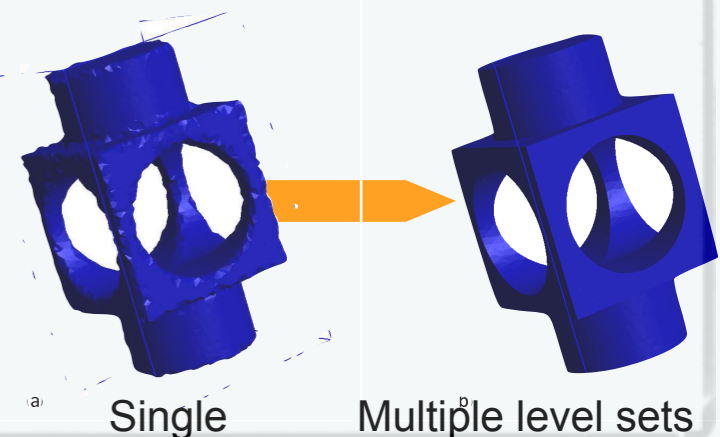
seed point(s) -  
requires **one single**  
global search

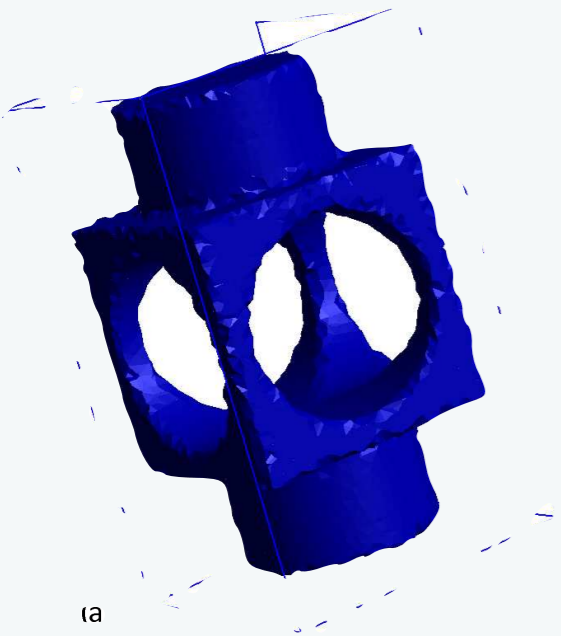
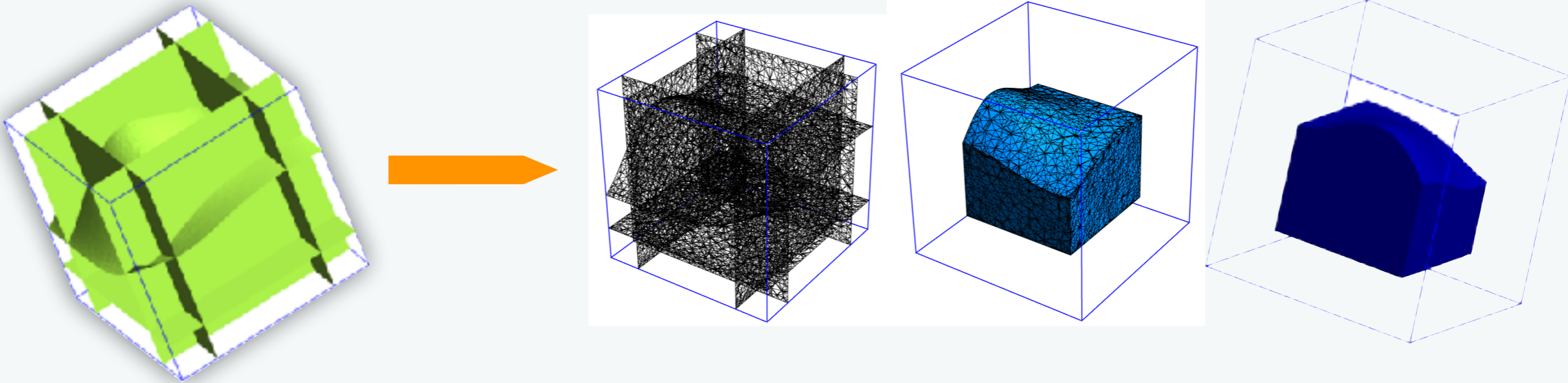


marching method

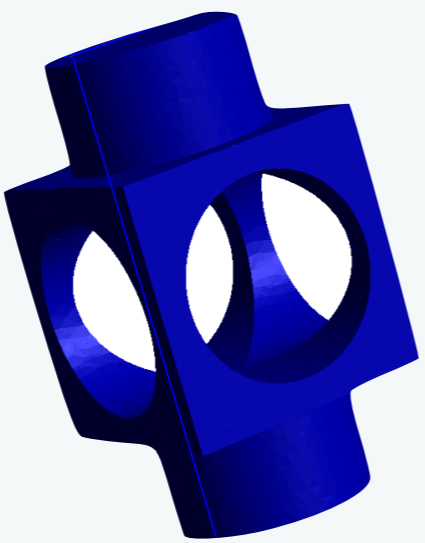
Level Set representation of a surface defined by a parametric function

Advance by CRP Henri Tudor in 2011  
(Moumnassi et al, CMAME DOI: 10.1016/j.cma.  
2010.10.002

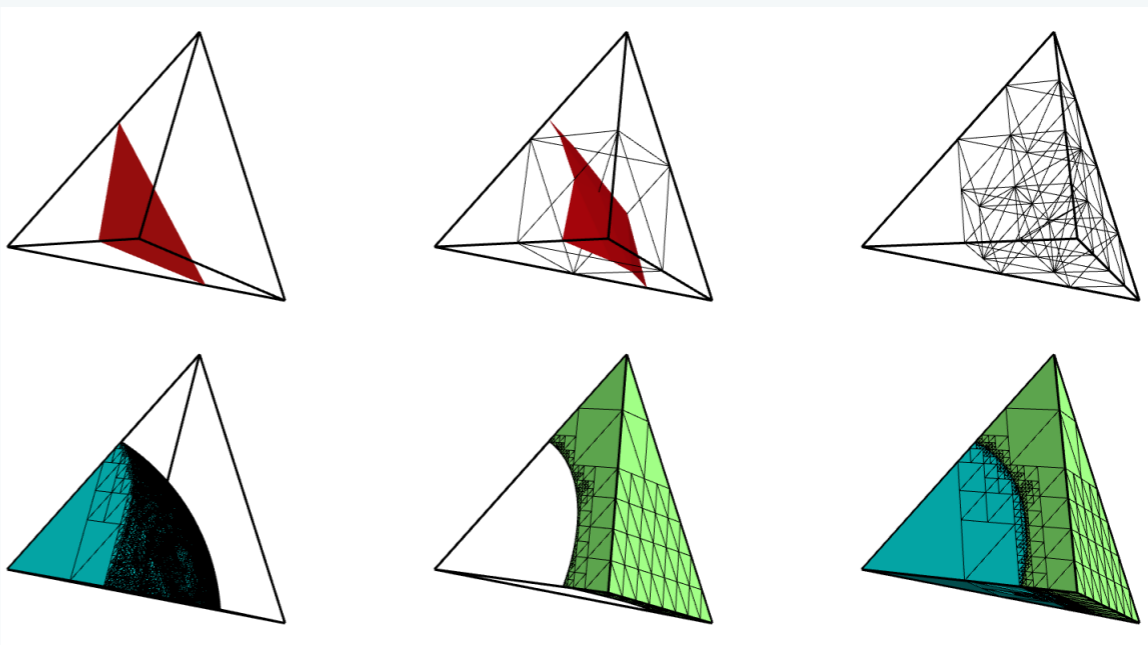




Single level set



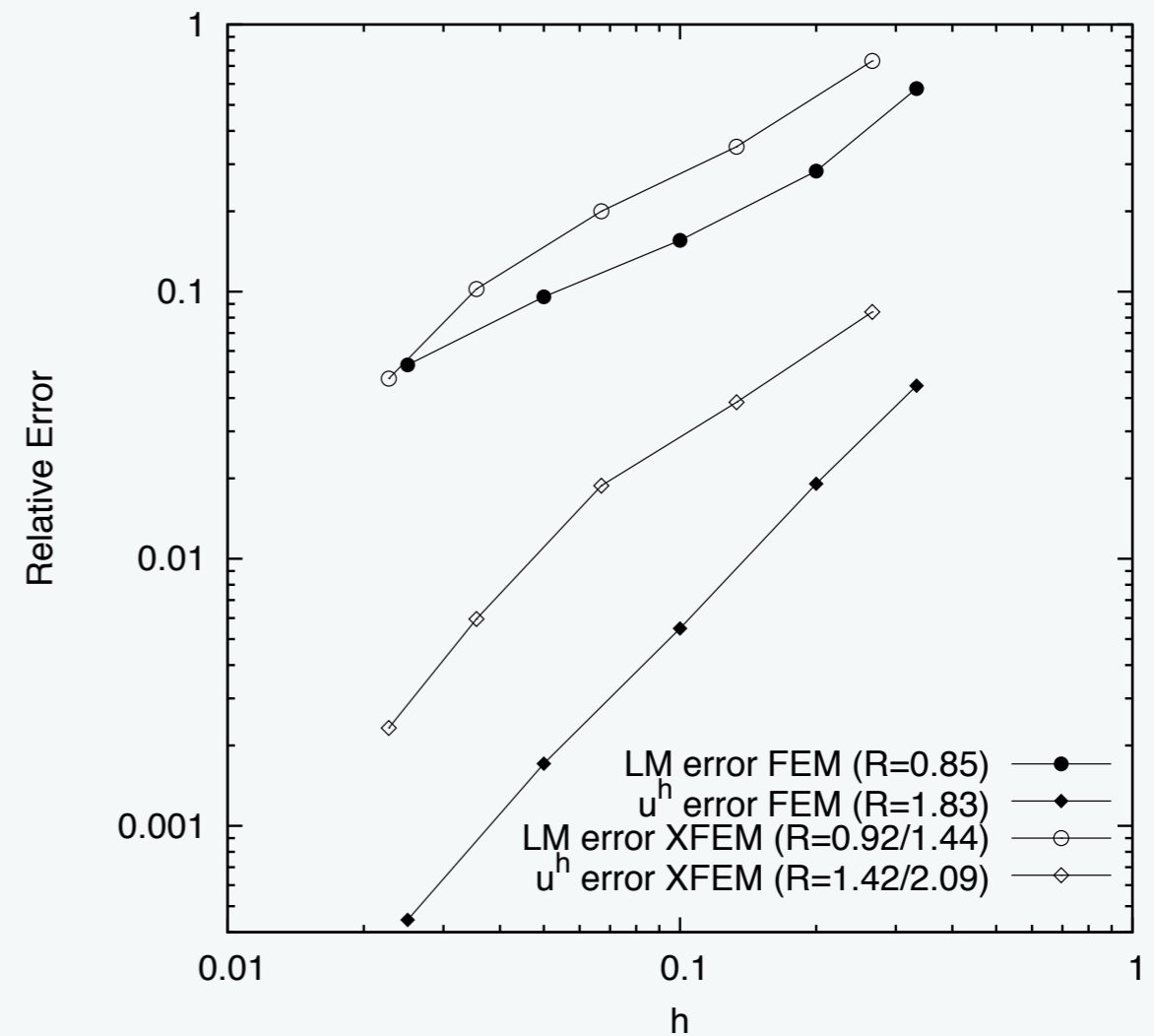
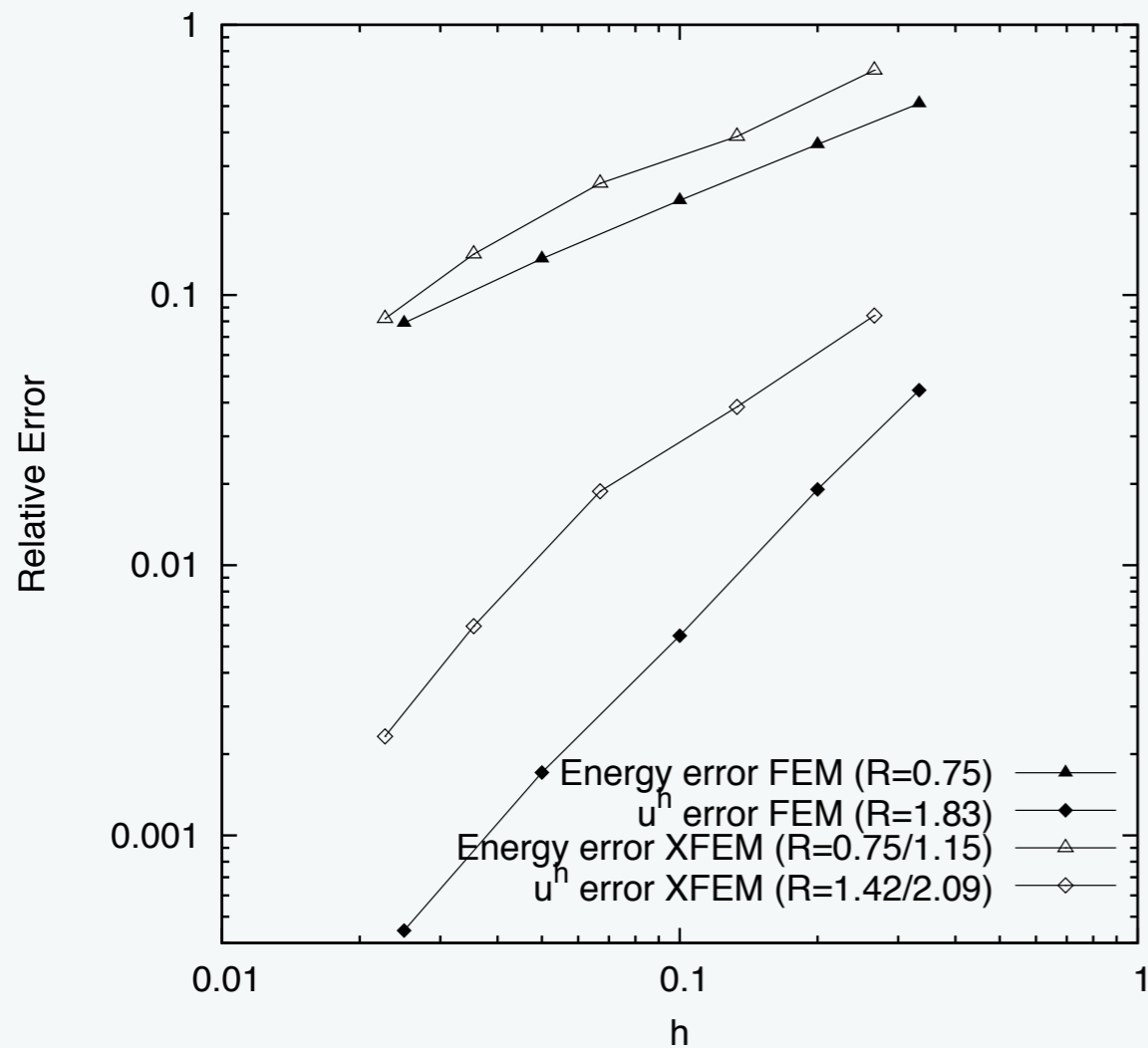
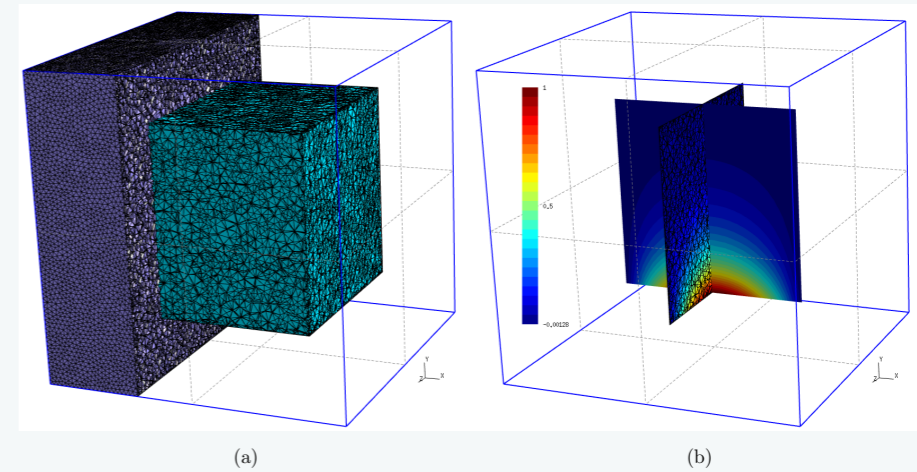
Multi level sets





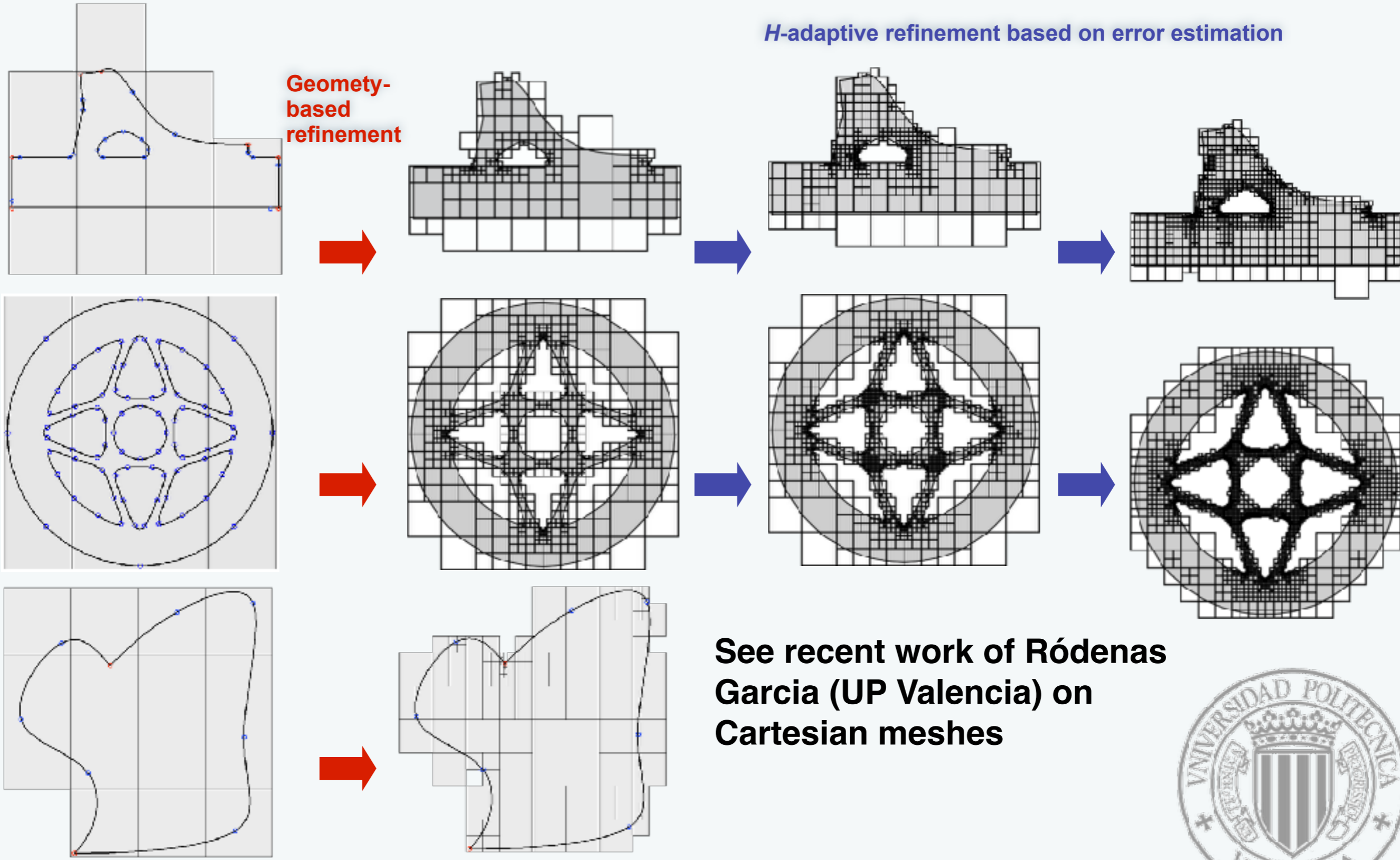
- Laplace equation on a cube
- convergence rates

- ➔ optimal
- ➔ requires proper Lagrange multiplier space to eradicate spurious oscillations



# Examples

*H*-adaptive refinement based on error estimation

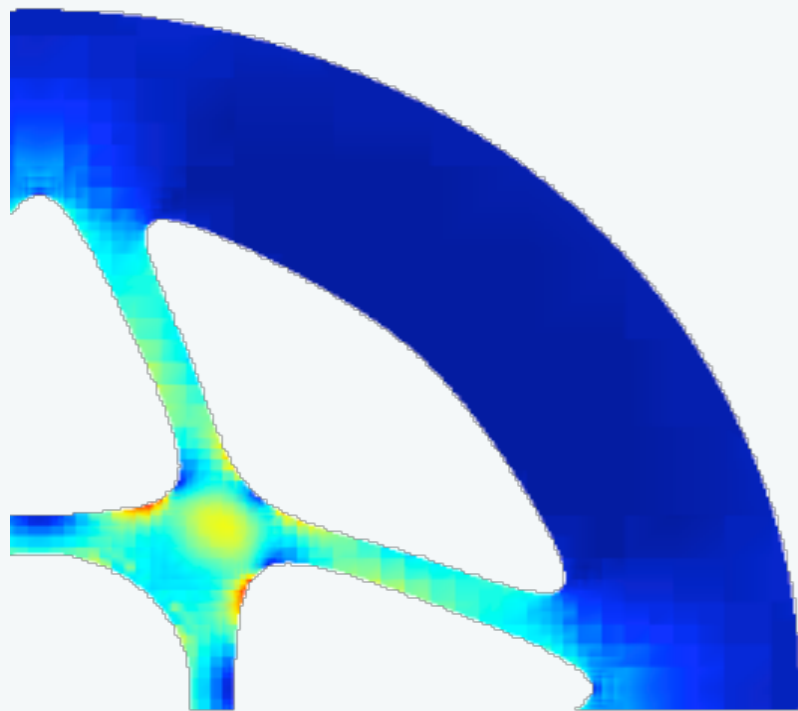


Geometry-based refinement

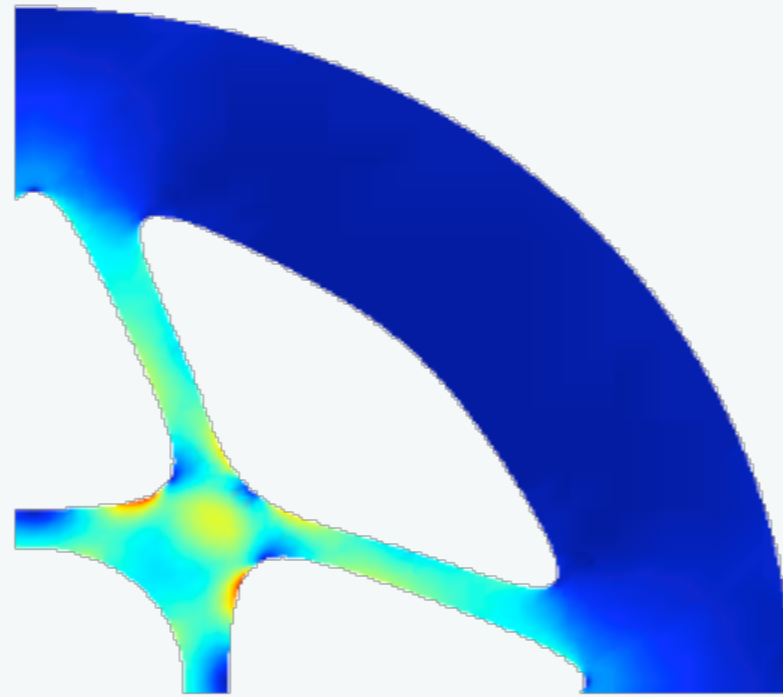
See recent work of Ródenas Garcia (UP Valencia) on Cartesian meshes



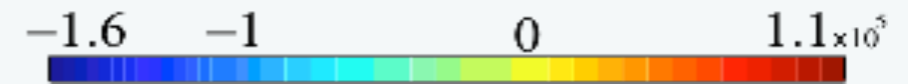
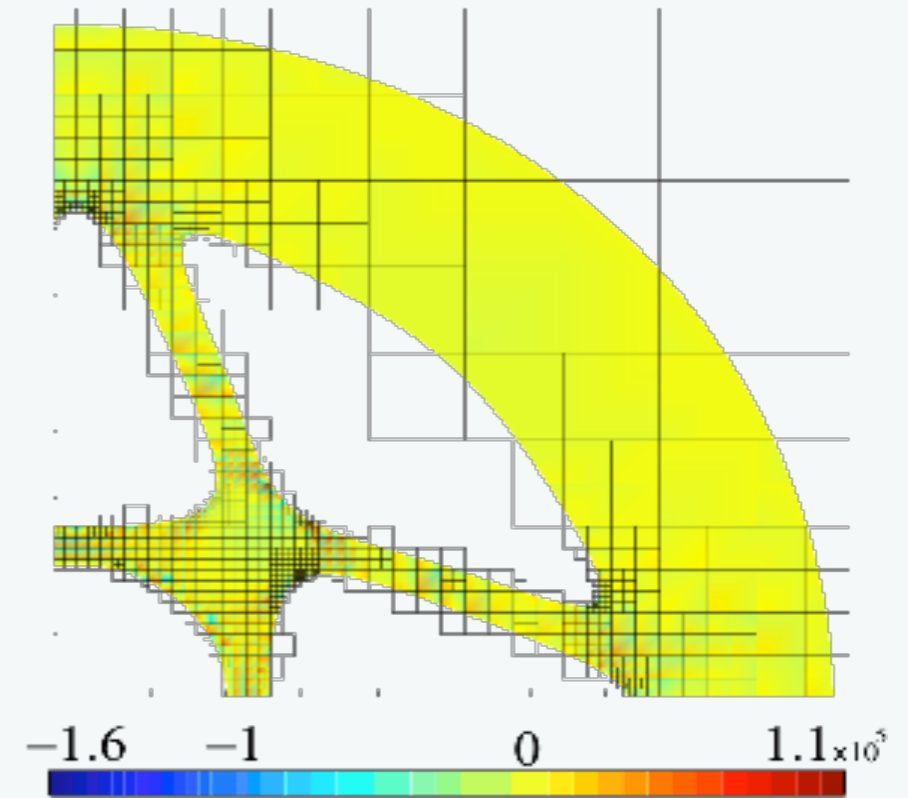
FEM



SPR-C

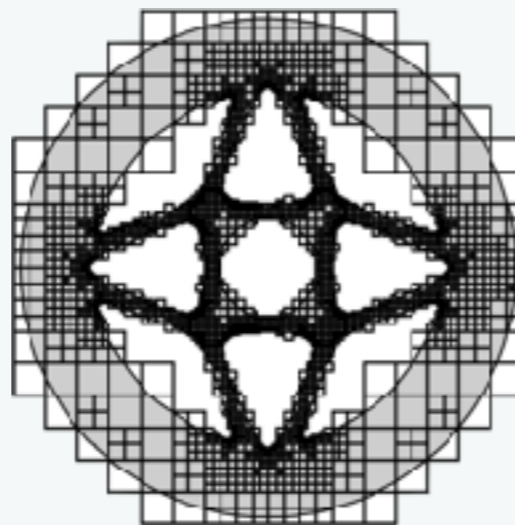
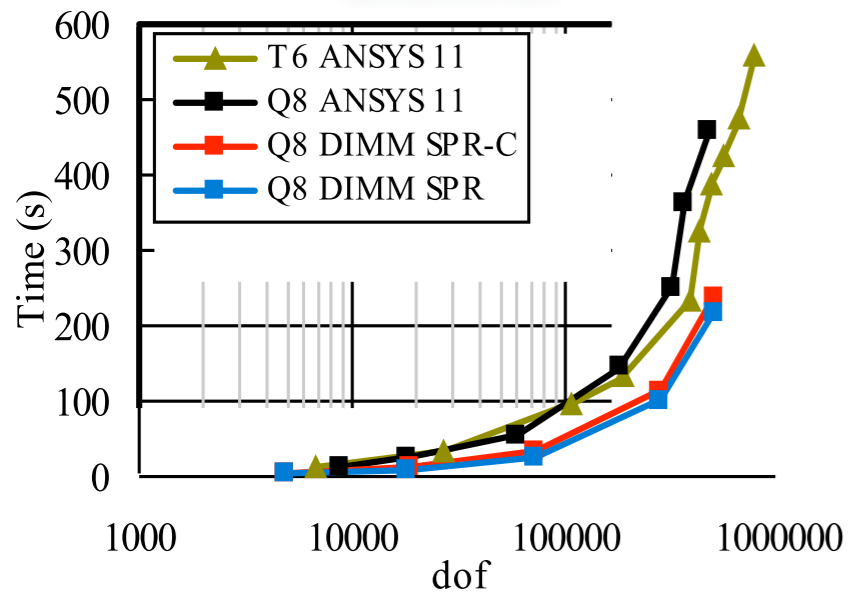


SPR-C-FEM



Quad8 uniform refinement

Processing time

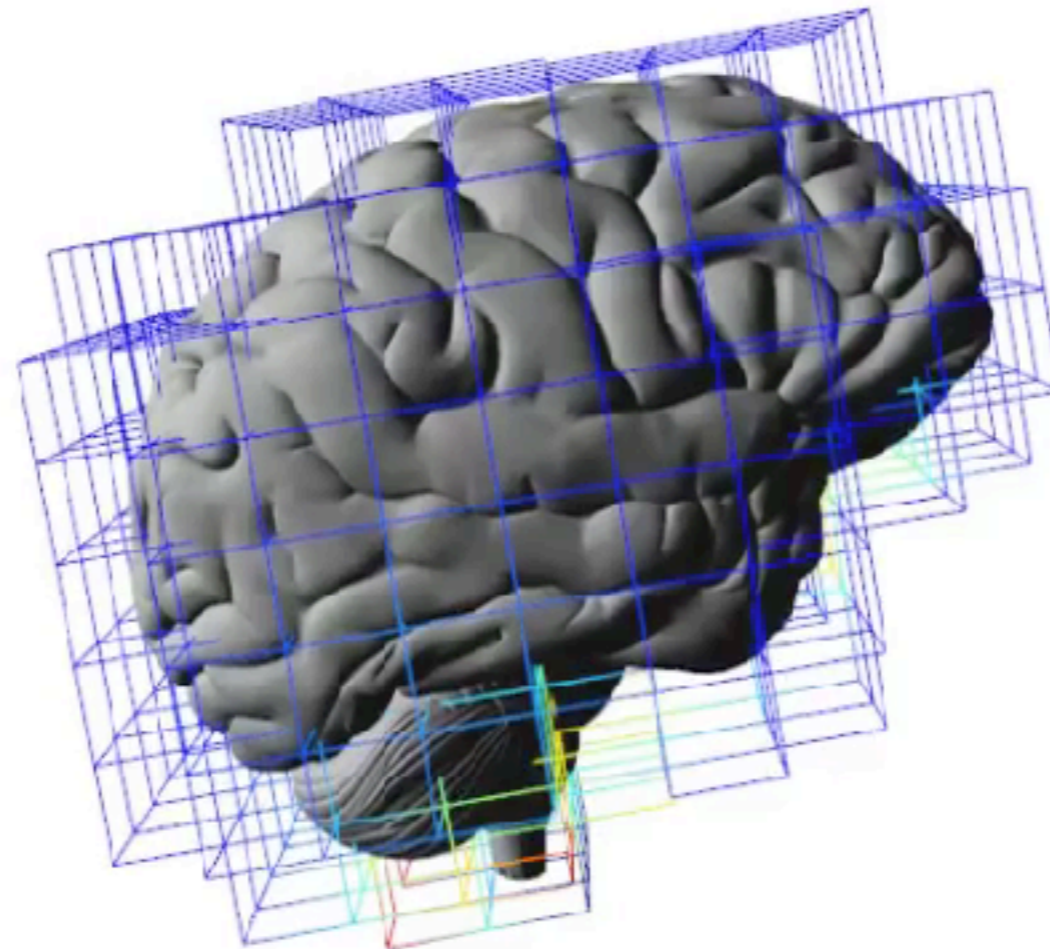


See recent work of Ródenas Garcia (UP Valencia) on Cartesian meshes

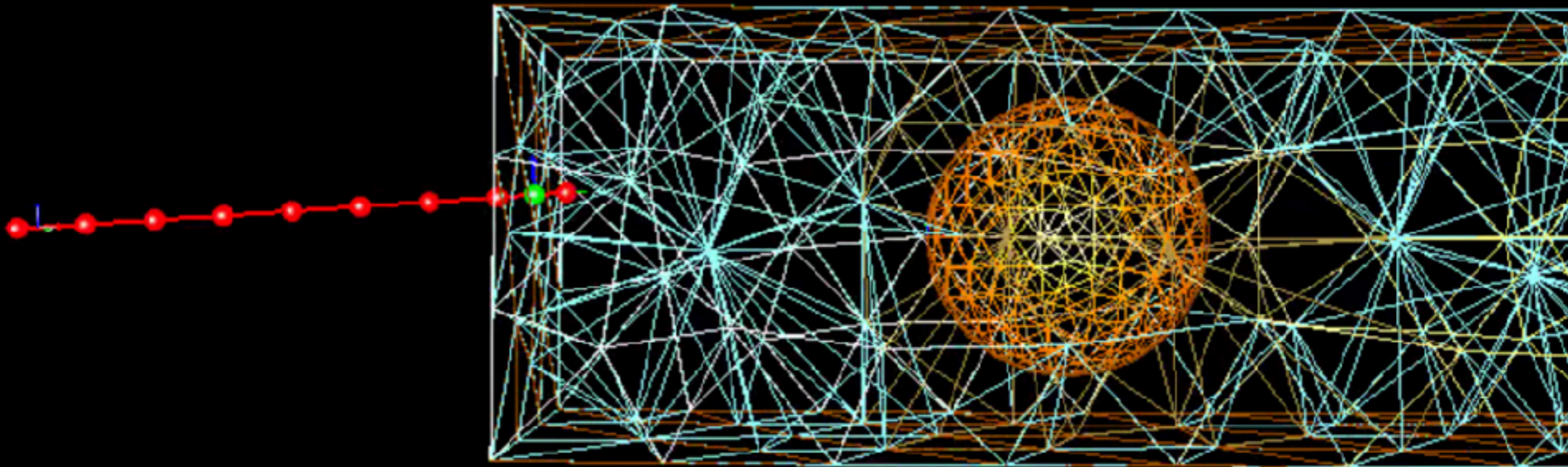


## *With implicit boundaries*

Brain shift occurs  
prior to cannula insertion

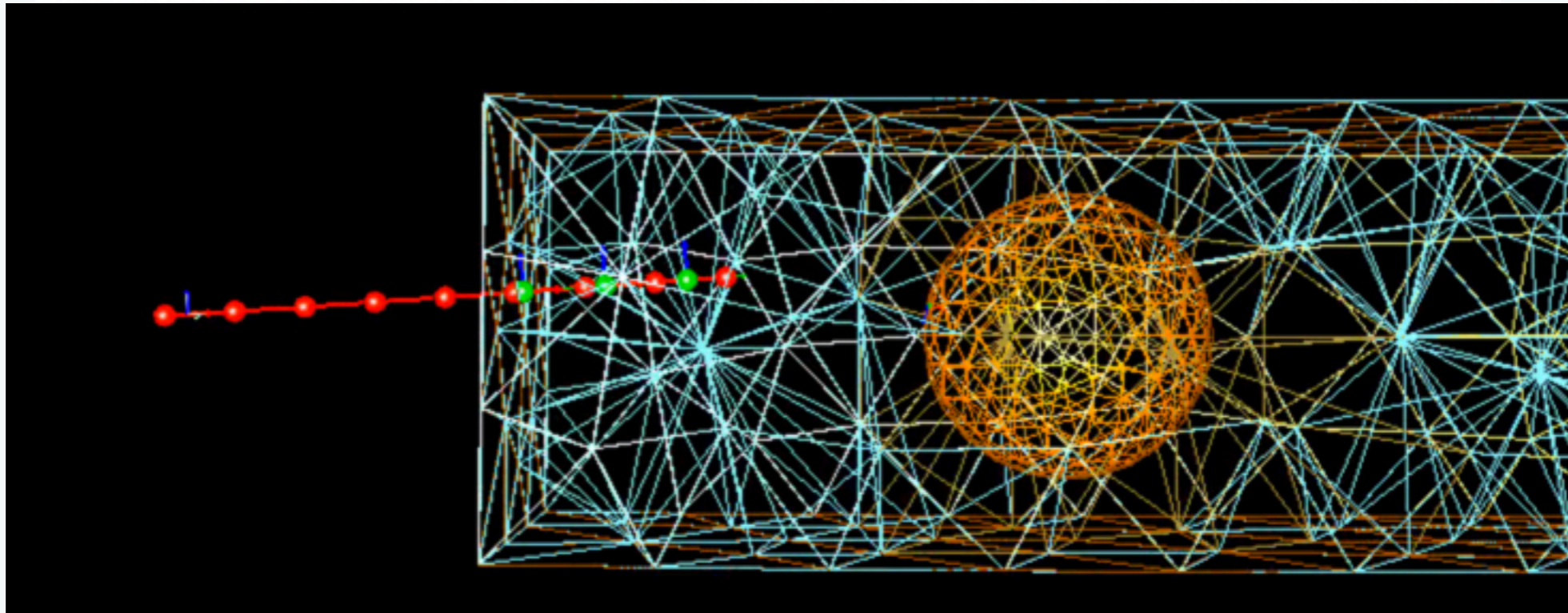


*With implicit boundaries*

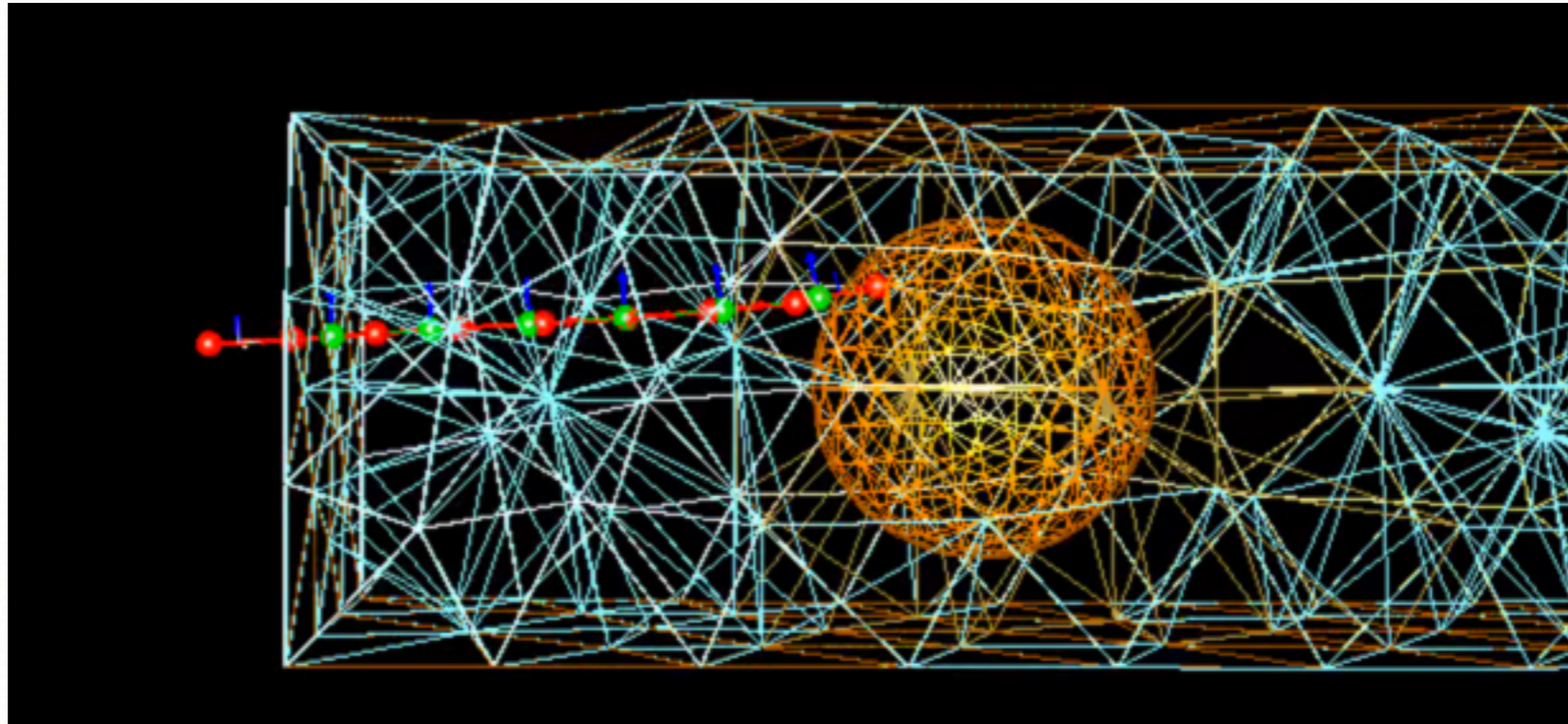


# Real-time needle insertion simulation

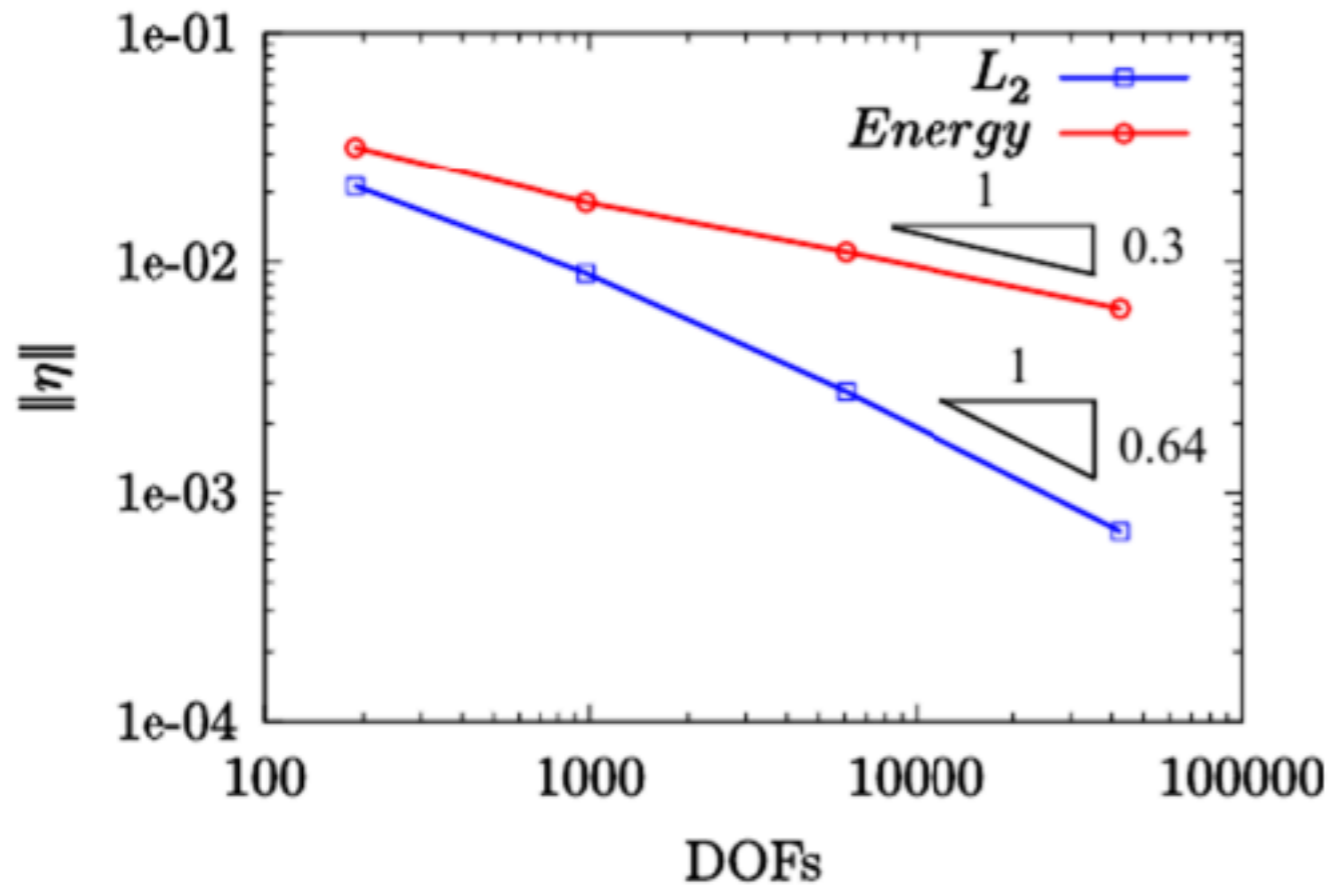
*With implicit boundaries*



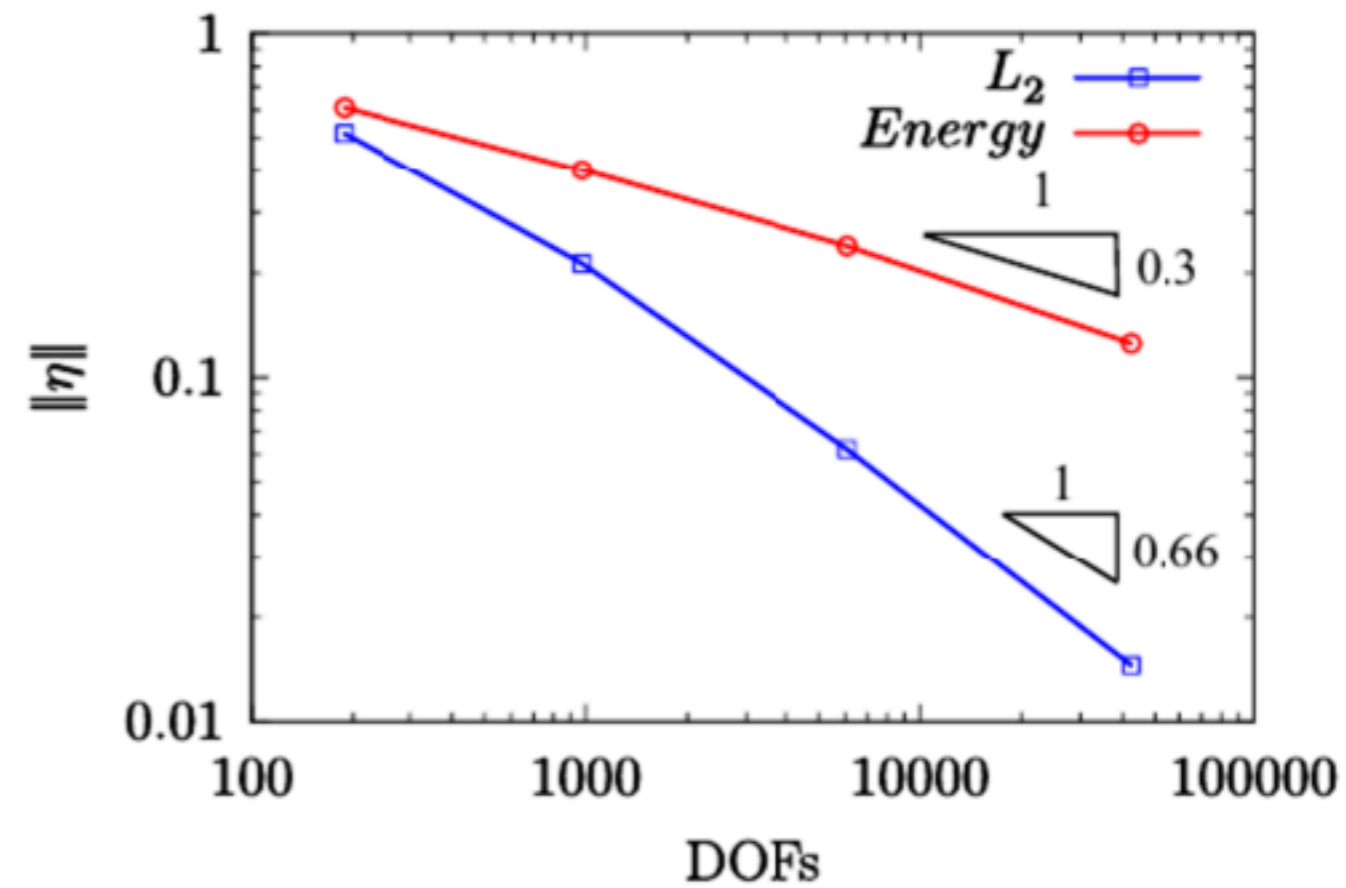
*With implicit boundaries*



*With implicit boundaries*



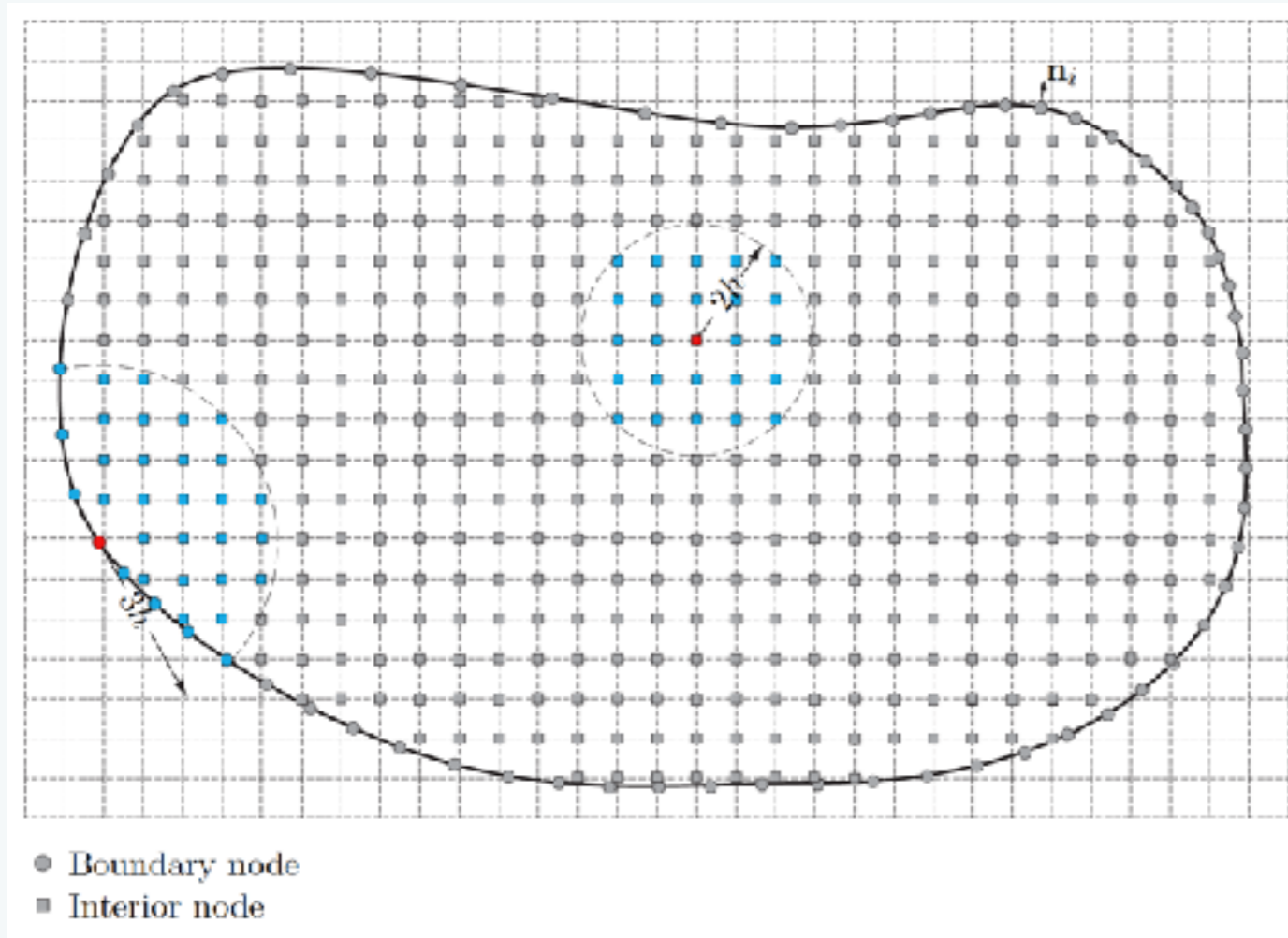
(a)



(b)



# Discretisation Correction of Particle Strength Exchange Collocation

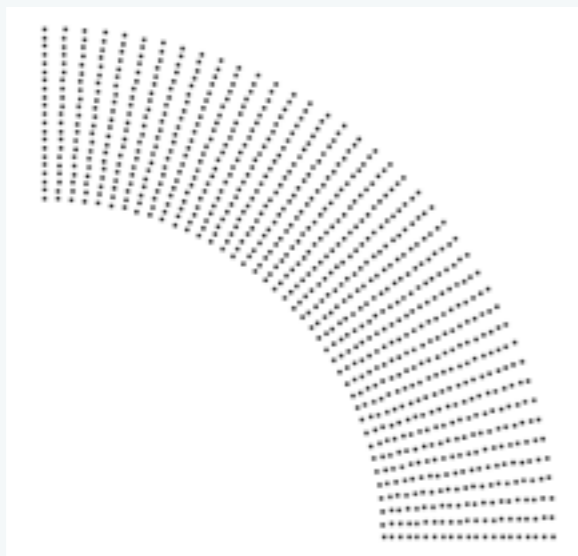
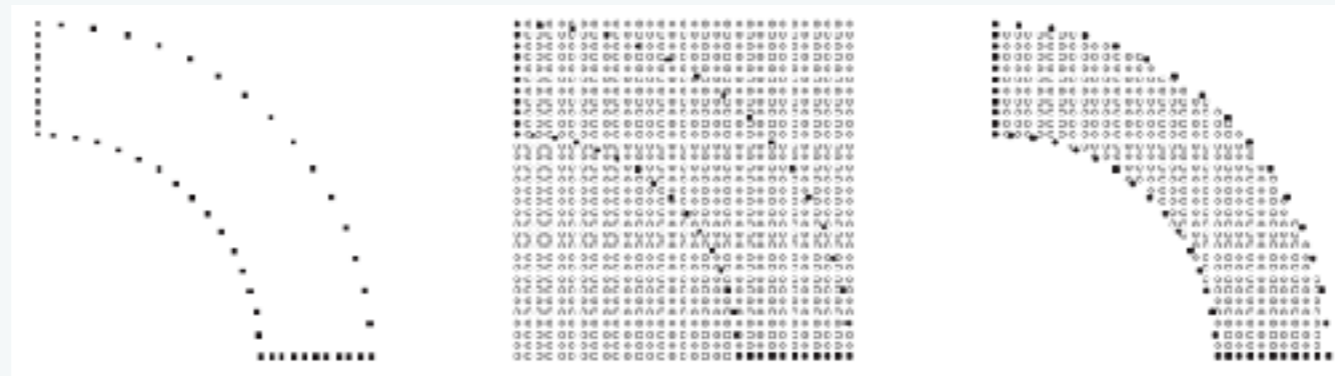


Key idea: use “generalized” finite differences

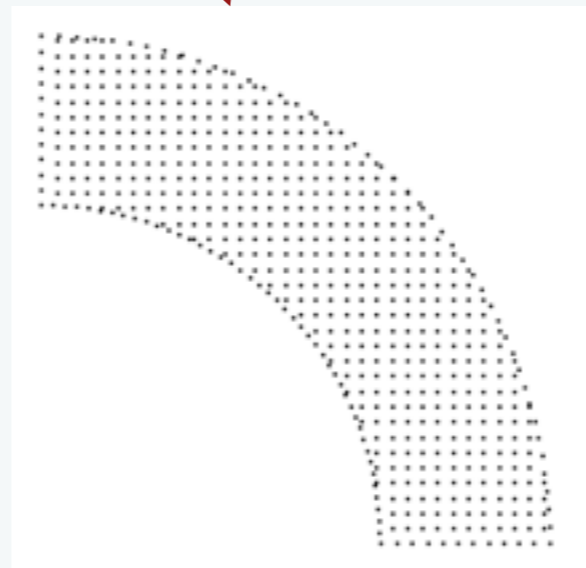
Key difficulty: stability and complex boundaries

Birte Schrader, Sylvain Reboux, and Ivo F Sbalzarini. Discretization correction of general integral PSE operators for particle methods. *Journal of Computational Physics*, 229(11):4159–4182, 2010.

K. Agathos et al. Stable immersed collocation method for elasto-static analysis directly from CAD [preprint available on [orbi.uni.lu](http://orbi.uni.lu)]



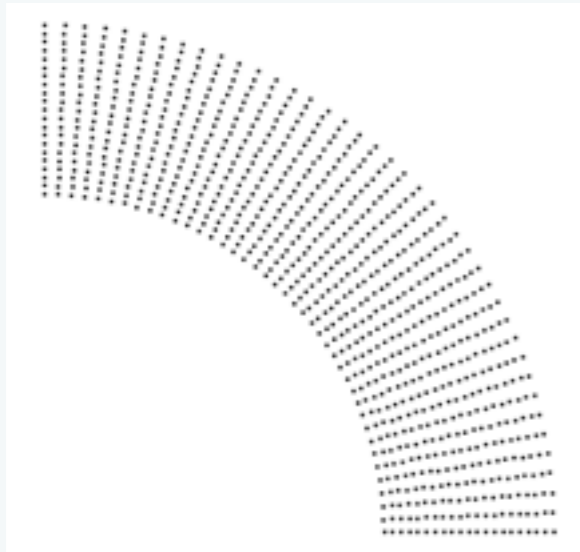
Symmetric



Cartesian



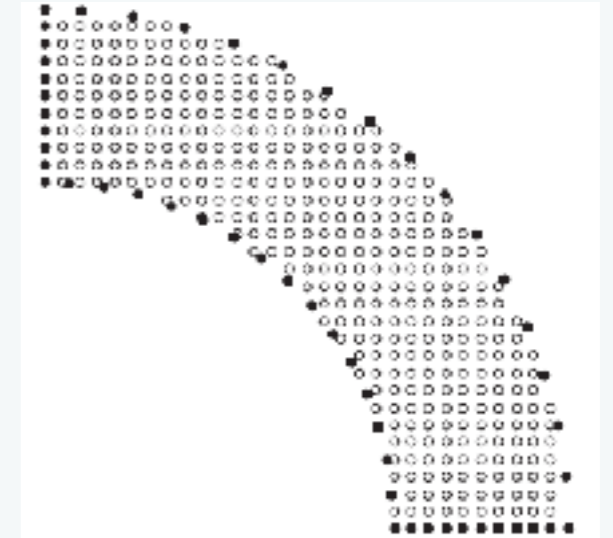
Hybrid



Symmetric



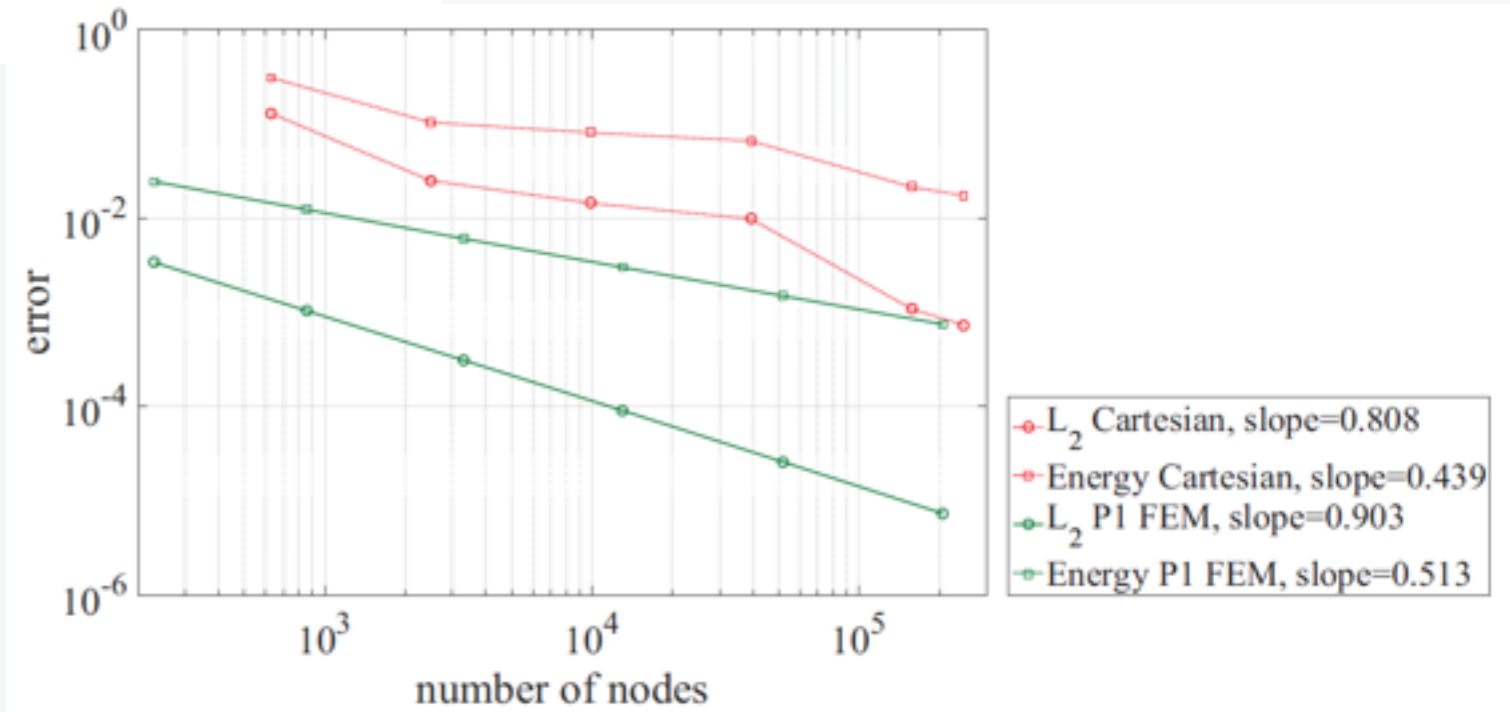
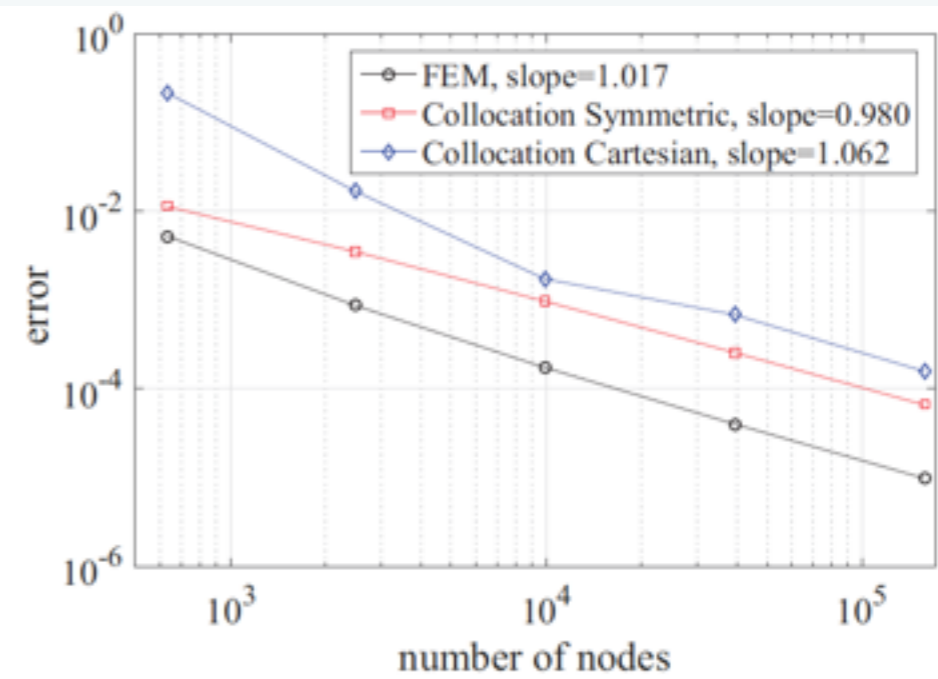
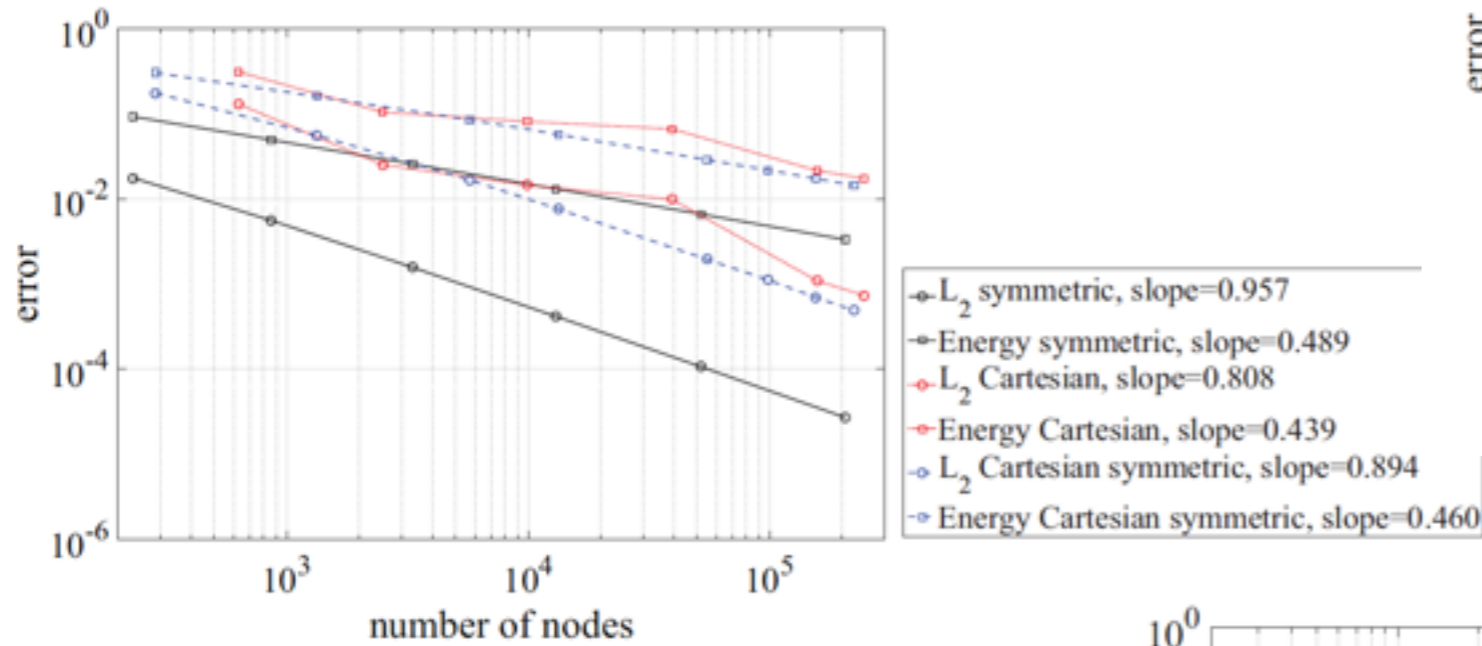
Hybrid



Cartesian

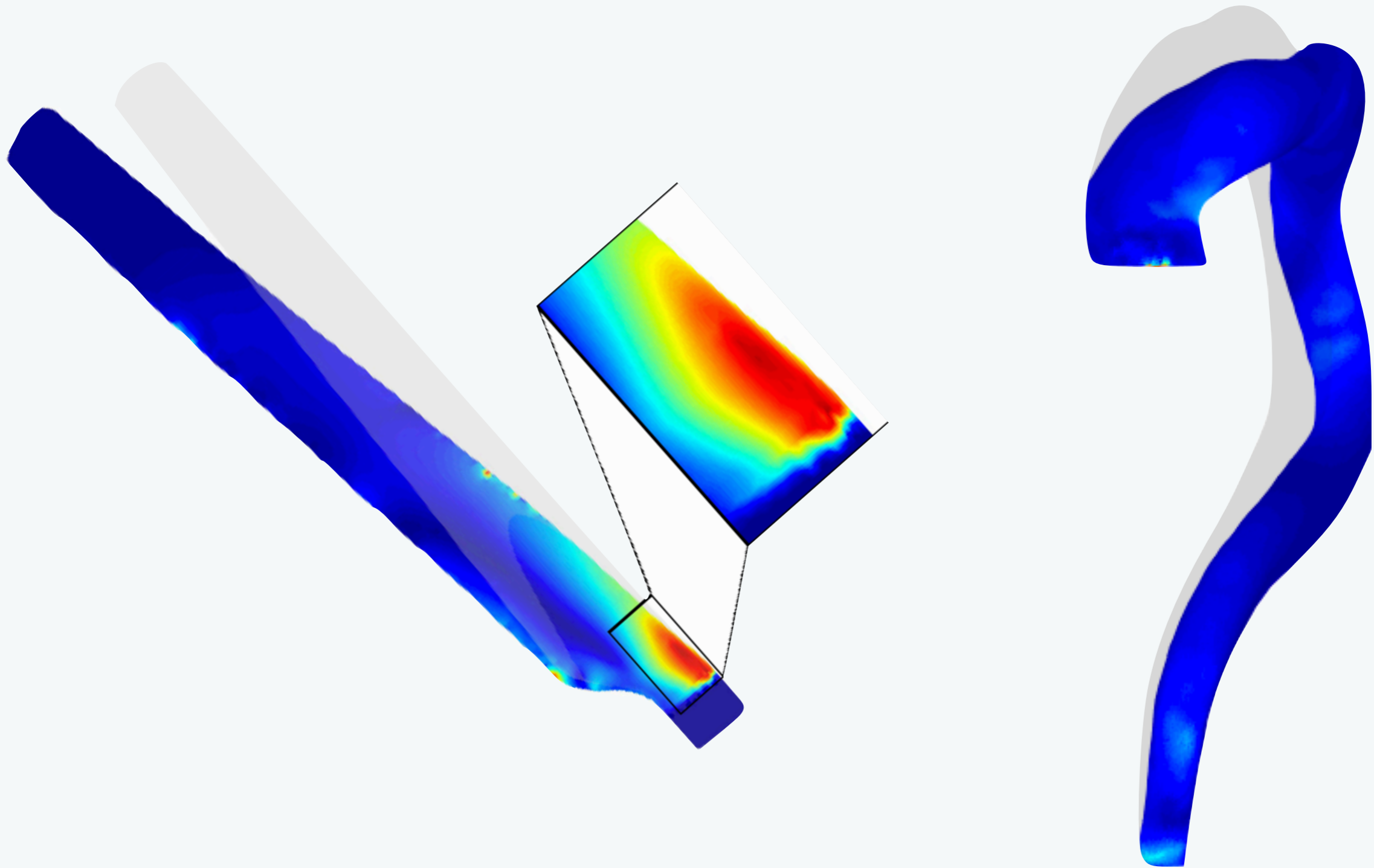
The symmetric node distribution is the most accurate whilst the Cartesian distribution is the worst, the Cartesian-symmetric distribution is intermediate.

Convergence rates of the collocation approach is similar to that of the P1 FEM we compared to whilst the error level is slightly higher. This corroborates results of the isogeometric point collocation method.



Top: Comparison between the different nodal distributions used. Bottom Comparison between the embedded Cartesian distribution and P1 nite elements.

## Wind turbine blade & aorta



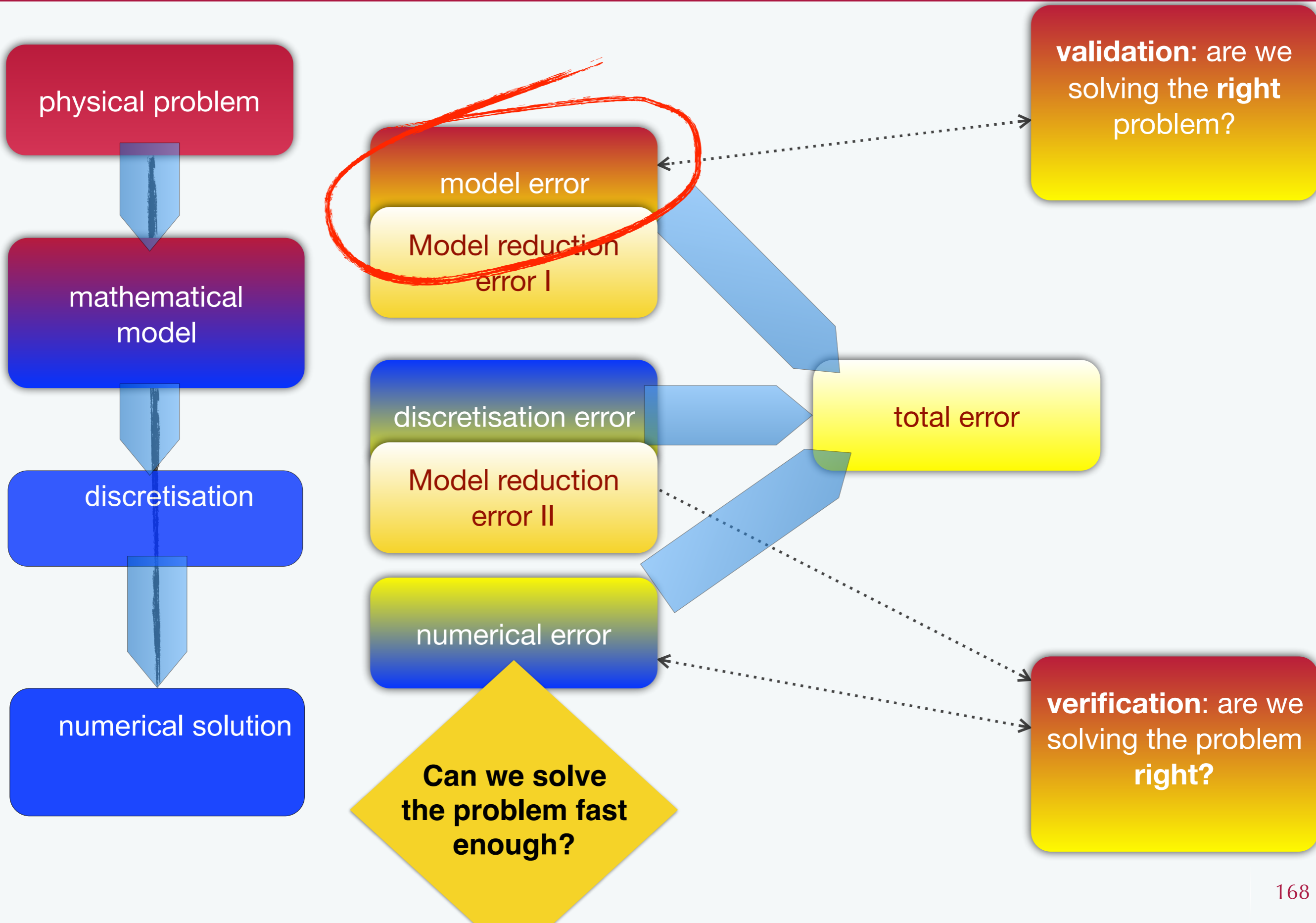
## Partial conclusions on methods decoupling geometry and field approximations

- ◆ There are numerous alternatives (immersed, CutFEM, structured XFEM, collocation...)
- ◆ Discussions on higher order boundaries (see XDMS2017 book of abstracts!)
- ◆ Using CAD geometries within a structured mesh/grid is a versatile approach

**Next: beyond discretisations... for a future lecture... how can we select the best model given (sparse) experimental data and quantify the uncertainties on the parameters of these models.**

**beyond discretisations... for a future lecture... how can we select the best model given (sparse) experimental data and quantify the uncertainties on the parameters of these models.**

# Modelling and simulation





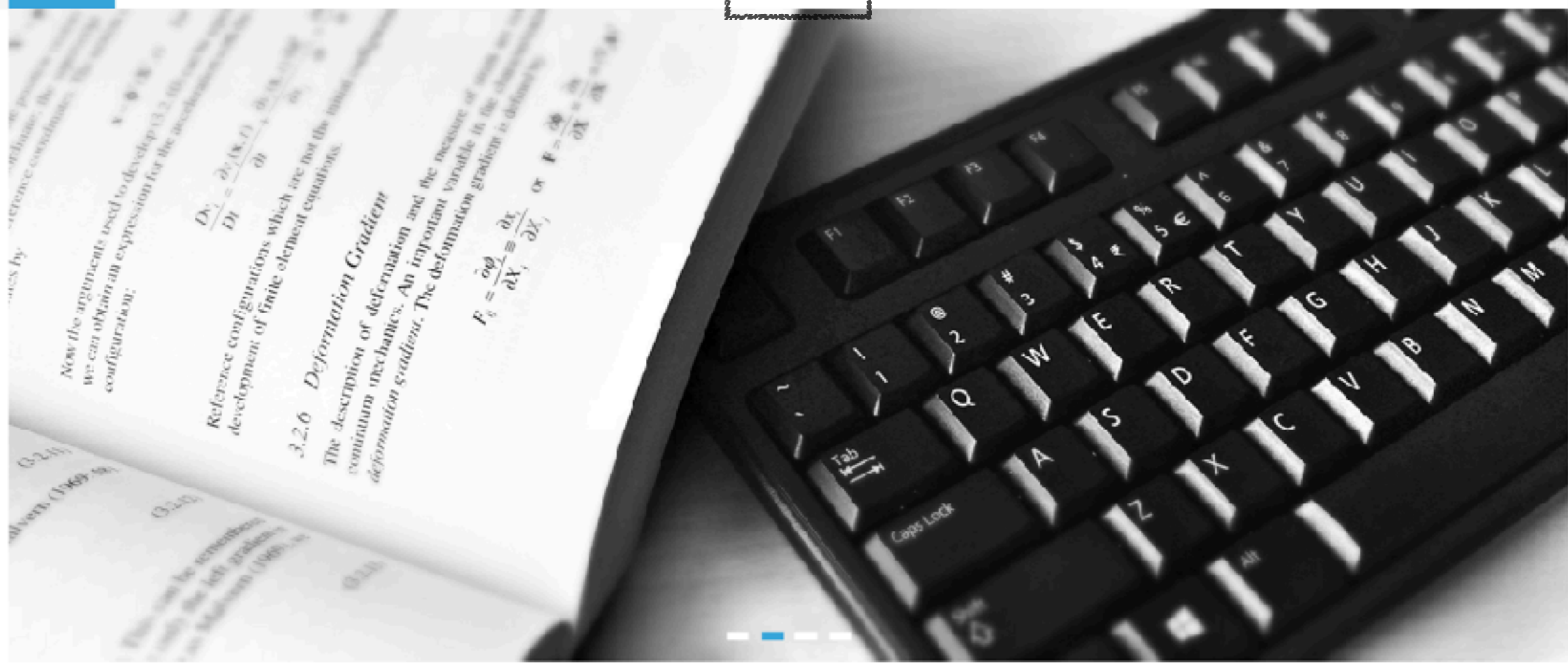


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The work of Stéphane Bordas was supported in part by the European Research Council under the European Union's S Grant Agreement n. 279578

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**Joined:** 2012-04-13 14:29:25

## Projects



### ElemFreGalerkin

A tutorial Galerkin meshfree code

*Last Updated: 2017-01-29*



### OpenXfem++

OpenXfem++ is an XFEM (eXtended Finite Element Method) written in C++.

*Last Updated: 2017-01-28*



### XFEM

XFEM implementation in MATLAB

*Last Updated: 2017-02-08*



### ciGen

ciGen is a short C++ code to generate cohesive interface elements.

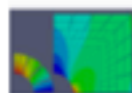
*Last Updated: 2017-01-25*



### igabem

Isogeometric boundary element analysis with matlab

*Last Updated: 2017-03-02*



### igafem

Open source 3D Matlab Isogeometric Analysis Code

*Last Updated: 2017-02-05*



### igafemgui

*Last Updated: 2017-05-10*

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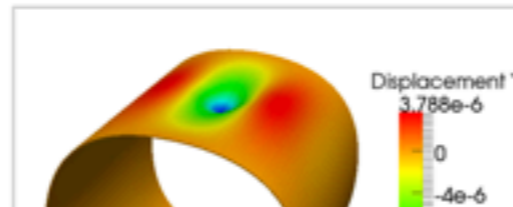
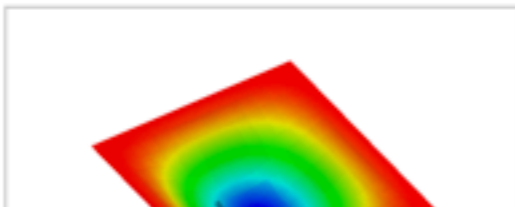
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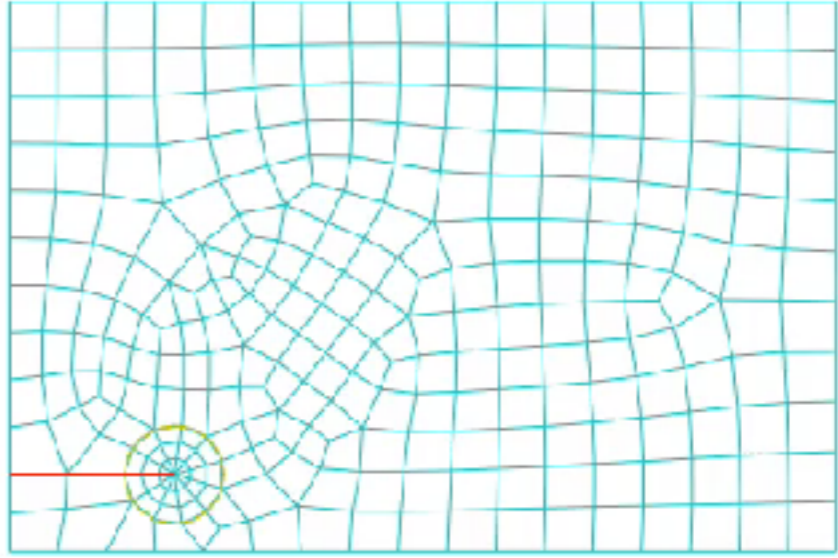
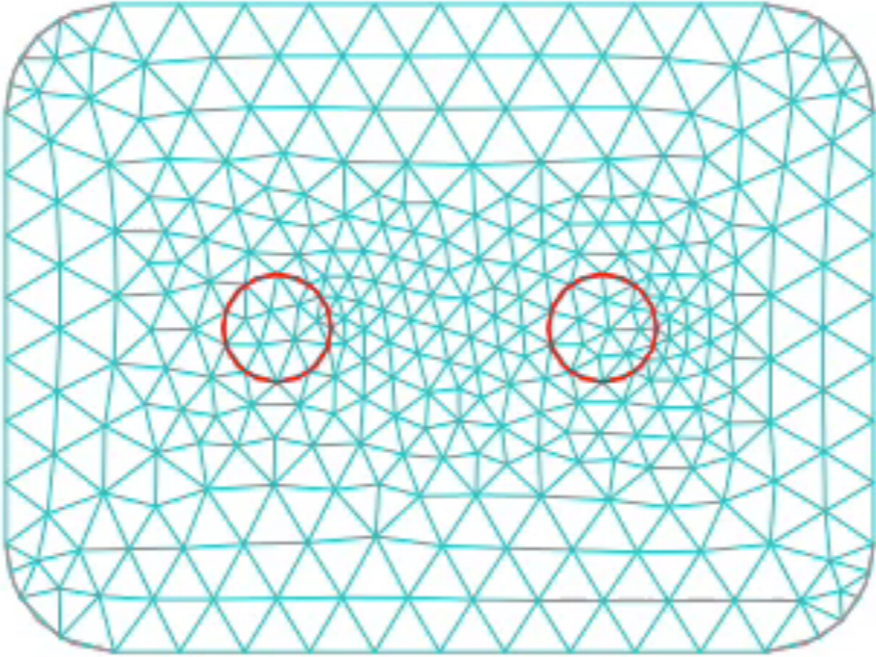
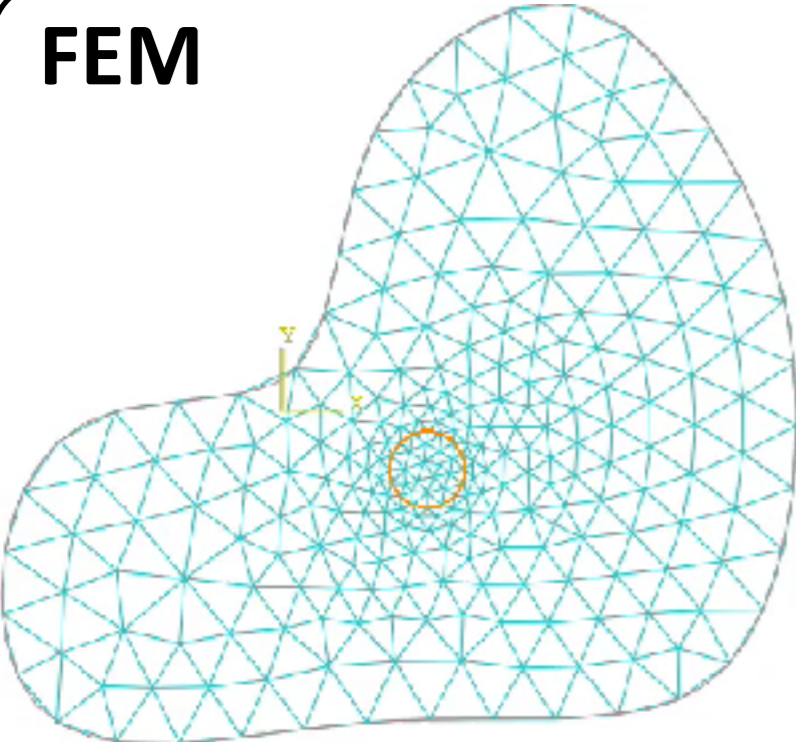
freeends



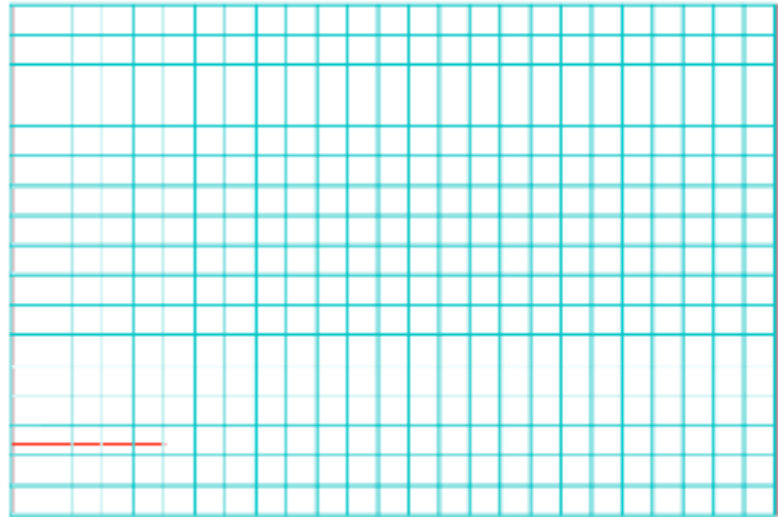
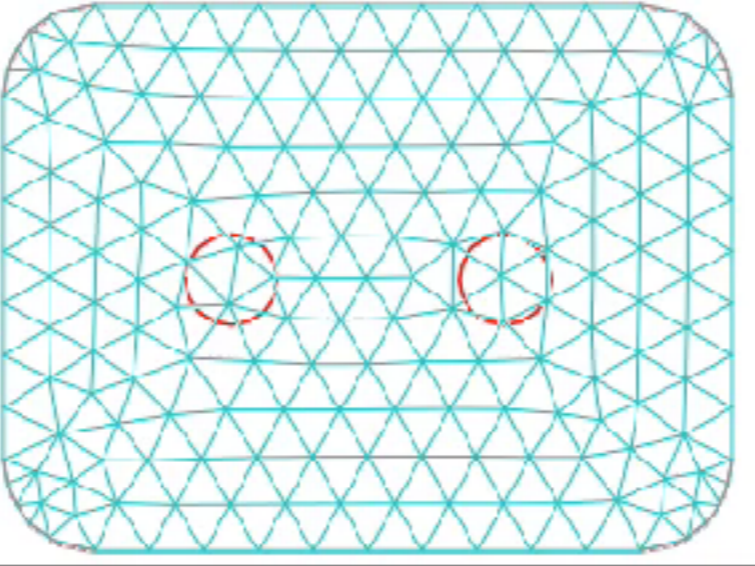
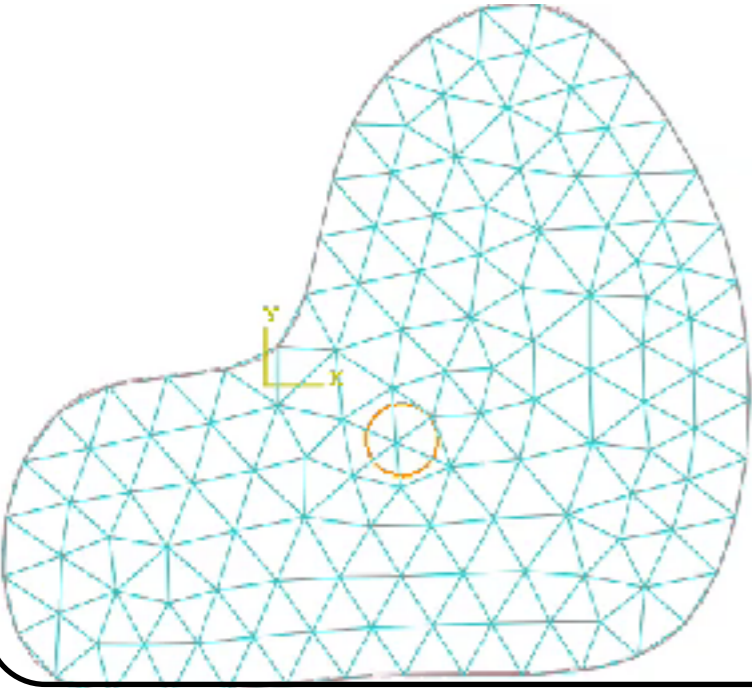
**beyond discretisations... for a future lecture... how can we select the best model given (sparse) experimental data and quantify the uncertainties on the parameters of these models.**



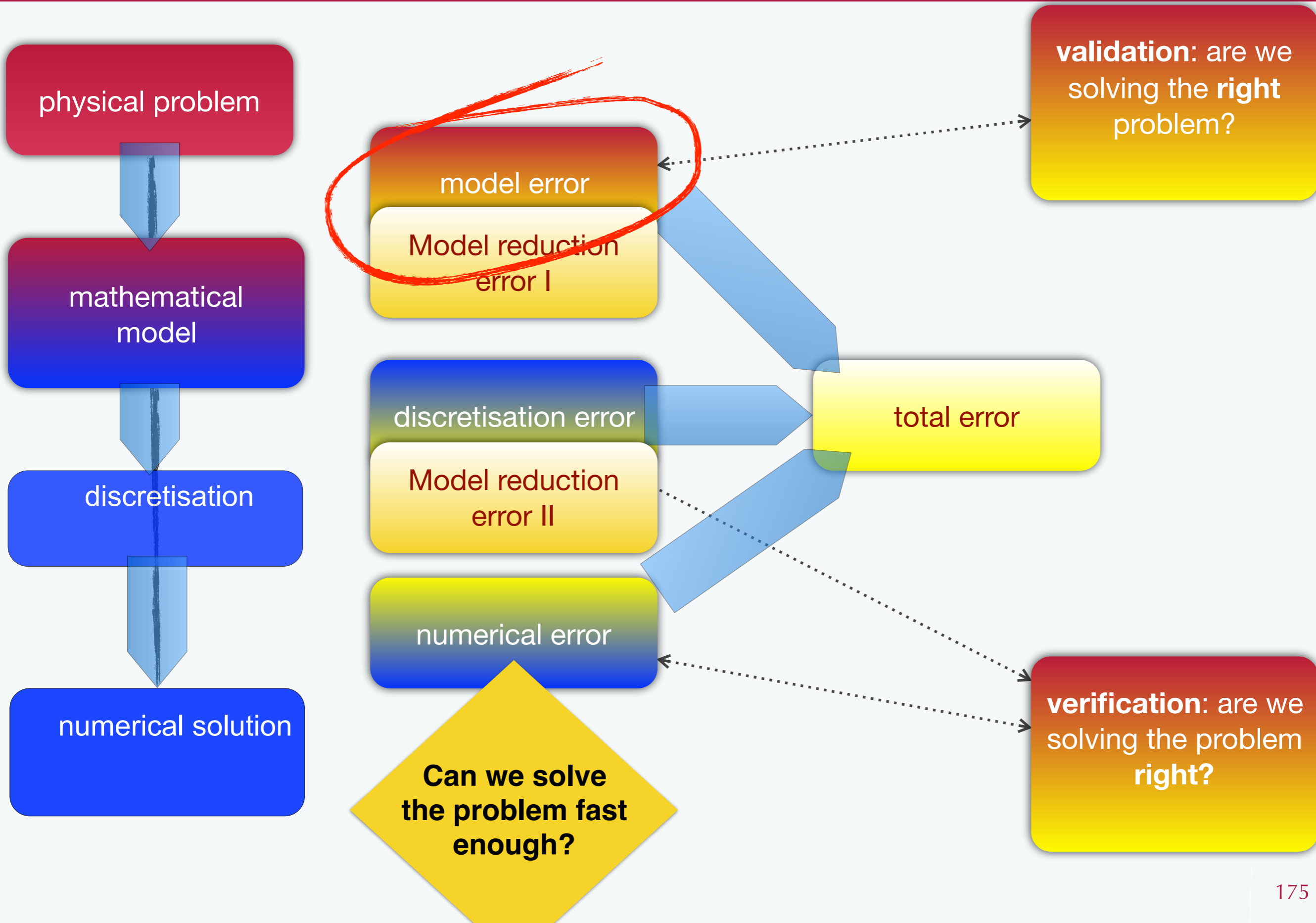
**FEM**

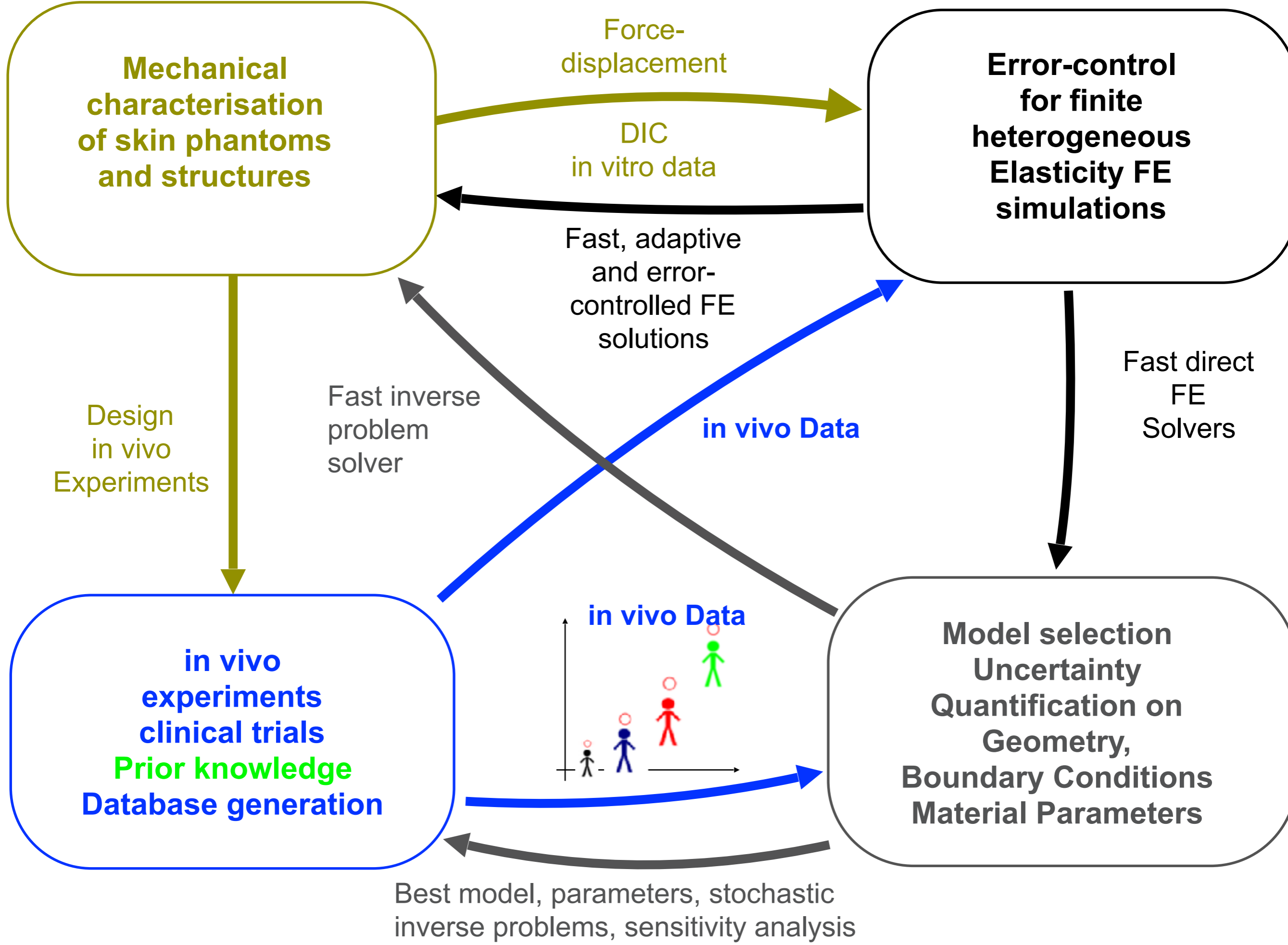


**XFEM**



# Modelling and simulation







# Ingredient #1 - Error control

Error-control  
for finite  
heterogeneous  
Elasticity FE  
simulations

# Controlling the Error on Target Motion through Real-time Mesh Adaptation: Application to Deep Brain Stimulation

H. P. Bui, S. Tomar, H. Courtecuisse, M. Audette, S. Cotin and S. P. A. Bordas

## Ingredient #2 - Uncertainty quantification

Model selection  
Uncertainty  
Quantification on  
Geometry,  
Boundary Conditions  
Material Parameters

# General framework for uncertainty quantification

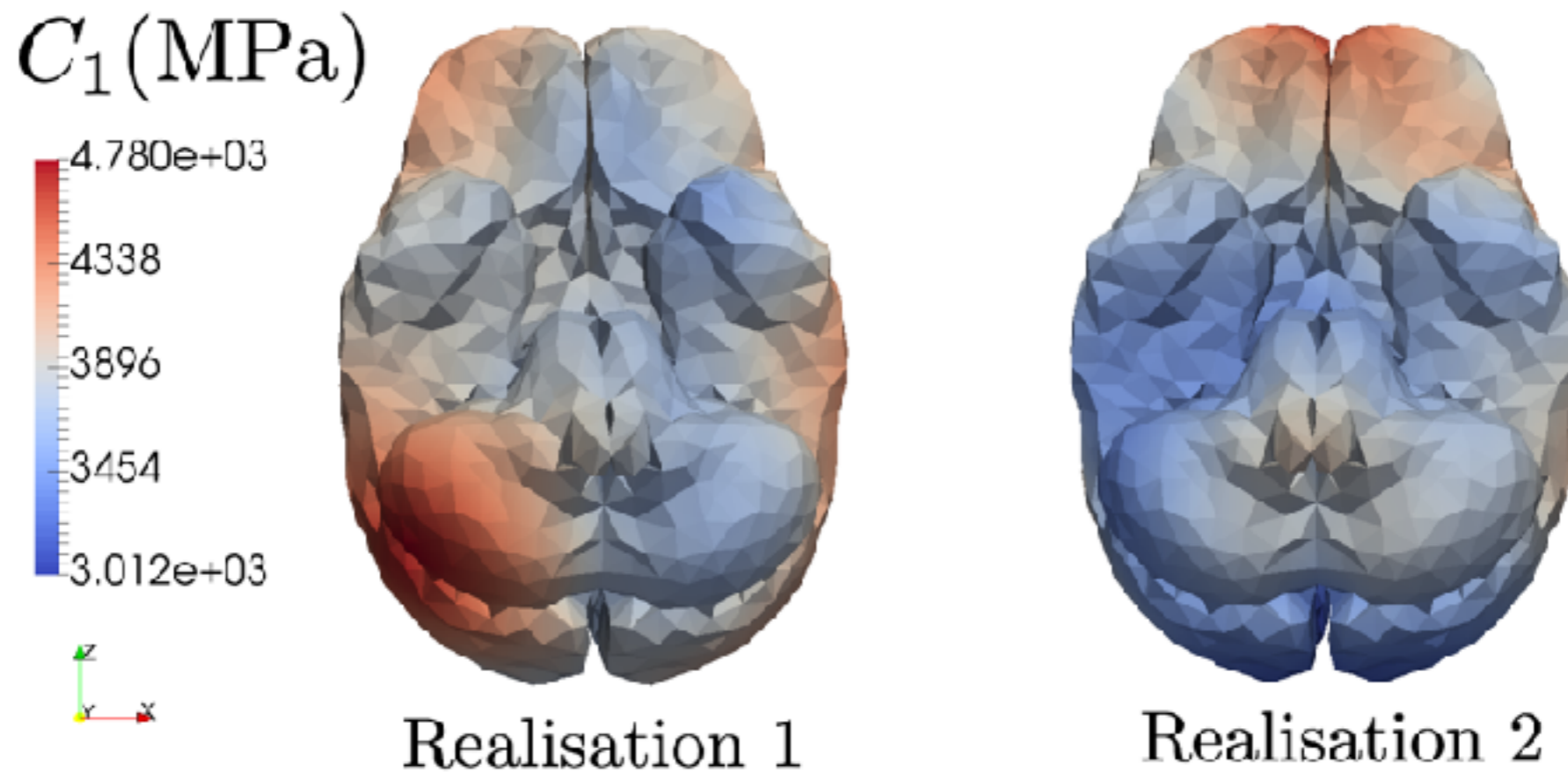
- ▶ Stochastic non-linear system:  $F(\mathbf{u}, \boldsymbol{\omega}) = \mathbf{0}$
  - ▶ Probability space:  $(\Omega, \mathcal{F}, P)$
  - ▶ Random parameters:  $\boldsymbol{\omega} = (\omega_1, \omega_2, \dots, \omega_M)$
- 
- ▶ Objective: provide statistical data for the solution of the problem.
  - ▶ Integration (to determine the expected value of a quantity of interest):

$$E[\Psi(u(\boldsymbol{\omega}))] = \int_{\Omega} \Psi(u(\boldsymbol{\omega})) dP(\boldsymbol{\omega})$$

# Random Fields

- ▶ Different methods: Karhunen–Loève expansion [Adler 2007], Fast Fourier transform [Nowak 2004].

## Randoms fields

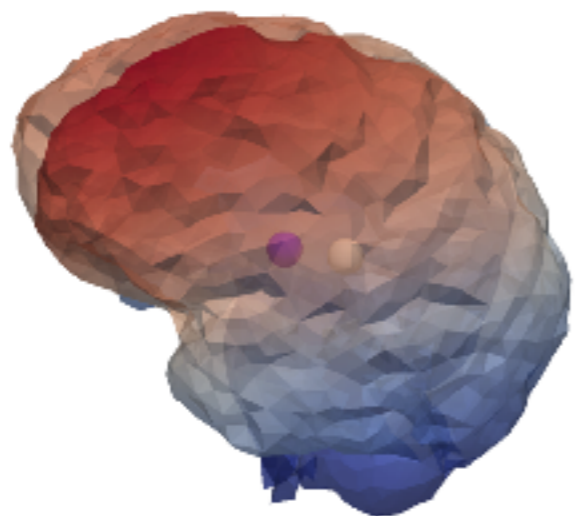
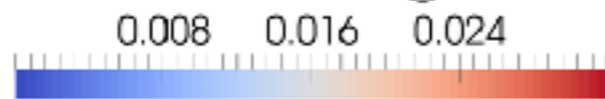


Two realisations of RF, with a log-normal distribution, for the parameter  $C_1$  (in MPa).

# Stochastic FE analysis of brain deformation

## Numerical results (8 RV, Holzapfel model)

Displacement magnitude (m)

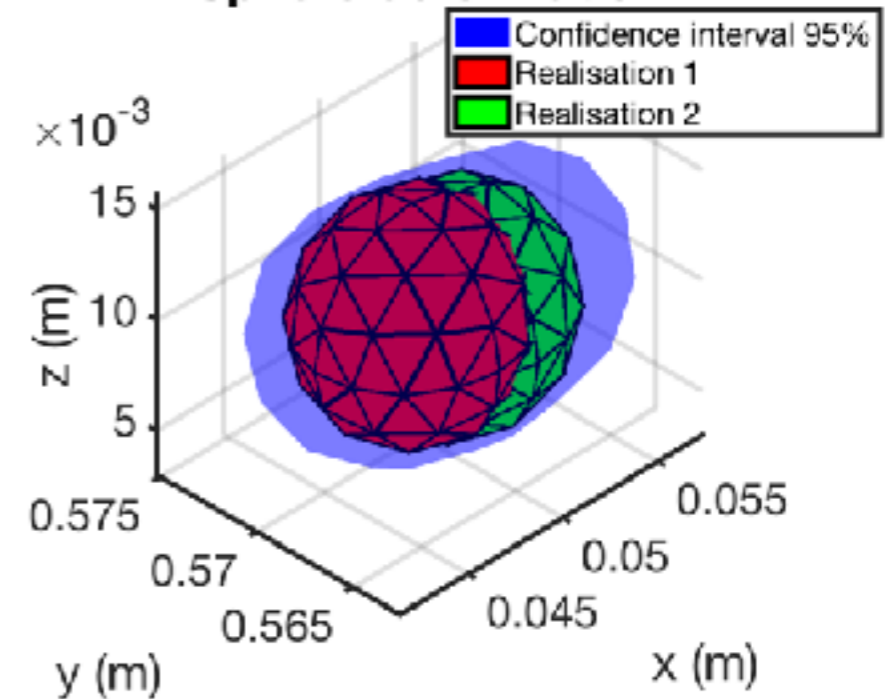


- Initial
- Deformed



Brain deformation with random parameters  
1 MC realisation.

**Sphere deformation**



Confidence interval 95%  
MC simulations.

# Numerical results: convergence

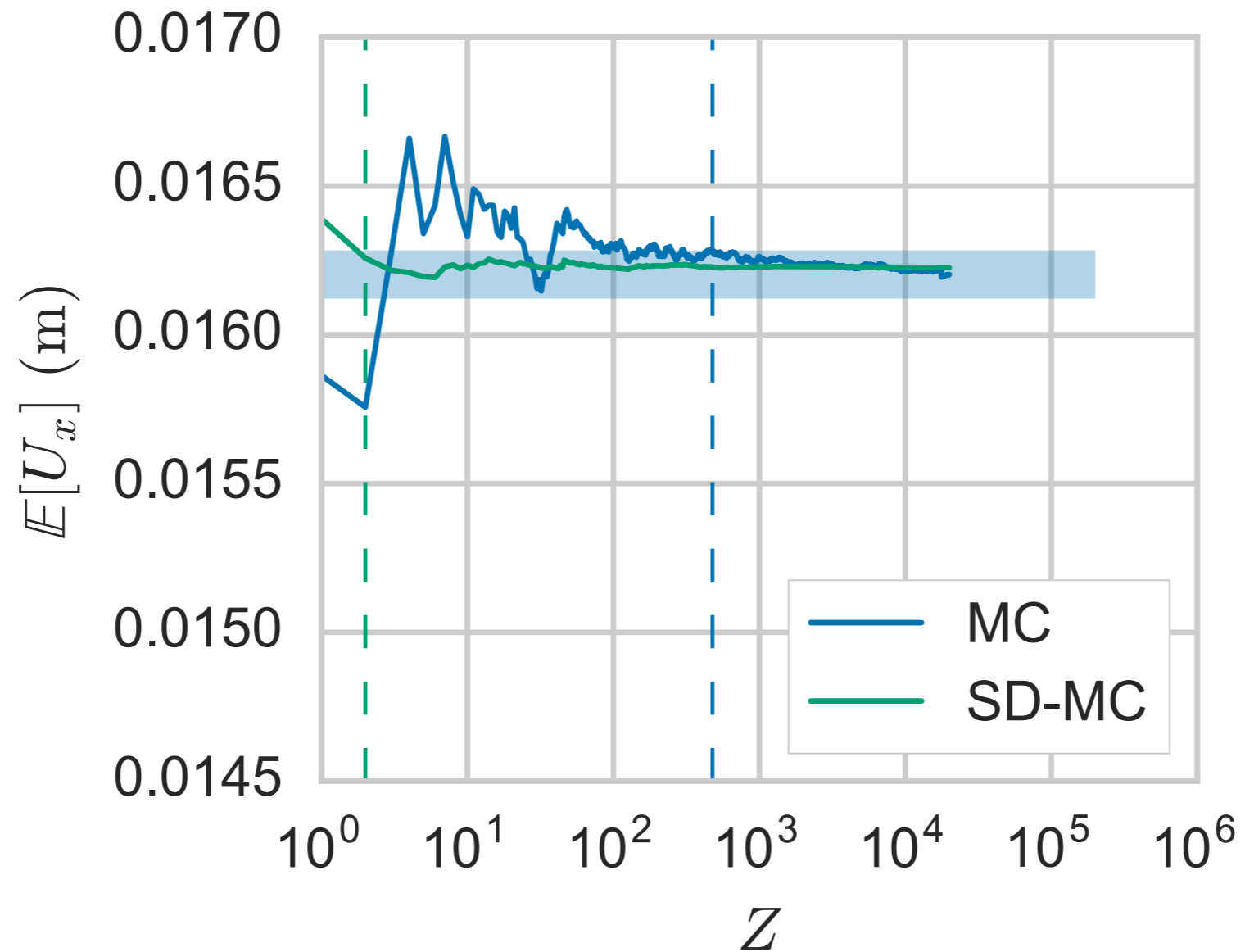
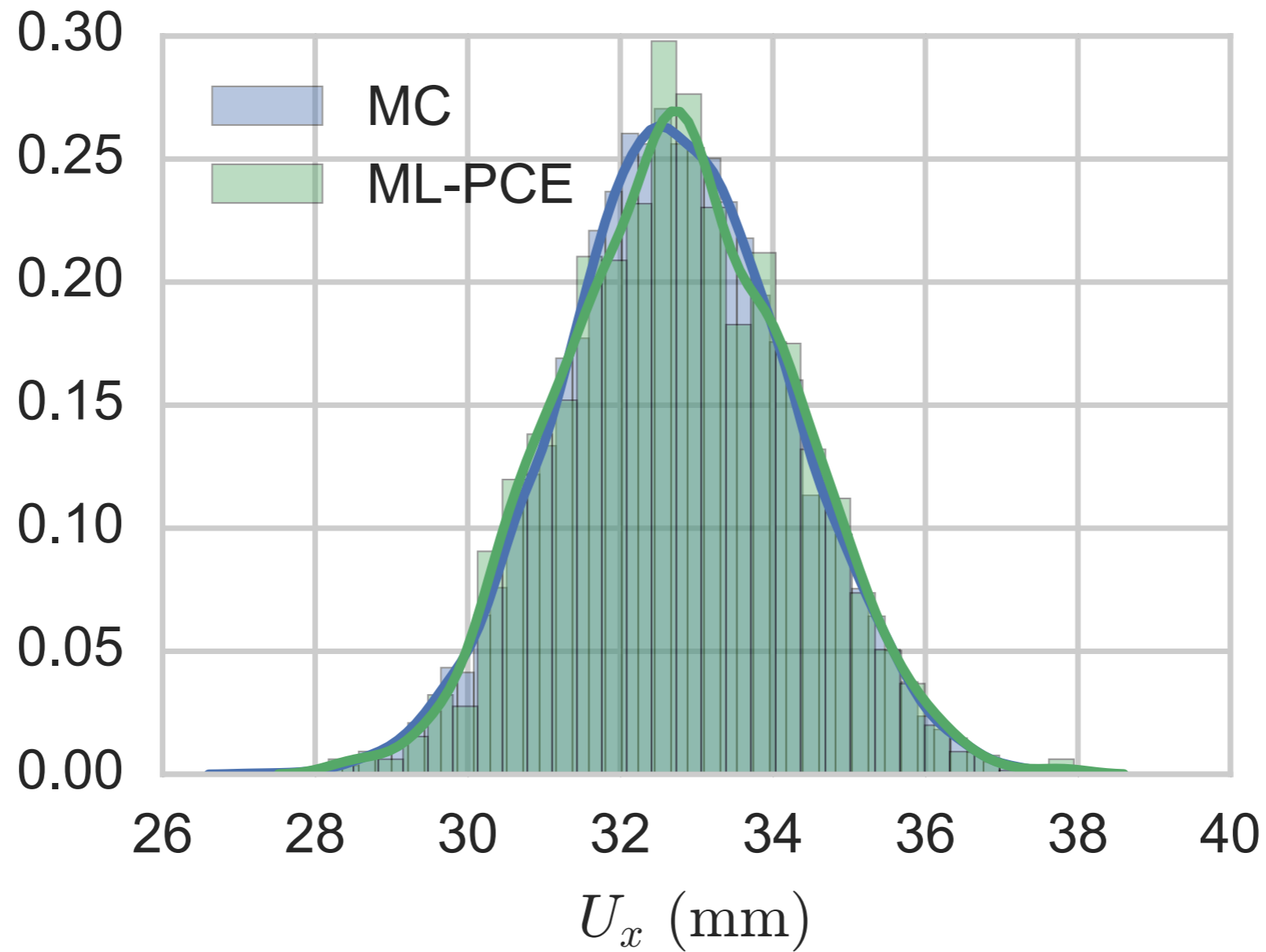


Fig. Center of the sphere: expected value of the displacement in the x direction as a function of  $Z$ .

Numerical results (8 RV, Holzapfel model)  
ML Monte-Carlo technique: ML-PCE

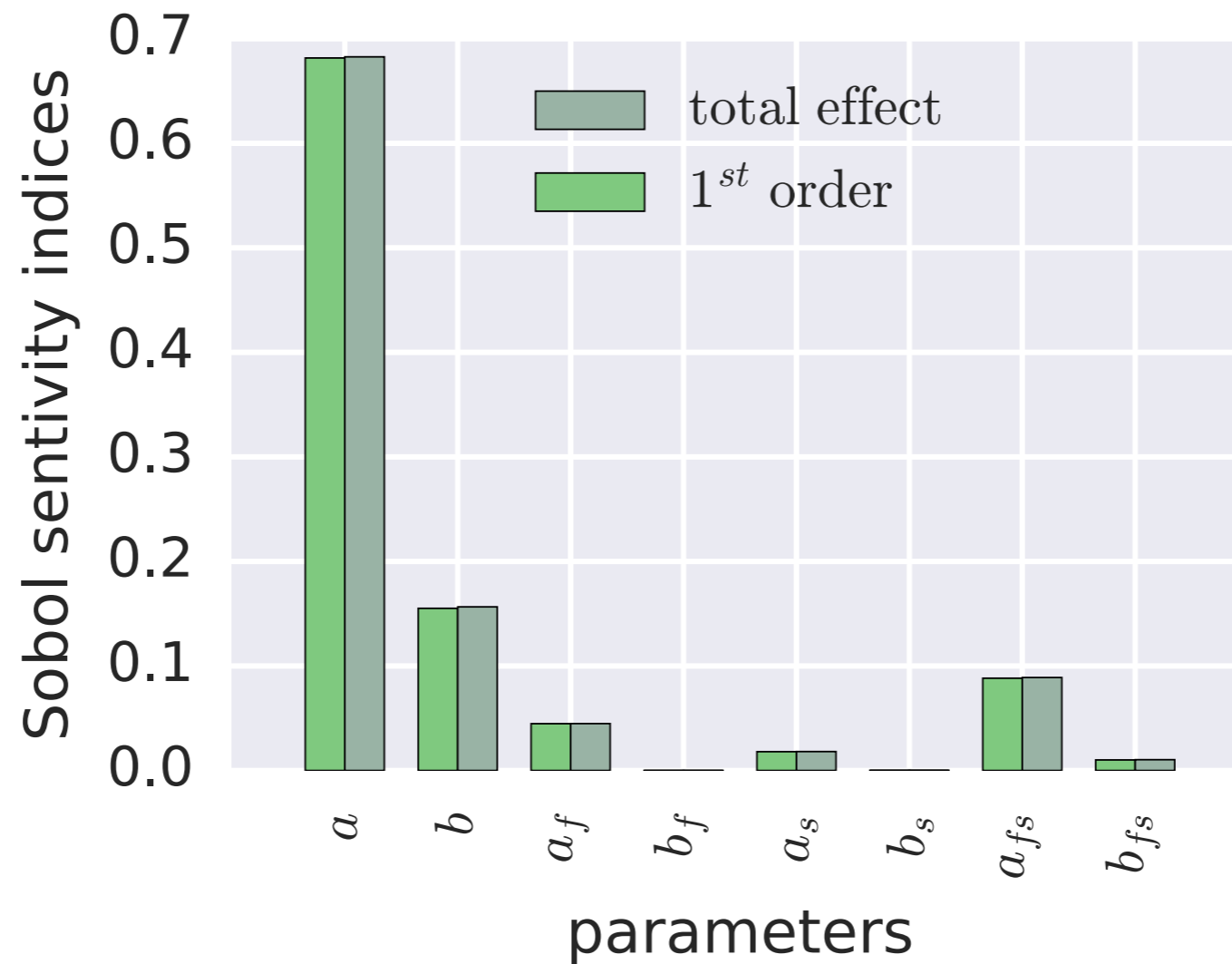


Histogram (MC and MC-PCE methods).



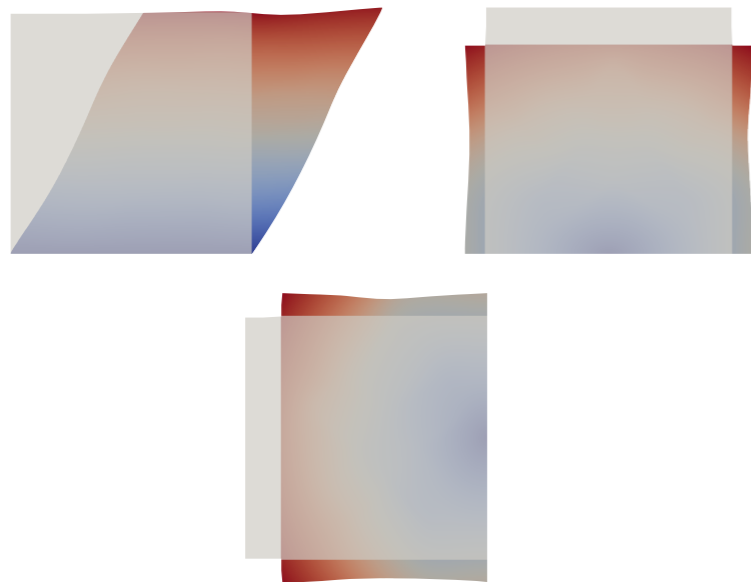
# Global sensitivity analysis

► Sobol sensitivity indices [Sobol 2015, Saltelli 2002]



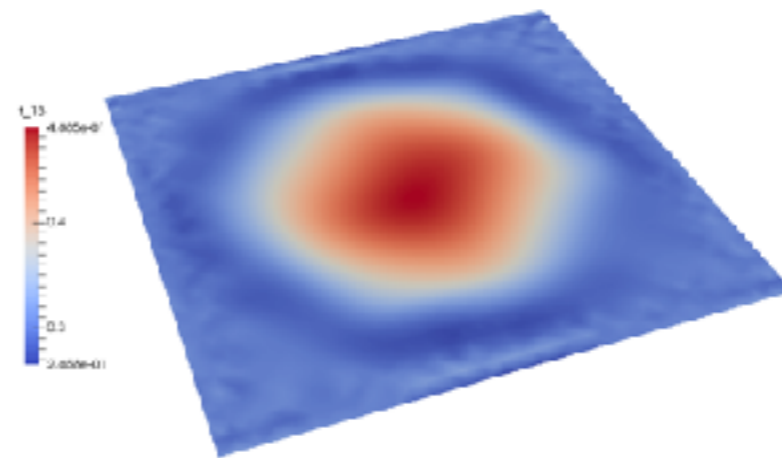
Quantity of interest: displacement magnitude of the target.

# Bayesian testbed for characterising hyperelastic materials

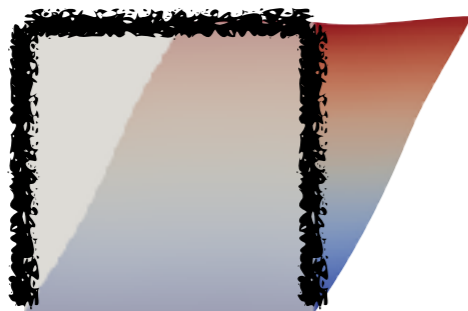


Experimental results

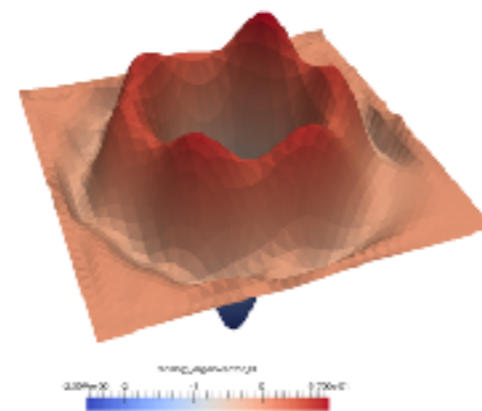
$$\pi_{\text{posterior}}(x | y) \propto \pi_{\text{likelihood}}(y | x) \pi_{\text{prior}}(x)$$



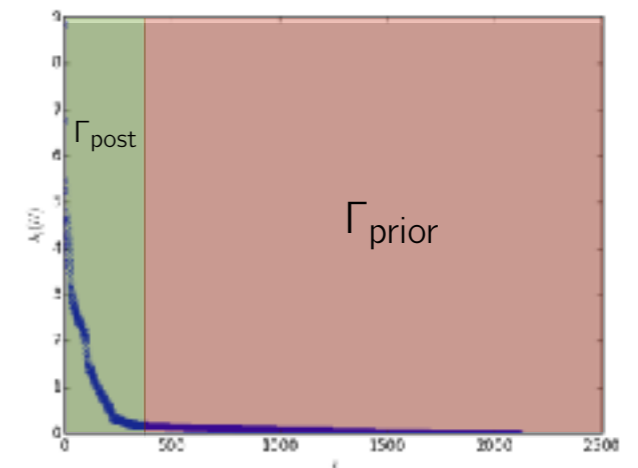
Parameter recovery

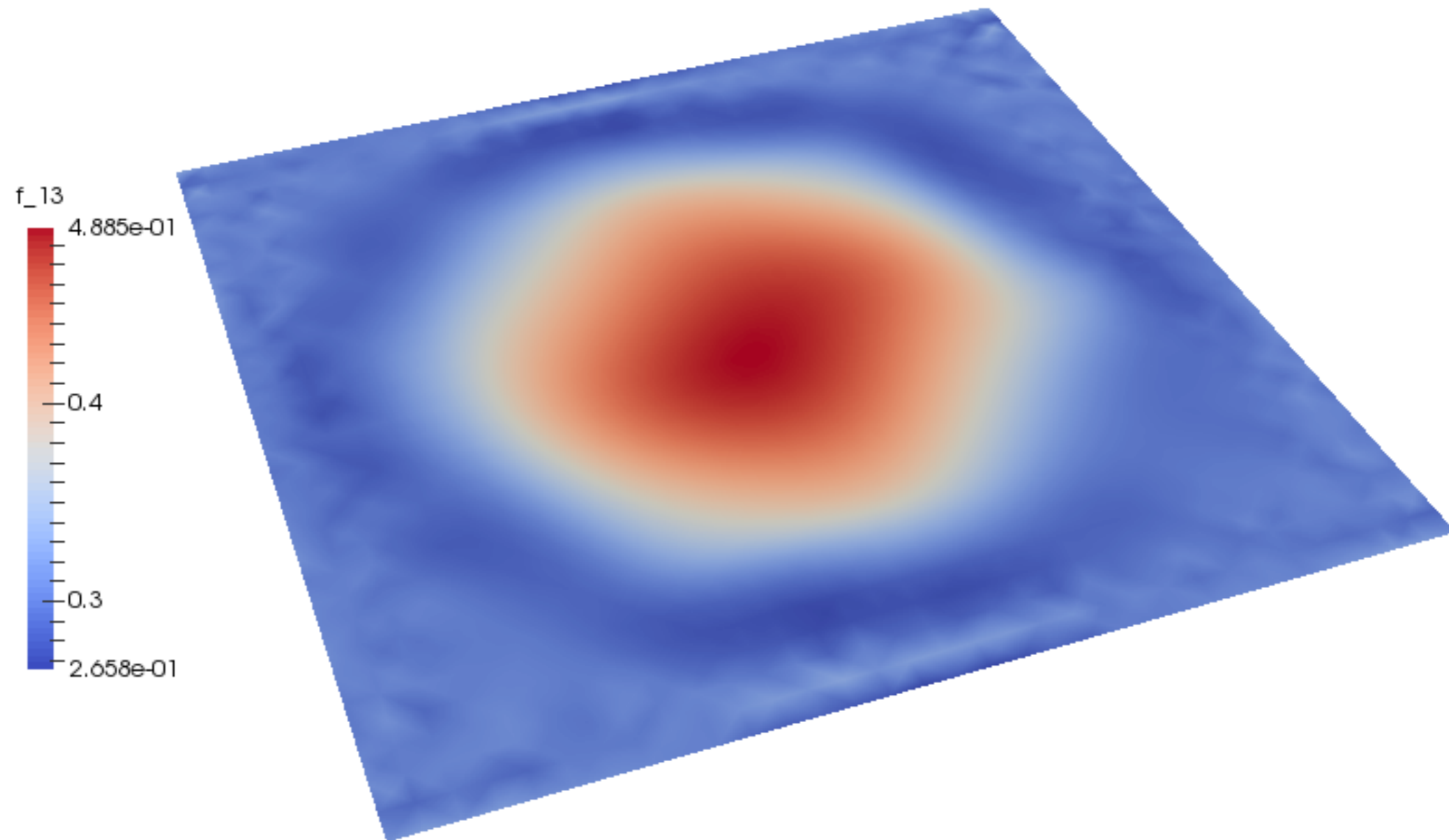


Uncertain and partial data

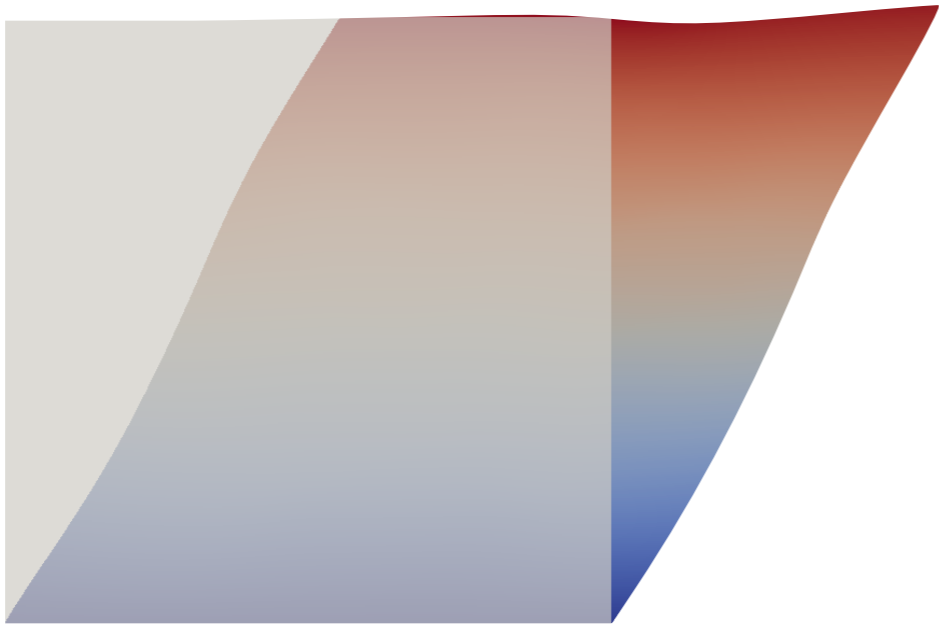


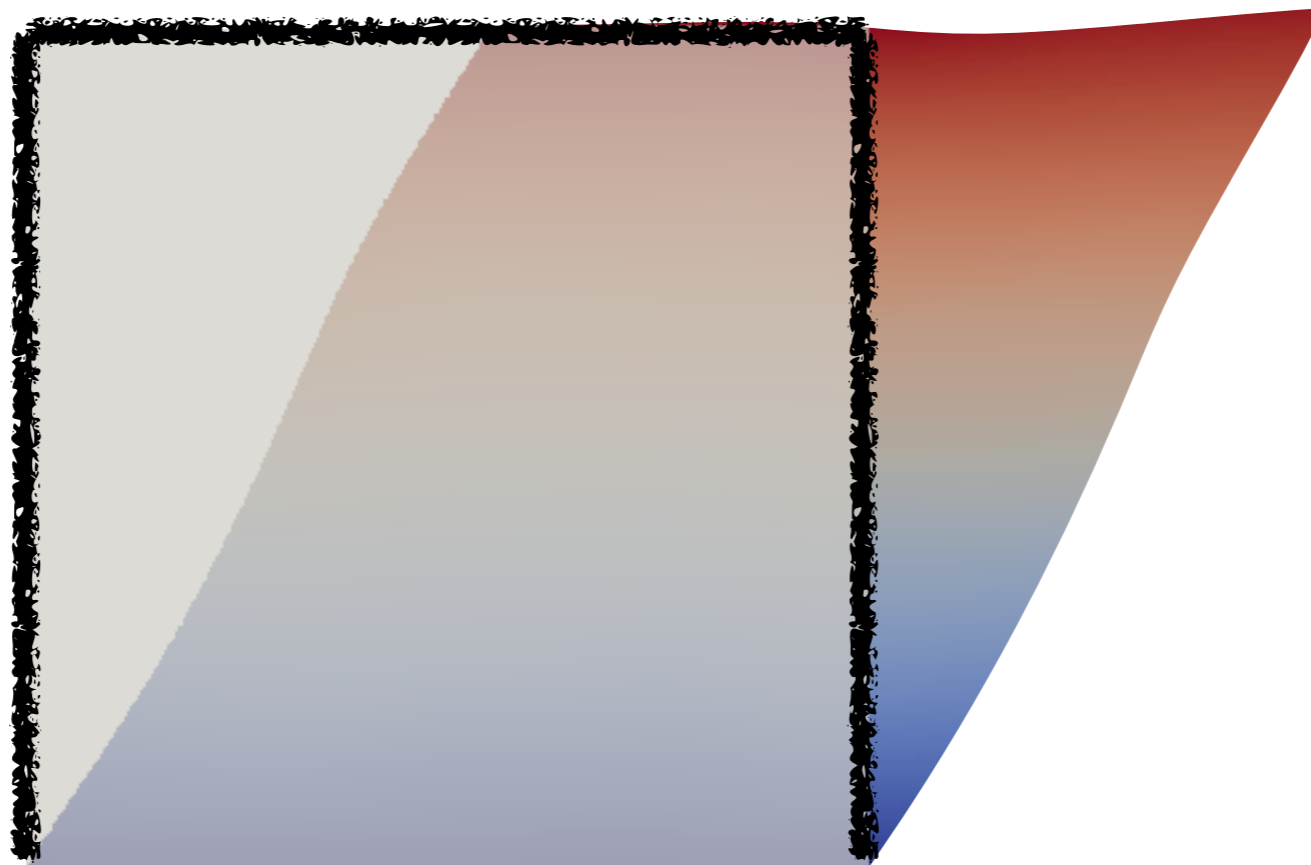
Quantification of uncertainty

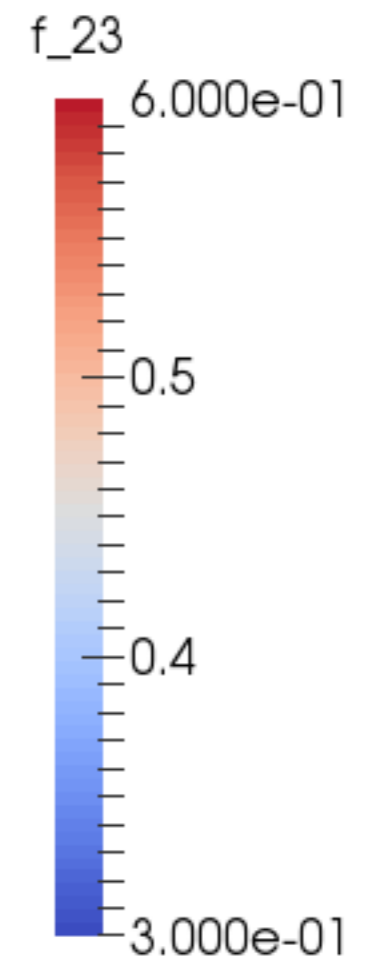
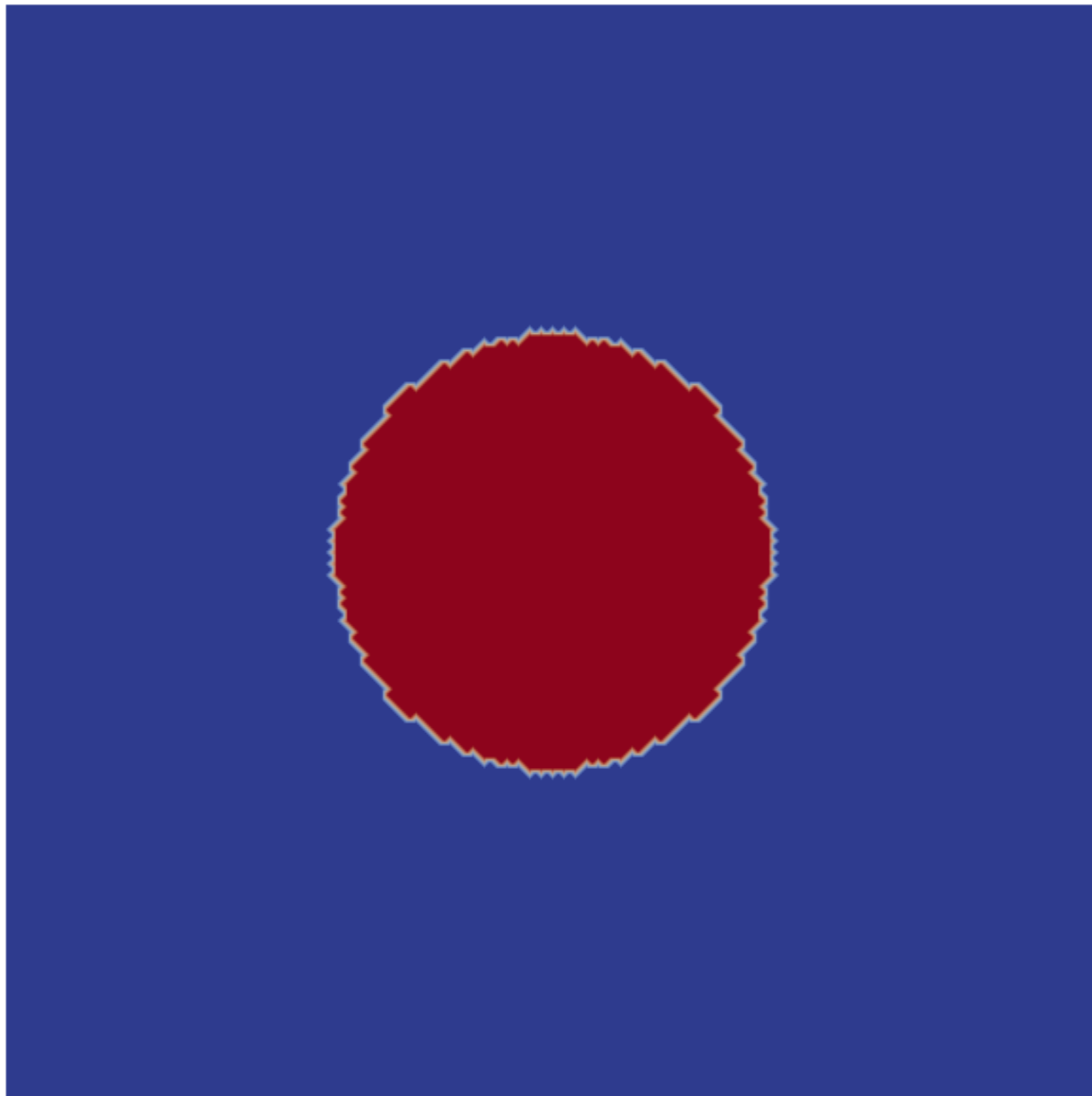


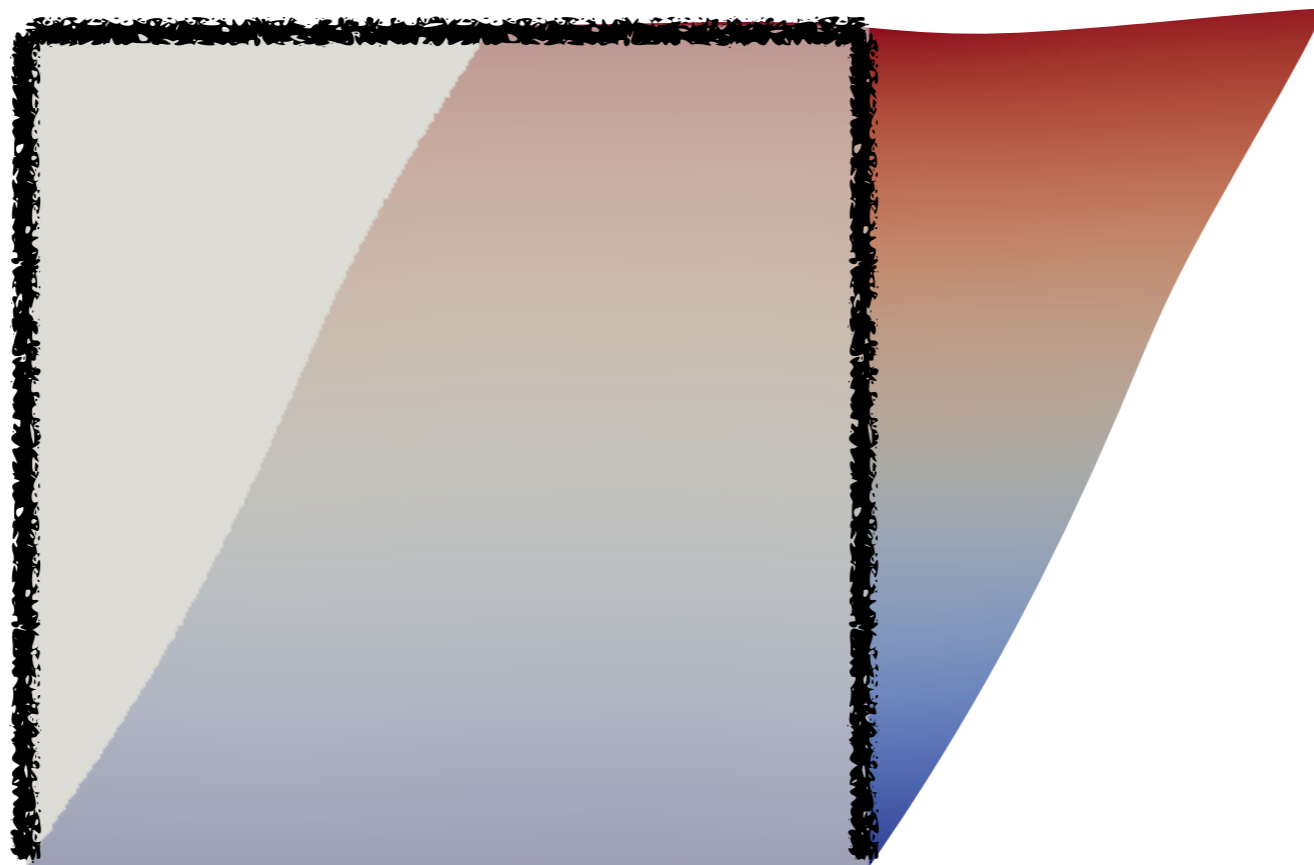


$X_{\text{map}}$









Q: What can we infer about the material parameters inside the domain, just from displacement observations on the outside?

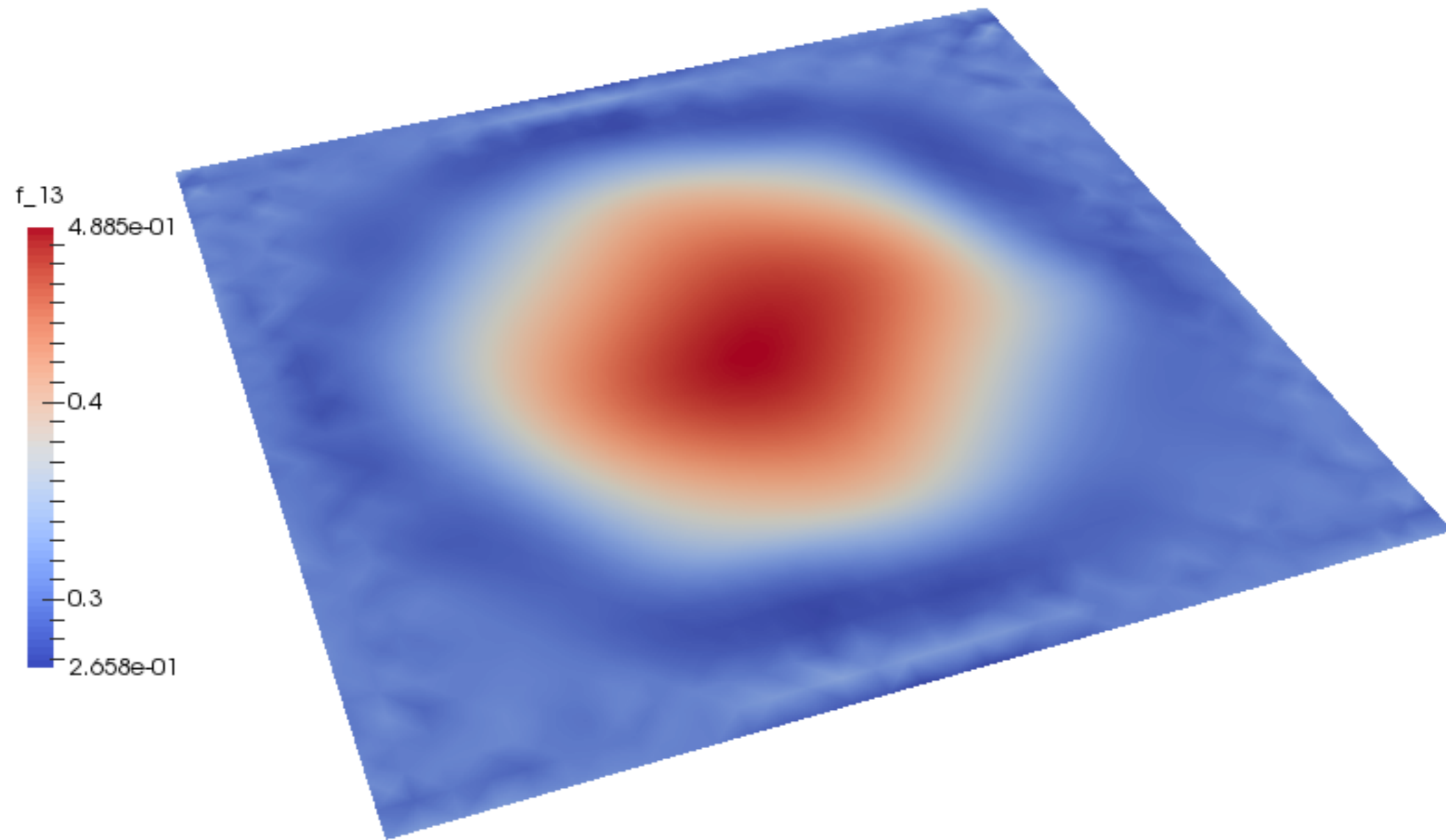
Q: Which parameters am I most uncertain about?



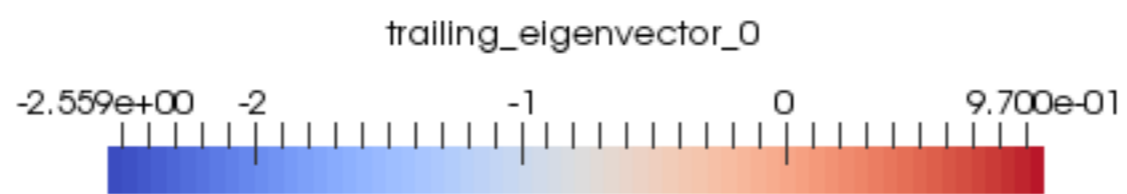
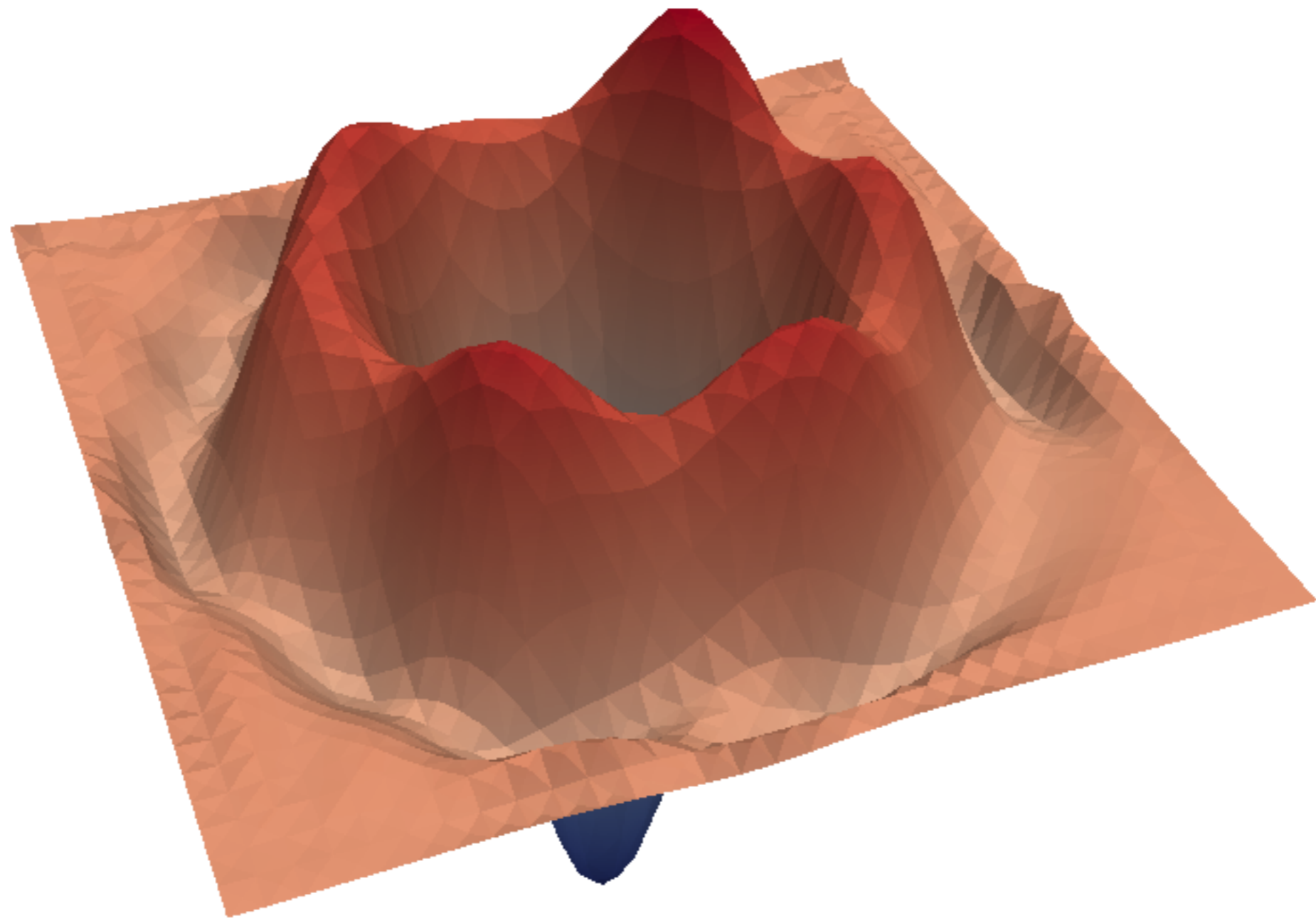
# Bayes Theorem

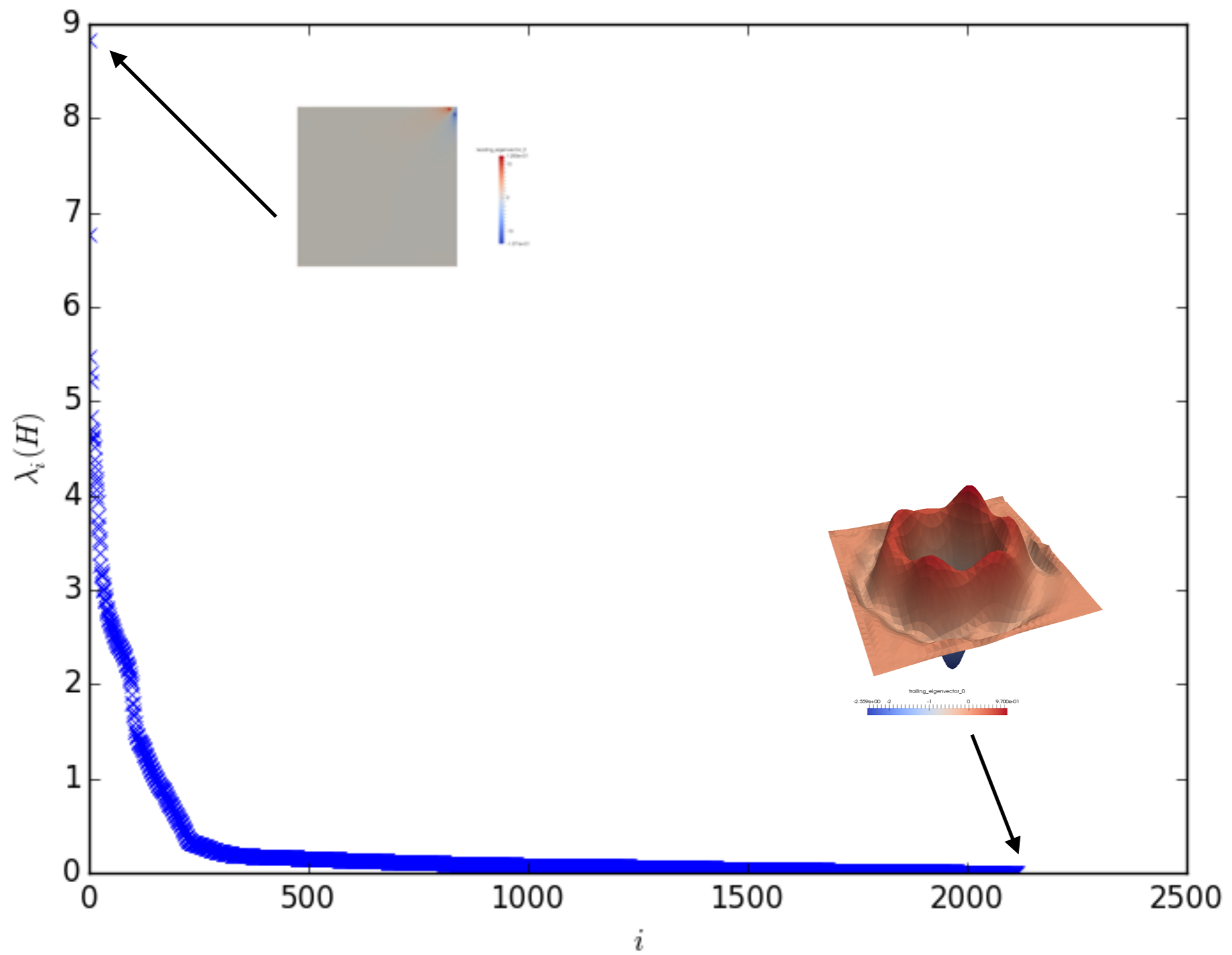
$$\pi_{\text{posterior}}(x | y) \propto \pi_{\text{likelihood}}(y | x)\pi_{\text{prior}}(x)$$

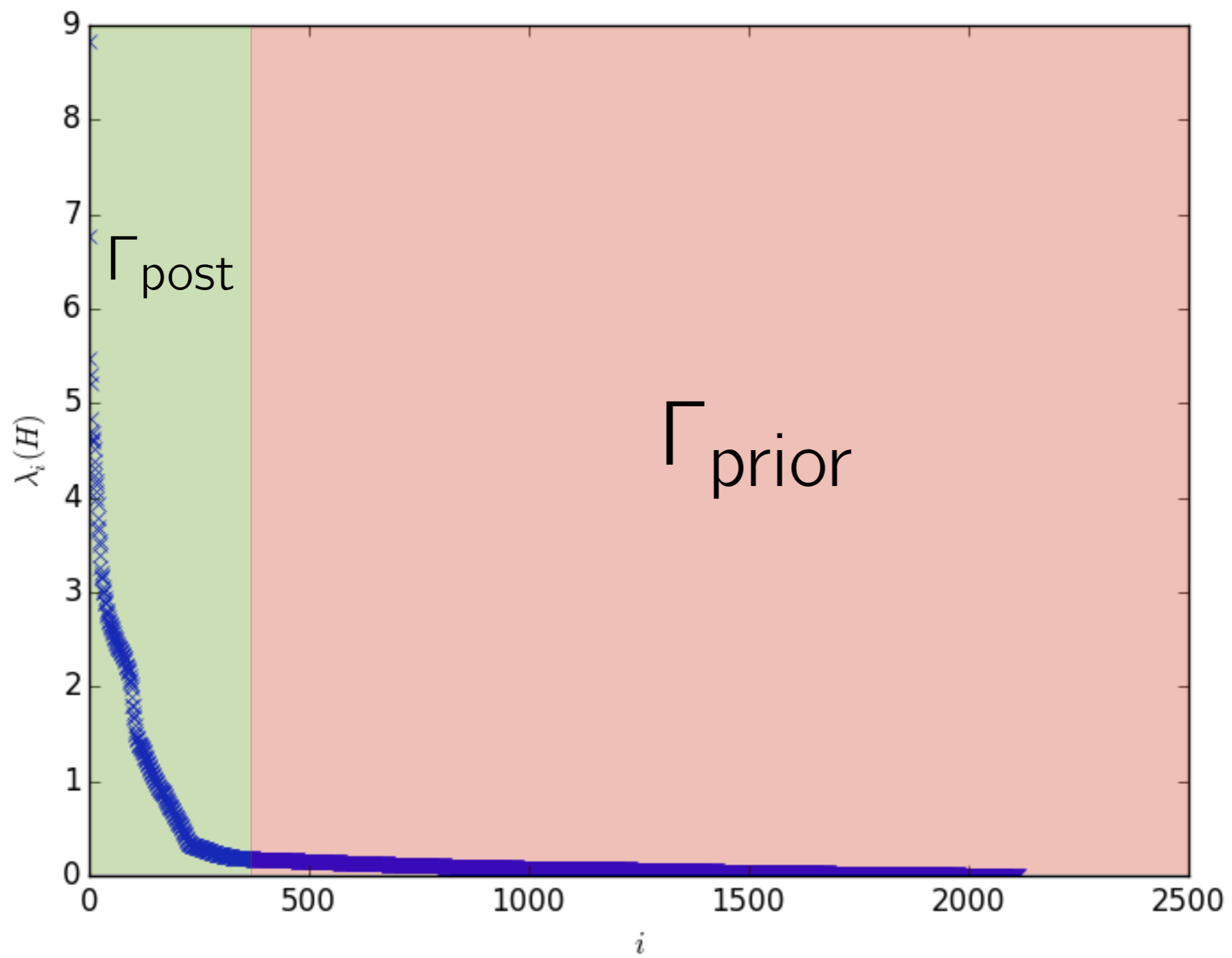
**Goal:** Given the observations, find the posterior distribution of the unknown parameters.



$X_{\text{map}}$



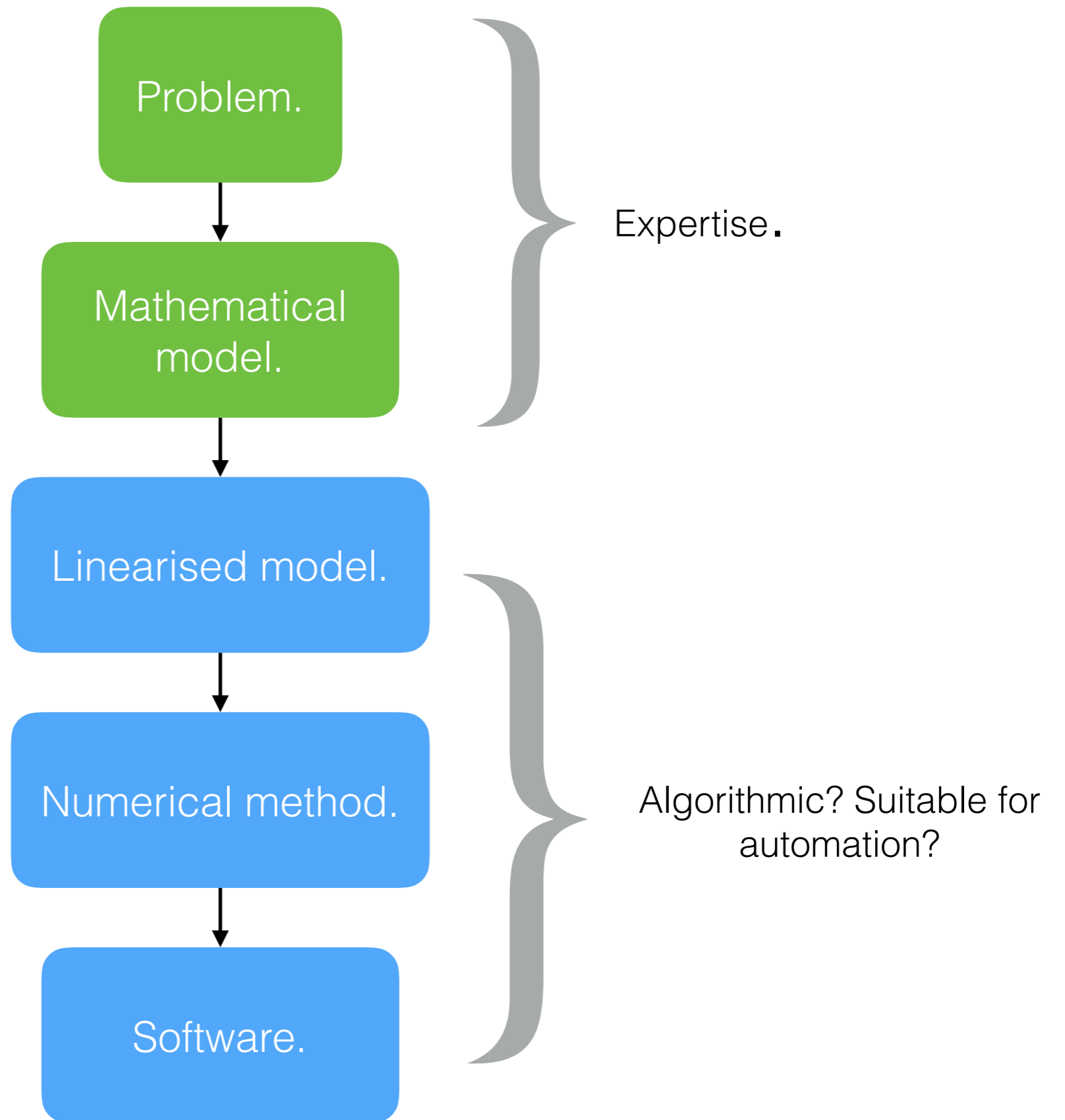






Alnæs, Bletcha, Hake, Johannson, Kehlet, Logg, Oelgaard, Richardson, Ring, Rognes, Wells...

- Key idea: implement high-level description of finite element models in the Unified Form Language.
- Let algorithms take over the tedious/difficult work of linearisation and transforming maths into lower-level languages.



## Stress measure

$$\mathbf{S} = \frac{t^3}{12} \left( 2\mu \mathbf{K} + \frac{2\mu\lambda}{2\mu + \lambda} \text{tr}(\mathbf{K}) \mathbf{I} \right)$$

`mu = Constant(0.3)`

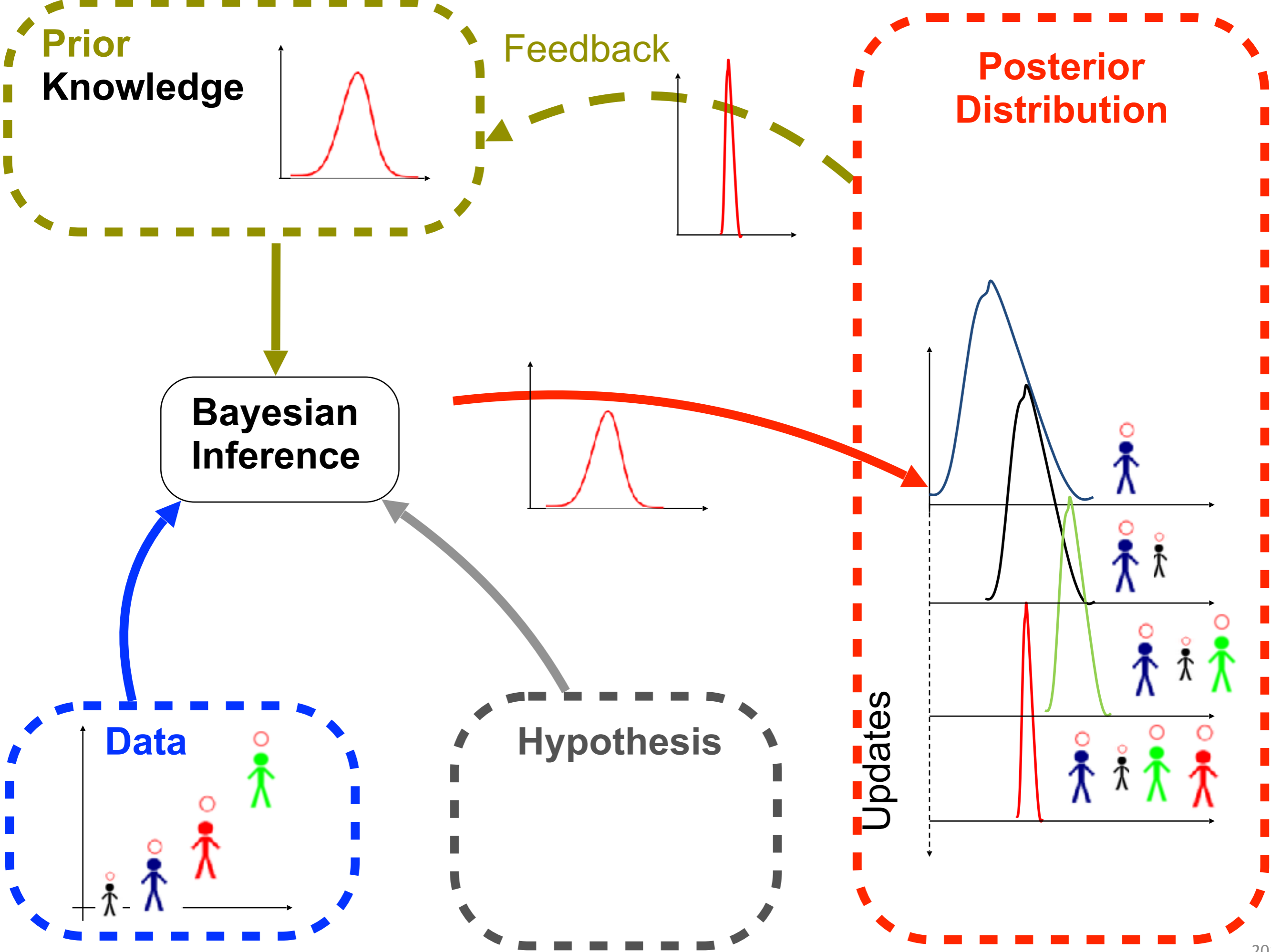
```
S = (t**3/12) * (2.0*mu*K + \
(2.0*mu*lambda) / (2.0*mu + lambda) *tr(K) *Identity(2))
```

## Bending energy

$$E_b = \frac{1}{2} \int_{\Omega} \mathbf{S} : \mathbf{K} \, dx$$

```
E_b = 0.5*inner(S, K) *dx
```





# Elastography under uncertainty

## ELASTOGRAPHY

*Elastography* is any method that can be used to extract quantitative or qualitative data about *elastic modulus distributions* from images of elastic solids (Parker, Doyley, and Rubens, 2011).

## WHY?

- ▶ Tumorous tissue is *significantly stiffer* than healthy tissue.
- ▶ If we can detect that change in stiffness we a useful extra imaging modality for cancer diagnosis.
- ▶ There is growing clinical evidence that elastography is useful (Parker, Doyley, and Rubens, 2011).

# Elastography under uncertainty

## QUESTIONS AND ISSUES

- ▶ Imaging modalities are *corrupted by noise*. How can we take this noise into account? How does it affect the results?
- ▶ If we only have *surface observations* of an object, how much do we really know about the parameters *inside*?
- ▶ The displacements of soft-tissues are related to the the stiffness parameters by a complex set of non-linear PDEs. Can we find the parameters in a *reasonable amount of time*?

# MODEL PROBLEM

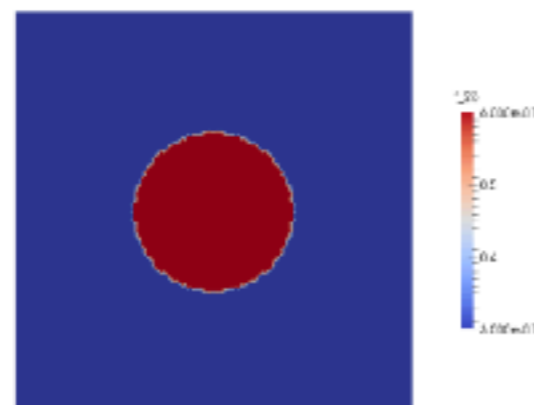
Given displacement observations on the surface of a block of soft tissue, possibly containing a stiff tumor, what can we infer about the material parameters of the tissue inside? How sure are we about what we infer?

## FIGURE 1



Left: Three virtual experimental results from applying three different loads to the same non-homogeneous block of soft tissue. We are only given the observations on the exterior surface, and they are corrupted by random white noise.

## FIGURE 2



Left: The true material parameter field used to generate the experimental data in Figure 1. A stiff circular tumour is surrounded by softer healthy tissue.

# Elastography under uncertainty

## METHODOLOGY

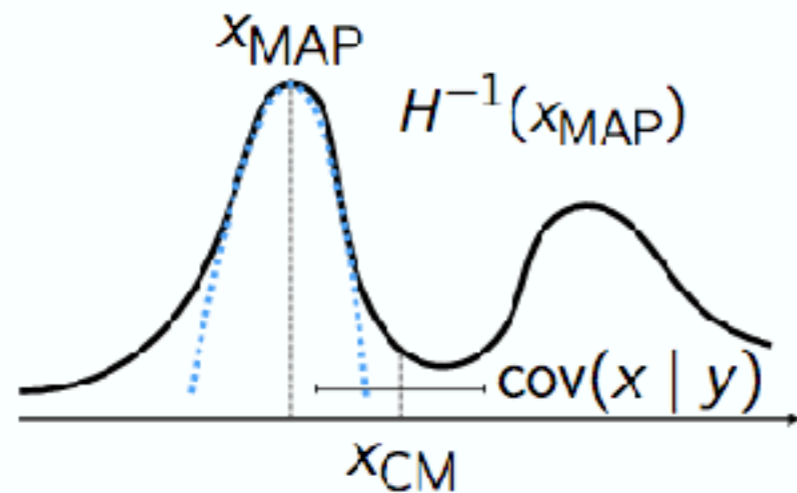
- ▶ We use the Bayesian framework for statistical inference (Stuart, 2010).
- ▶ Allows for rigorous statistical quantification of uncertainty arising from:
  - ▶ Partial observations.
  - ▶ Noisy instruments.
  - ▶ Model inadequacy.
- ▶ Soft tissue modelled by a fully non-linear hyperelastic PDE.
- ▶ Flexible Gaussian noise and prior modelling.
- ▶ We use derivatives of the finite element model to find the most likely material parameters and approximate the covariance structure.

# Elastography under uncertainty

## FIGURE 3

$$\pi_{\text{posterior}} \sim \mathcal{N}(x_{\text{MAP}}, \mathbf{H}^{-1})$$

$$\pi_{\text{posterior}}^{\text{approx}} \sim \mathcal{N}(x_{\text{MAP}}, \mathbf{H}^{-1}(x_{\text{MAP}}))$$



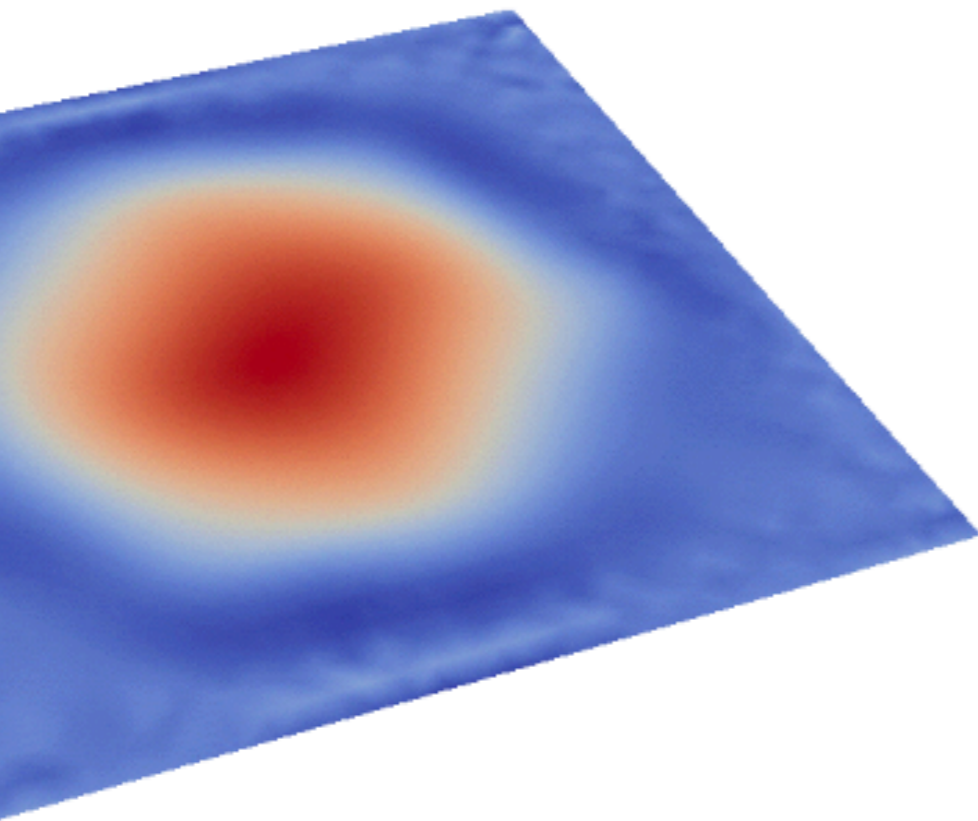
Left: The Bayesian posterior encodes the probability of the all possible parameters given our experimental observations. We find the *maximum a posteriori* point through gradient-driven optimisation. We construct a *Gaussian approximation* of the covariance structure at this point.

# Elastography under uncertainty

## COMPUTATIONAL TECHNIQUES

- ▶ Automatic construction of forward and adjoint models with dolfin-adjoint (Farrell et al., 2013). *Easy to change physical model.*
- ▶ Efficient algebraic multigrid preconditioning of forward and adjoint models. *Forward runs dominate overall cost, reduce as much as possible.*
- ▶ Gauss-Newton Conjugate-Gradient method to find maximum a posteriori point. *Scales well on mesh refinement.*
- ▶ Matrix-free Krylov-Schur algorithm for principal component analysis of prior pre-and-post-conditioned Hessian of likelihood. *Fixed cost for given observations/model.*
- ▶ Optimal low-rank update from prior to posterior covariance (Spantini et al., 2014). *Reduces Hessian actions/forward model runs.*

# Elastography under uncertainty

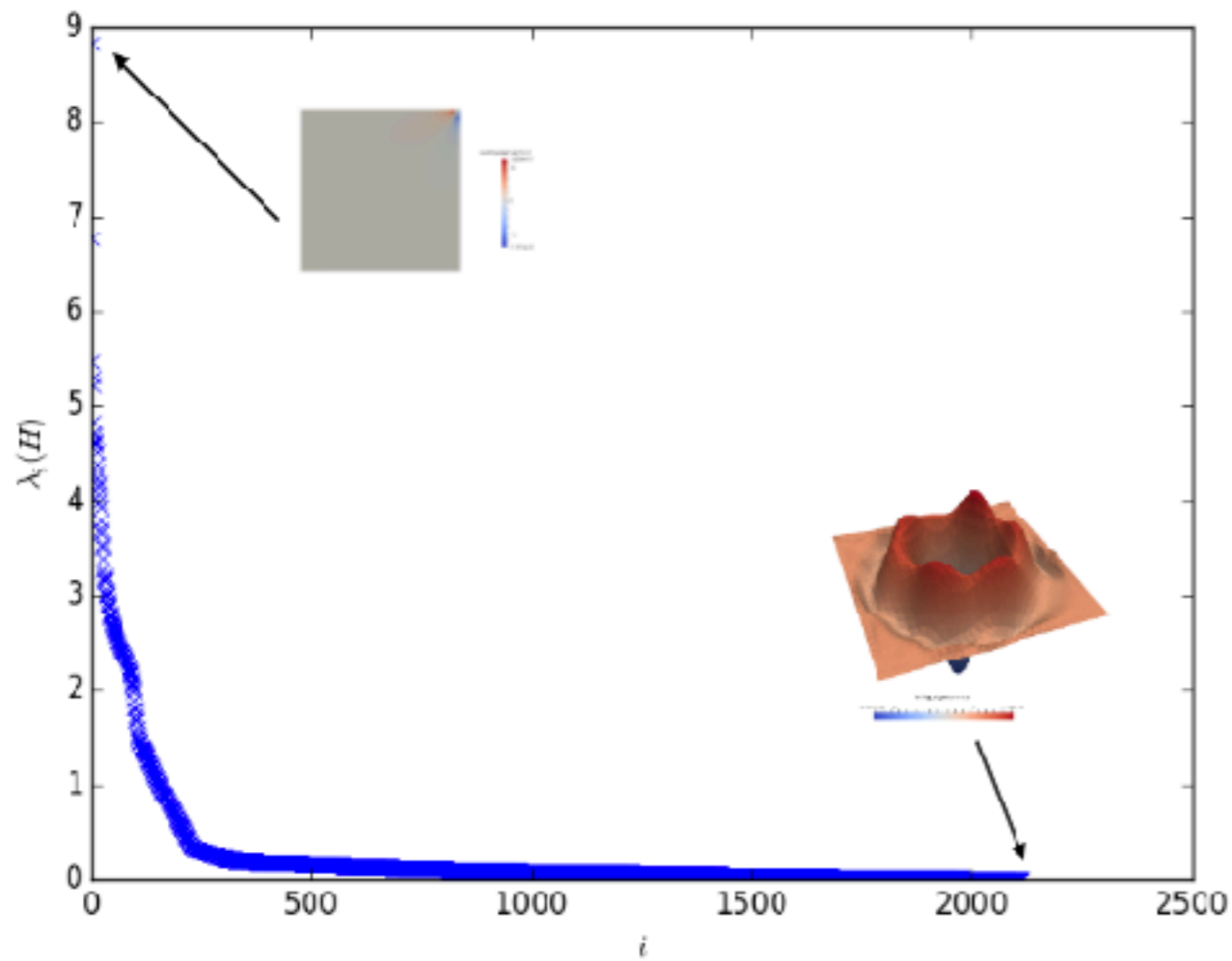


Left: Recovered MAP point, cf. Figure 1.  
We *can* detect the stiff inclusion inside the object just from the noisy surface observations.

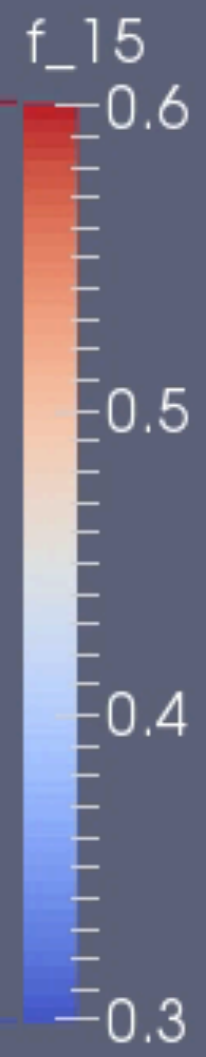
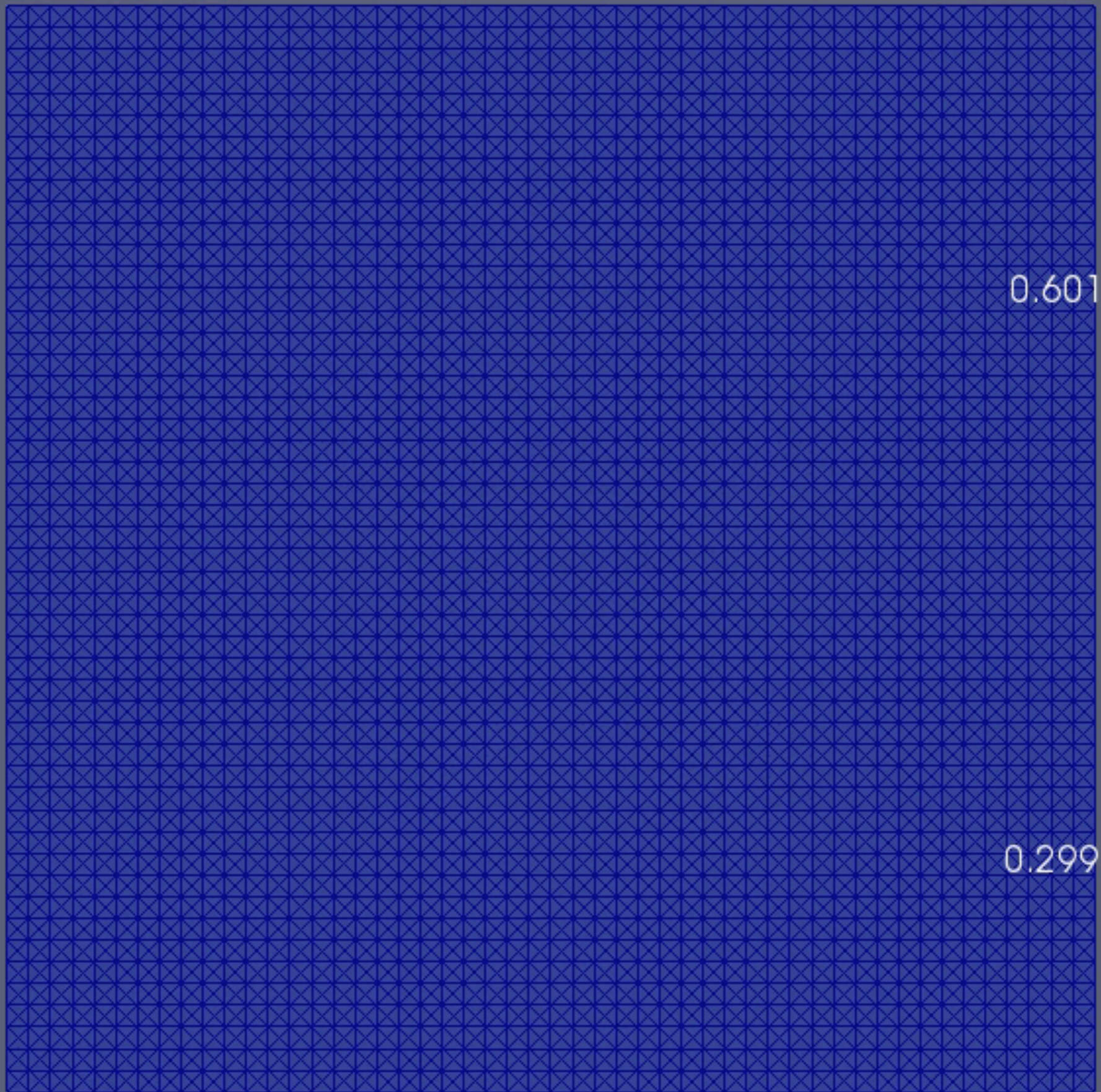


# Elastography under uncertainty

## FIGURE 5



Left: Low-rank structure of spectrum of posterior covariance. Data is only informative on low-rank subspace of original parameter space. Top left eigenvector points towards direction in parameter space most-constrained by the observations, bottom right towards least-constrained.



**Thank you for your attention!**

You can **download** the **slides** of my plenary at ECCOMAS-XDMS 2017 here <http://hdl.handle.net/10993/31487> or [http://orbilu.uni.lu/bitstream/10993/31487/1/XDMS\\_2017\\_Bordas.pdf](http://orbilu.uni.lu/bitstream/10993/31487/1/XDMS_2017_Bordas.pdf)

and the slides of **this presentation** here:

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[http://orbilu.uni.lu/bitstream/10993/31487/4/XDMS\\_2017\\_Bordas\\_AverageResolution\\_withLinks.pdf](http://orbilu.uni.lu/bitstream/10993/31487/4/XDMS_2017_Bordas_AverageResolution_withLinks.pdf)

or/and email me [stephane.bordas@alum.northwestern.edu](mailto:stephane.bordas@alum.northwestern.edu)

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Patient-Specific Data



Expert Knowledge



**Guidance**

Design of Implants & Prosthetics

Diagnosis

Surgical Training

Prognosis

Medical Devices

Planning

Monitoring

<p>Cardiovascular Devices</p> <p>u </p>	<p>Scoliosis</p> <p></p>	<p>Eye surgery</p> <p></p>	<p>Neurology</p> <p></p>	<p>Spine Braces</p> <p>u </p>
<p>Hip growth</p> <p></p>	<p>Prostate Cancer</p> <p></p>	<p>Intraoperative radiotherapy</p> <p>u </p>	<p>Surgical guidance</p> <p></p>	<p>Soft organ diagnosis</p> <p></p>
<p>Dental prostheses</p> <p></p>	<p>Breast Cancer</p> <p></p>	<p>Surgical navigation</p> <p>u </p>	<p>Surgical planning</p> <p></p>	<p><b>Apps</b></p>



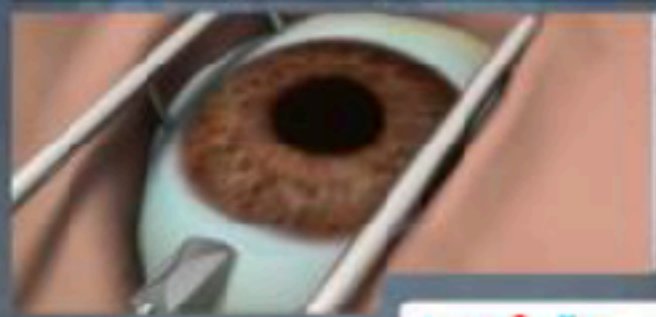
Patient-Specific Data



Expert Knowledge



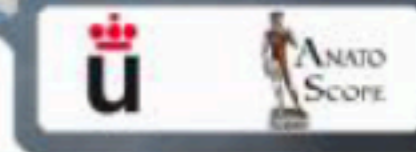
Eye surgery



Neurology



Spine Braces



Intraoperative radiotherapy



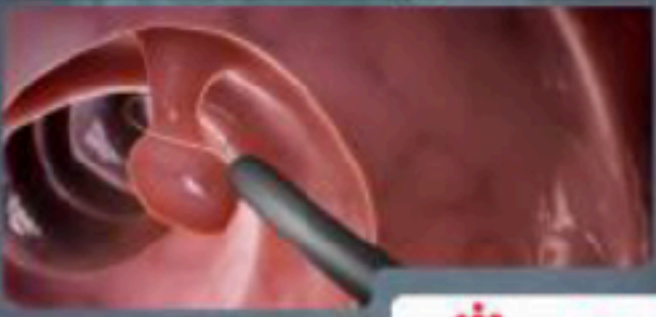
Surgical guidance



Soft organ diagnosis



Surgical navigation



Surgical planning



Apps

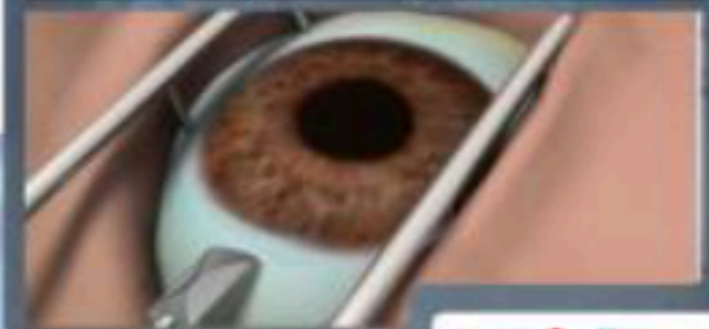
Cardiovascular Devices



Scoliosis



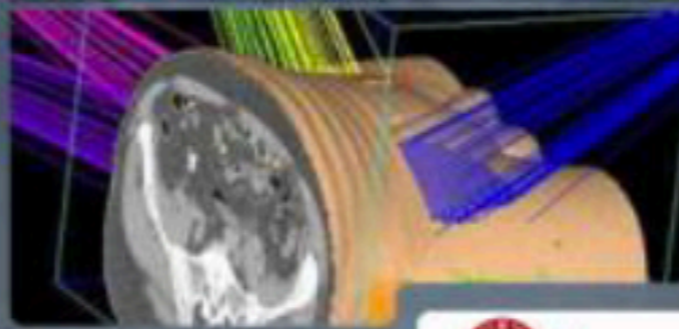
Eye surgery



Hip growth



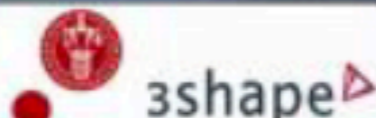
Prostate Cancer



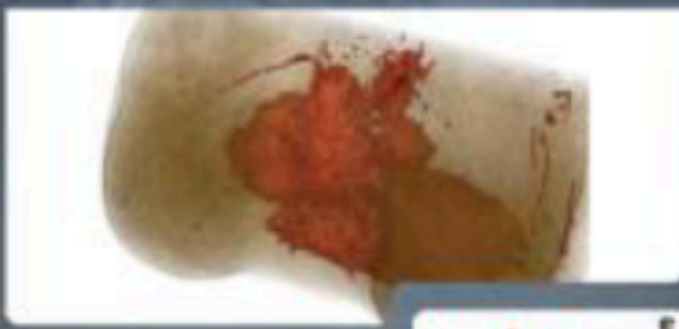
Intraoperative radiotherapy



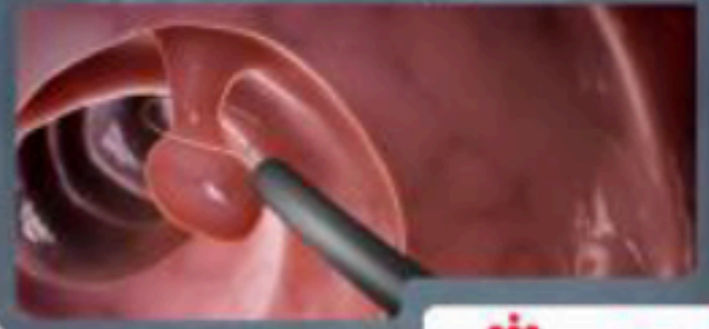
Dental prostheses



Breast Cancer



Surgical navigation







# EPSRC

Pioneering research and skills



## Acknowledgements



European Research Council



### **Multi-scale fracture and model order reduction**

Pierre Kerfriden, Lars Beex, Jack Hale, Olivier Goury, Daniel Alves Paladim, Elisa Schenone, Davide Baroli, Thanh Tung Nguyen, Hoang Khac Chi, Timon Rabczuk

### **Advanced discretisation techniques**

Elena Atroshchenko, Danas Sutula, Xuan Peng, Haojie Lian, Peng Yu, Qingyuan Hu, Sundararajan Natarajan, Nguyen-Vinh Phu

### **Error estimation**

Pierre Kerfriden, Satyendra Tomar, Daniel Alves Paladim, Andrés Gonzalez Estrada

### **Biomechanics applications**

Alexandre Bilger, Hadrien Courtecuisse, Bui Huu Phuoc

## *Fracture of homogeneous materials*

[https://publications.uni.lu/bitstream/10993/10039/1/2013stressAnlaysiaWithoutMeshingIGABEM3D\\_ICE.pdf](https://publications.uni.lu/bitstream/10993/10039/1/2013stressAnlaysiaWithoutMeshingIGABEM3D_ICE.pdf)

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