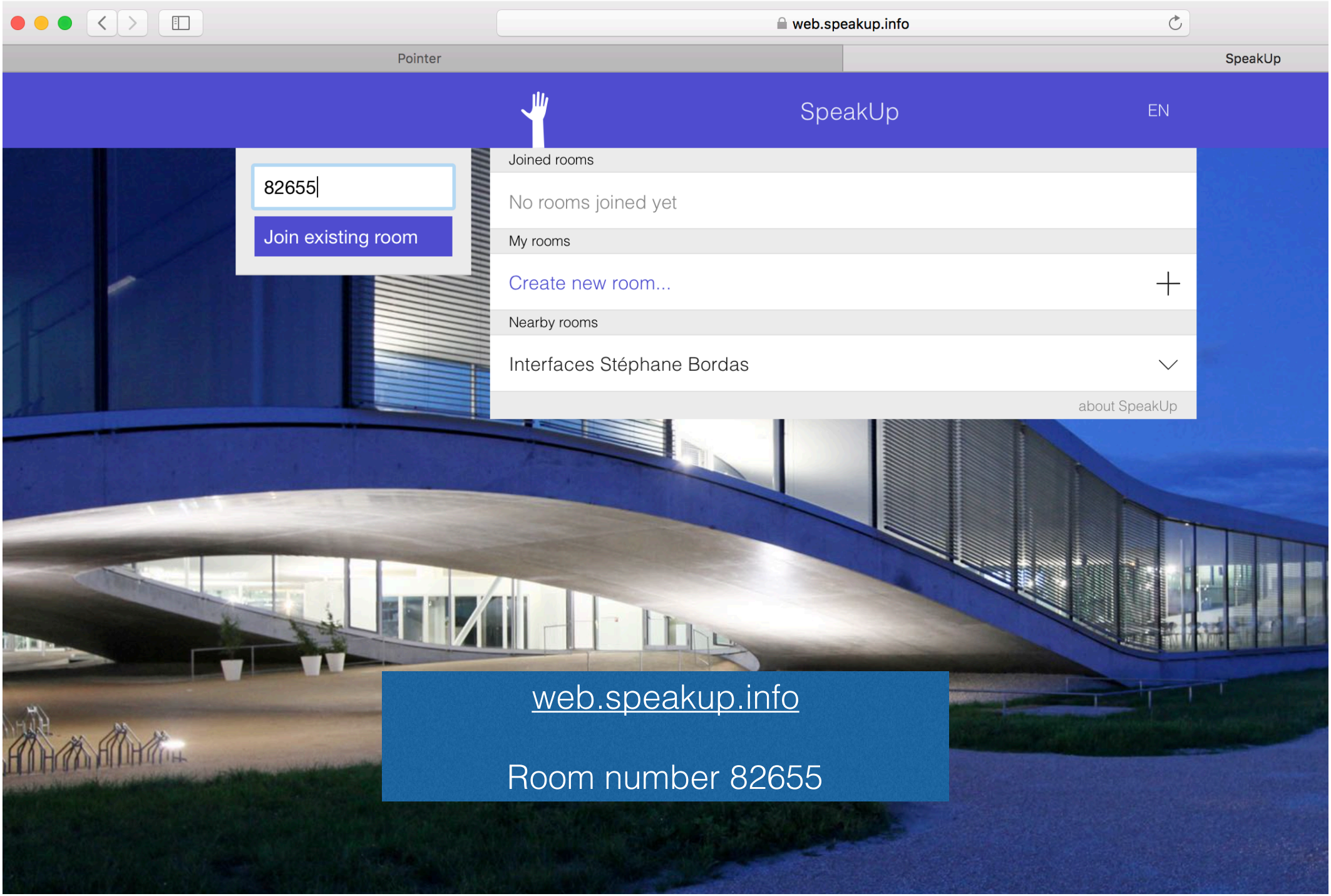
Numerical methods for free boundary problems

and data-driven modelling

Stéphane P.A. Bordas, University of Luxembourg and Cardiff University

Oxford Engineering Mechanics Seminar 2018 03 05


web.speakup.info
Pointer
SpeakUp
SpeakUp
EN
82655
Join existing room
Joined rooms
No rooms joined yet
My rooms
Create new room...
Nearby rooms
Interfaces Stéphane Bordas
about SpeakUp
web.speakup.info
Room number 82655

Computed in Luxembourg

Computational Sciences Luxembourg

UNIVERSITÉ DU LUXEMBOURG

Department of Computational Engineering & Sciences

10 km
10 miles
ARDENNES
Clervaux
BELGIUM
Wiltz
Vianden
GERMANY
Diekirch
MULLERTHAL
Echternach
LUXEMBOURG
Grevenmacher
LUXEMBOURG
Moselle
MOSELLE
VALLEY
Petange
Differdange
Modorf-les-Bains
Esch
Budelange
FRANCE
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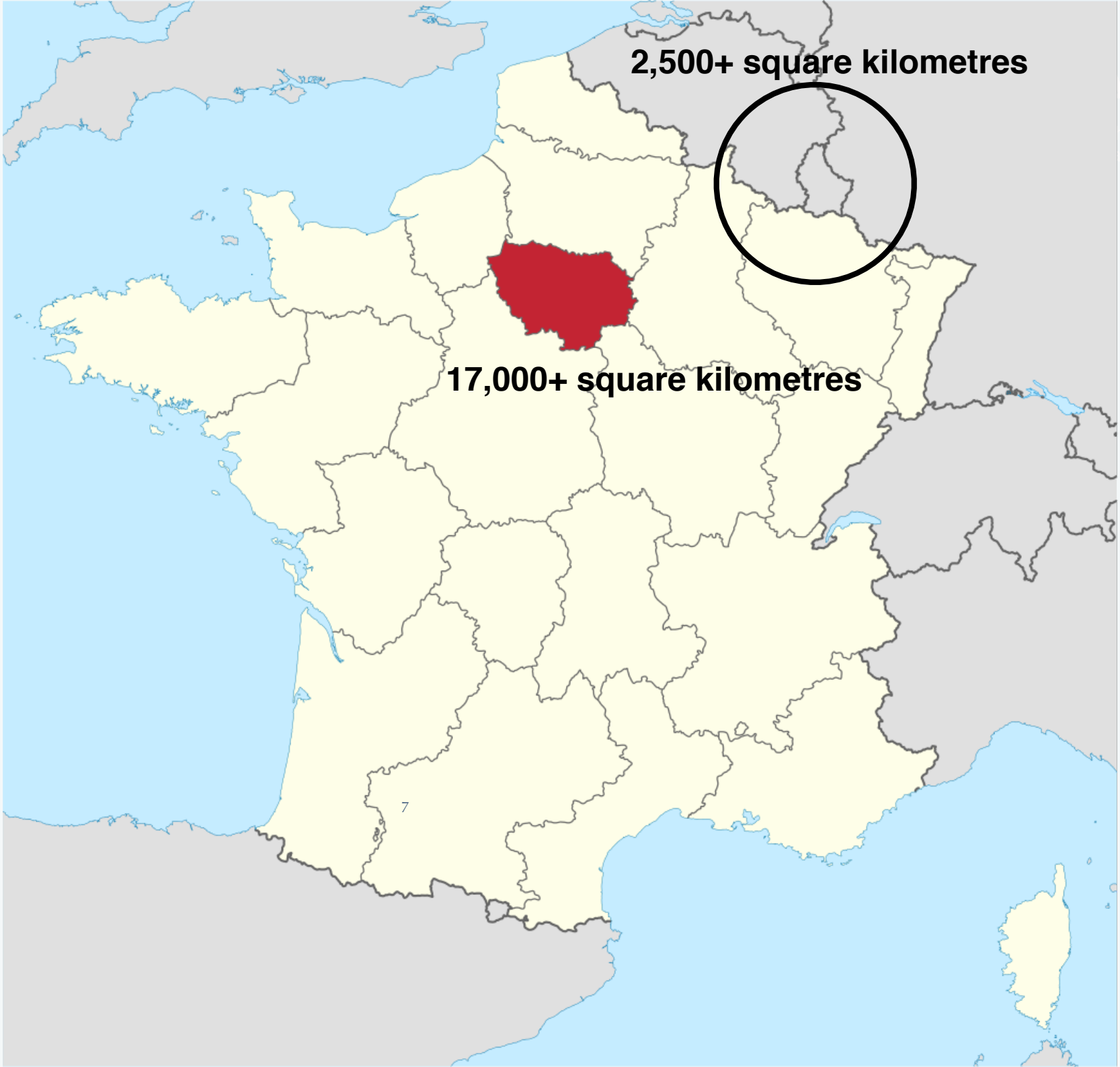
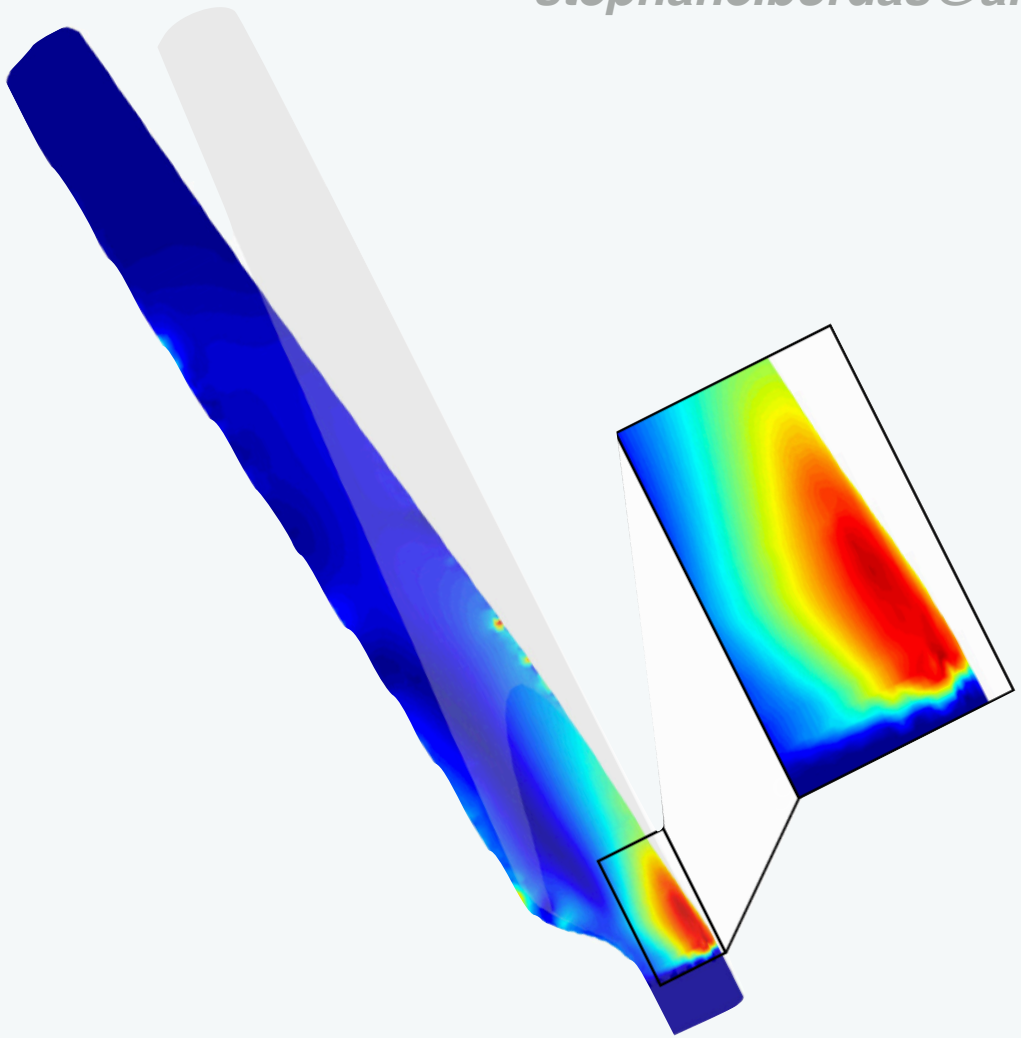
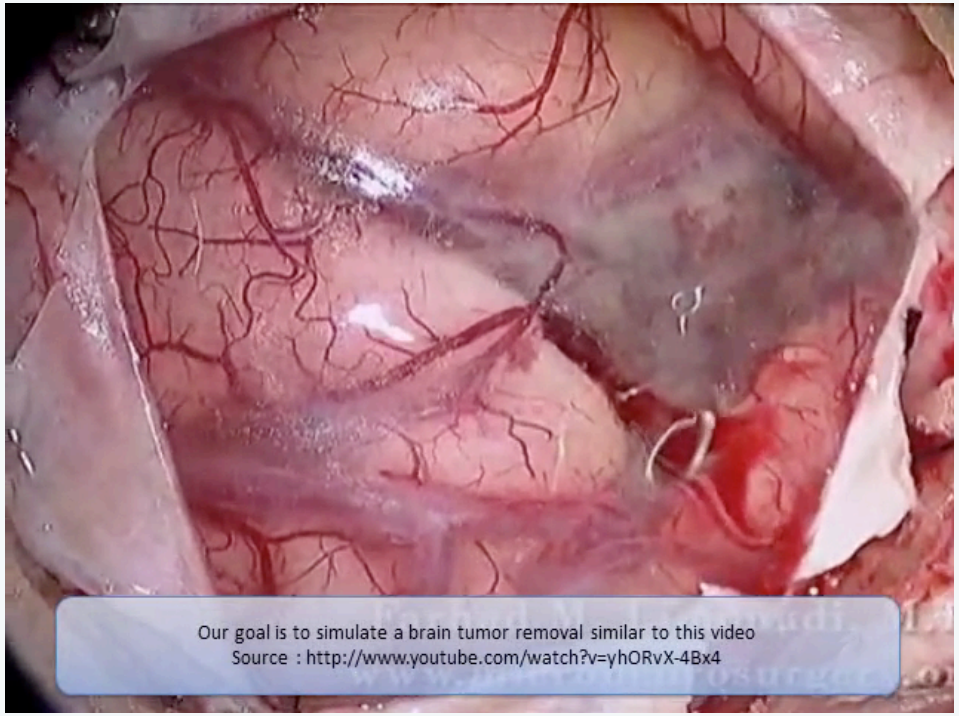

2,500+ square kilometres
17,000+ square kilometres

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

Numerical Methods for Free Boundary Problems

Stéphane P.A. Bordas
stephane.bordas@alum.northwestern.edu





"Free boundary problems deal with solving partial differential equations (PDEs) in a domain, a part of whose boundary is unknown in advance; that portion of the boundary is called a free boundary”

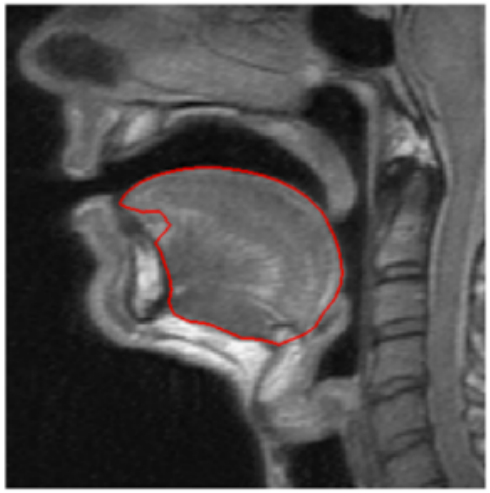
Avner Friedman (Friedman, 2000).

Mathematical Modelling

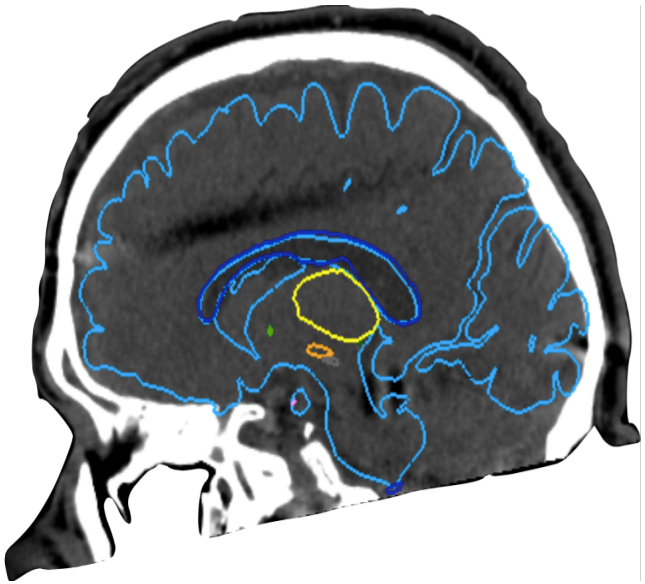
Continuous Problem

Mathematical Modelling

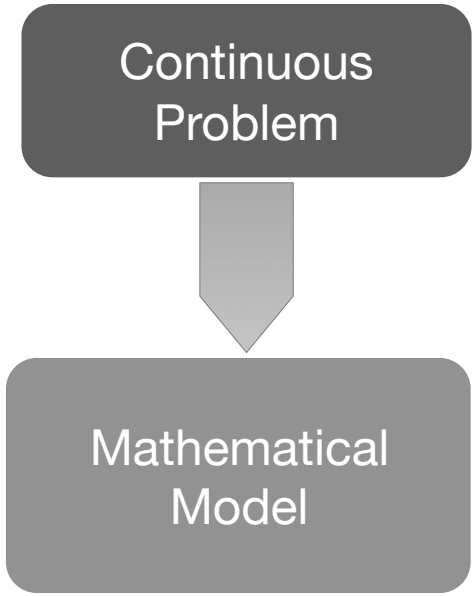
Continuous Problem



Bijar, Rohan, Perrier & Payan 2015



Mathematical Modelling



Mathematical Modelling

Continuous Problem

Mathematical Model

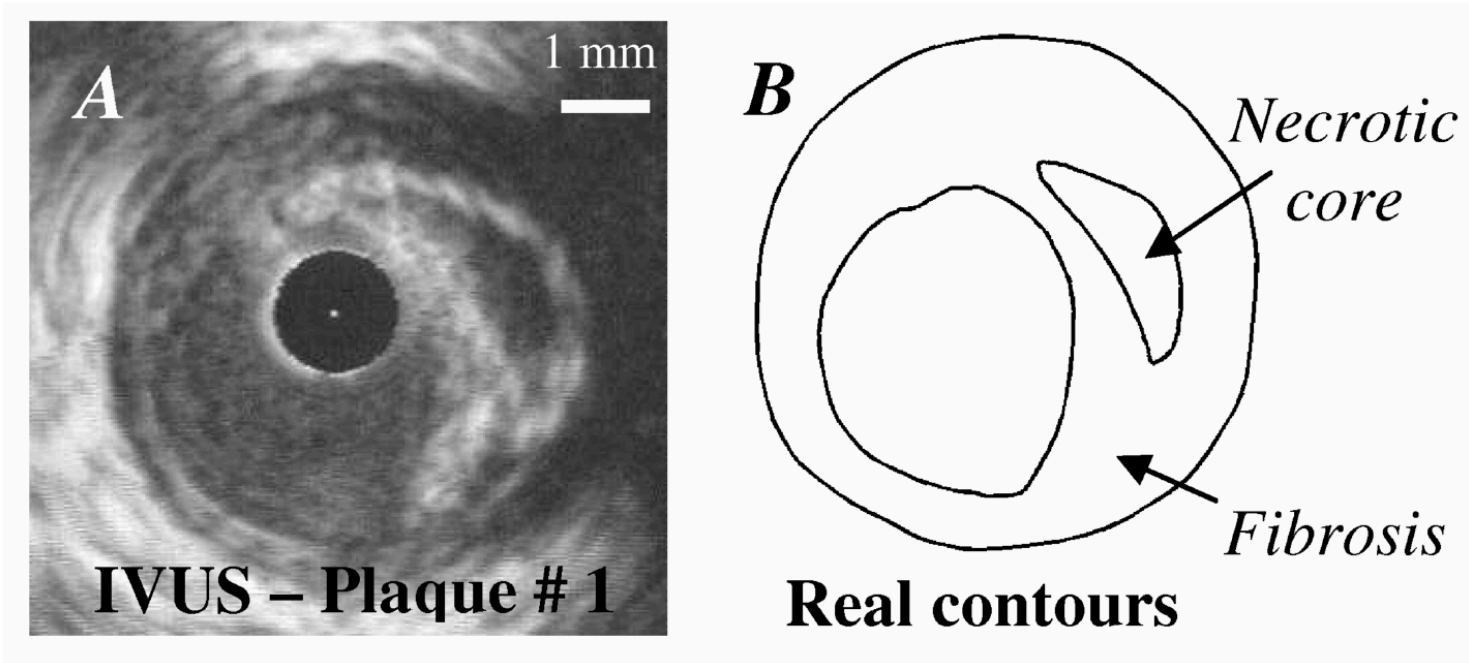
$$\min_{\mathbf{u}\in\mathbf{V}} \frac{1}{2}\int_\Omega \boldsymbol{\sigma}(\mathbf{u},\beta) : \boldsymbol{\varepsilon}(\mathbf{u})\, d\mathbf{x} - \int_\Omega \mathbf{g}\cdot\mathbf{u}\, d\mathbf{x}$$

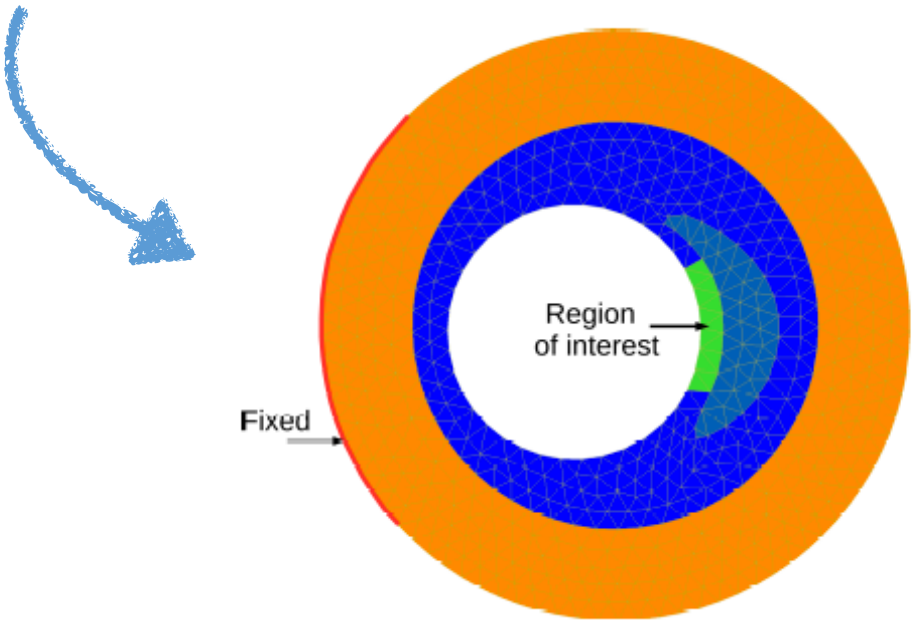
with $$\boldsymbol{\sigma}(\mathbf{u},\beta) = \underbrace{\boldsymbol{\sigma}_P(\mathbf{u})}_{\text{passive material}} + \underbrace{\boldsymbol{\sigma}_A(\beta)}_{\text{muscular activation}} \quad \begin{cases} \boldsymbol{\sigma}_A(\beta) = \beta T e_A \otimes e_A \\ e_A : \text{ fiber direction} \\ T : \text{ tension} \\ \beta : \text{ activation} \end{cases}$$

Mathematical Modelling

Continuous Problem

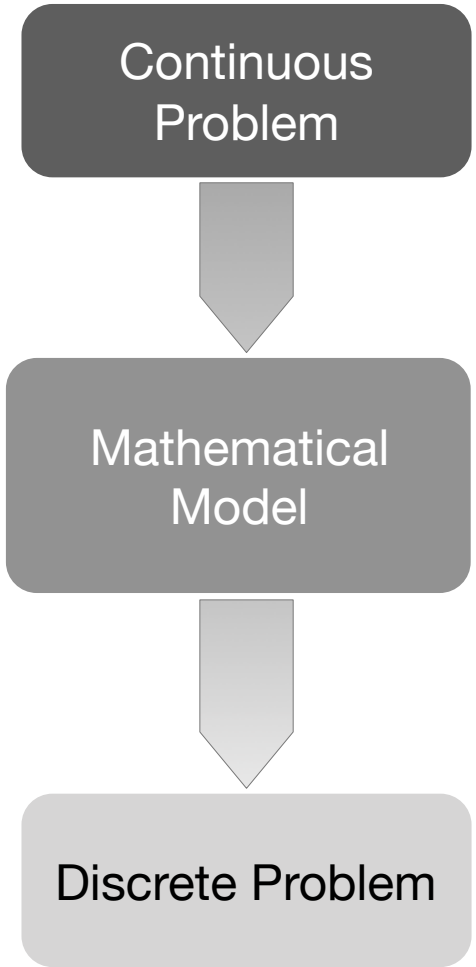
Mathematical Model





Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg and Cardiff University

Mathematical Modelling



Mathematical Modelling

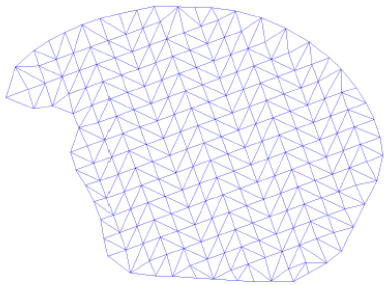
Continuous Problem

↓

Mathematical Model

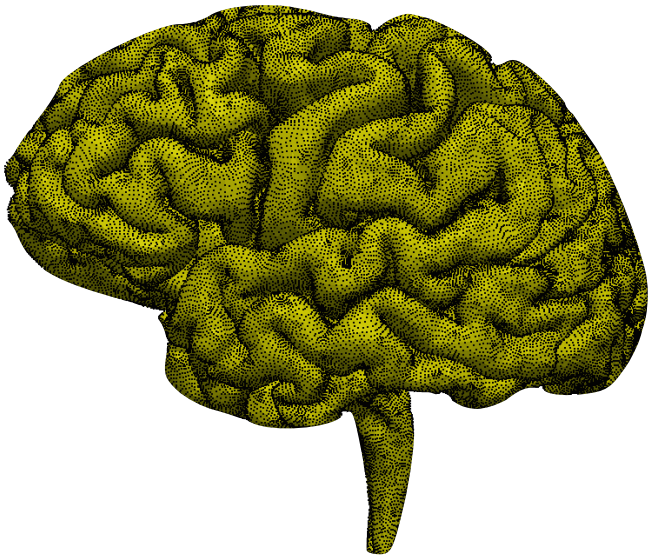
↓

Discrete Problem



Finite element mesh
of a tongue with F. Chouly et al.

Hexahedral mesh of a brain
with Bruno Lévy, Inria



Meshless brain discretization
with Bruno Lévy, Inria

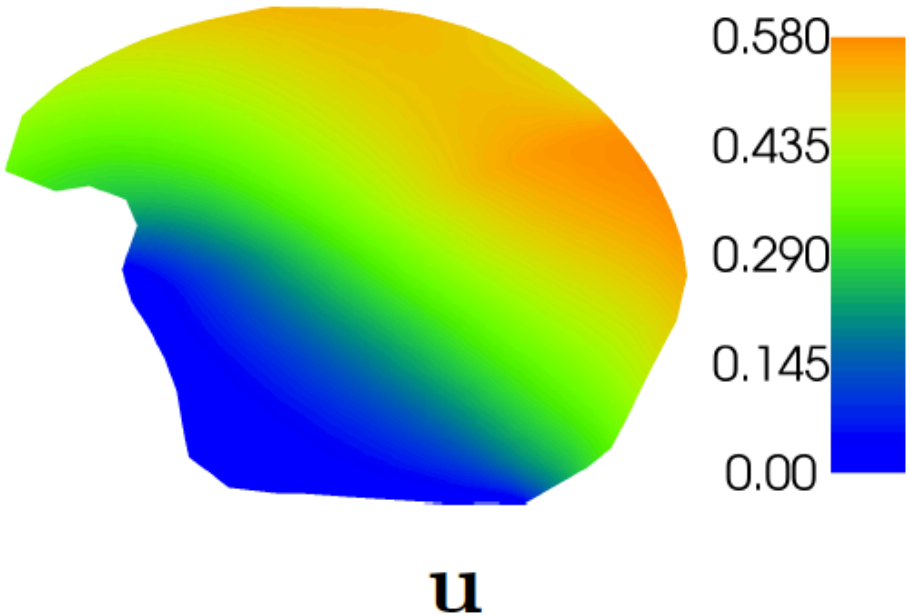
Mathematical Modelling

Continuous Problem

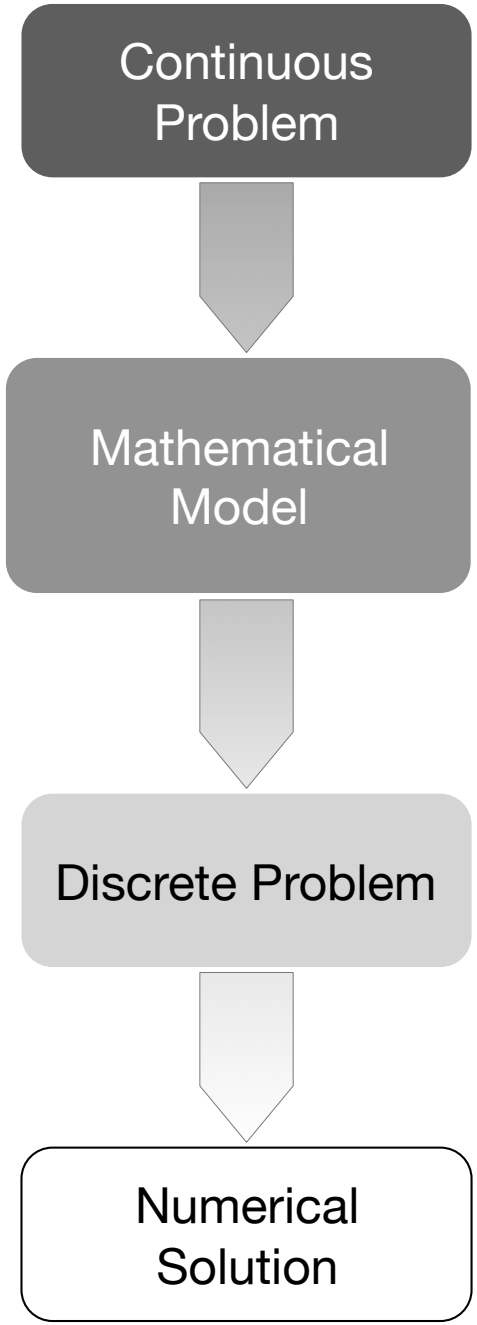
Mathematical Model

Discrete Problem

Numerical Solution



Mathematical Modelling



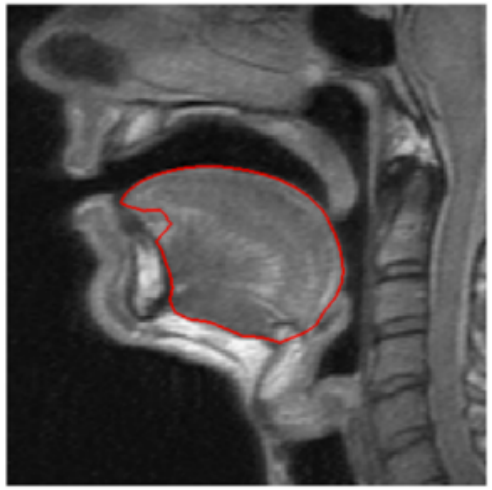
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution



Bijar, Rohan, Perrier & Payan 2015

$$\neq$$

$$\min_{\mathbf{u}\in\mathbf{V}} \frac{1}{2}\int_\Omega \boldsymbol{\sigma}(\mathbf{u},\beta) : \boldsymbol{\varepsilon}(\mathbf{u})\, d\mathbf{x} - \int_\Omega \mathbf{g}\cdot\mathbf{u}\, d\mathbf{x}$$

Mathematical Modelling

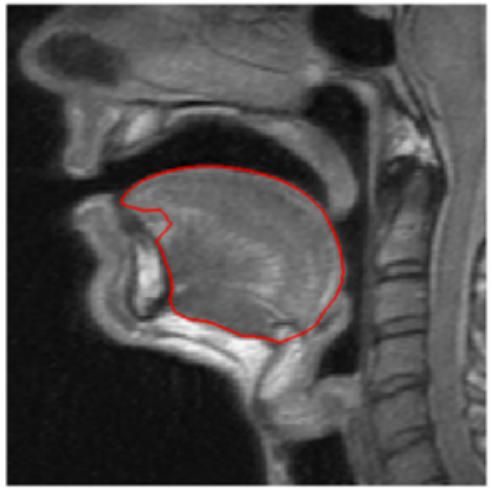
Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error



Bijar, Rohan, Perrier & Payan 2015

$$\neq$$

$$\min_{\mathbf{u}\in\mathbf{V}} \frac{1}{2}\int_\Omega \boldsymbol{\sigma}(\mathbf{u},\beta) : \boldsymbol{\varepsilon}(\mathbf{u})\, d\mathbf{x} - \int_\Omega \mathbf{g}\cdot\mathbf{u}\, d\mathbf{x}$$

Physical Problem
Constitutive Model
Material Parameters

Mathematical Modelling

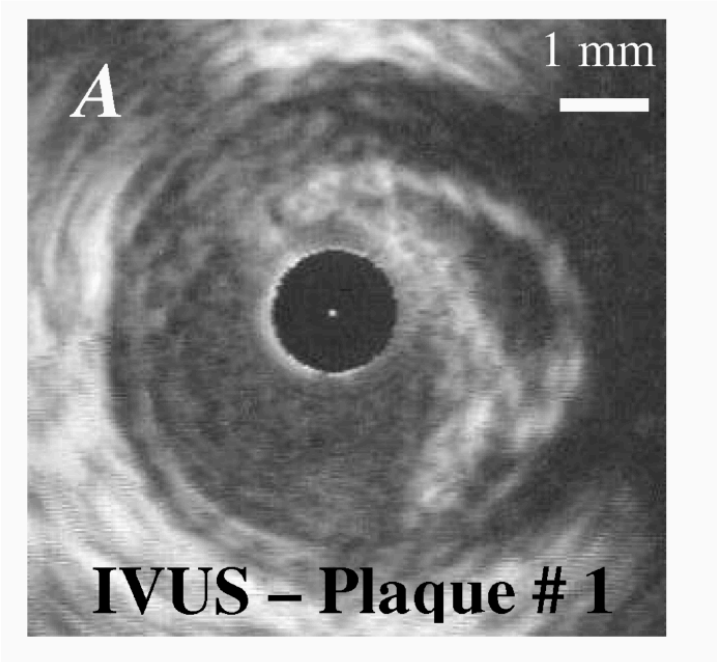
Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error



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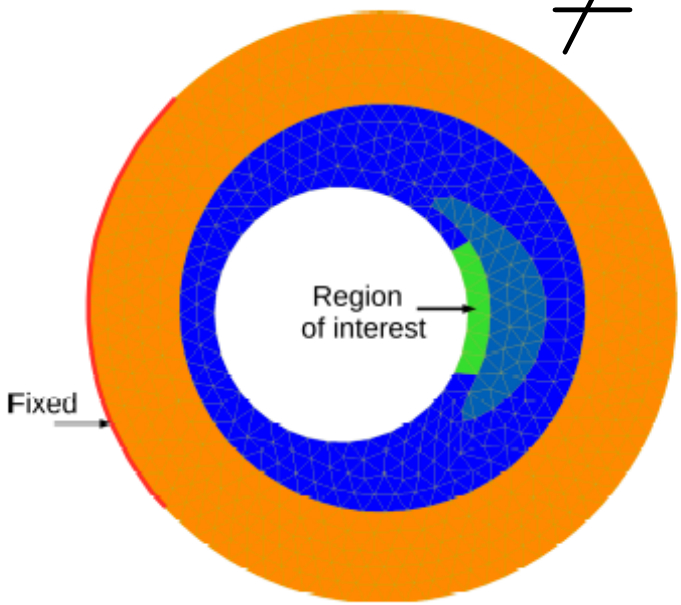


Geometry
Boundary conditions

Mathematical Modelling

Continuous Problem

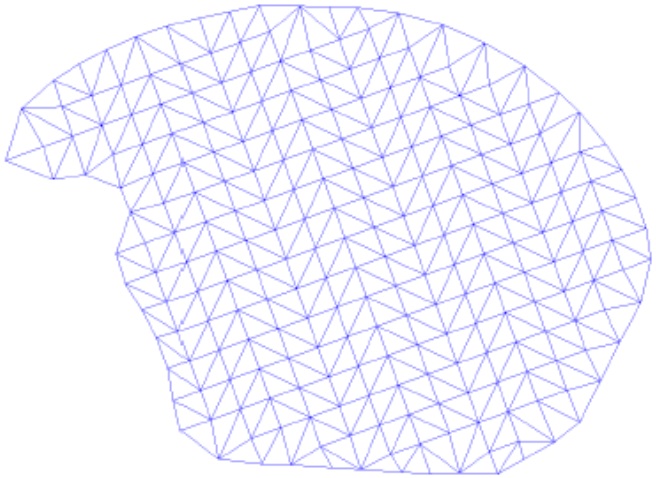
Mathematical Model

Discrete Problem

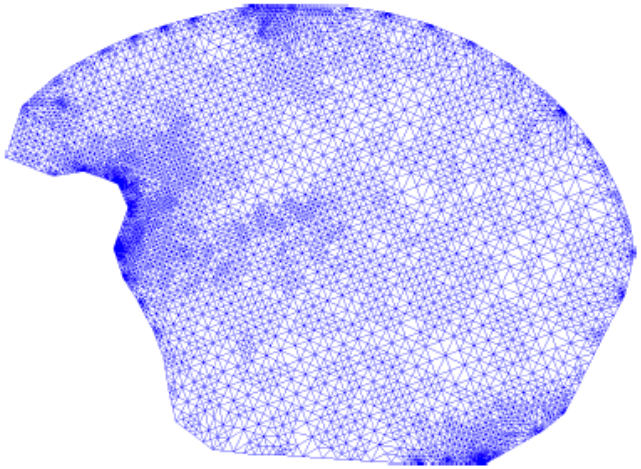
Numerical Solution

Model Error

Discretization Error



vs.



Mathematical Modelling

Continuous Problem

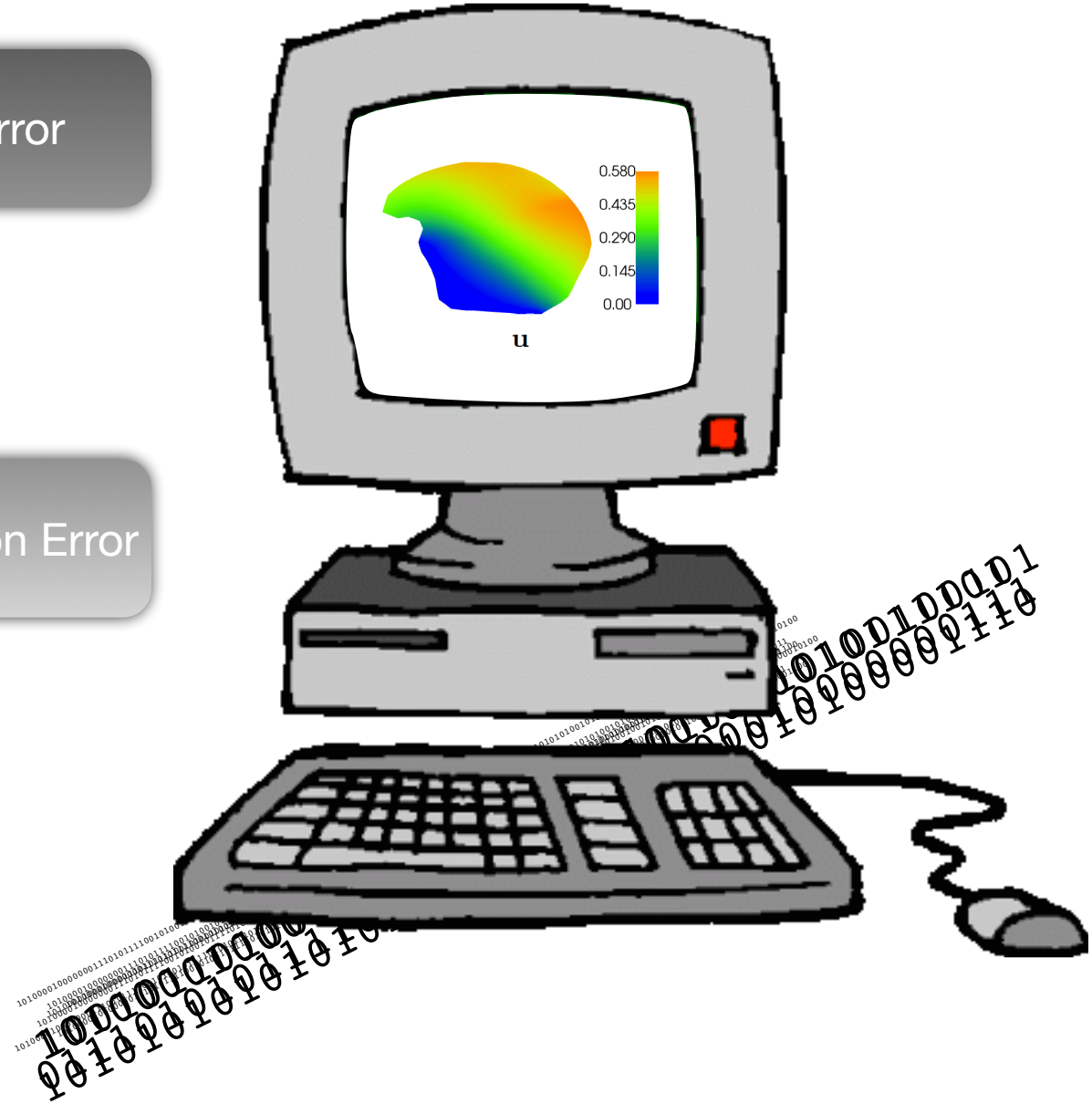
Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Discretization Error



Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

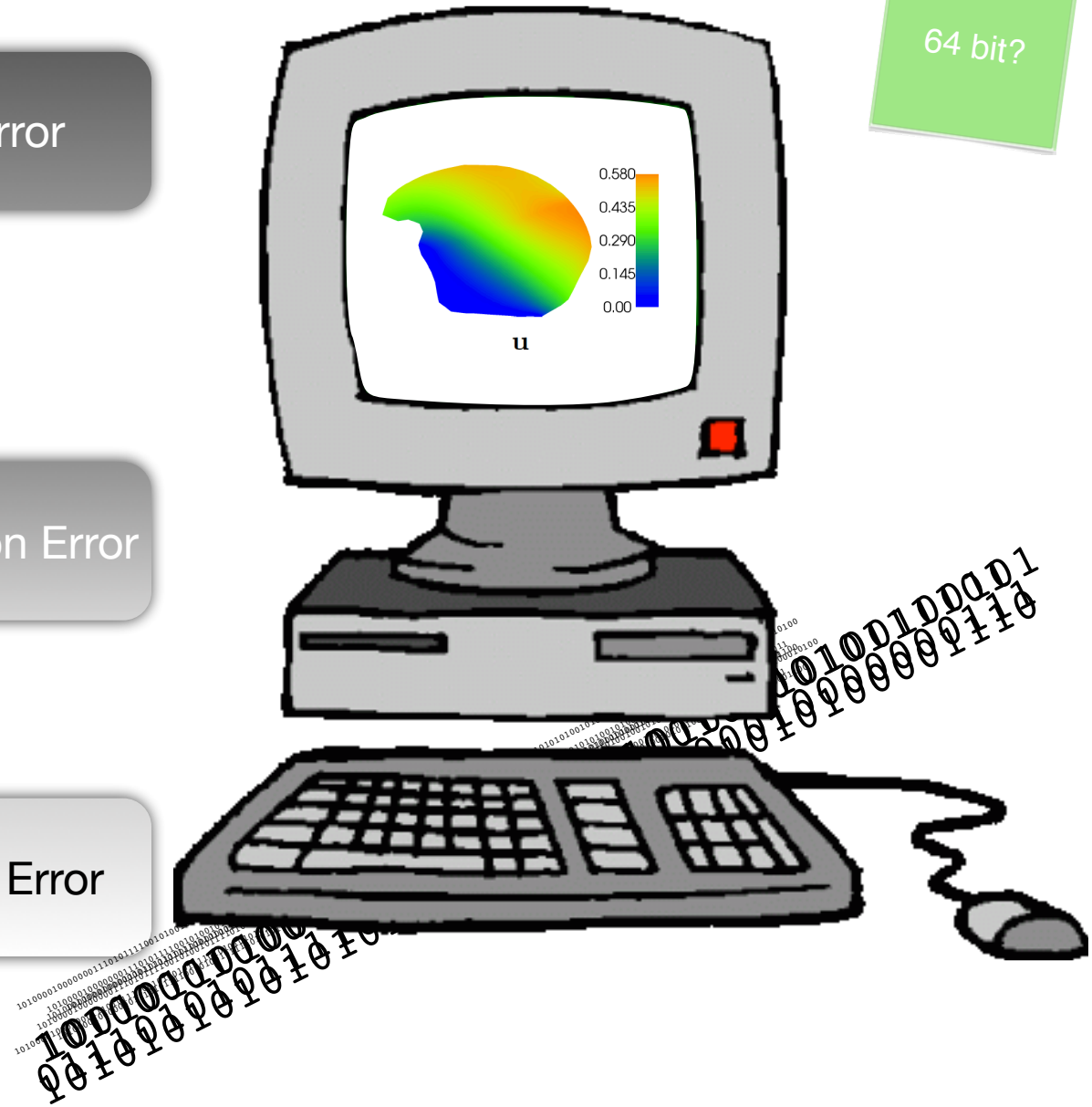
Model Error

Discretization Error

Numerical Error

32 bit?

64 bit?



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Mathematical Modellin

Continuous Problem

Mathematical Model

Discrete Problem

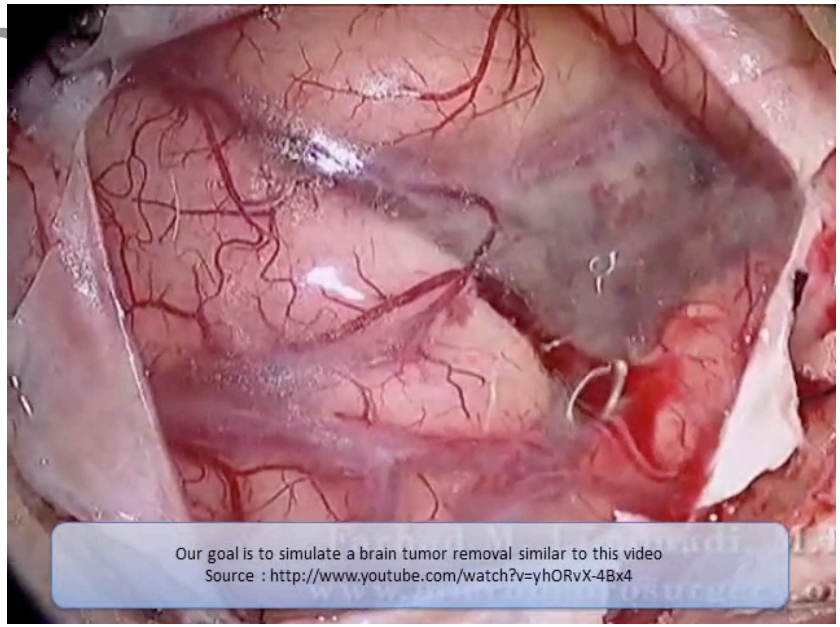
Numerical Solution

Model Error

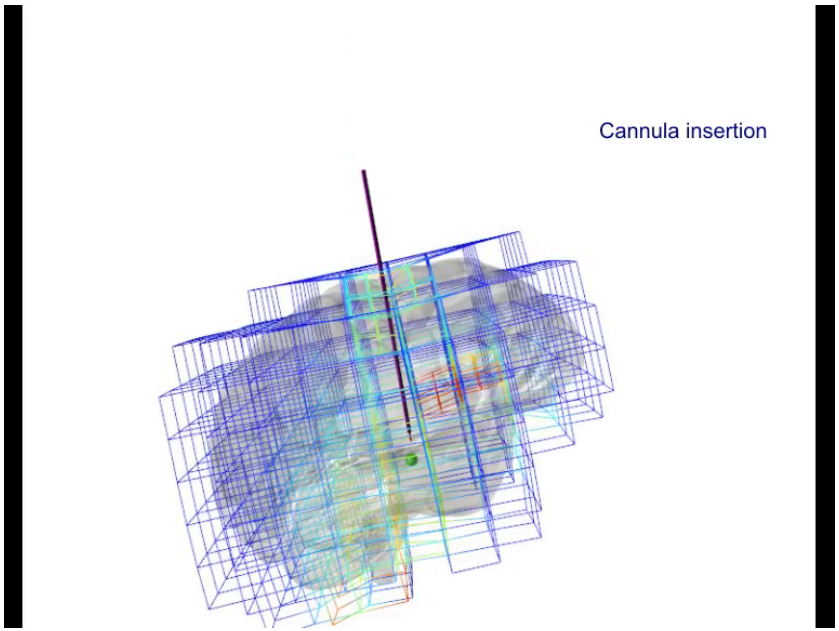
Discretization Error

Numerical Error

Total Error



Reality vs. Simulation



Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Are we solving the right problem?

Total Error

Discretization Error

Numerical Error

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Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

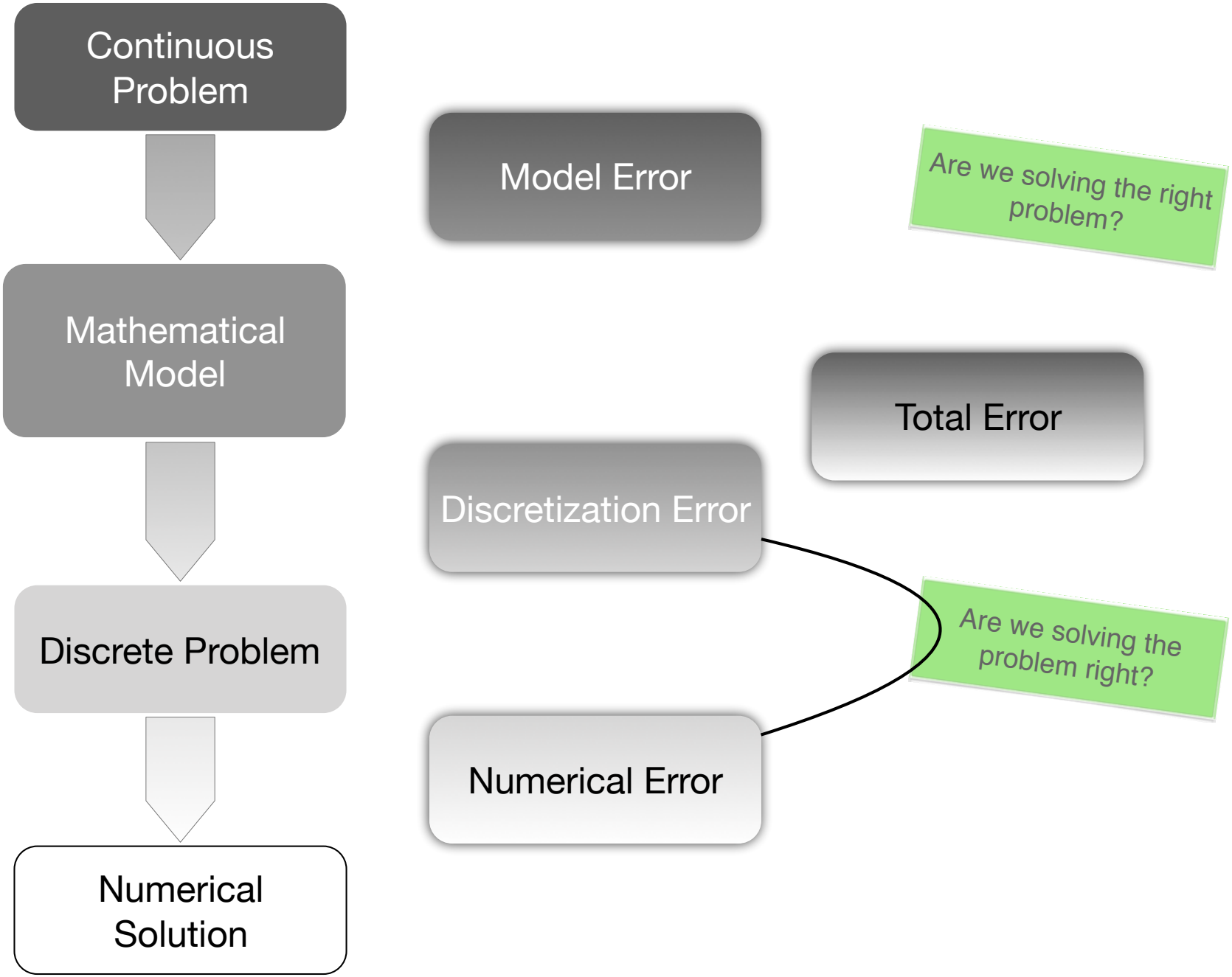
Are we solving the right problem?

Total Error

Discretization Error

Numerical Error

Mathematical Modelling



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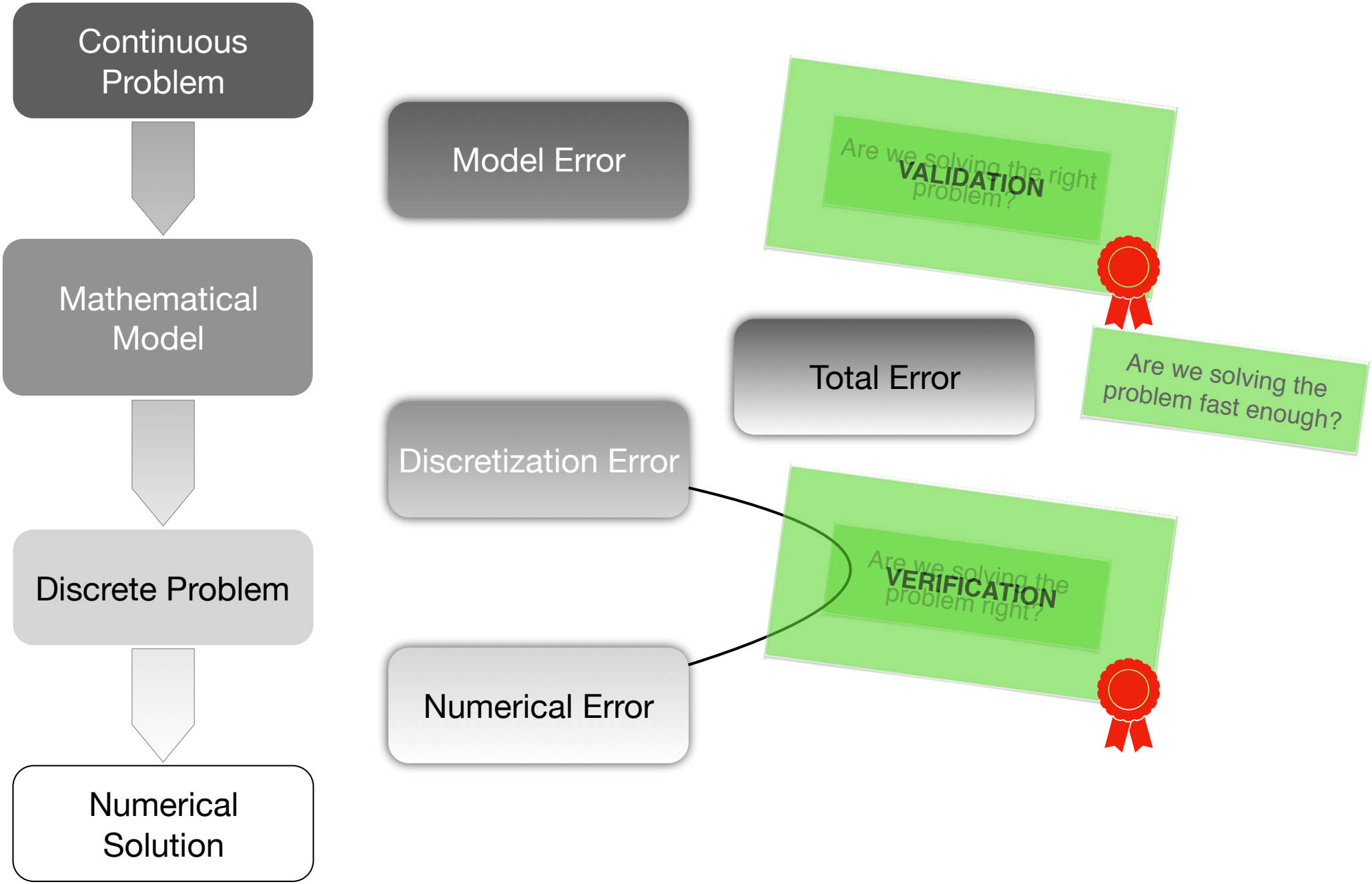
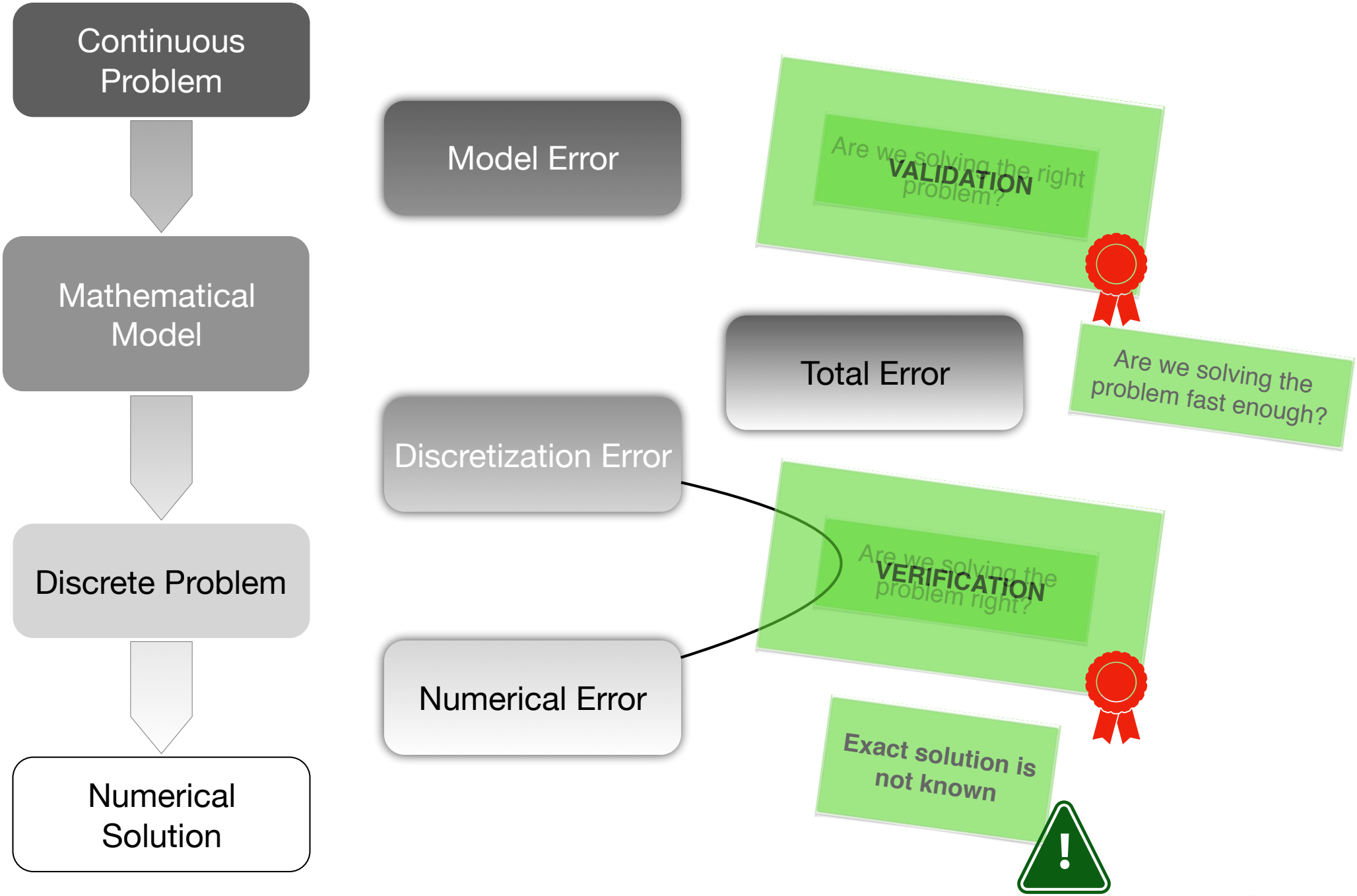


Mathematical Modelling



Computational Mechanics of Interfaces

with Engineering and Medical Applications

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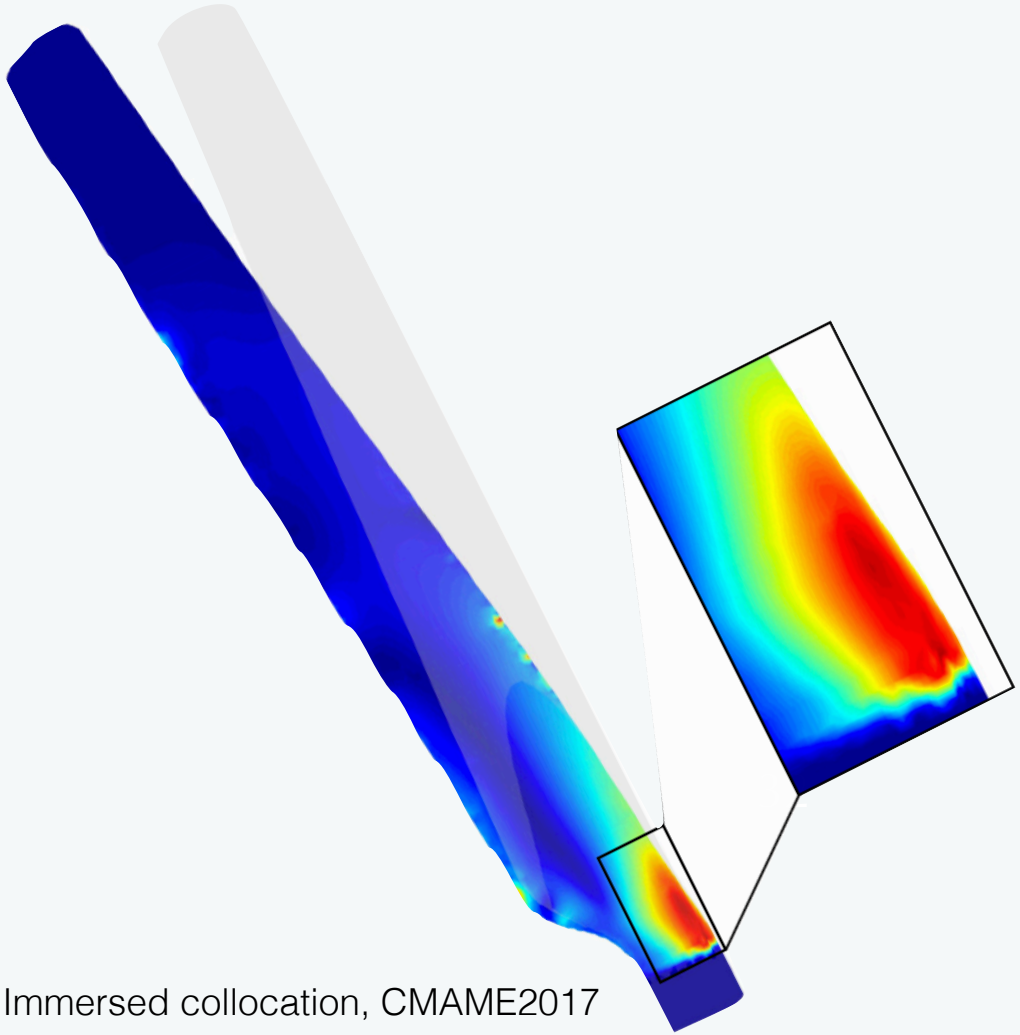
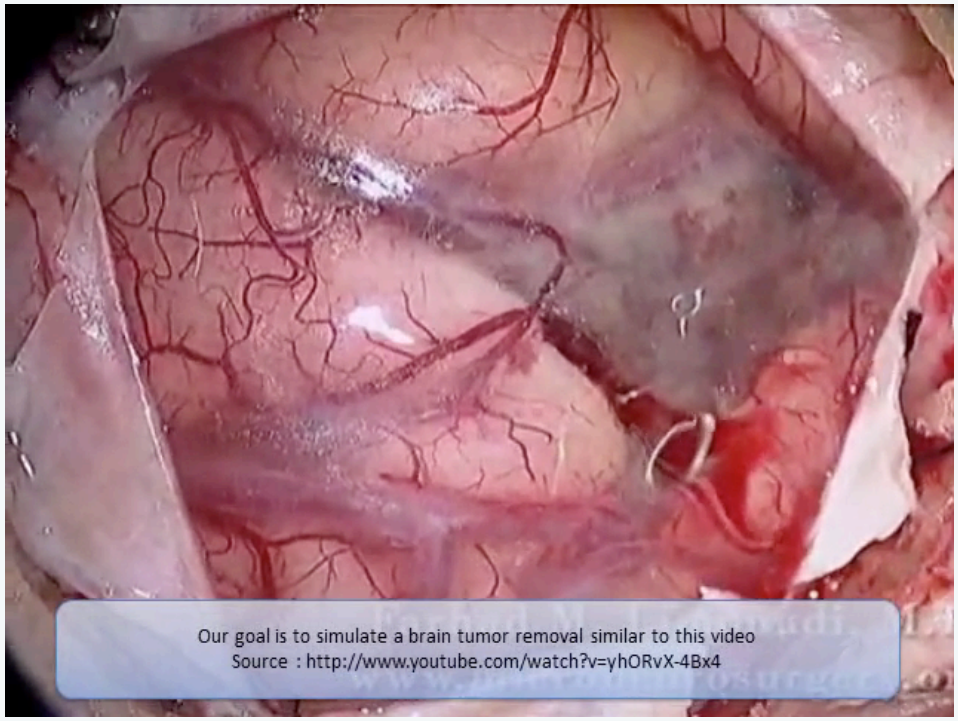
stephane.bordas@alum.northwestern.edu



Immersed collocation, CMAME2017



Real-time cutting, MEDIA2014, IEEE2017

Interface problems appear naturally

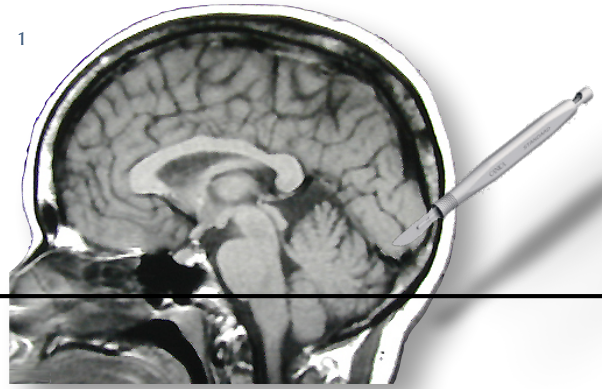
Discontinuities

1

Large scale

Small scale

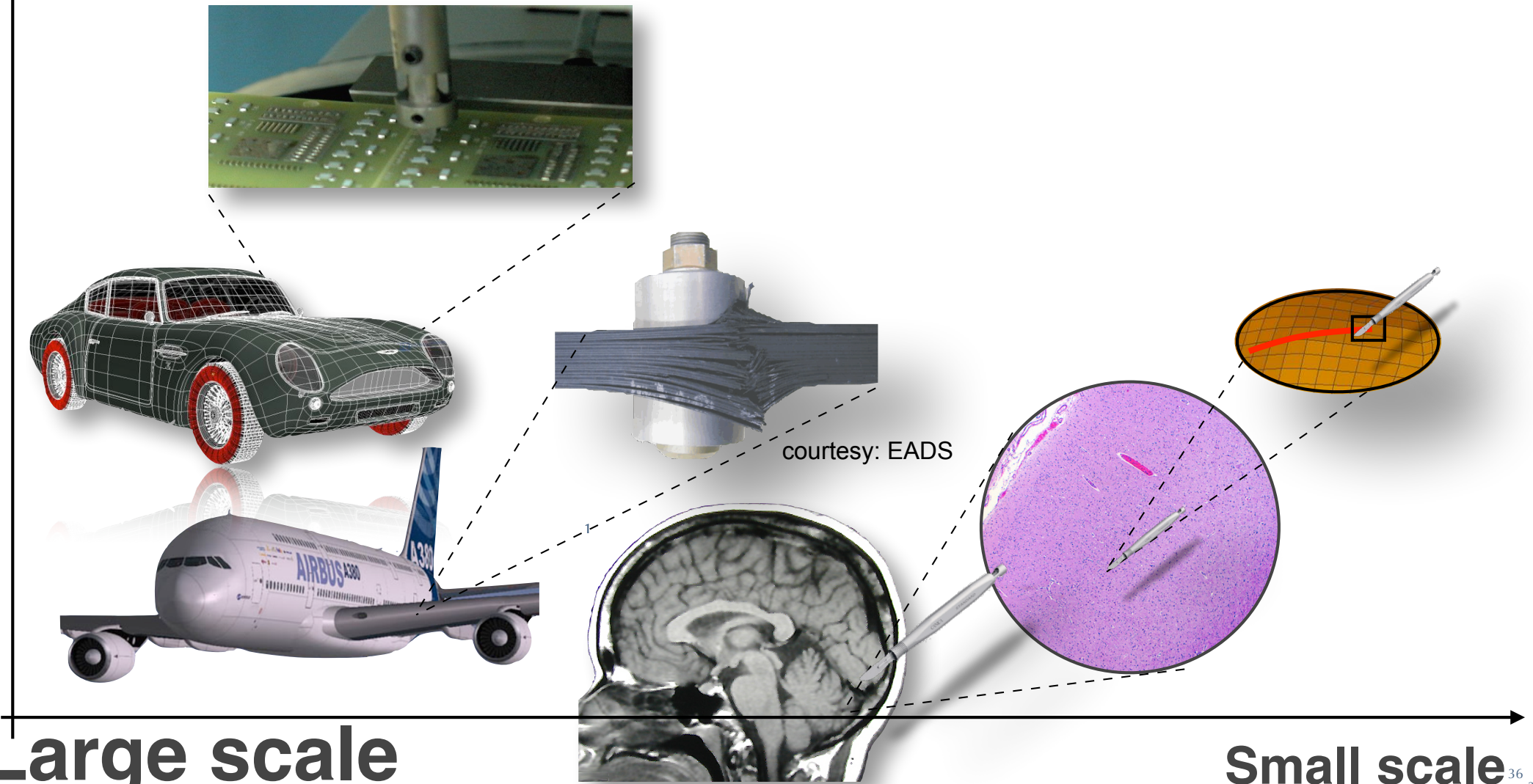
Discontinuities



Large scale

Small scale

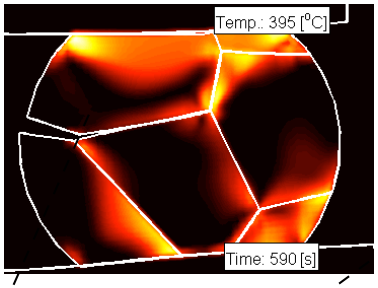
Discontinuities

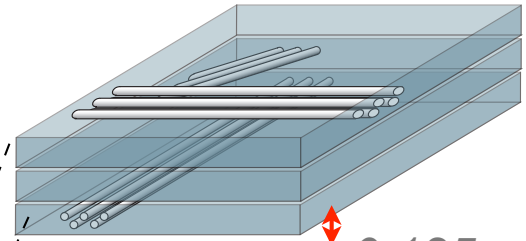


Large scale

Small scale

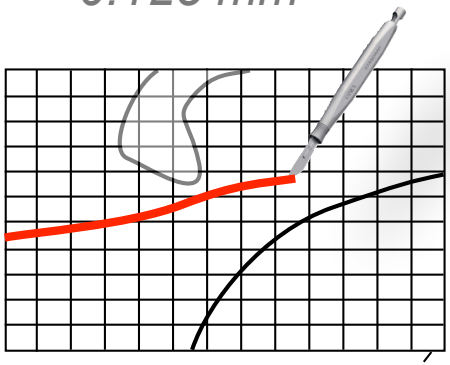
Discontinuities

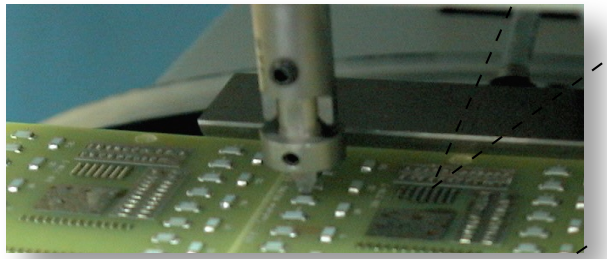


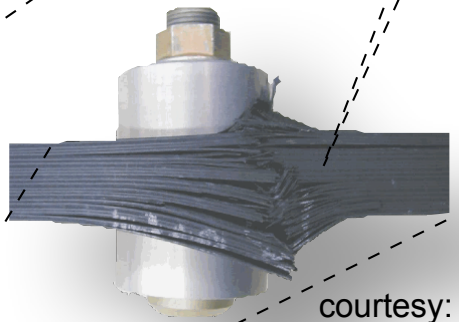


100 plies

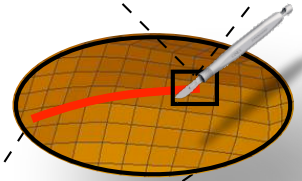
0.125 mm

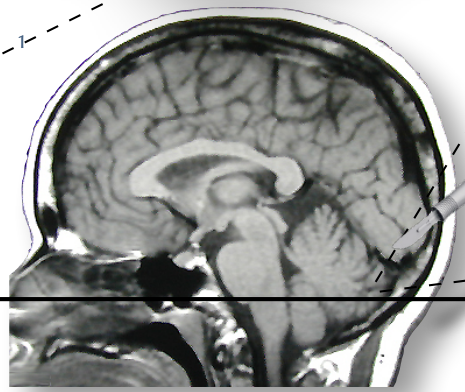


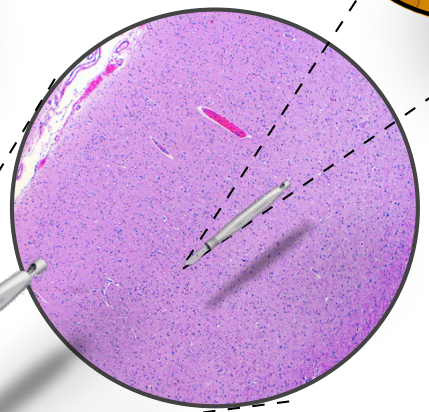




courtesy: EADS

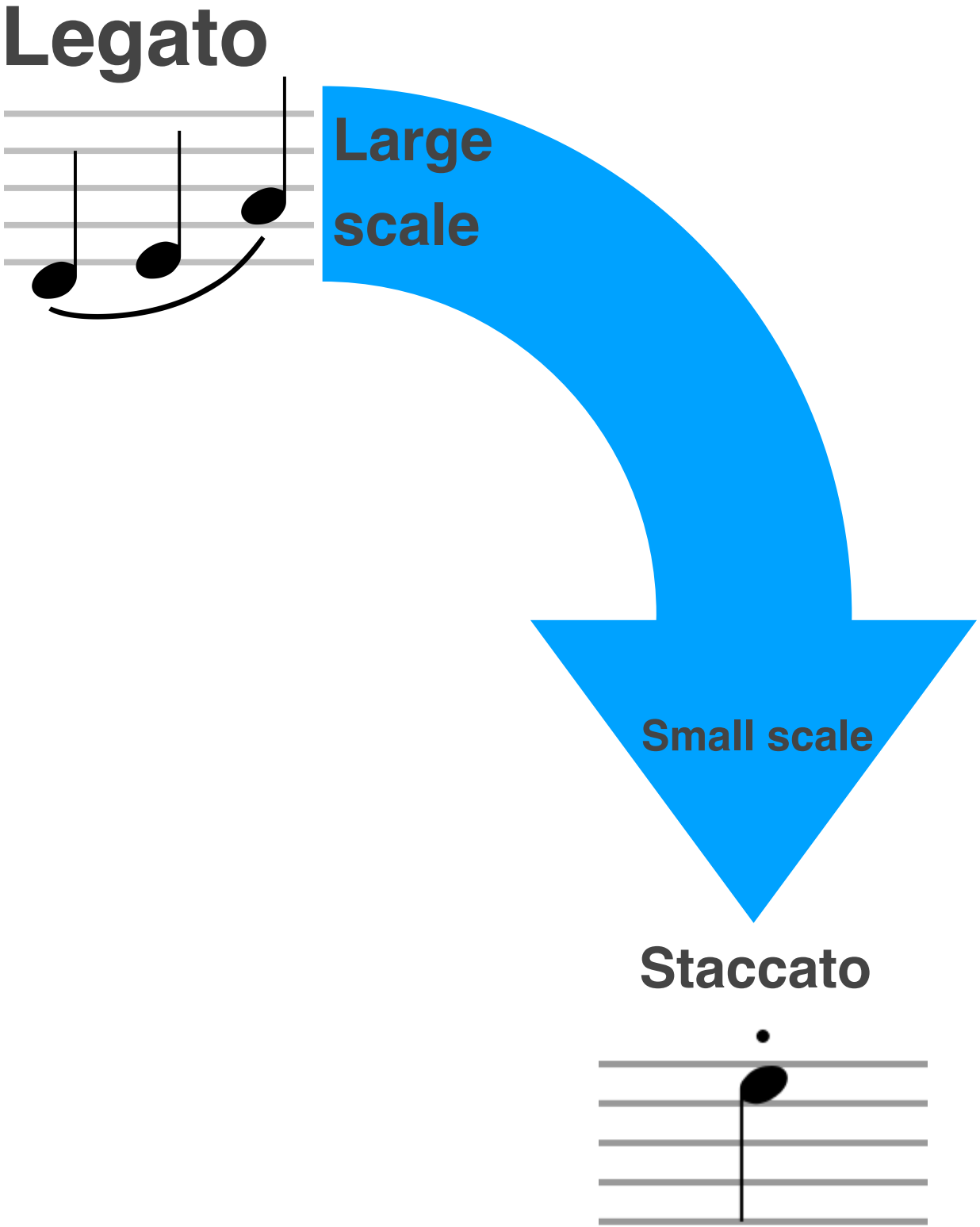




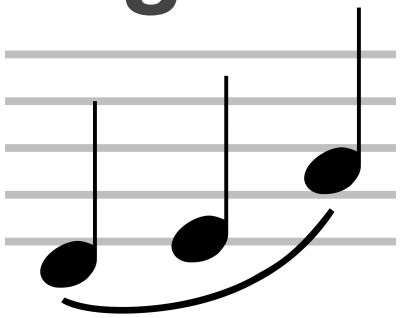


Large scale

Small scale

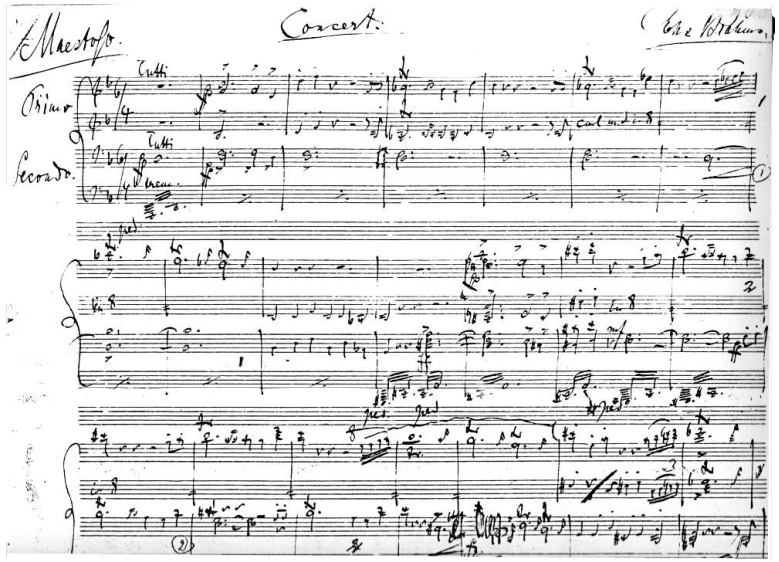

Legato
Large scale
Small scale
Staccato

Legato

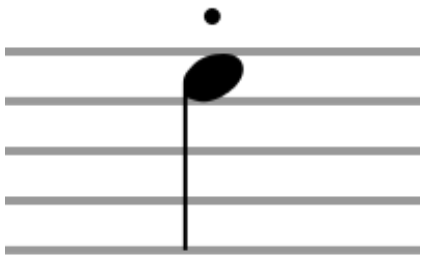


Large scale

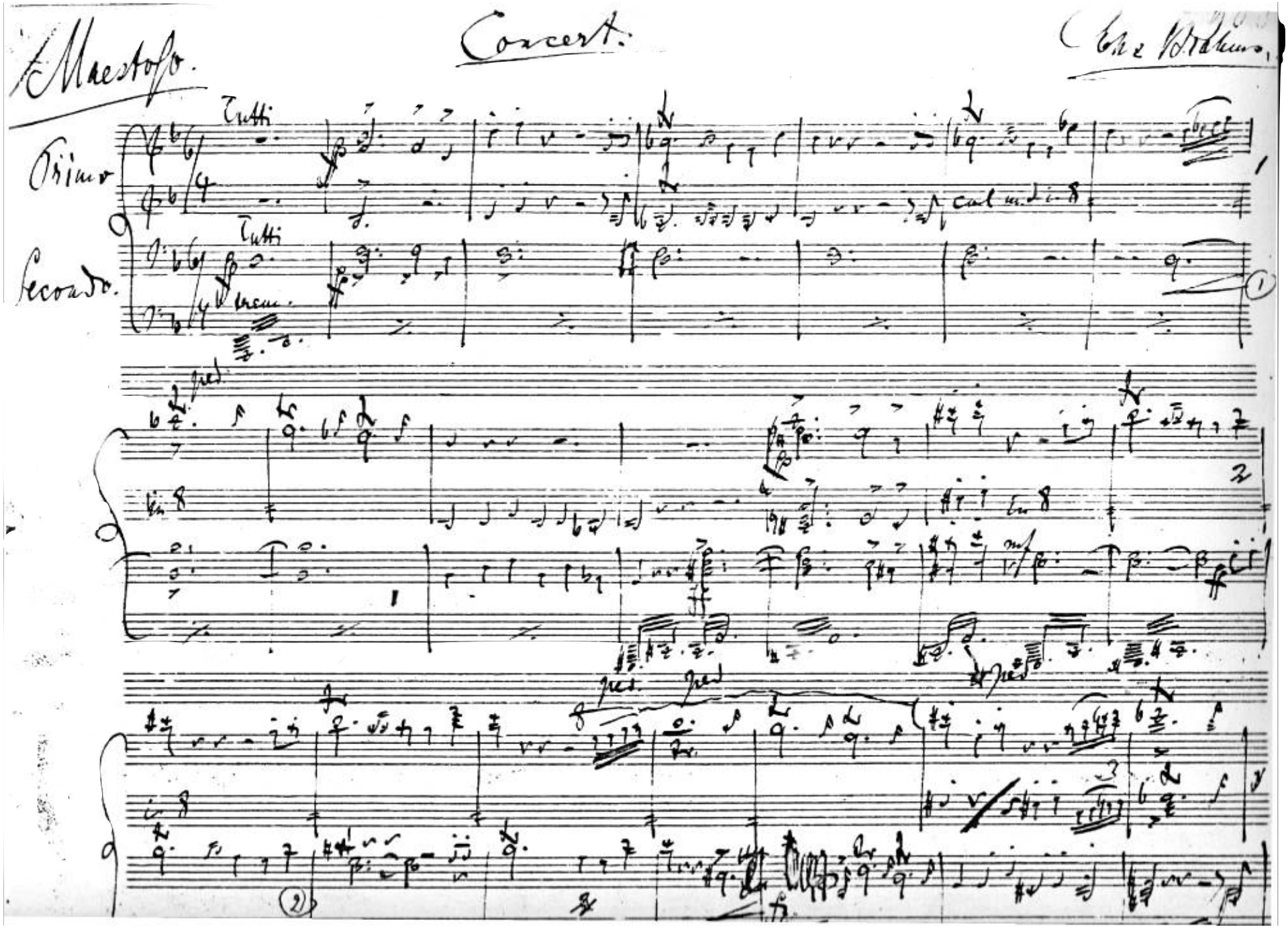
Small scale



Staccato

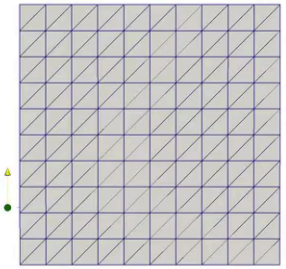


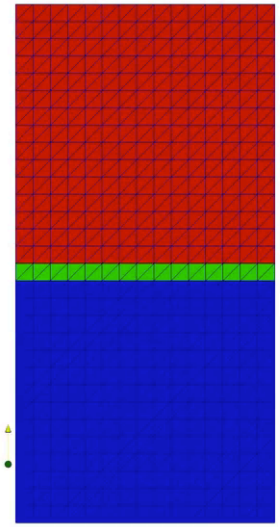
Music of materials

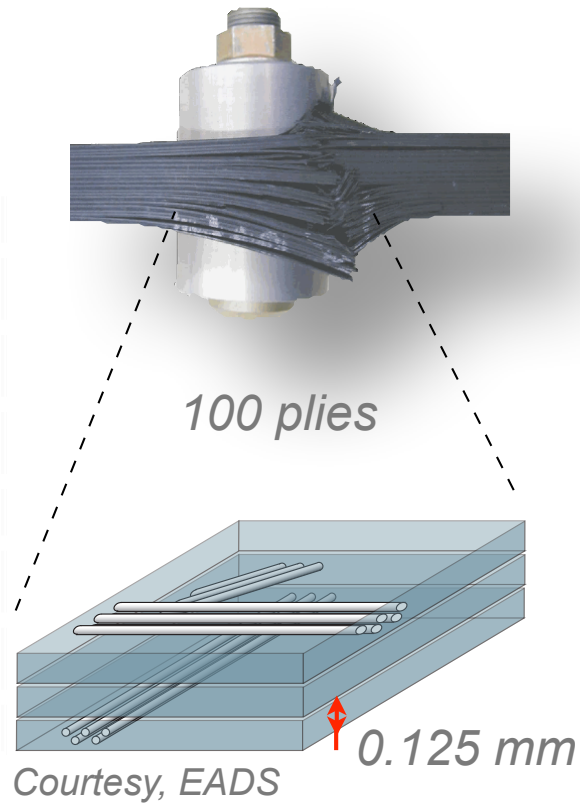


BRAHMS Piano Concerto Nr. 1, op. 15, Tibor HAZAY, Kurt BRASS St Gallen Orchestra

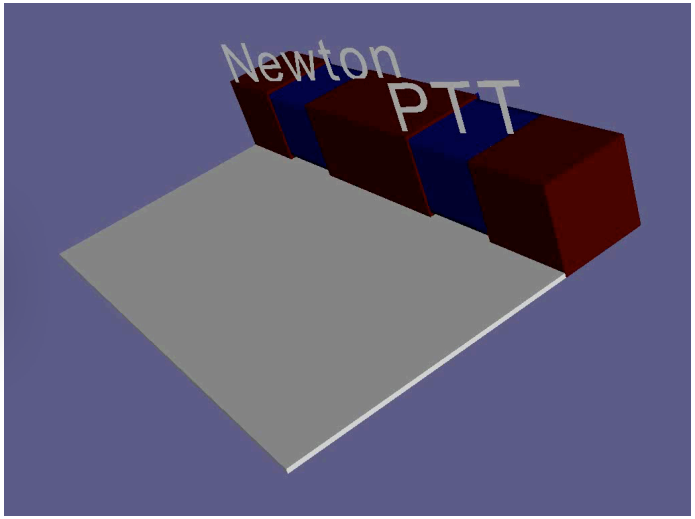
Phases

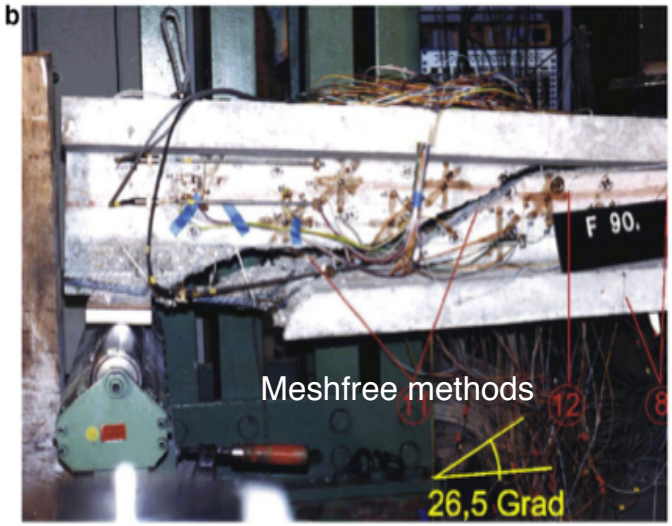


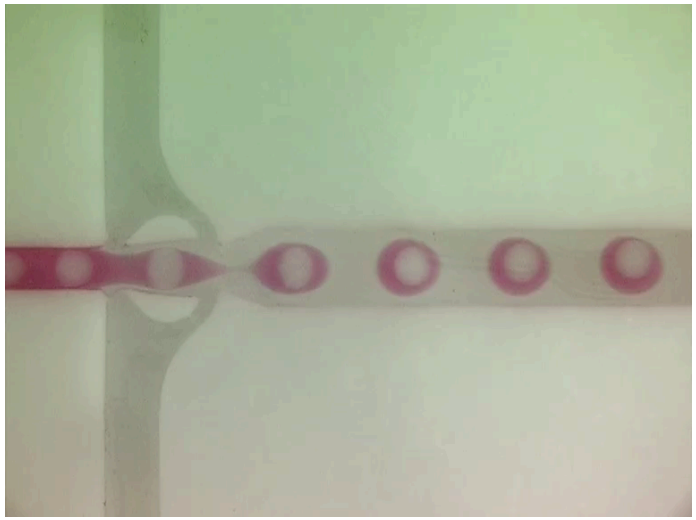




Courtesy, EADS



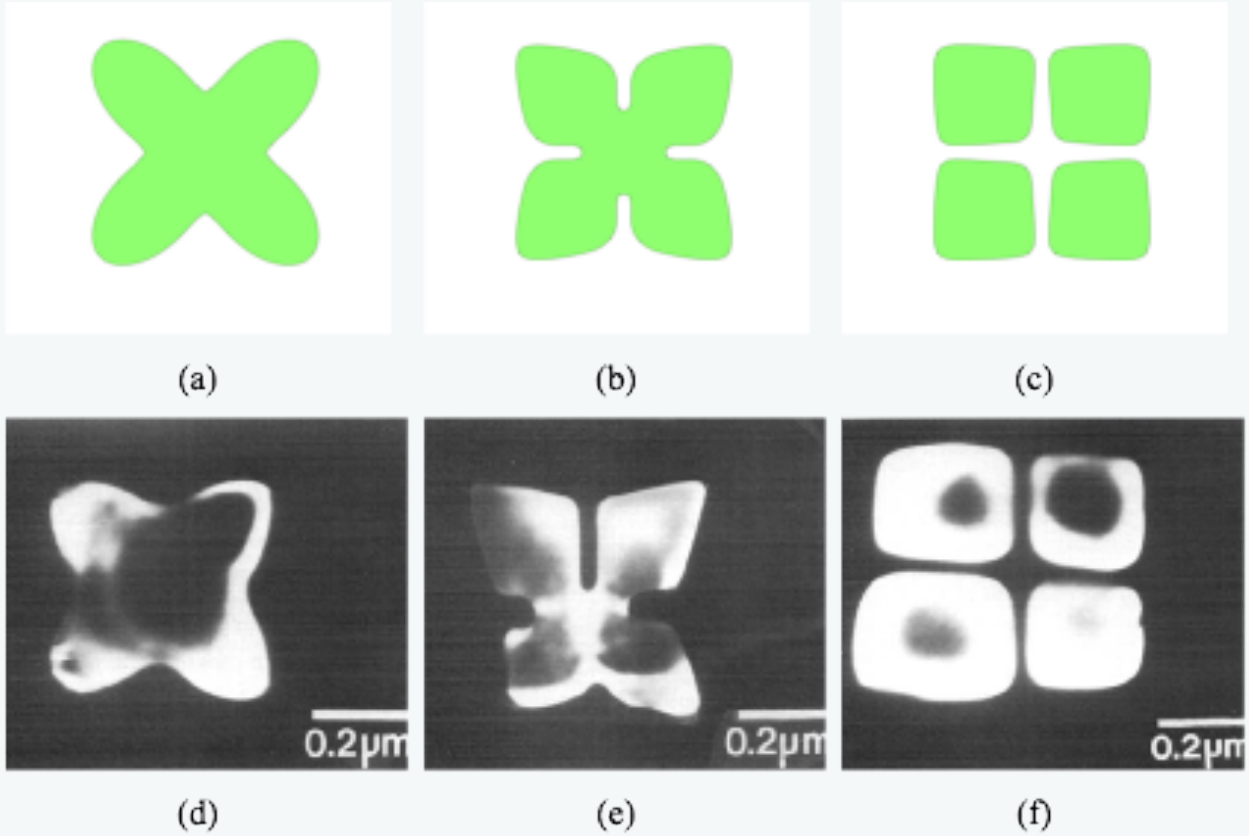




CMECH 2007, EFM2008 CAS 2009, with Timon Rabczuk and Goangseup Zi

Phases at the nano-scale

Surface effects are critical

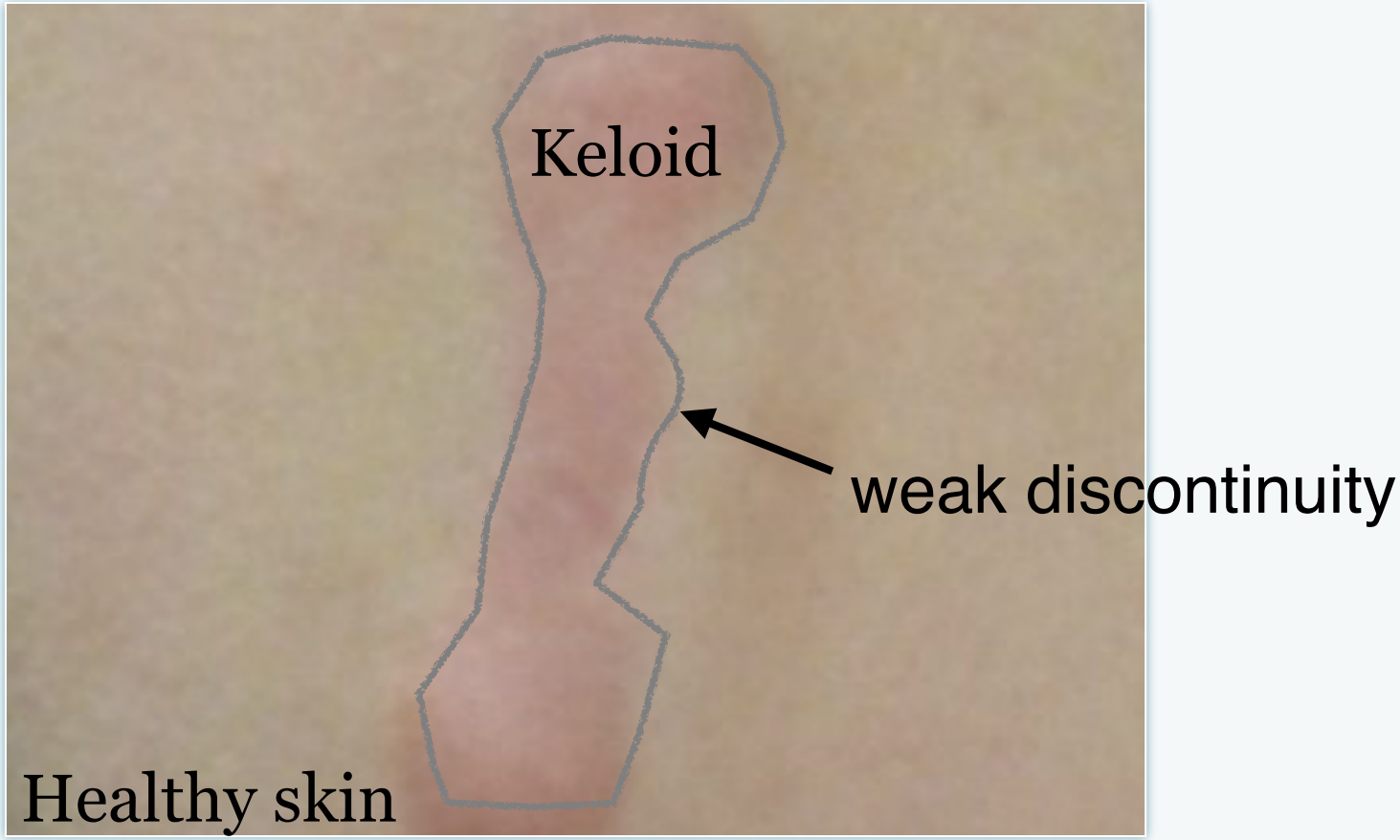


Equilibrium shapes of nano-heterogeneities (with X. Zhao, R. Duddu, J. Qu).

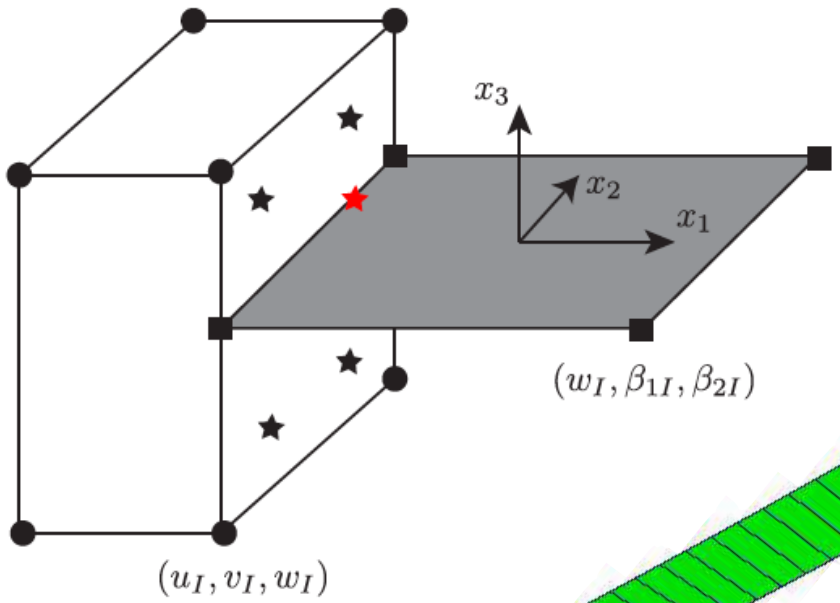
JMPS2015 http://orbilu.uni.lu/bitstream/10993/11024/1/manuscript%20-%20JMPS-D-12-00428.pdf
CMECH2013 http://orbilu.uni.lu/bitstream/10993/11022/1/Manuscript_XZHAO_CMECH_revision.pdf

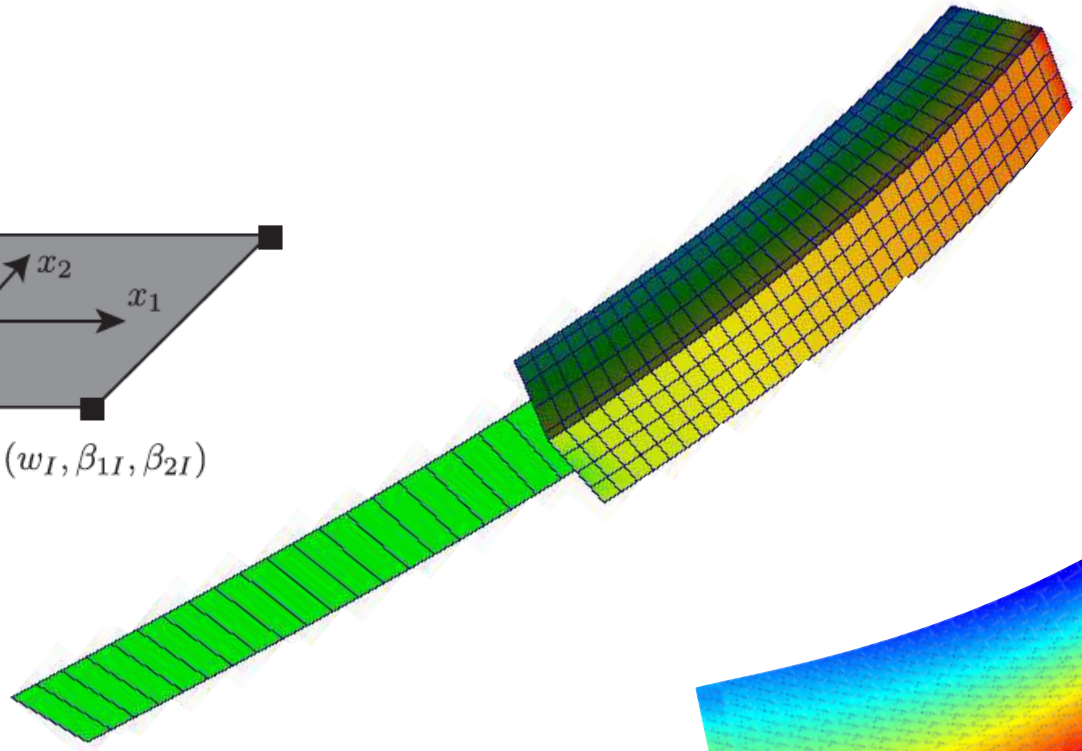
$$\bar{F} = \int_V W dV + \int_\Gamma \gamma dS + \lambda \left(\int_\Omega dV - V_0 \right)$$

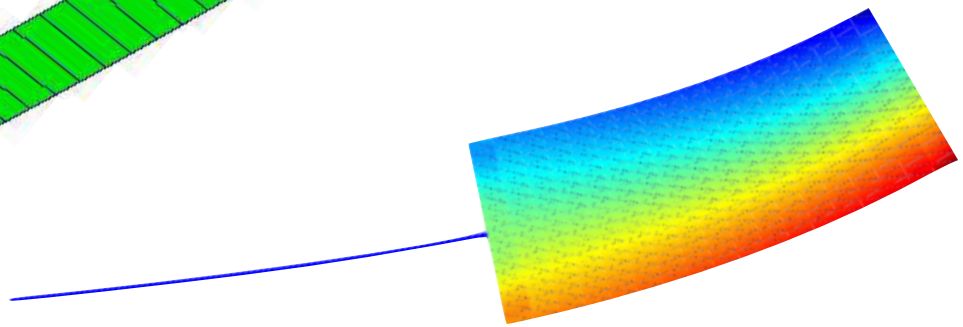
Keloid
Healthy skin


Keloid
weak discontinuity
Healthy skin

Kinematics interfaces

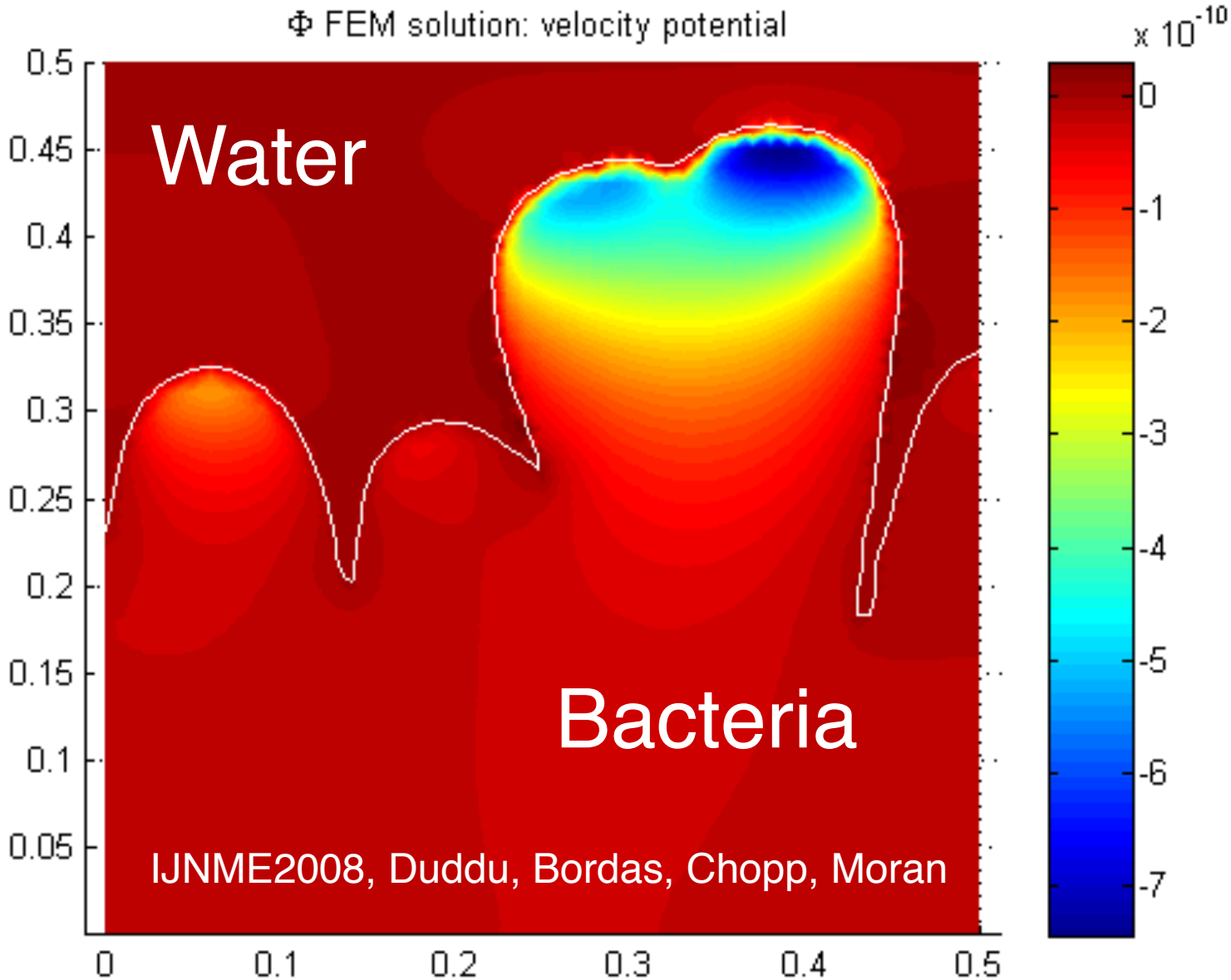




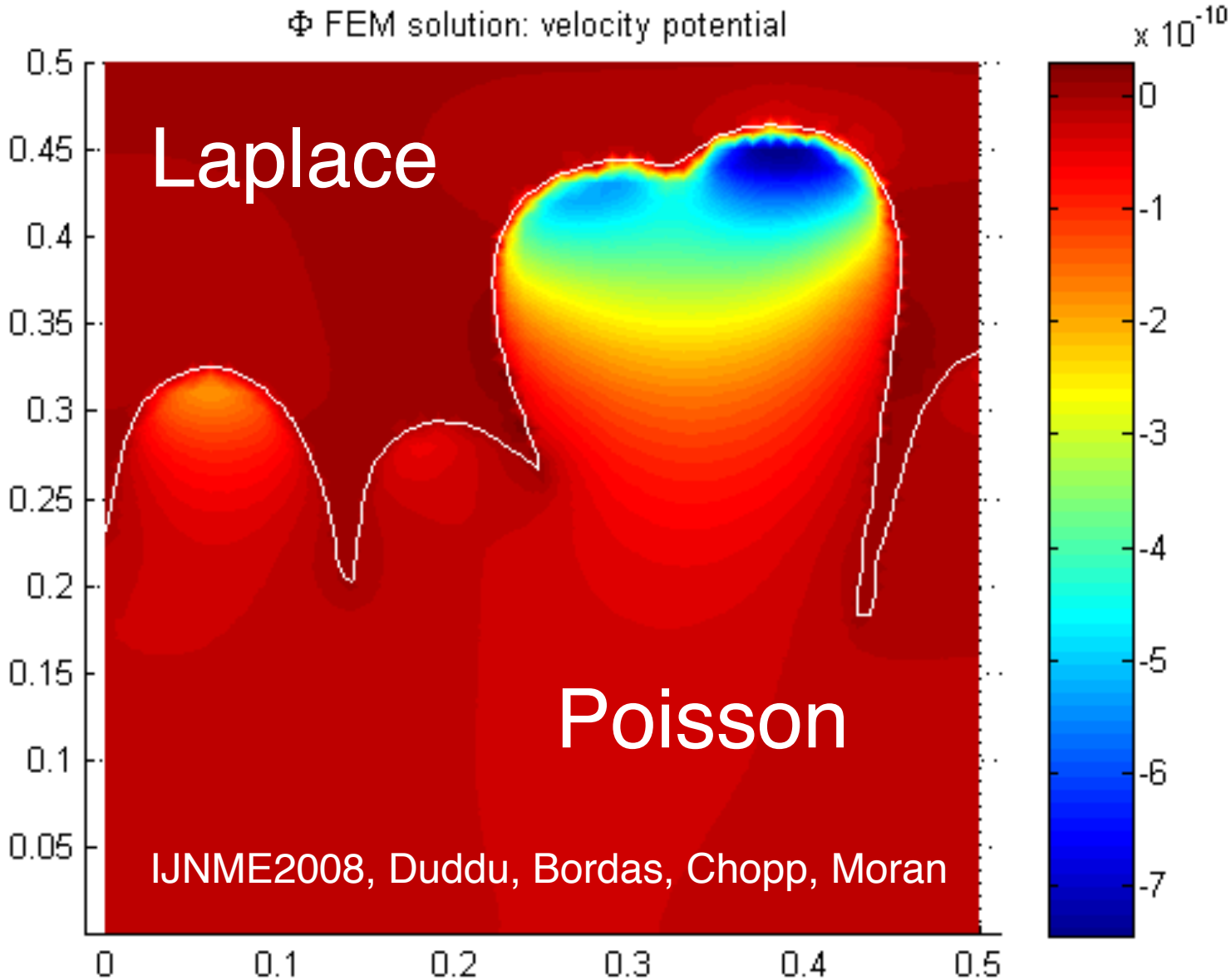


Interfaces between different PDEs

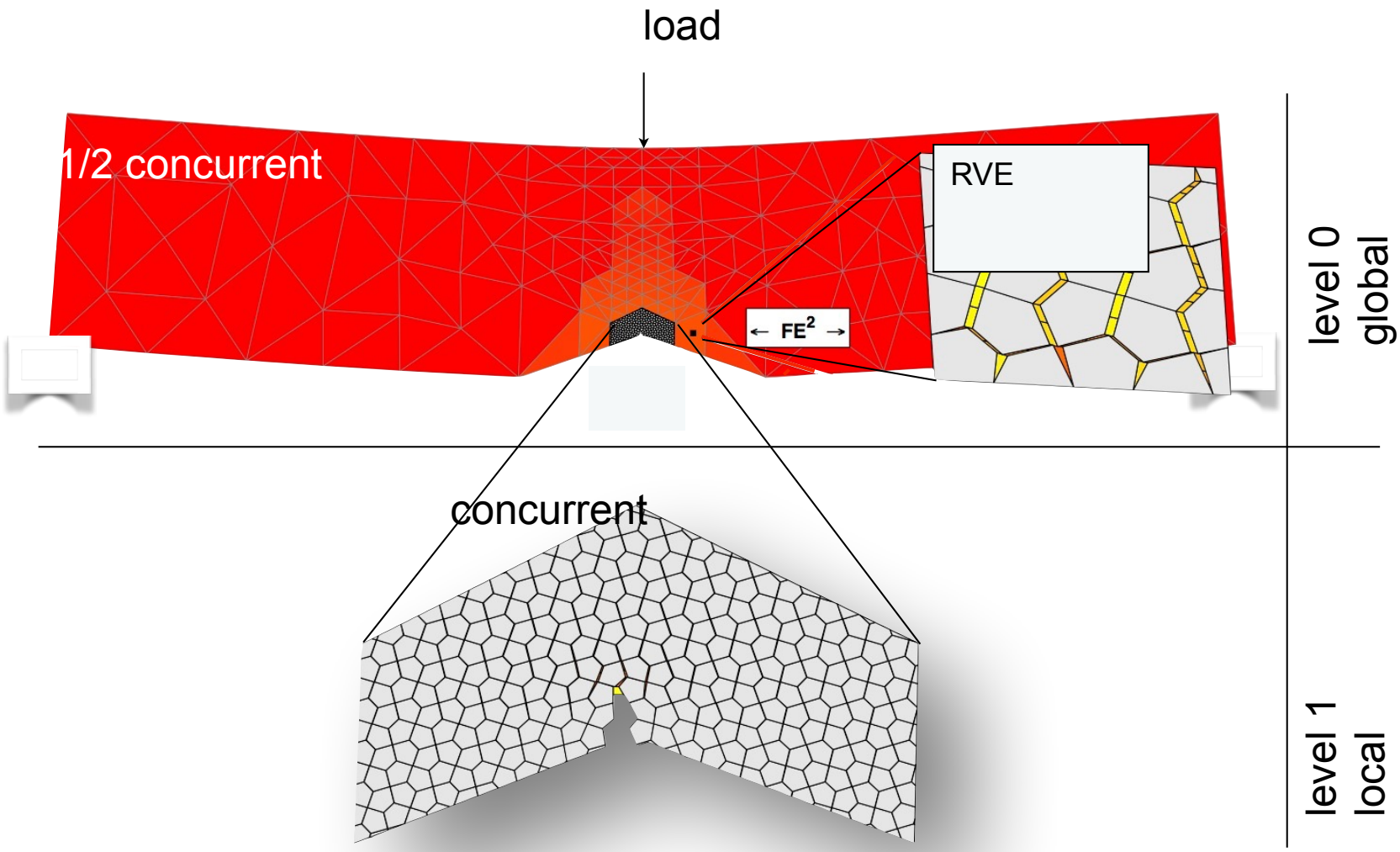
e.g. Biofilms



Interfaces between different PDEs

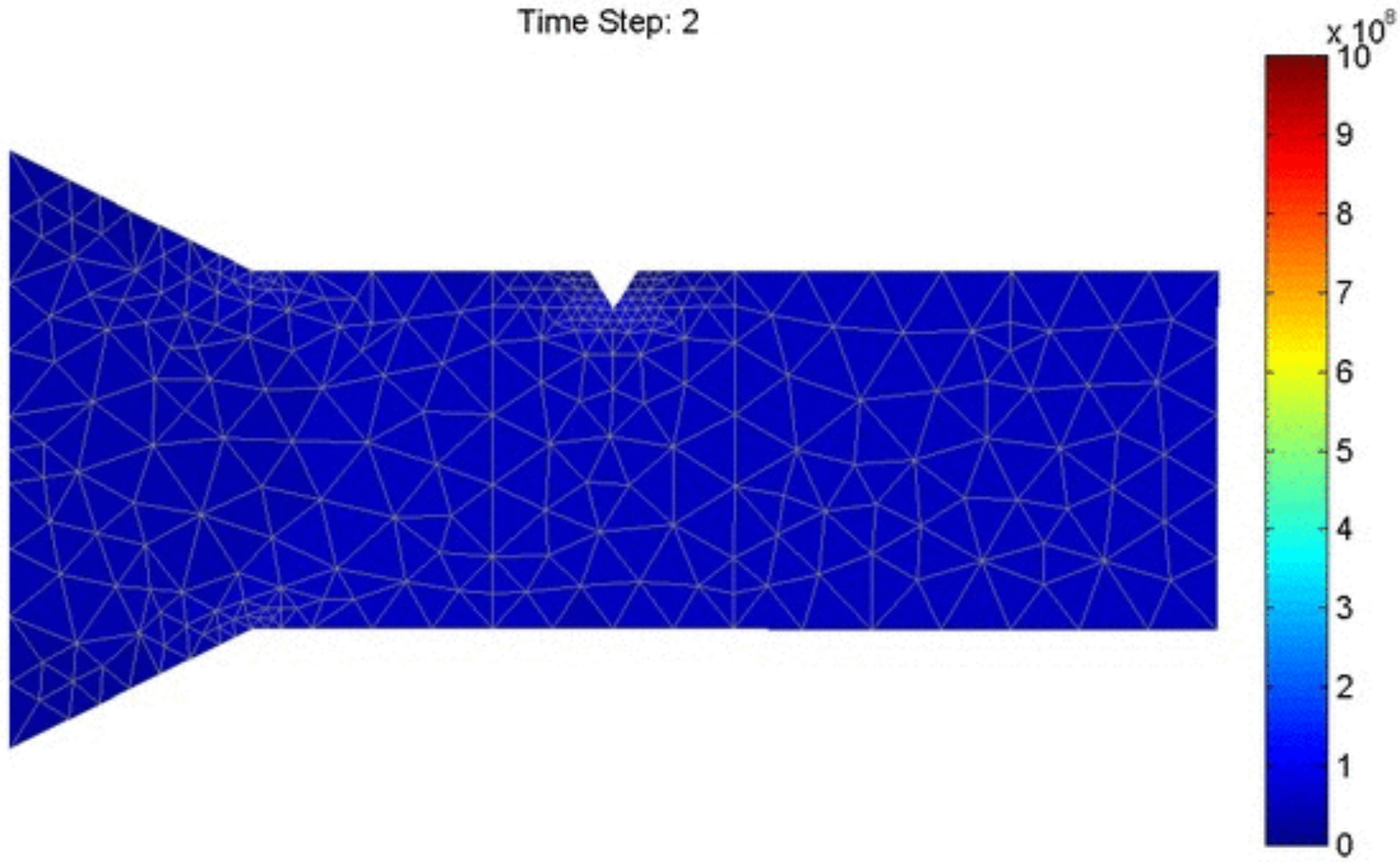


Interfaces between material models

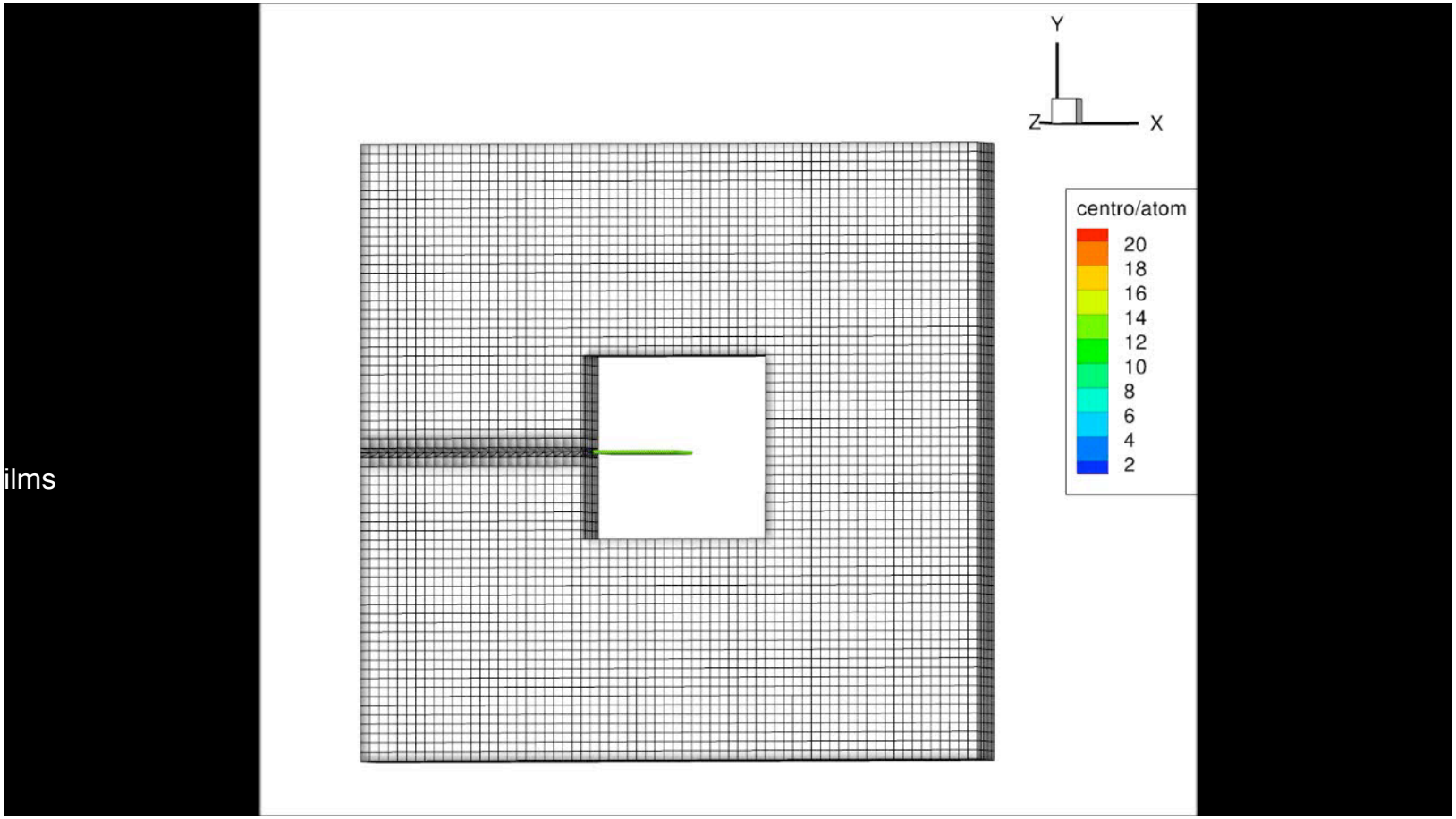


PhilMag15, Akbari
CMAME13,CMECH16, Goury
NMPDES13,CMAME15, Chi

Adaptive model selection



Molecular dynamics - continuum interfaces

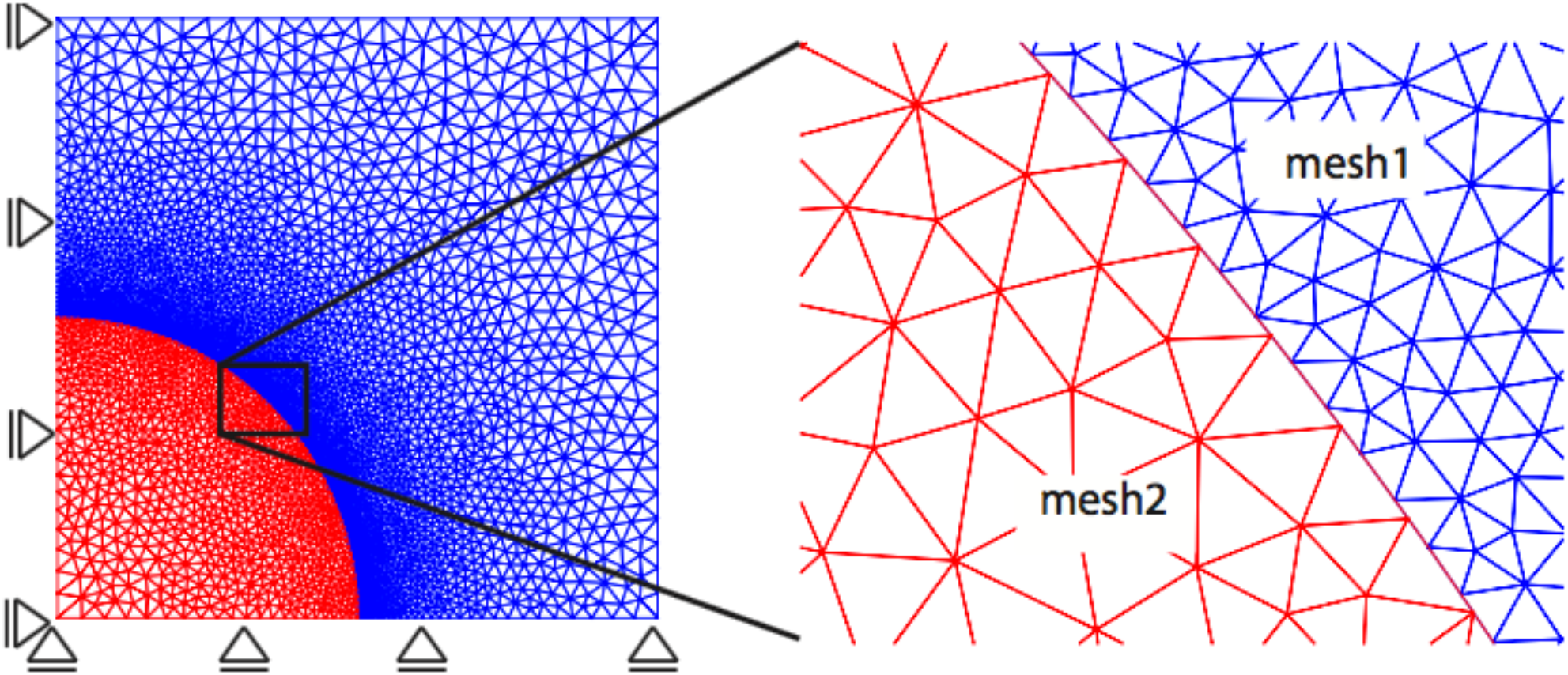


ilms

CMECH14, IJMSE13 Talebi

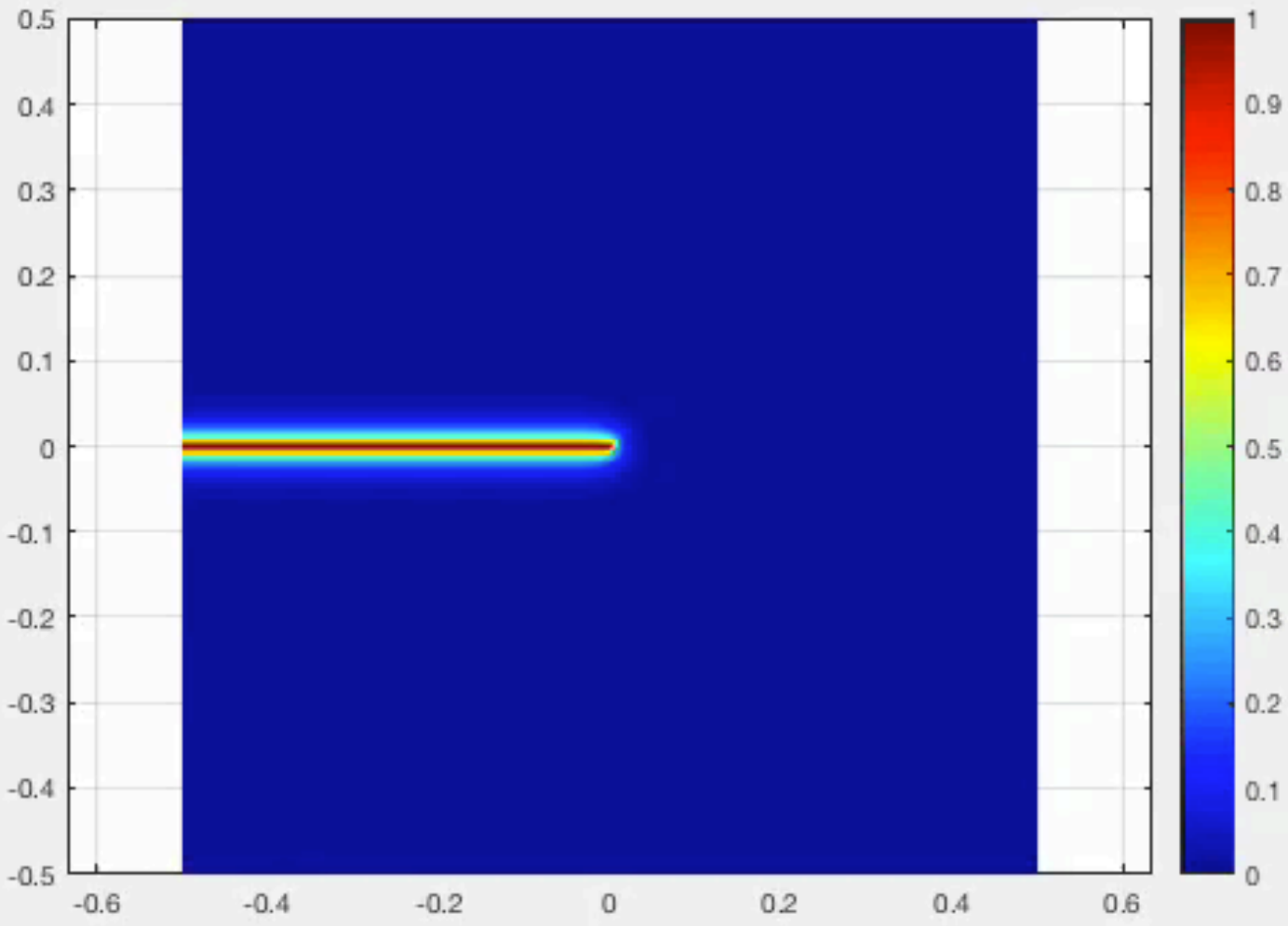
Interfaces between different discretizations

Example: non-matching meshes/discretisation



CMECH2014, CAD2014, CMECH2016, MatCompSim2016, CMAME2017, Nguyen-Vinh Phu
http://publications.uni.lu/bitstream/10993/13726/1/phu-meshless.pdf
https://orbilu.uni.lu/bitstream/10993/15234/1/bordasphu.pdf

Cracks and cuts



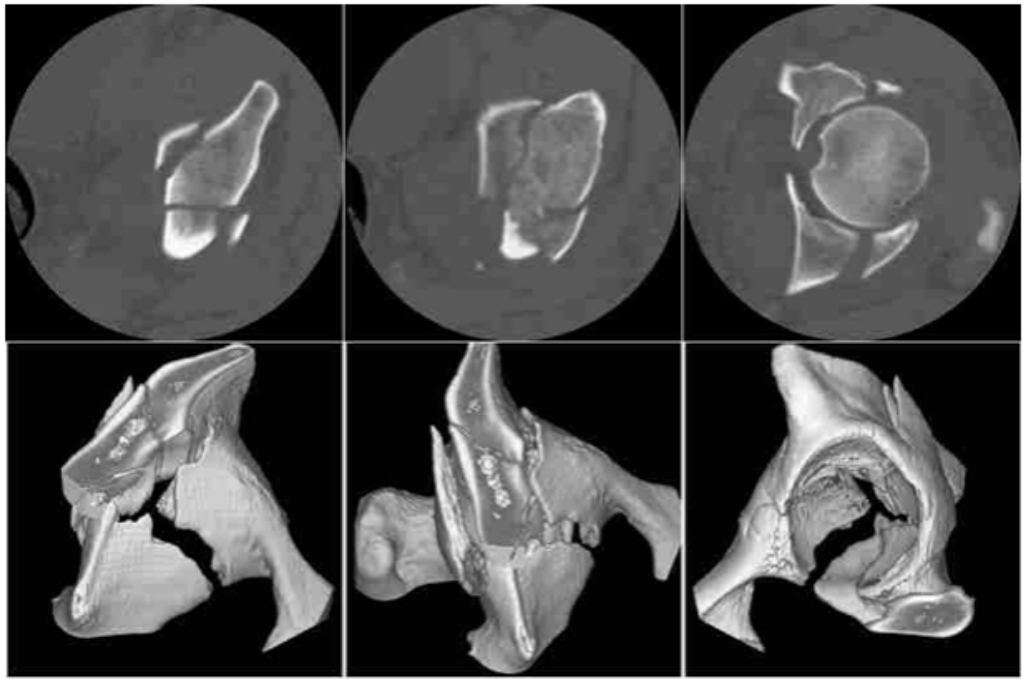
2017 Nguyen-Vinh Phu

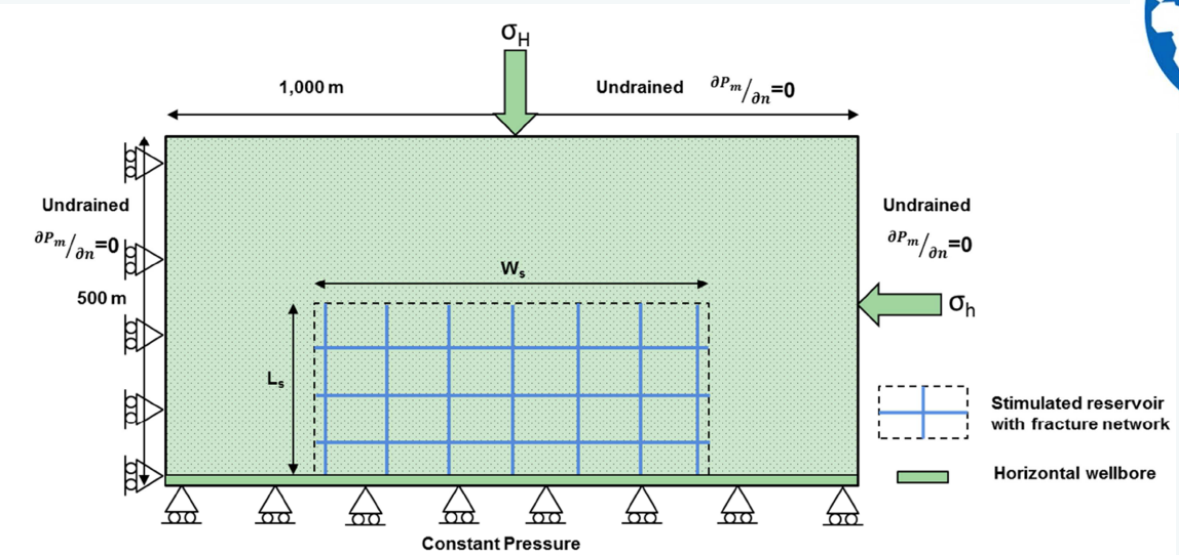
Shuttle crash, 2003

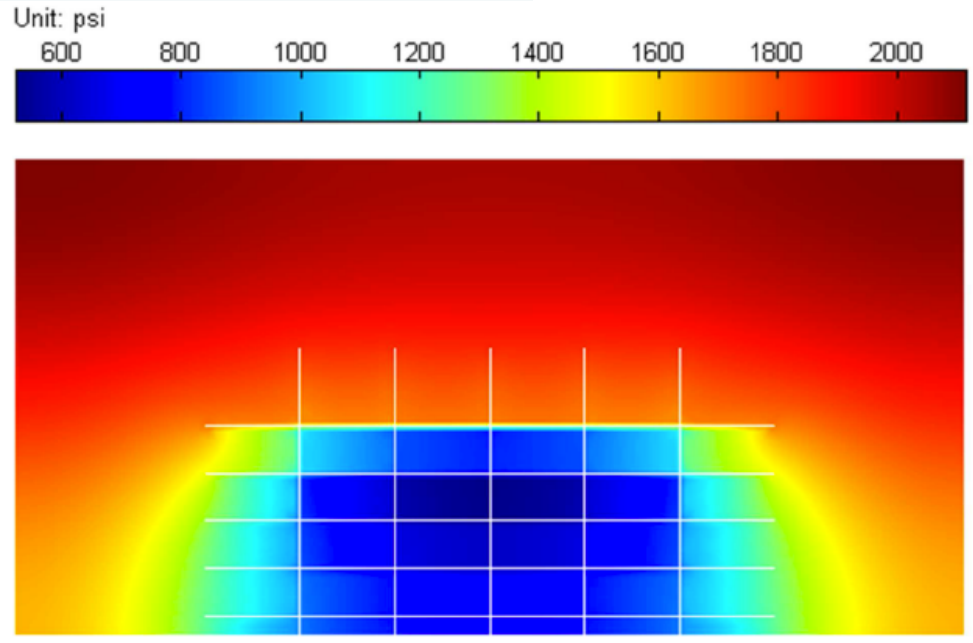
Landslide, Colorado

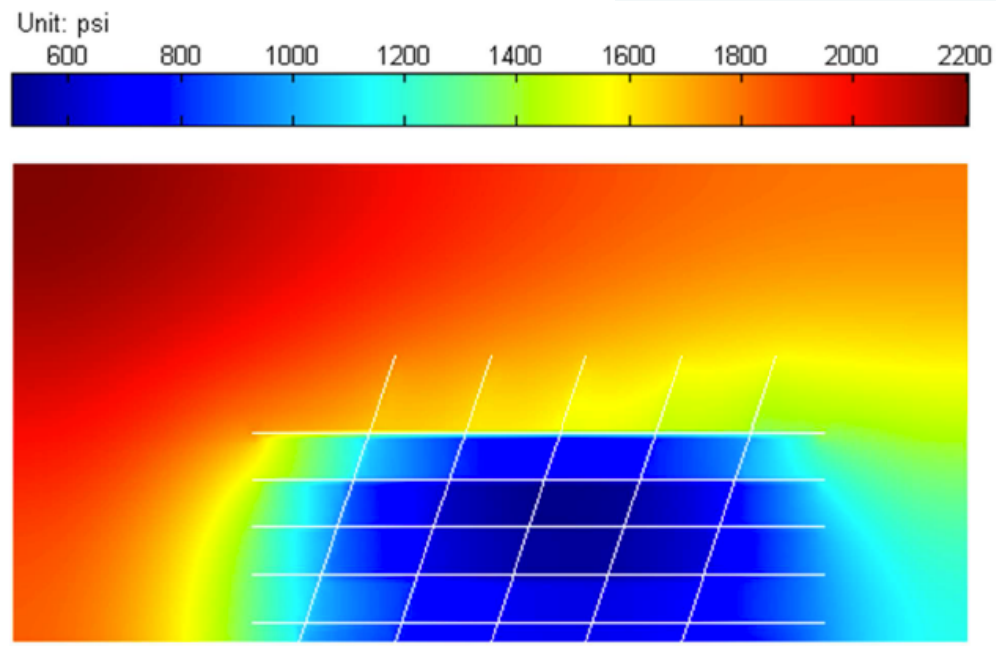
Taiwan earthquake, 2003

Fragmentation of concrete

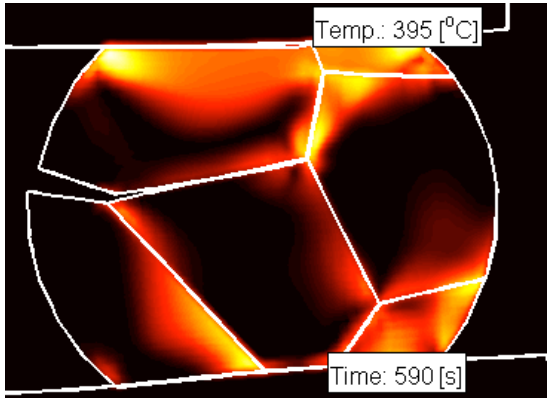



σH
1,000 m
Undrained
∂Pm/∂n=0
Undrained
∂Pm/∂n=0
500 m
Ws
Ls
Undrained
∂Pm/∂n=0
σh
Stimulated reservoir
with fracture network
Horizontal wellbore
Constant Pressure

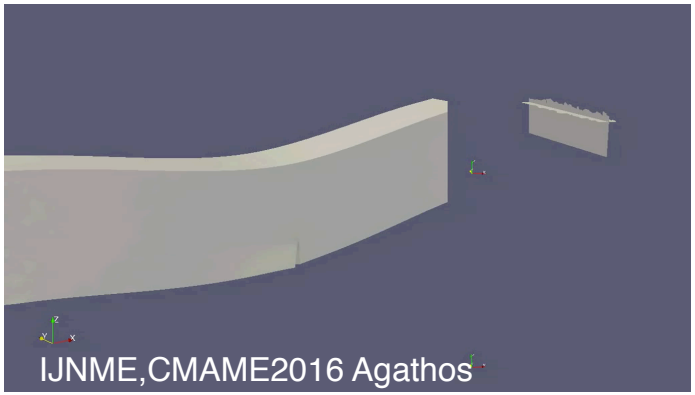

Unit: psi
600
800
1000
1200
1400
1600
1800
2000

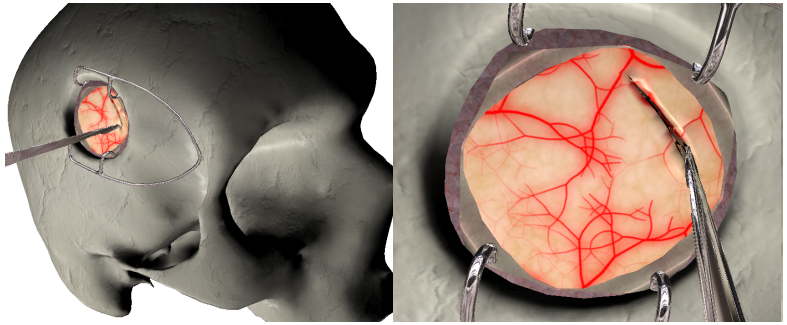

Unit: psi
600
800
1000
1200
1400
1600
1800
2000
2200

CRACKS & CUTS

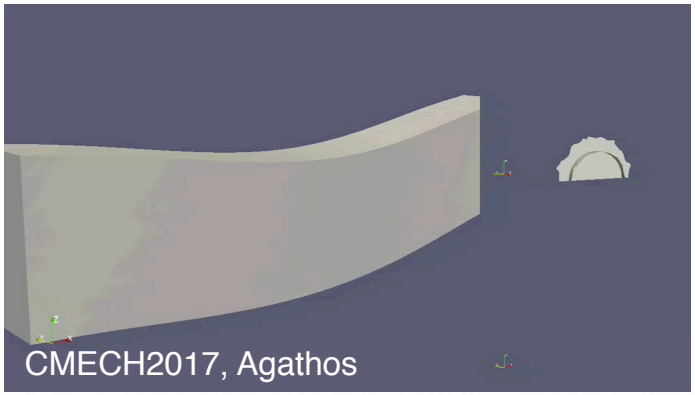


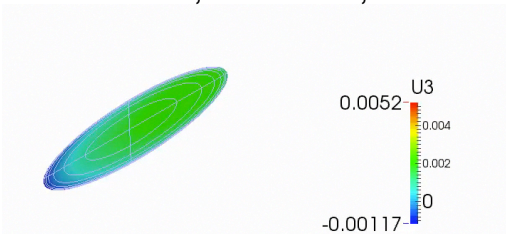
IJNME2011, CMS2012, Menk



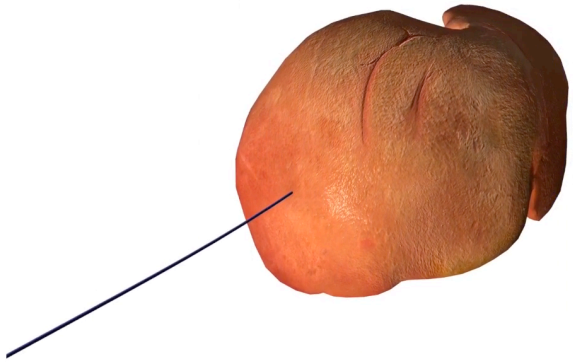


Real-time simulation of cutting during brain surgery
Med. Im. Anal. 2014 Courtecuisse



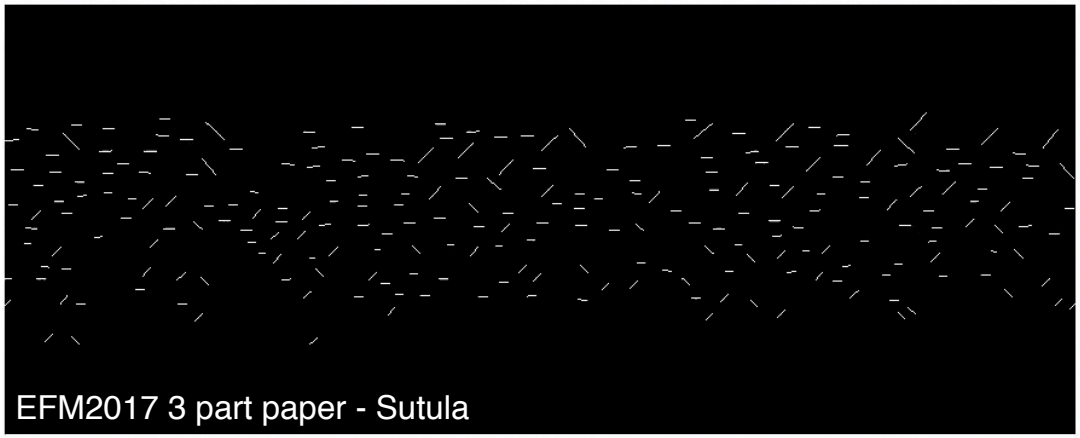


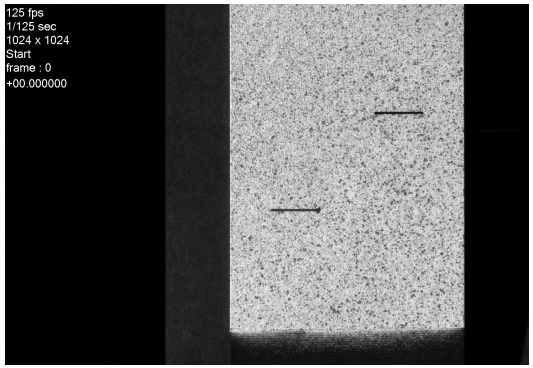
CMAME2016 Peng



Needle tissue interaction with breathing motion

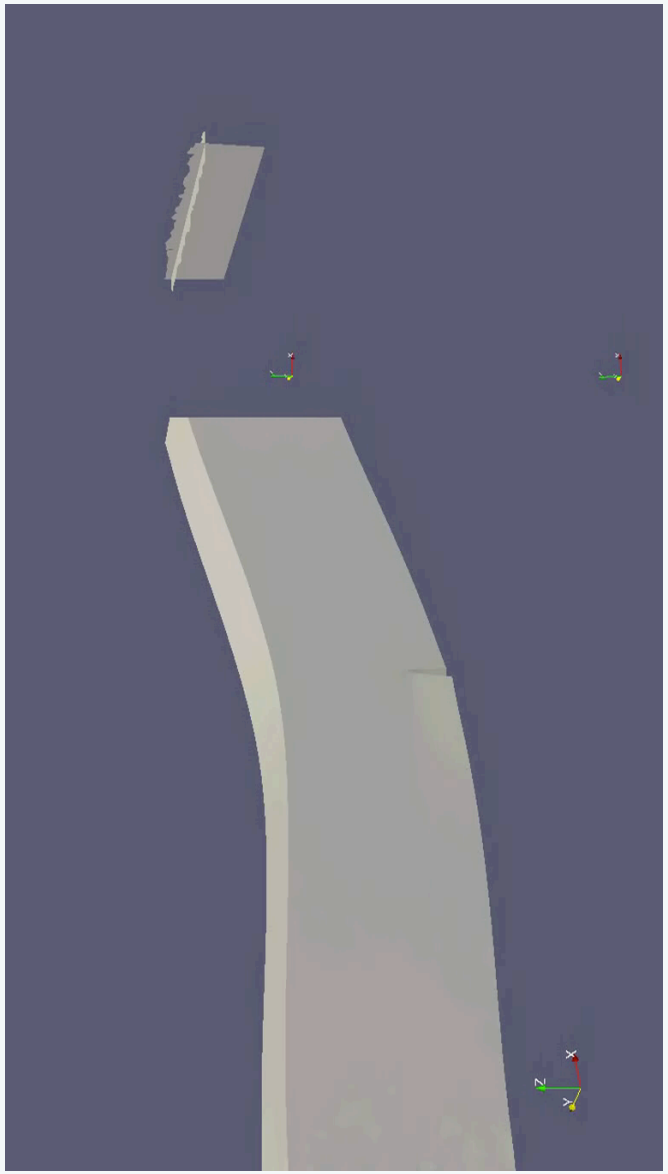
IEEE J. Biomed. Engng. 2017 Bui

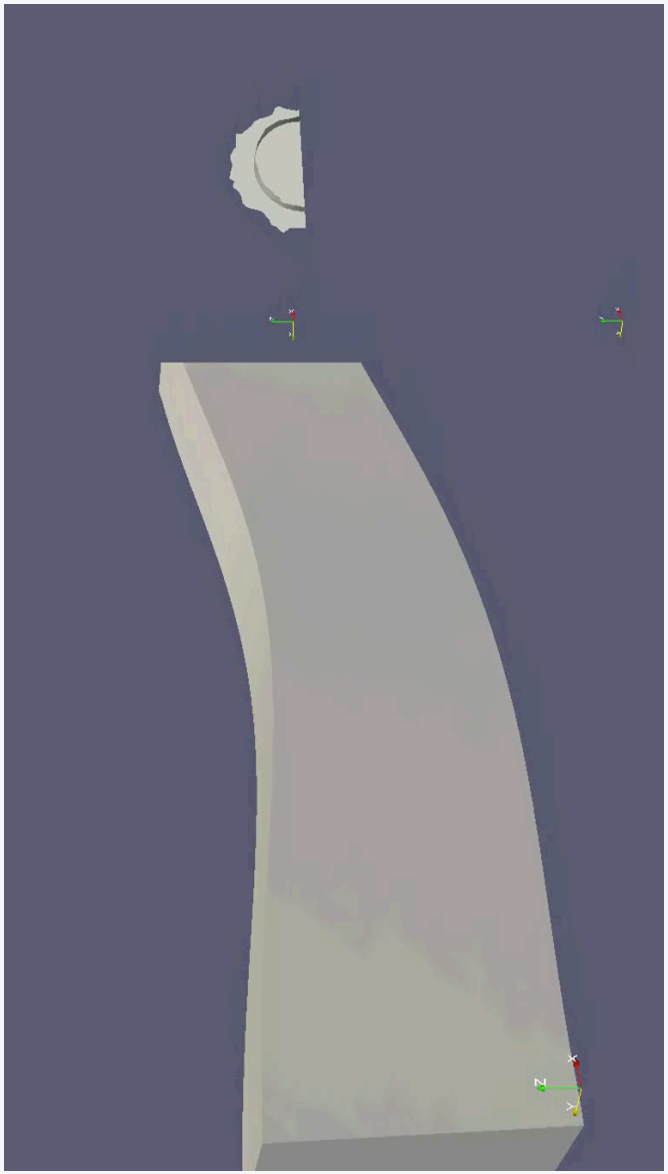




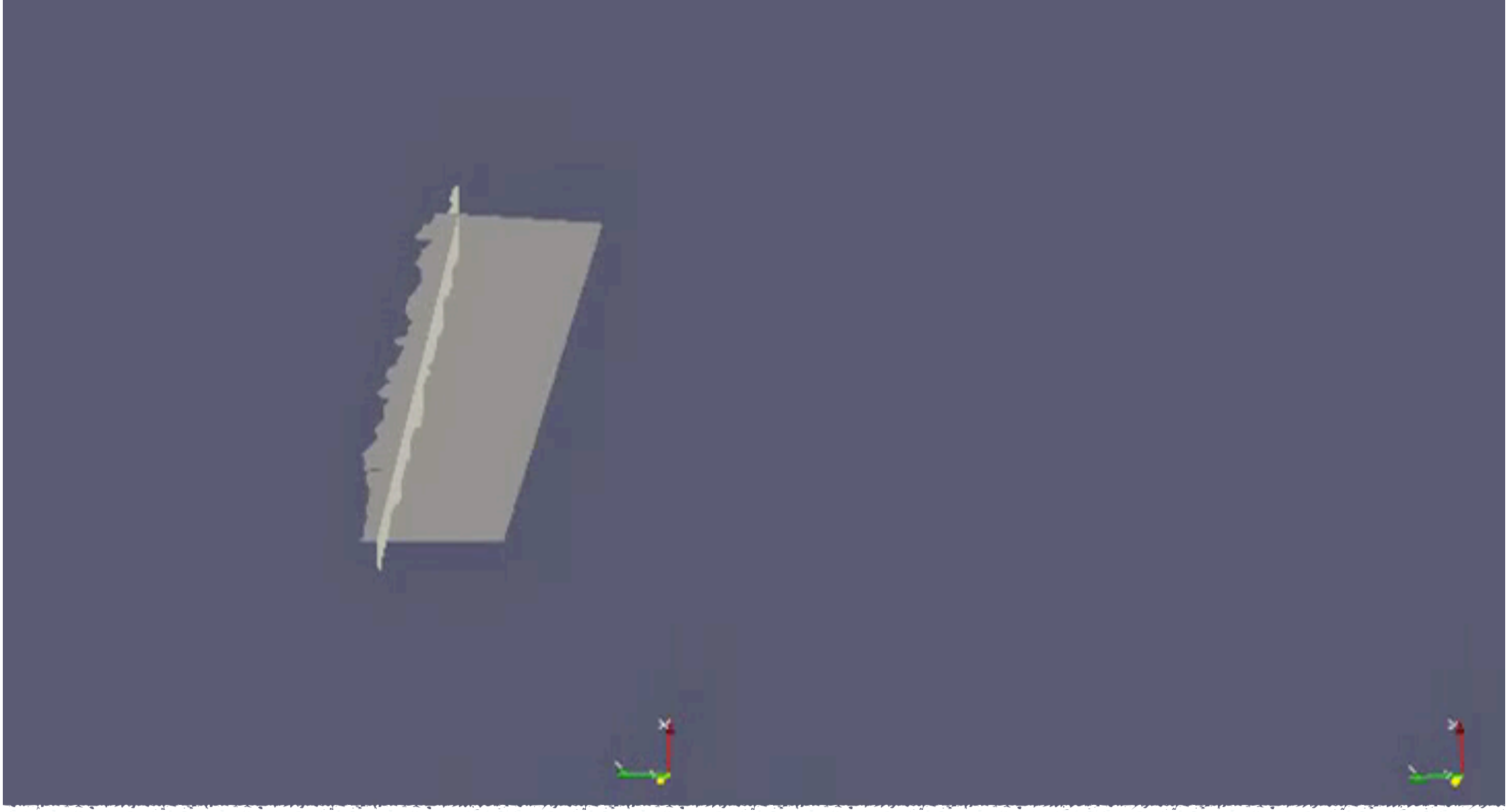
COST 2014, Cahill

Fracture of homogeneous materials

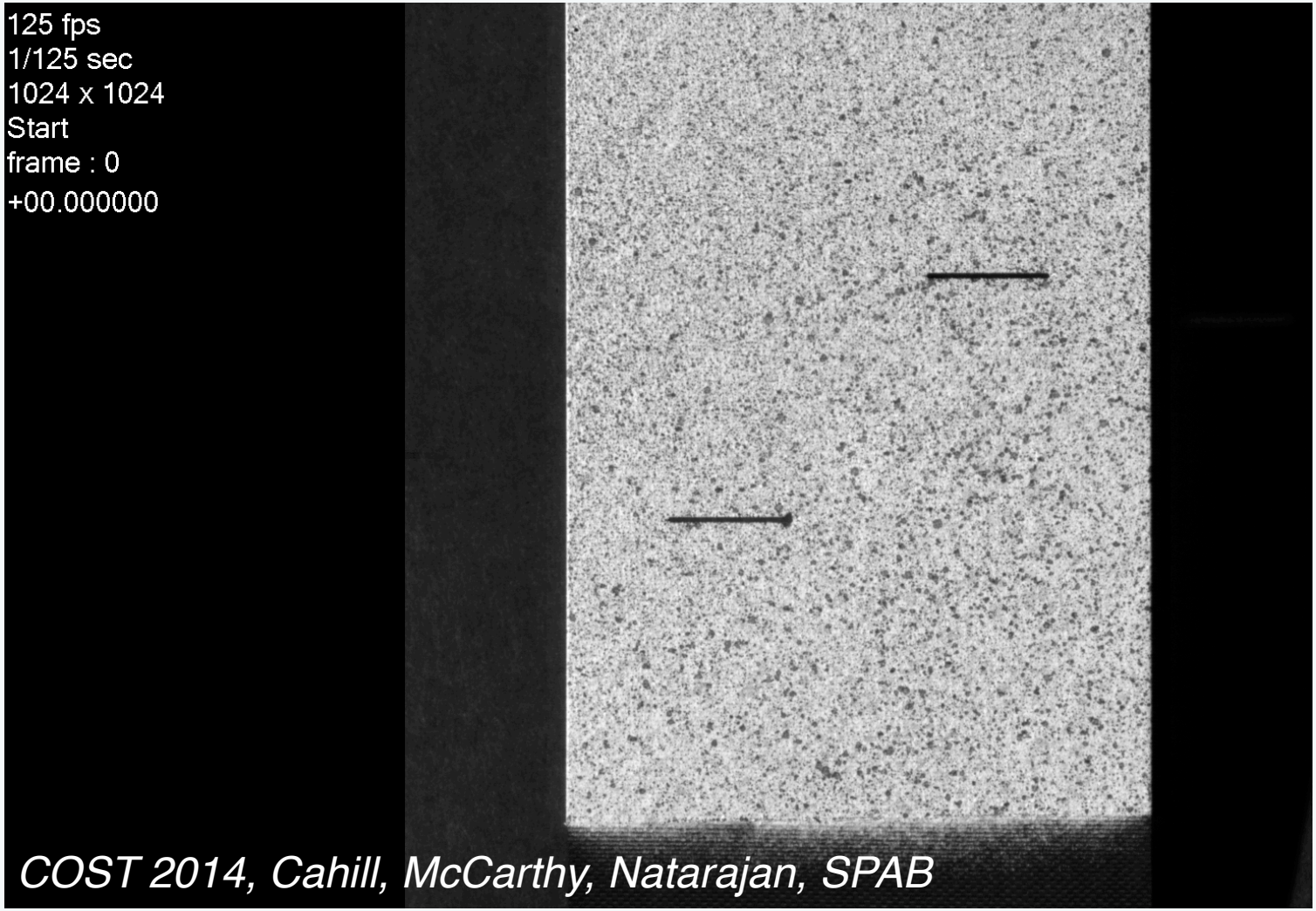




Agathos, Chatzi, Ventura, Talaslidis, SPAB: IJNME, CMAME2016, IJNME2017, CMECH18

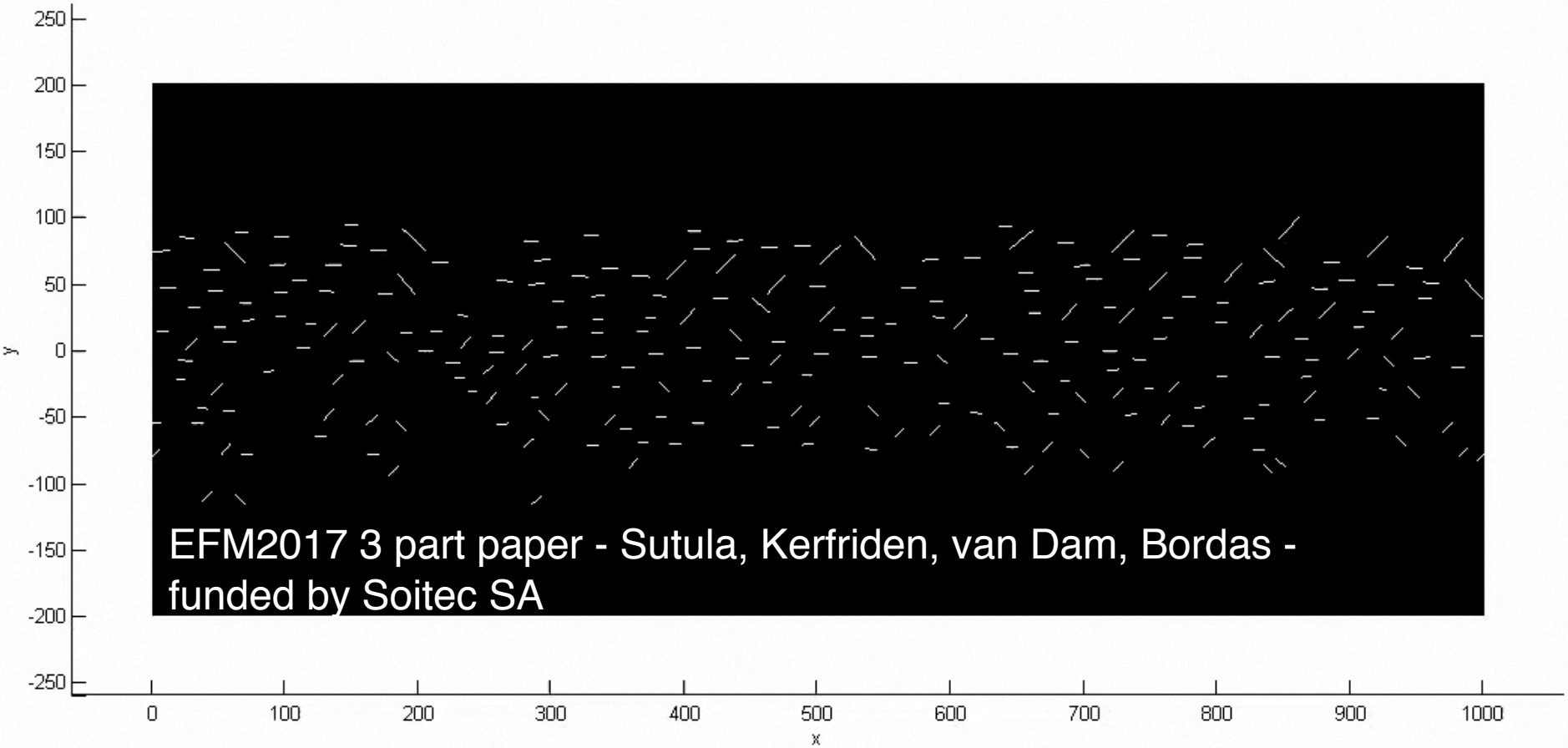


Composite failure

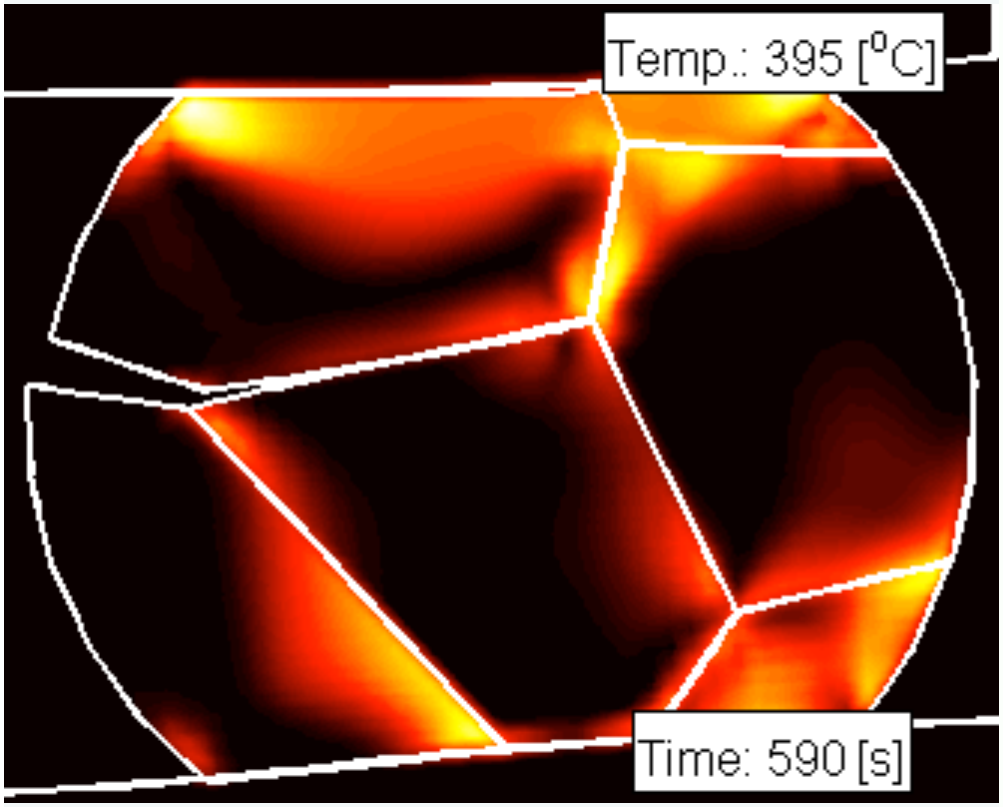


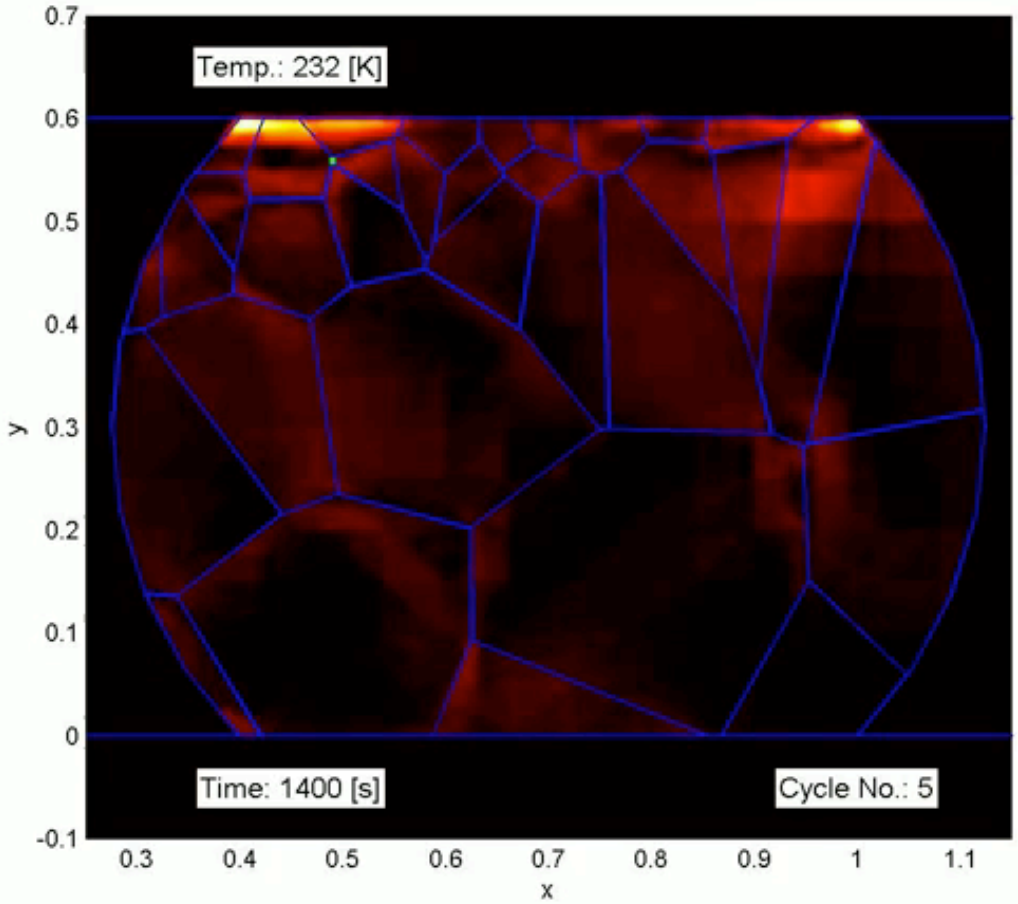
COST 2014, Cahill, McCarthy, Natarajan, SPAB

Energy-minimal multi-crack growth
300 cracks growing in Si due to H+ implantation (SmartCut TM)



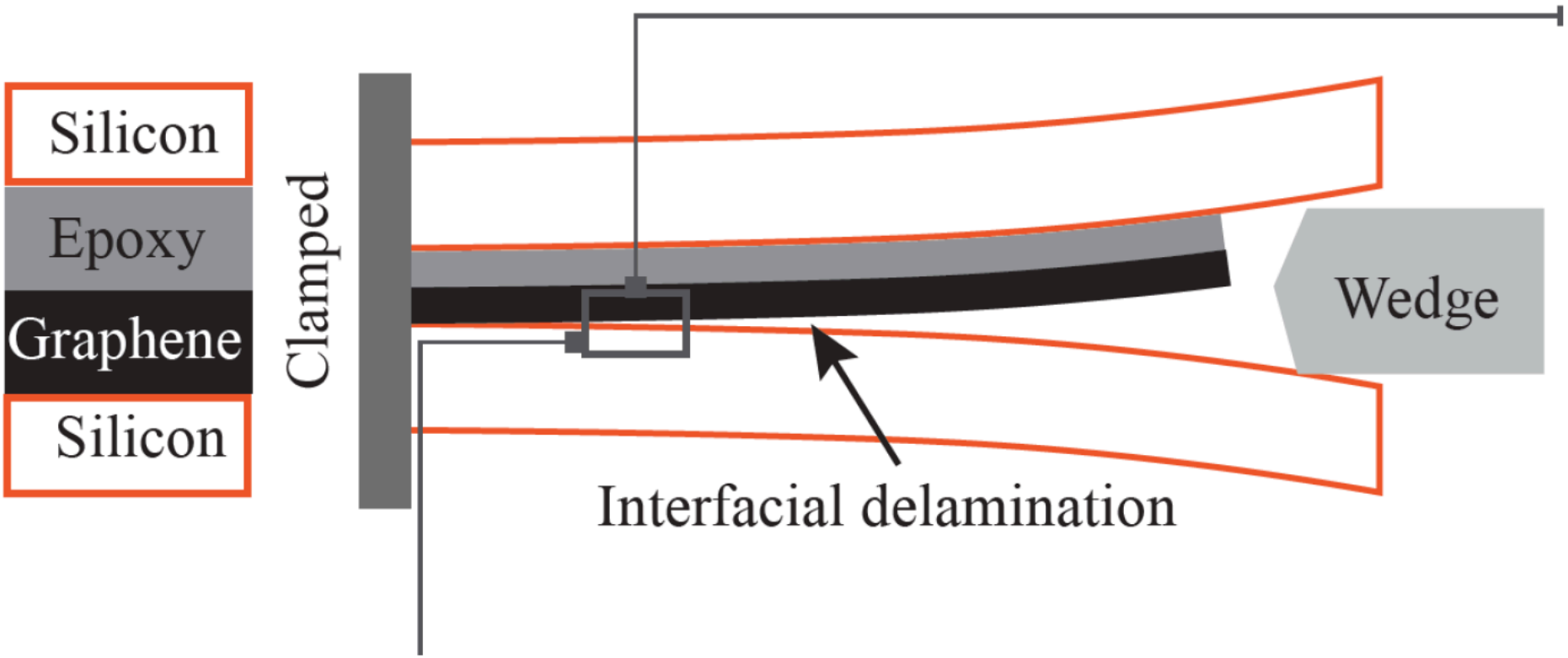
Polycrystalline failure (SnAgCu vs. SnPb)





IJNME2011, CMS2012, Menk & SPAB funded by Bosch GmbH

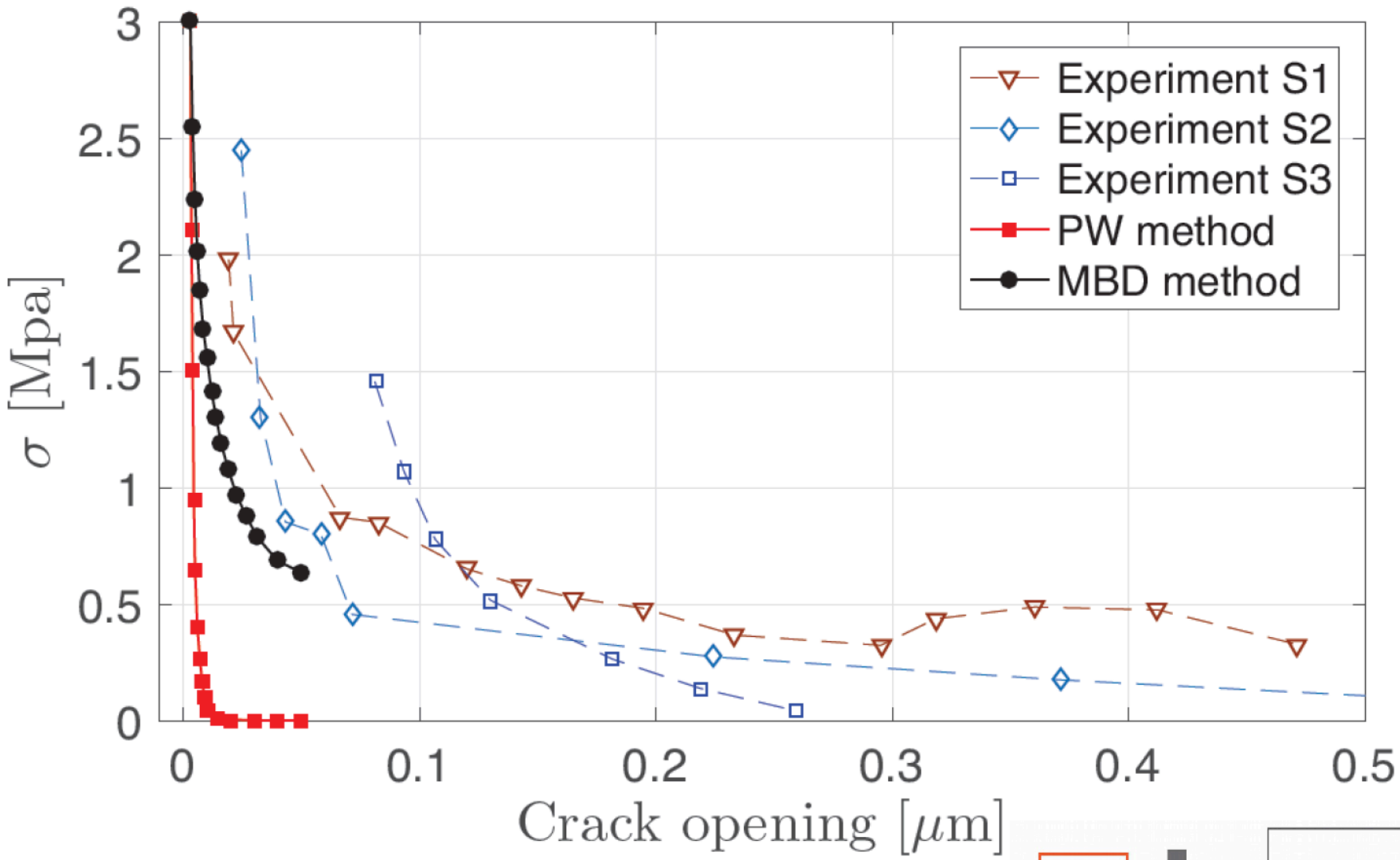
Ultra-long range delimitation mechanics

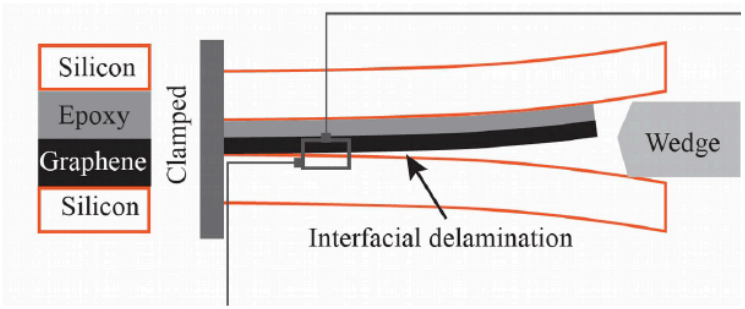


2018 APS - With Tkatchenko, Ambrosetti and Nguyen Thanh-Tung

S. R. Na, J.W. Suk, R. S. Ruoff, R. Huang, and K. M. Liechti,
Ultra long-range interactions between large area graphene and silicon,
ACS Nano 8, 11234 (2014).

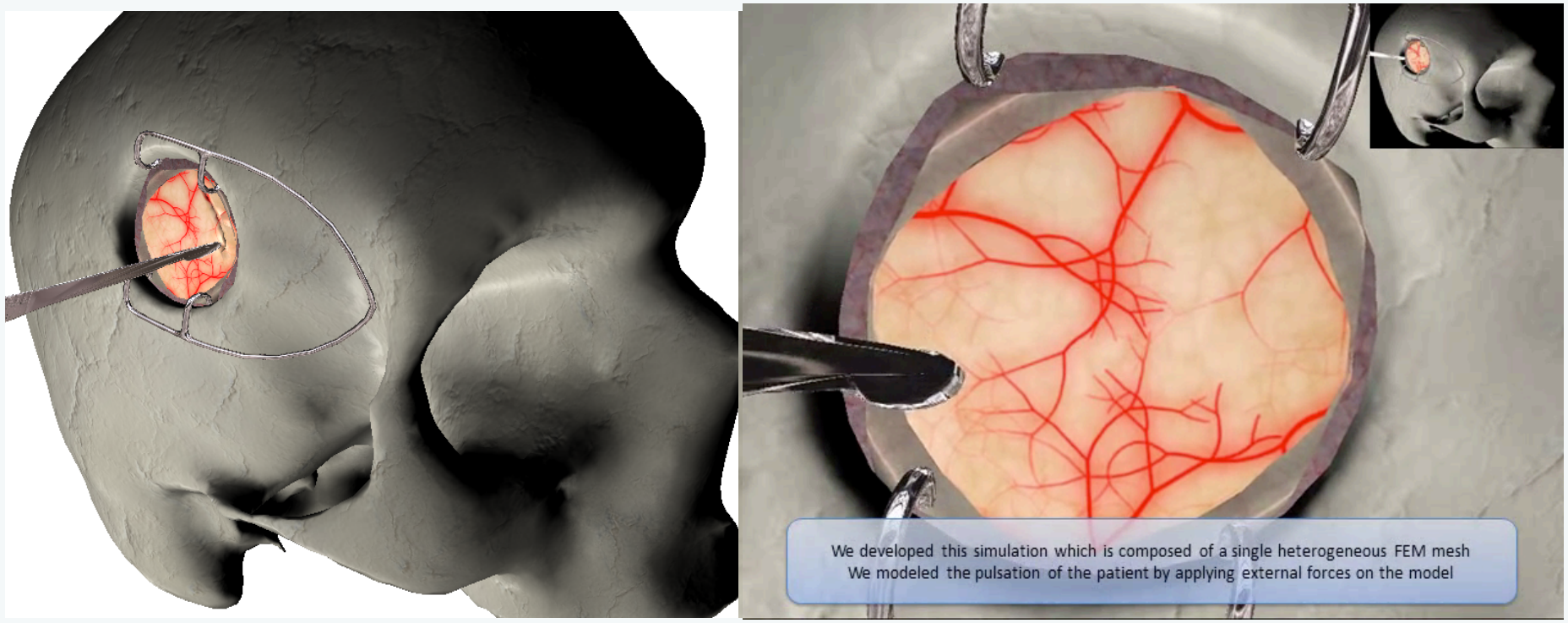
Ultra-long range delimitation mechanics





T. T. Nguyen, A. Ambrosetti, S. P. Bordas and A. Tkatchenko, *to be submitted*.

Cutting in soft tissue

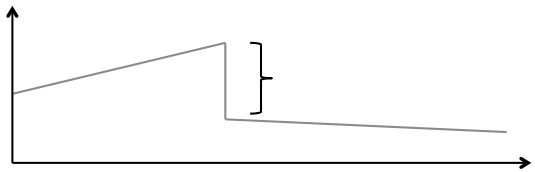


Real-time simulation of cutting during brain surgery
Med. Im. Anal. 2014 Courtecuisse, Cotin, SPAB et al.

Classification of Discontinuities

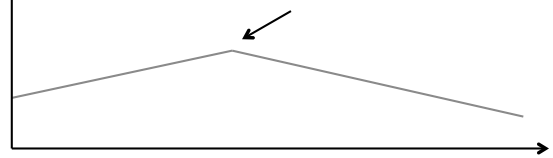
Strong discontinuities

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



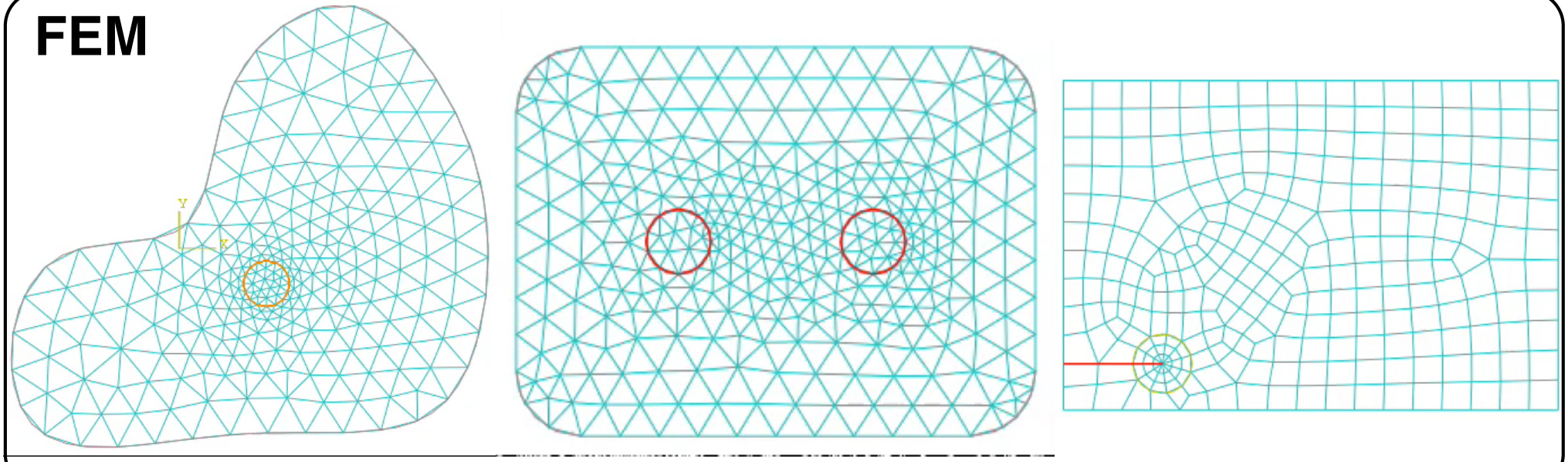
Weak discontinuities

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

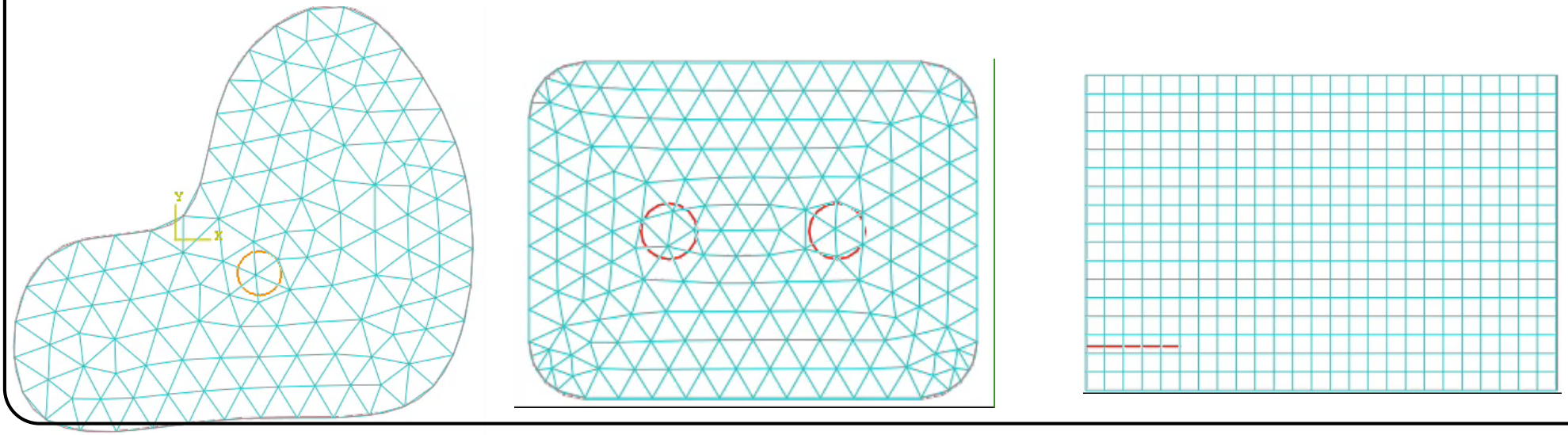


Discretization of interface problems

FEM



XFEM



Discretization of interface problems
Challenges

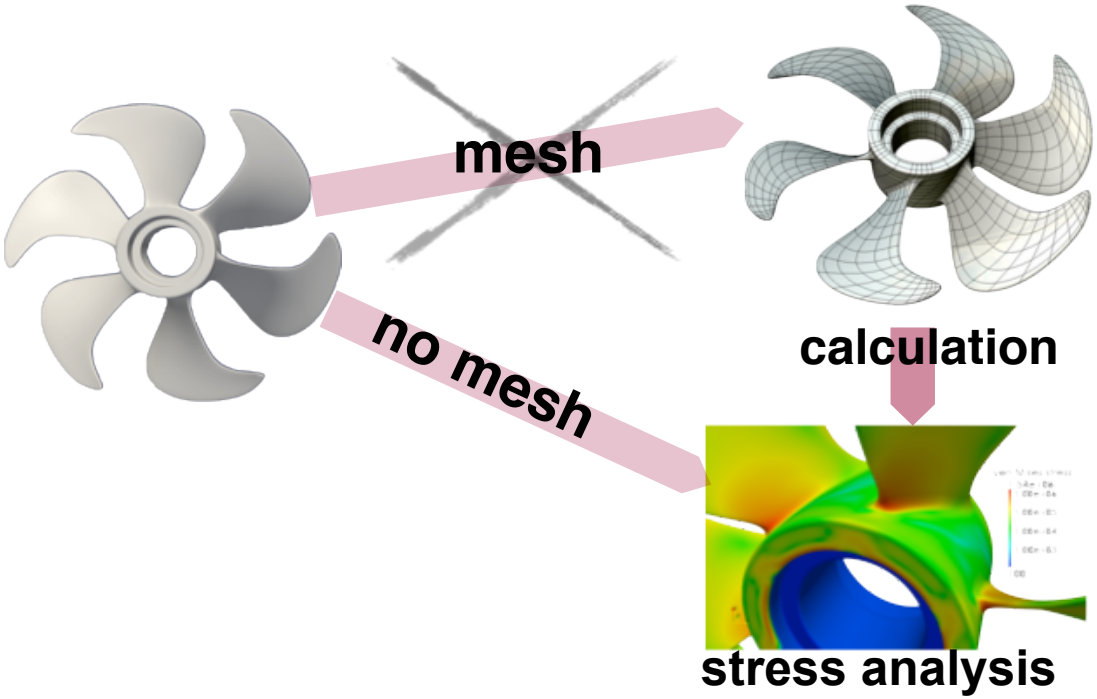
Evolving and complex geometries

Accurate calculations of front velocities

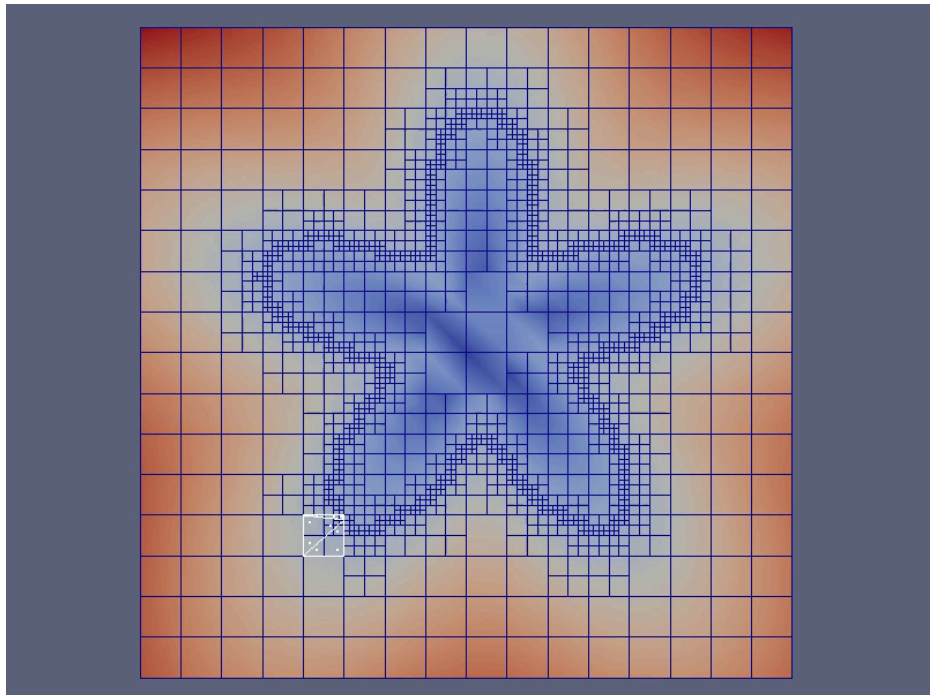
Error estimation and adaptivity

Time stepping schemes

Handling interfaces numerically



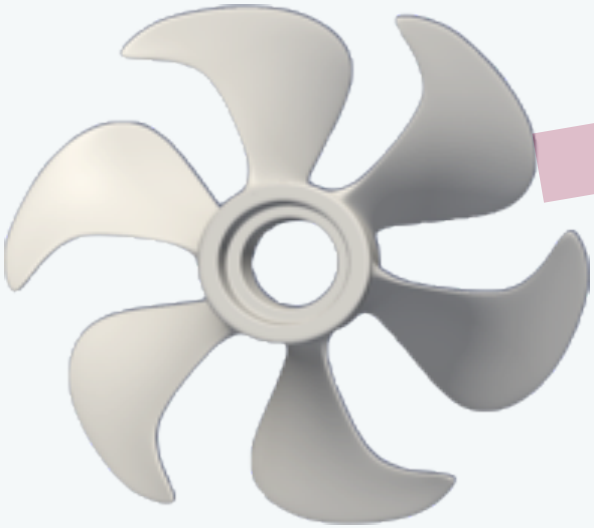
Coupling - isogeometric analysis



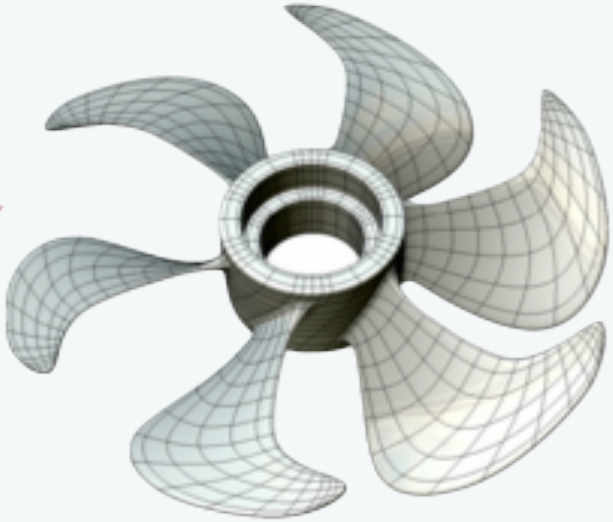
Decoupling - implicit interfaces

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

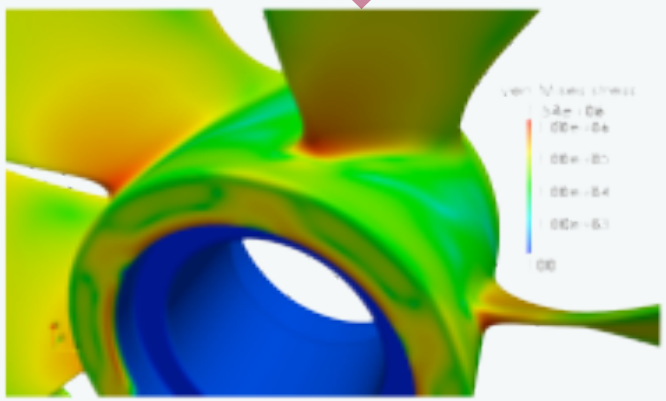
Isogeometric analysis



mesh

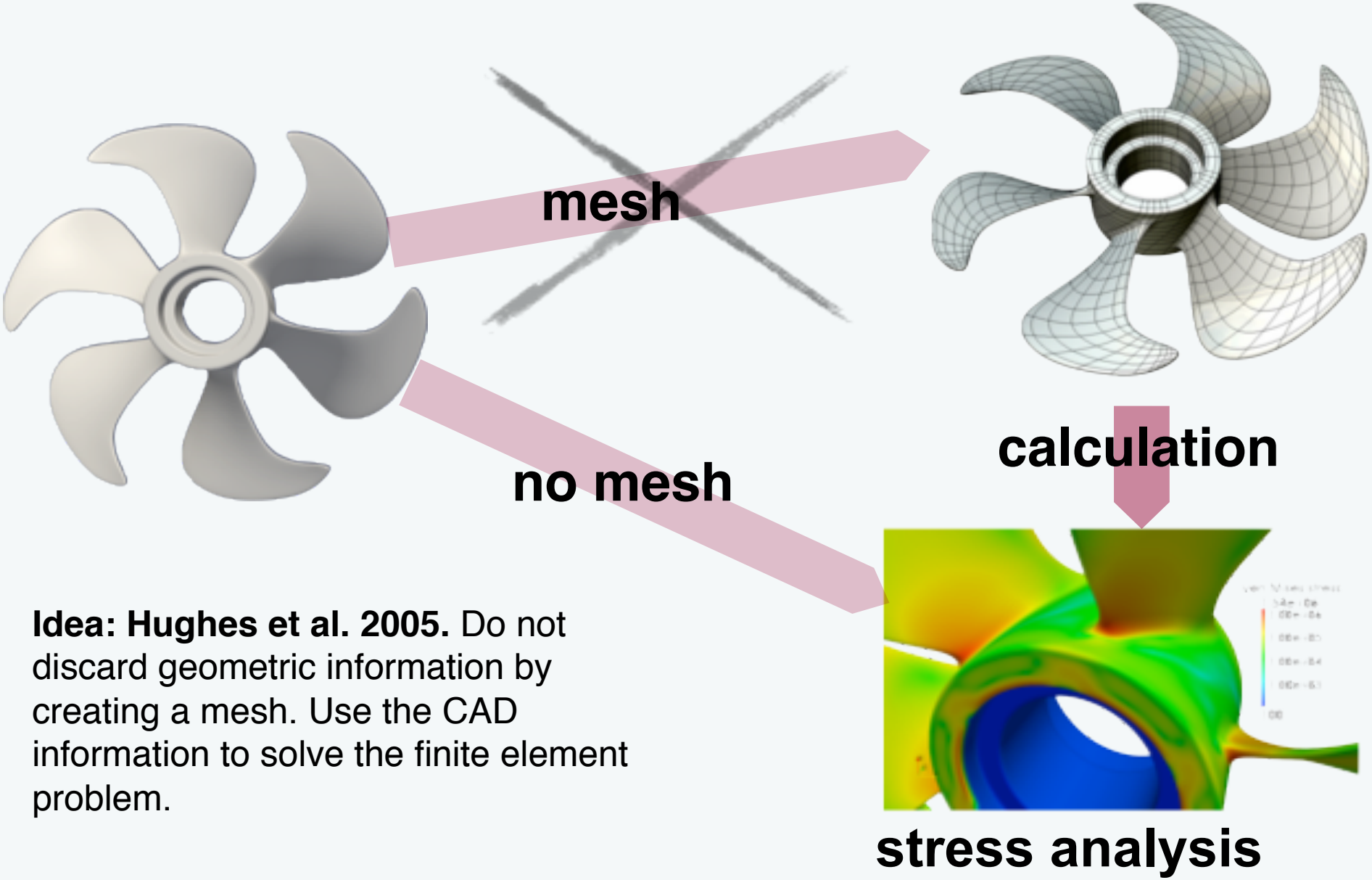


calculation



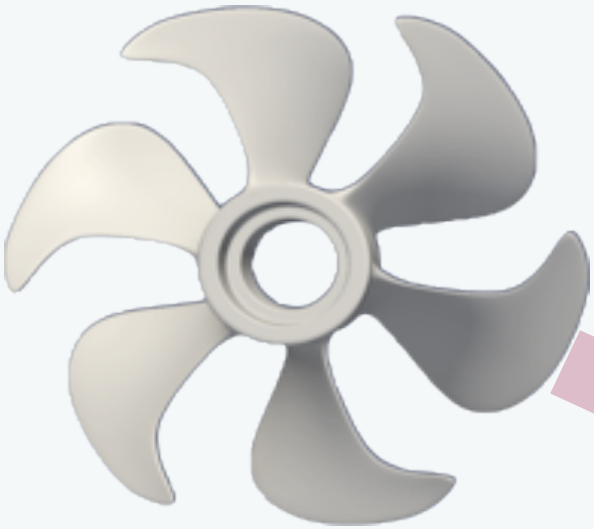
stress analysis

Isogeometric analysis

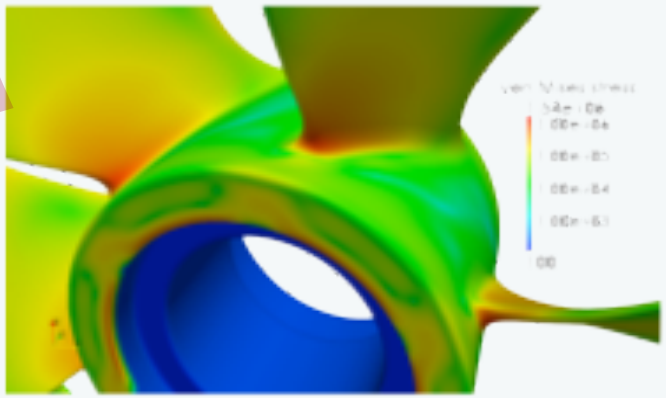


Idea: Hughes et al. 2005. Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.

Isogeometric analysis



direct calculation

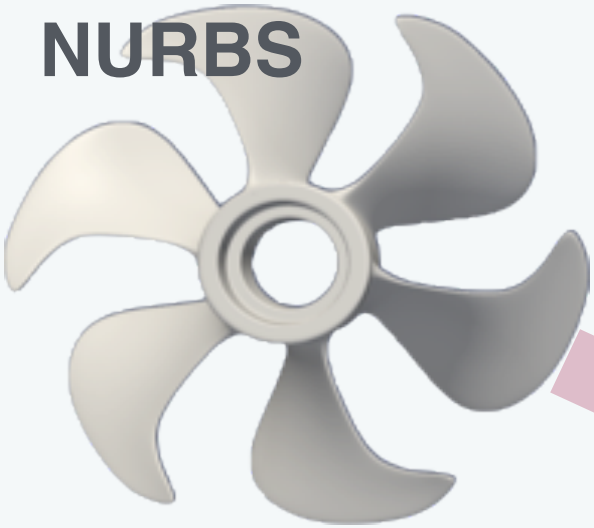


stress analysis

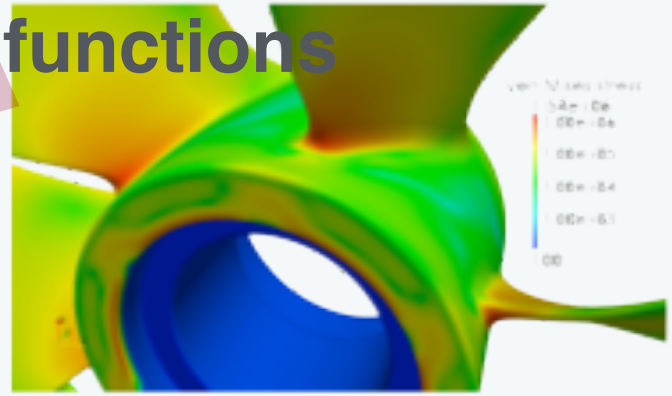
Idea: Hughes et al. 2005. Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.

Isogeometric analysis

CAD: described by NURBS



Use NURBS as FE basis functions



stress 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.

Coupling or decoupling

Question:
What is the performance of NURBS-based Isogeometric Analysis in Reducing the Mesh Burden?

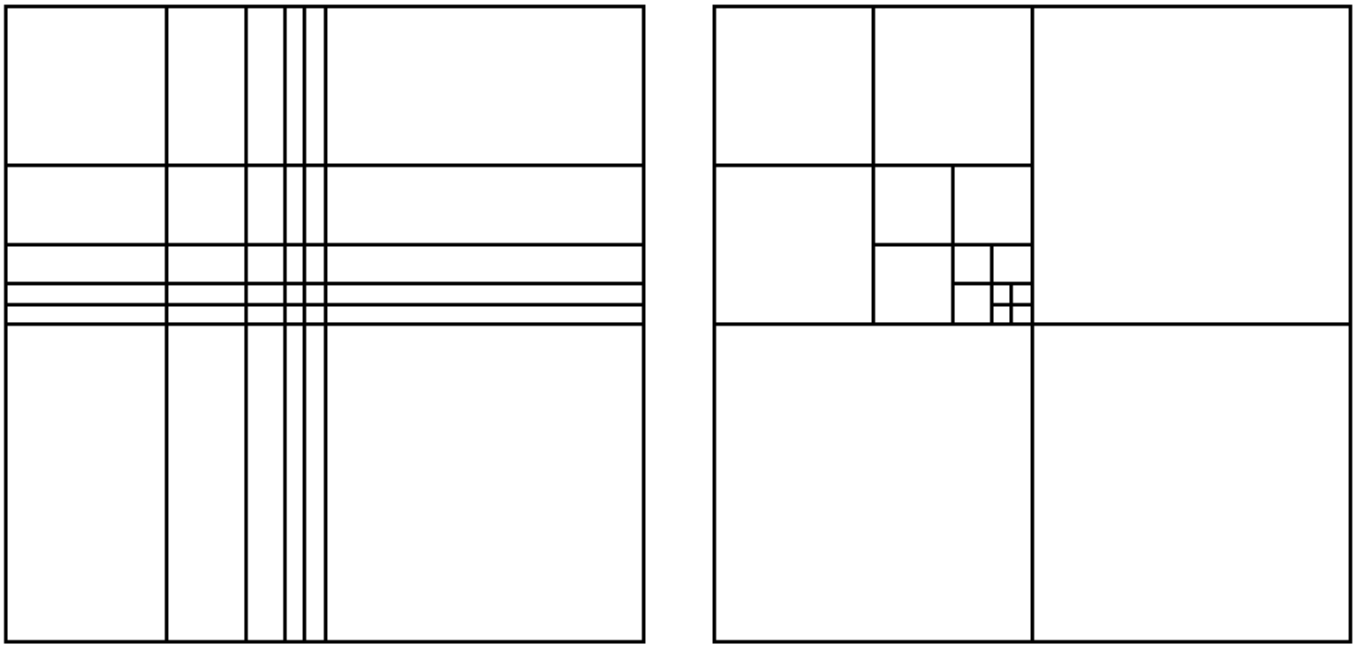
Isogeometric Finite Element Analysis

- [x] For shell-like domains
- [ ] For volumes (needs volume parameterisation)
- [ ] Coupling between multiple patches (Nitsche, Mortar…)

Adaptivity

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

Mesh refinement in NURBS-IGA



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

GIFT approach

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, 2018, accepted [preprint available on arXiv]

Permalink: http://hdl.handle.net/10993/31469

Numerical observations - no proof…

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

GIFT - key features

- ☑ 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 approximation 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…)

GIFT - key features

- ☑ 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

IGABEM vs. IGAFEM

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)

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.

Isogeometric Boundary Element Analysis

☑ For shell-like domains

☑ For volumes

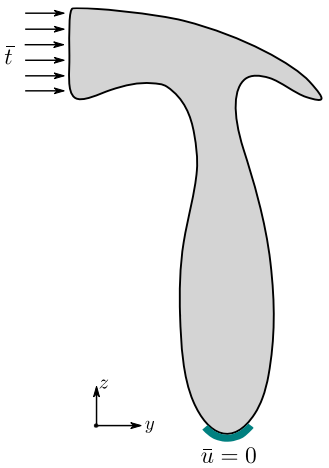
Fracture mechanics directly from CAD

X. Peng, et al. (2017). *IJF*, 204(1), 55–78.
X. Peng, et al. (2017). *CMAME*, 316, 151–185.

Handling (complex) interfaces numerically

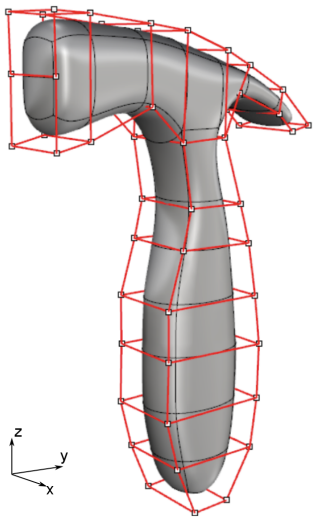
Example applications
Isogeometric Boundary Element Analysis (IGABEM)

Shape optimisation



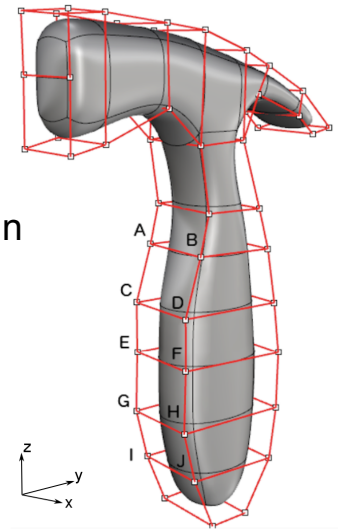
Problem definition

Model construction with CAD



Control points

Design points selection in control points



Design points

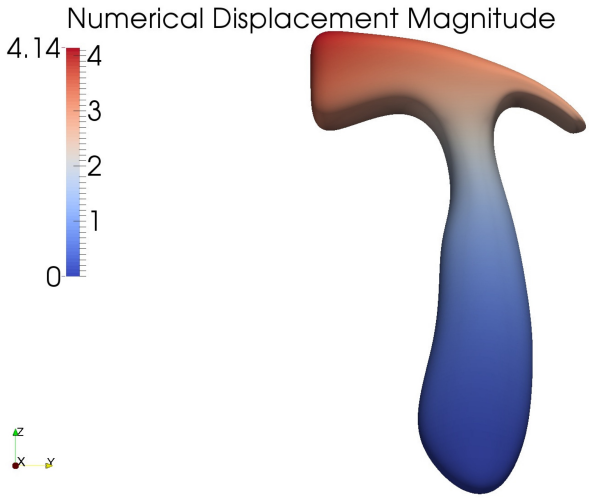
Objective function: $\int_S t_i u_i \mathrm{d}S$

Volume constraint: $V - V_0 \leq 1$

Side constraints:

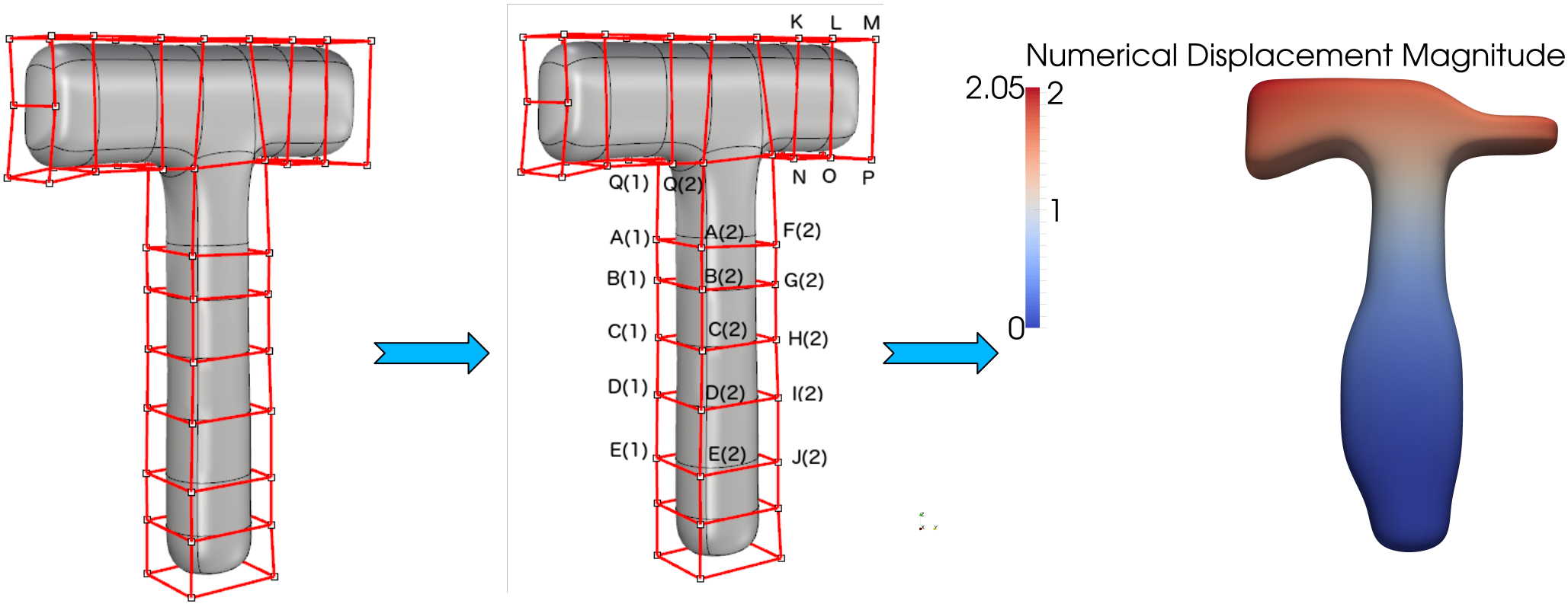
Design variable	Lower bound	Upper bound	Initial value
t_1	0	4	2.45
t_2	0	4	1.25
t_3	0	4	1.33
t_4	0	4	1.28
t_5	0	4	2.30

Structural analysis;
Sensitivity analysis;
gradient-based optimizer



Optimized solution

Shape optimization



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.
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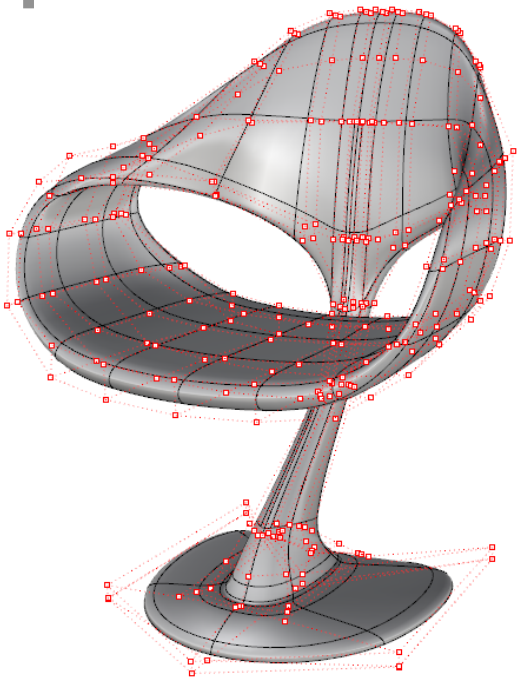
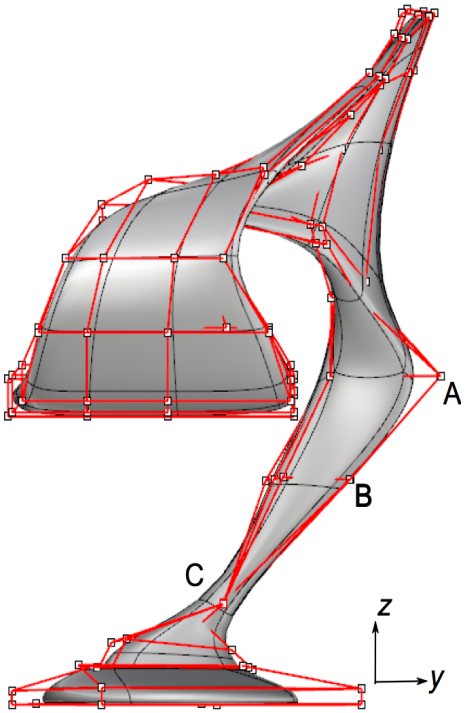
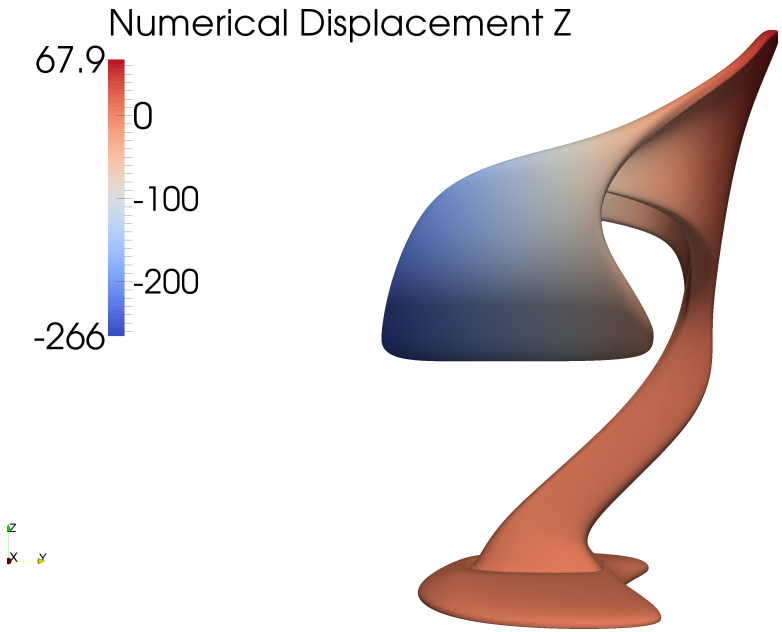
Shape optimization



Construct the geometric model
(imported from Rhino)



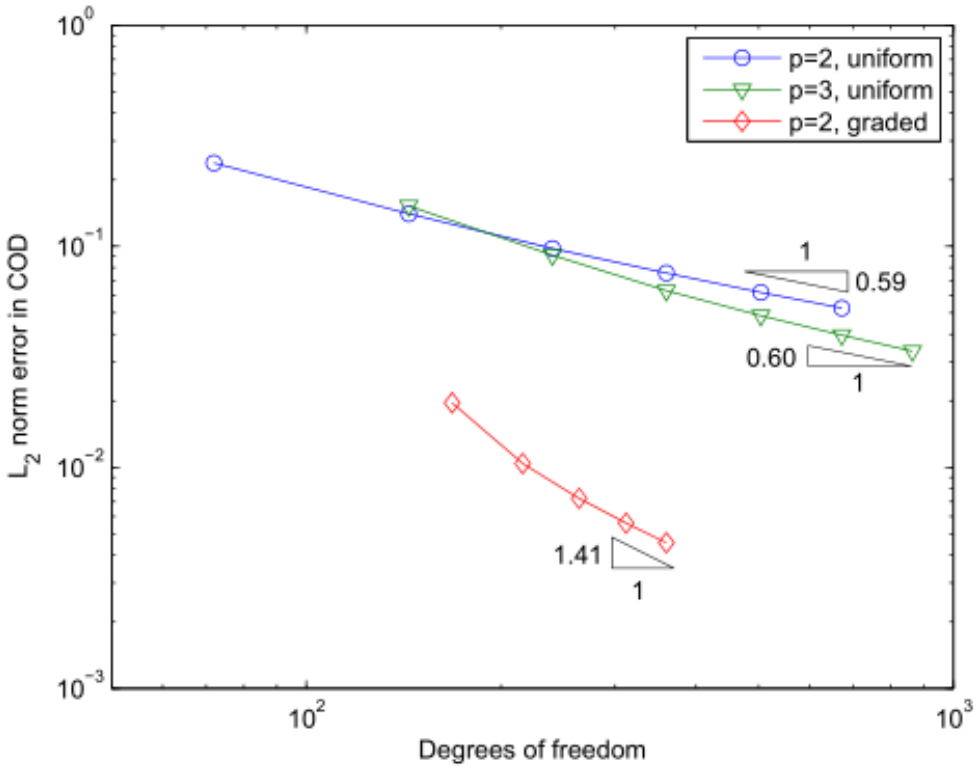
Select design points from
control points



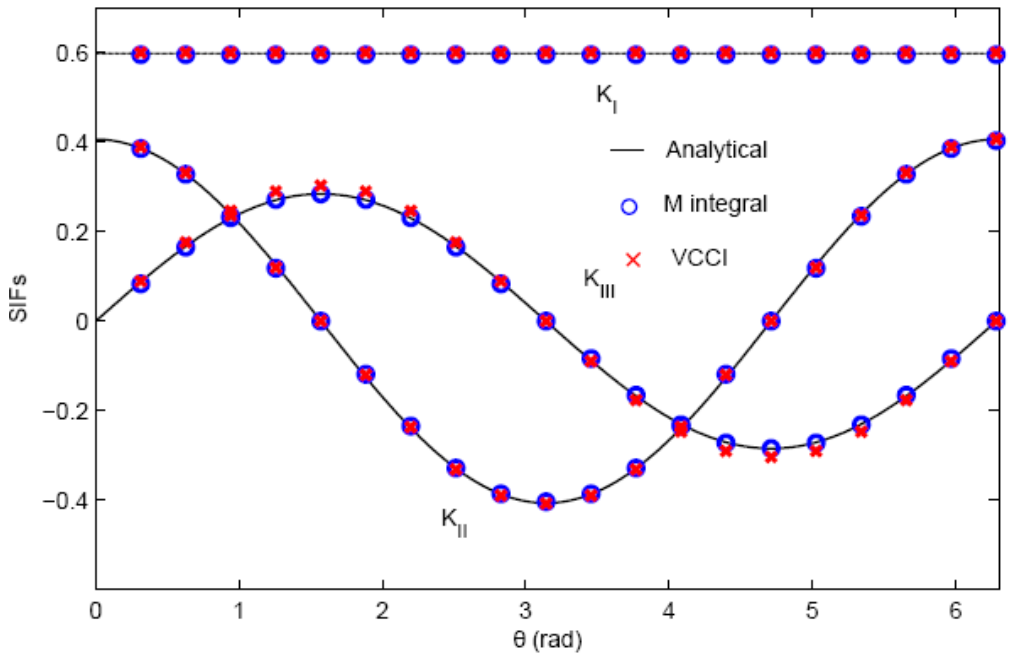
Find optimized solution

Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg and Cardiff University

Penny crack under tension



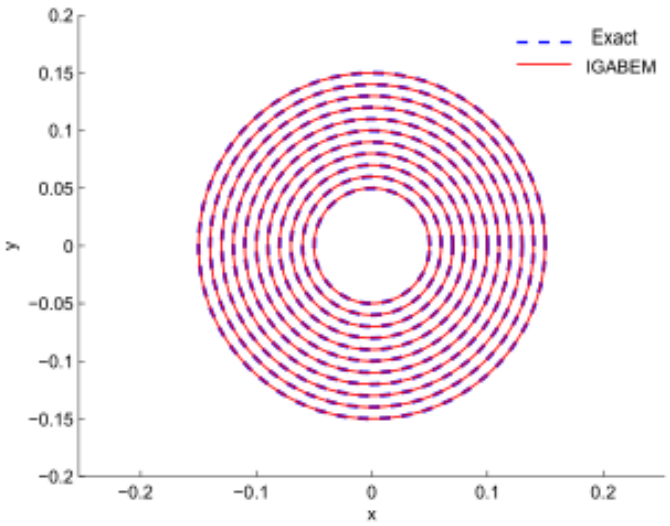
L_2 norm error of COD for penny-shaped crack



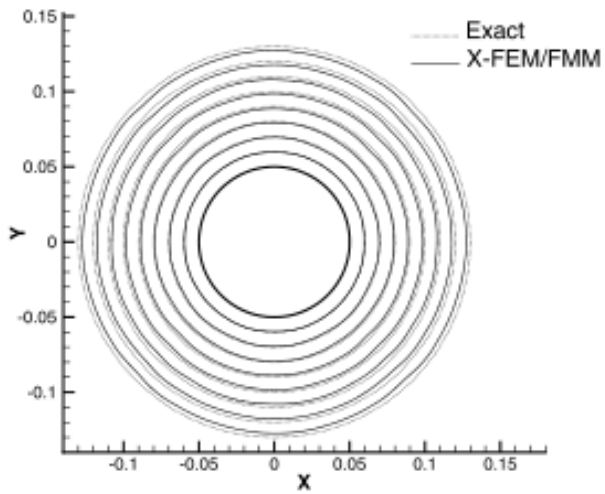
stress intensity factors for penny crack with $\varphi = \pi/6$

Fracture mechanics directly from CAD
X. Peng, et al. (2017). *IJF*, 204(1), 55–78.
X. Peng, et al. (2017). *CMAME*, 316, 151–185.

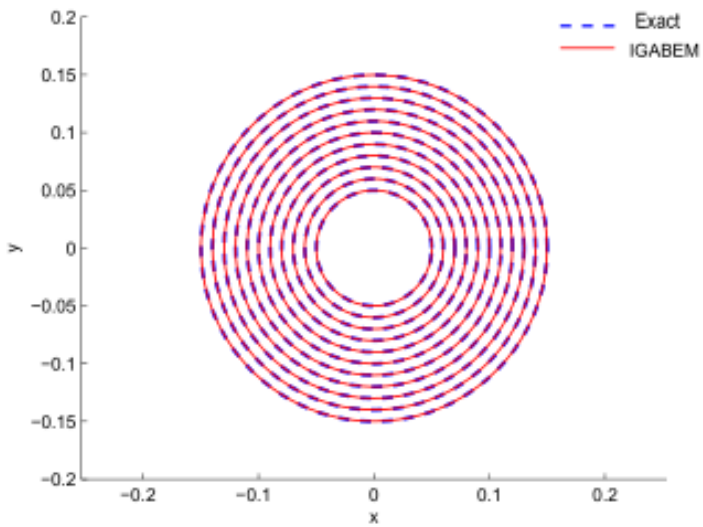
Penny crack growth



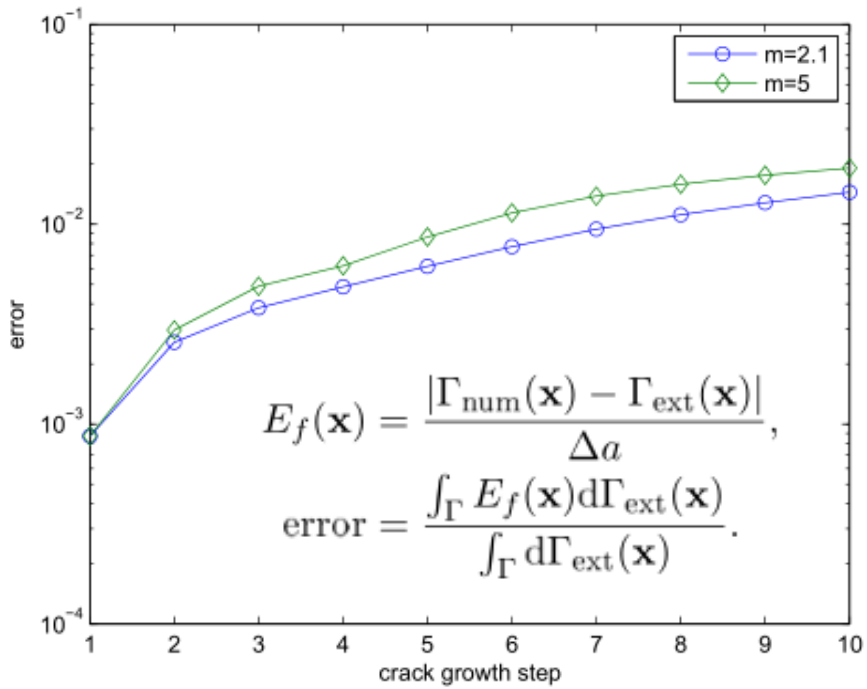
(a) IGABEM, $m = 2.1$



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

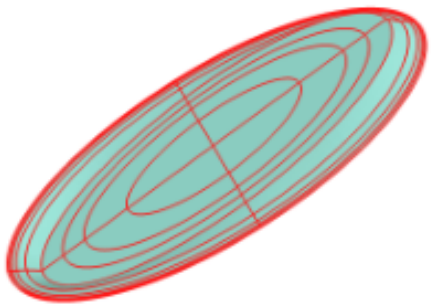


(c) IGABEM, $m = 5$

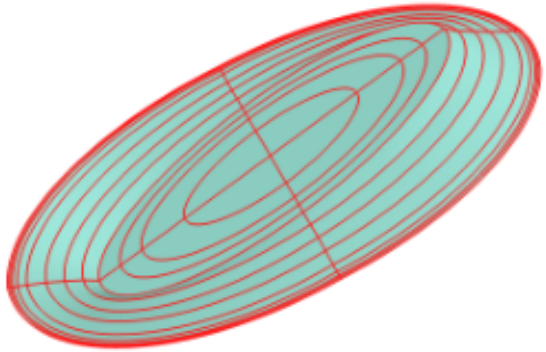


Relative error of the crack front for in each crack growth step by IGABEM

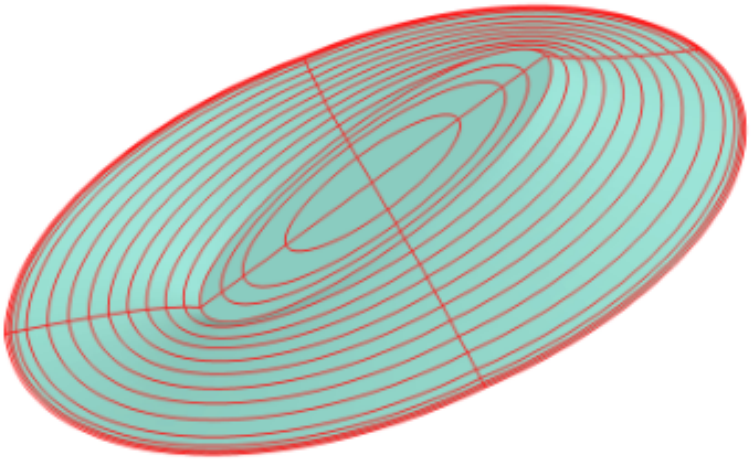
Inclined penny crack growth



(a) Step 2



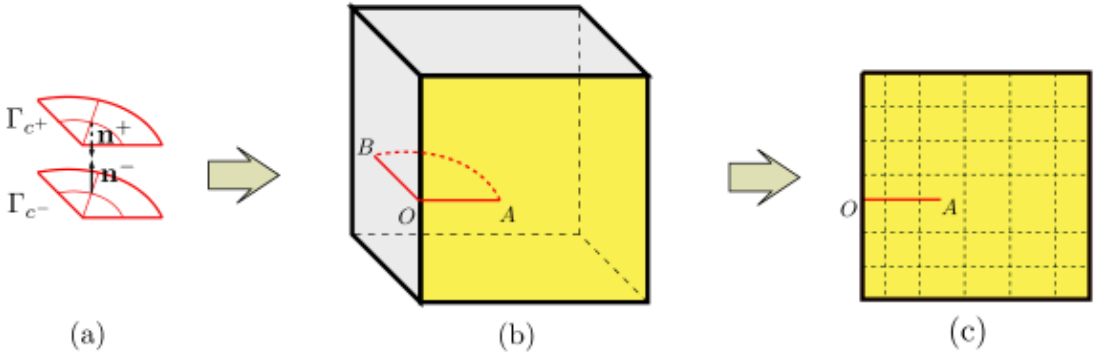
(b) Step 5



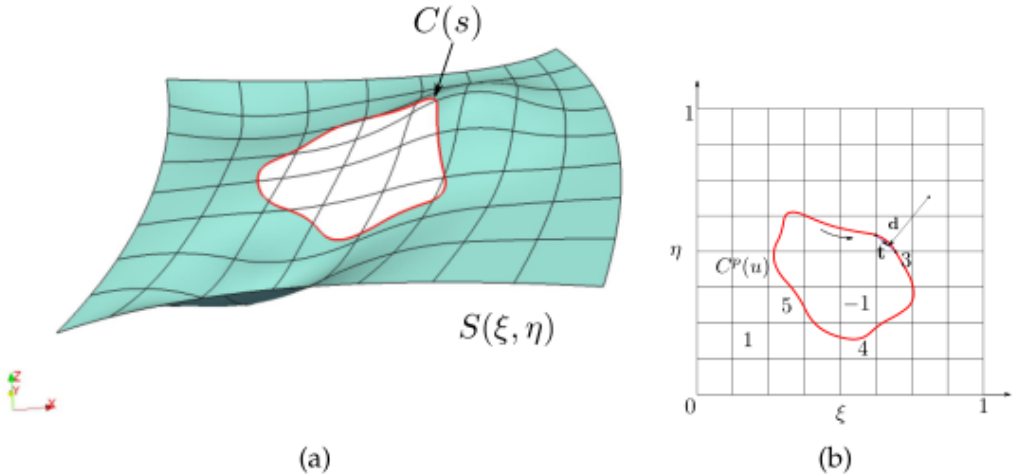
(c) Step 10

Fracture mechanics directly from CAD
X. Peng, et al. (2017). *IJF*, 204(1), 55–78.
X. Peng, et al. (2017). *CMAME*, 316, 151–185.

Surface cracks



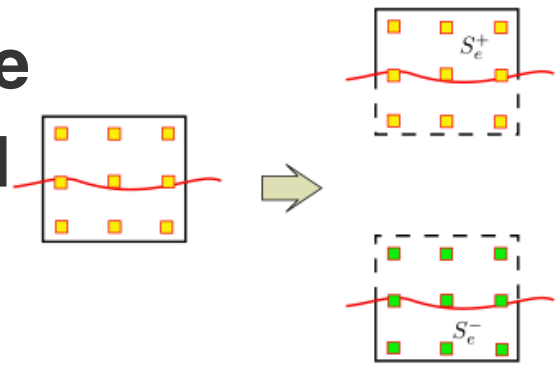
Surface discontinuity is introduced



Trimmed NURBS technique

Crack = trimming curve

Phantom node method



(a)

(b)

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

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

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

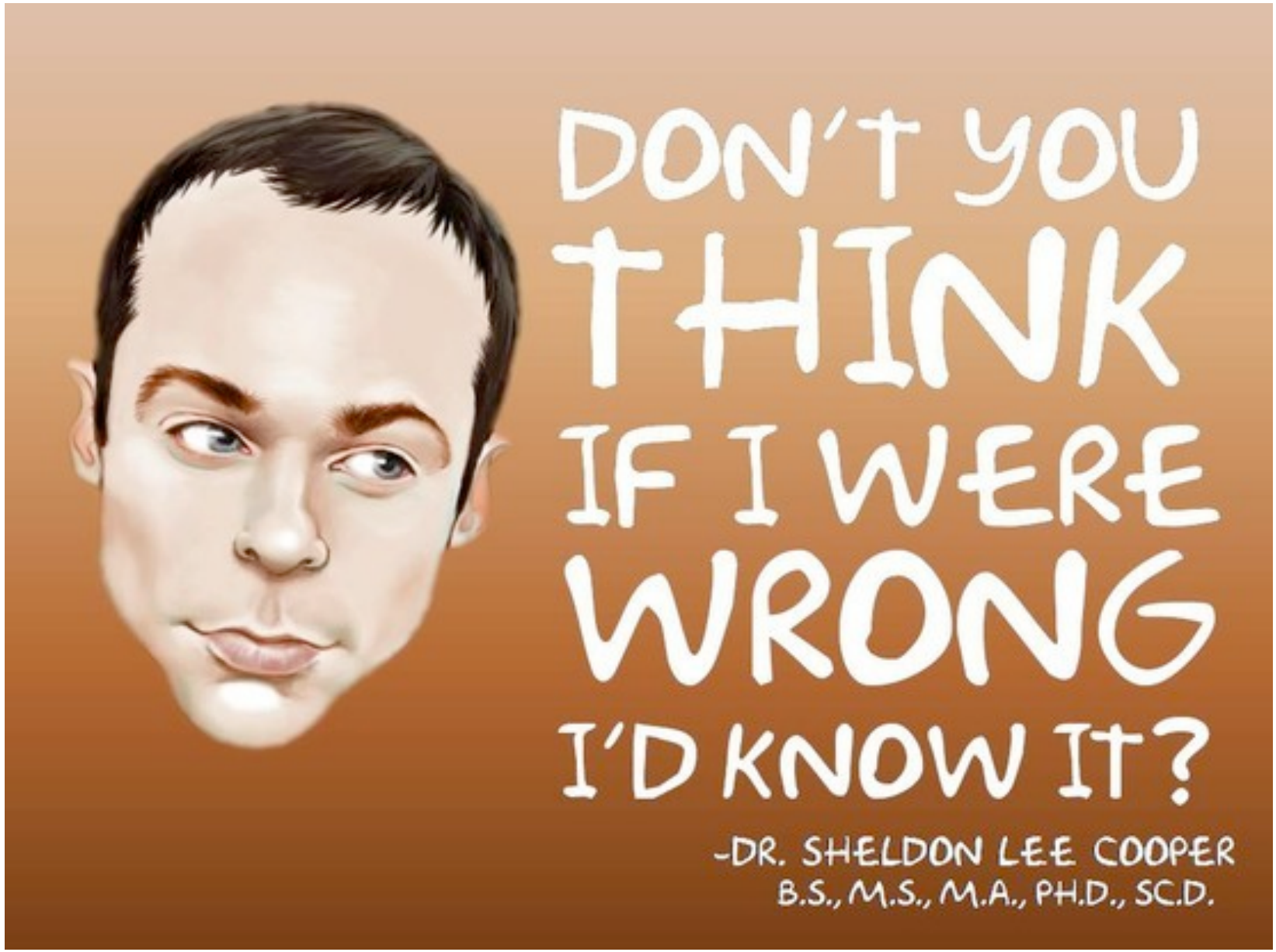
1.Adjoint methods for a large number of design variables and a small number of constraints.

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

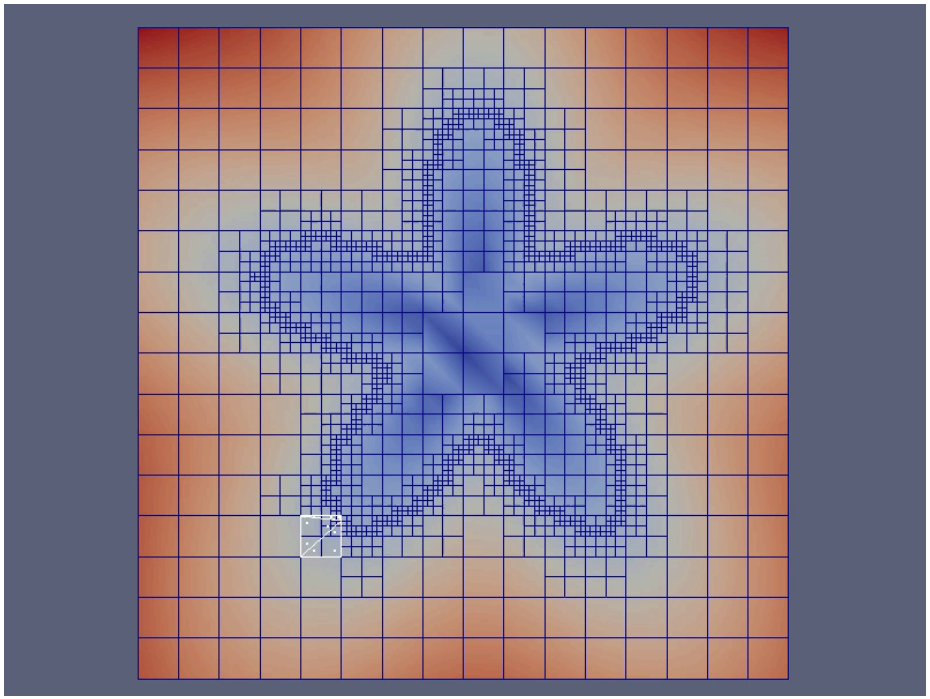
3.Combined with the gradient-less solver.

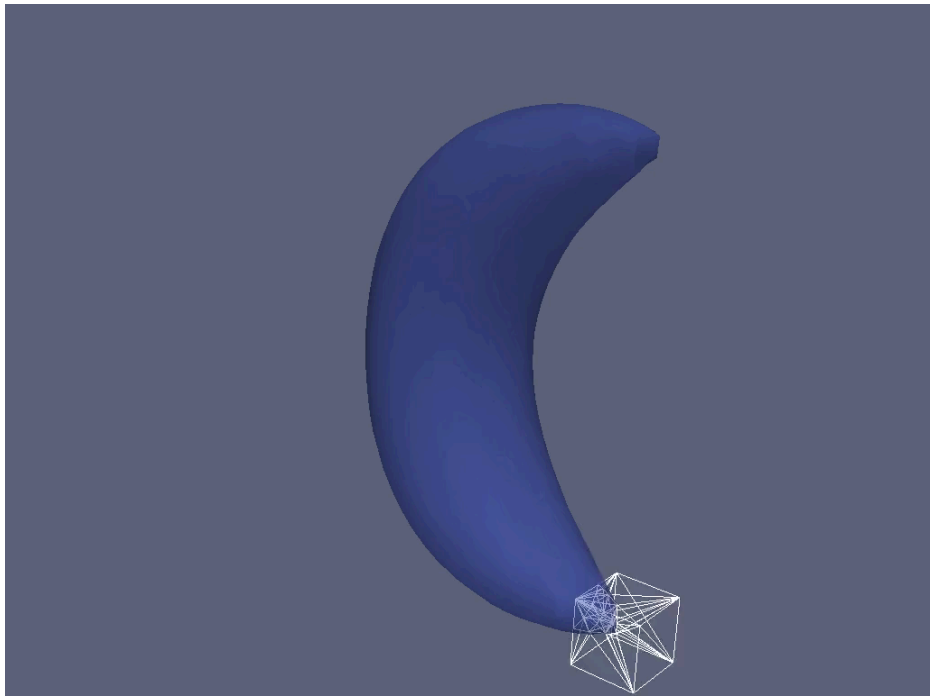
4.Using PHT-splines.

5.GIFT-IGABEM optimization.


DON'T YOU
THINK
IF I WERE
WRONG
I'D KNOW IT?
-DR. SHELDON LEE COOPER
B.S., M.S., M.A., PH.D., SC.D.

Decoupling geometry and approx.

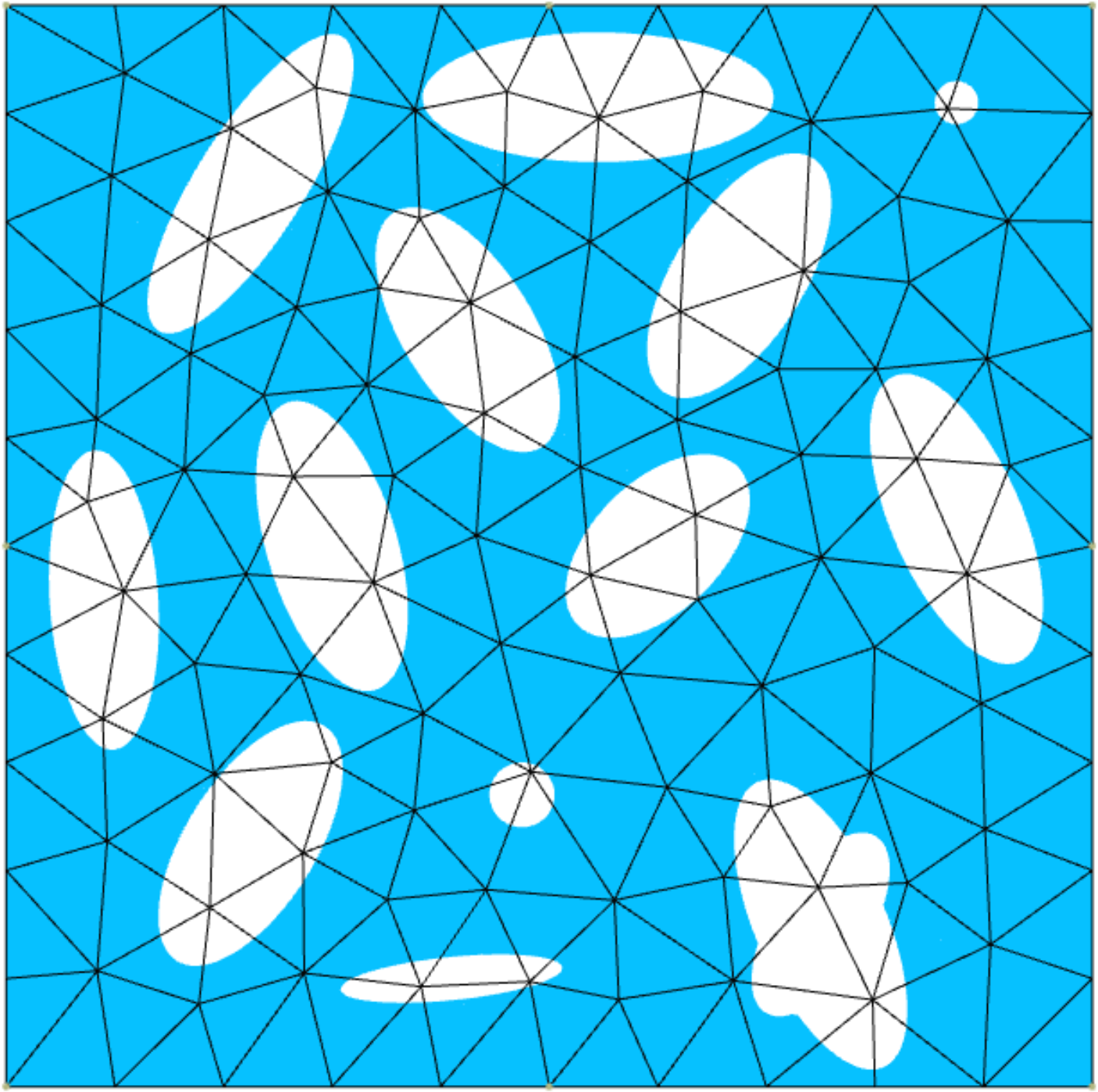


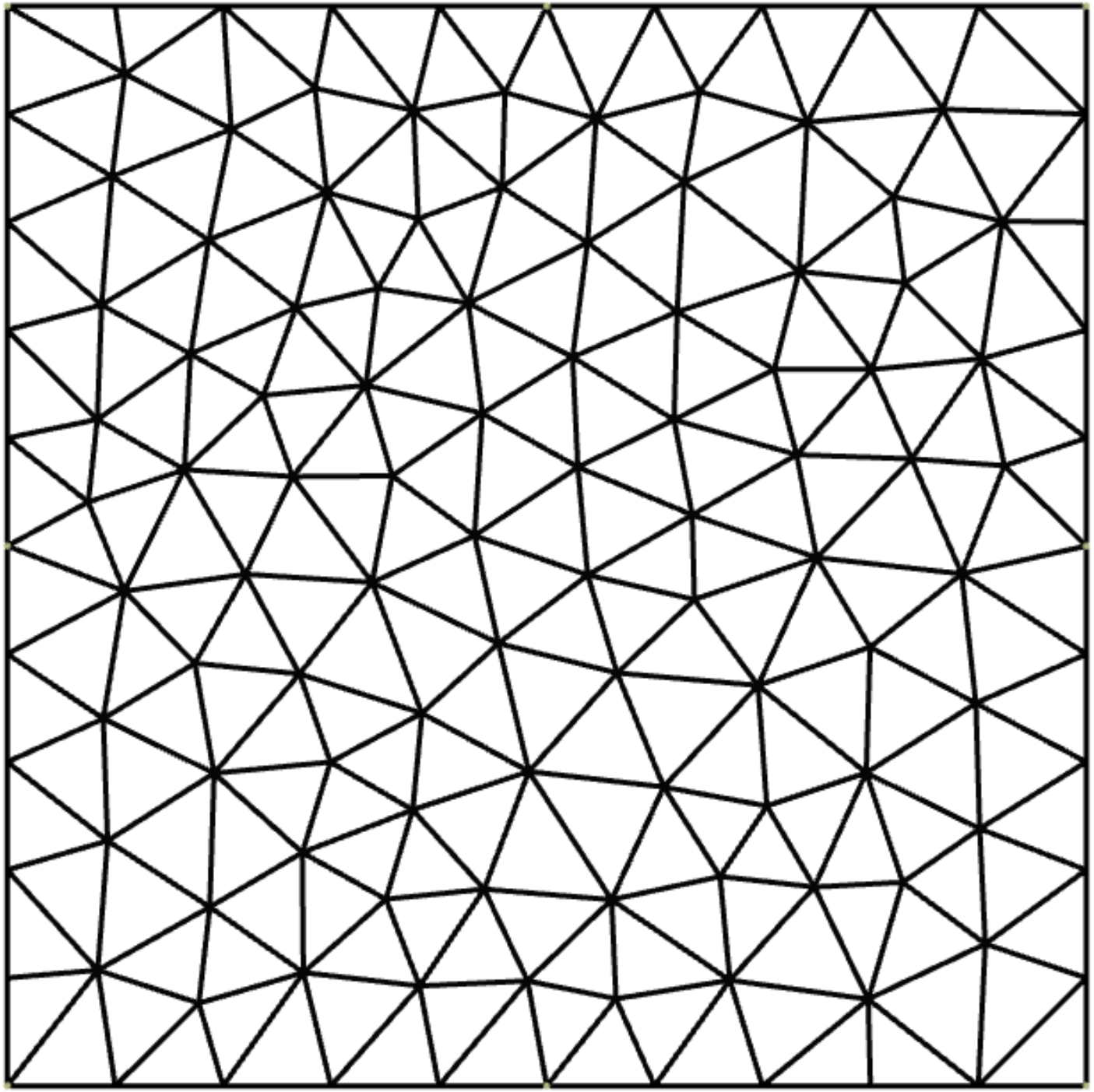


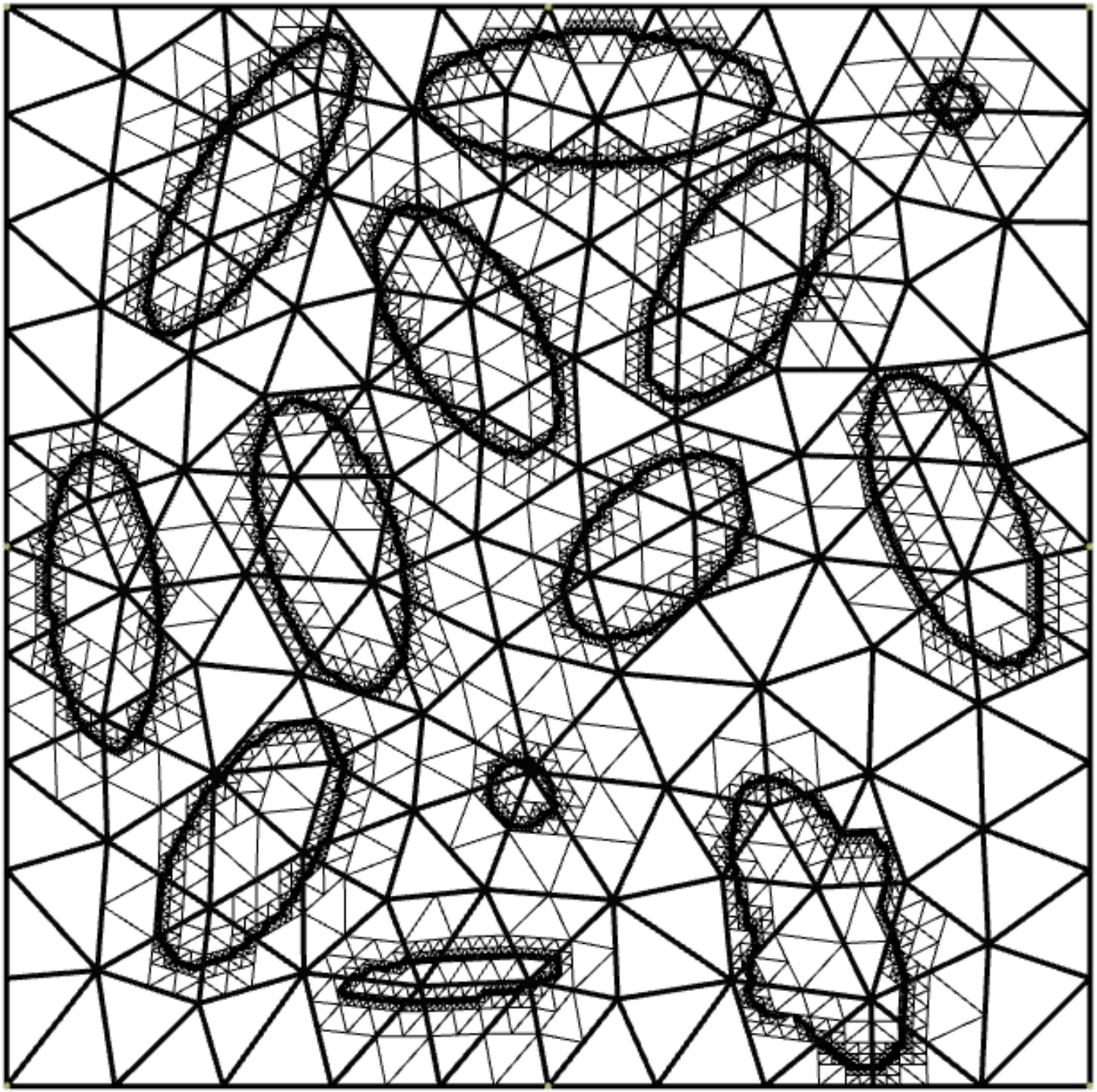
Question: for which problems are we better off coupling/decoupling the geometry from the field approximation?

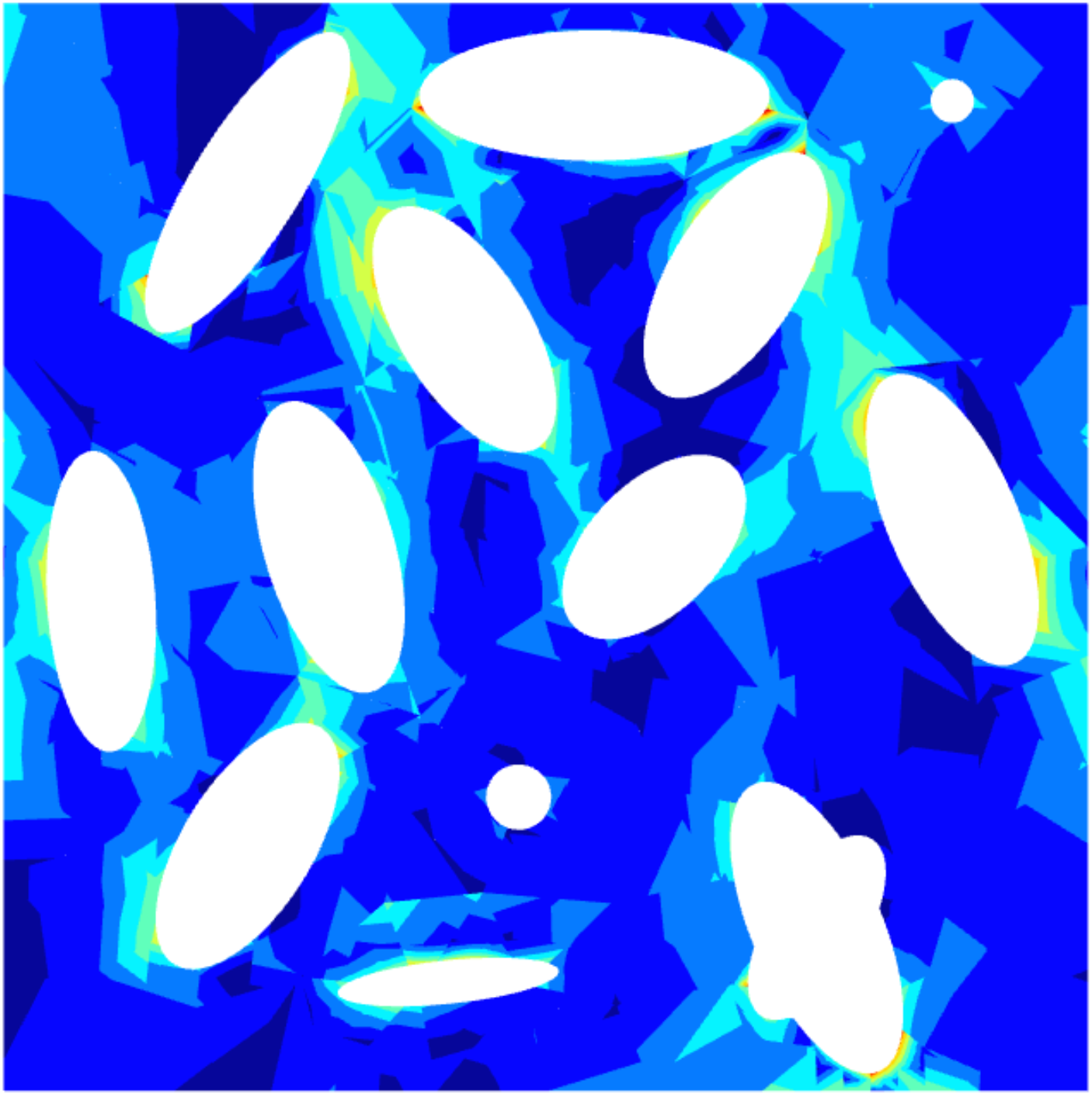
Implicit surfaces

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) CMAME192.28 (2003): 3163-3177. (Single level set)
T. Belytschko IJNME 56.4 (2003): 609-635. (Structured XFEM)
…

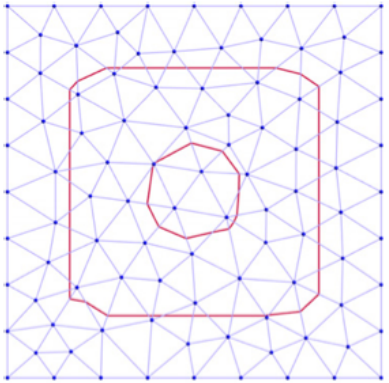




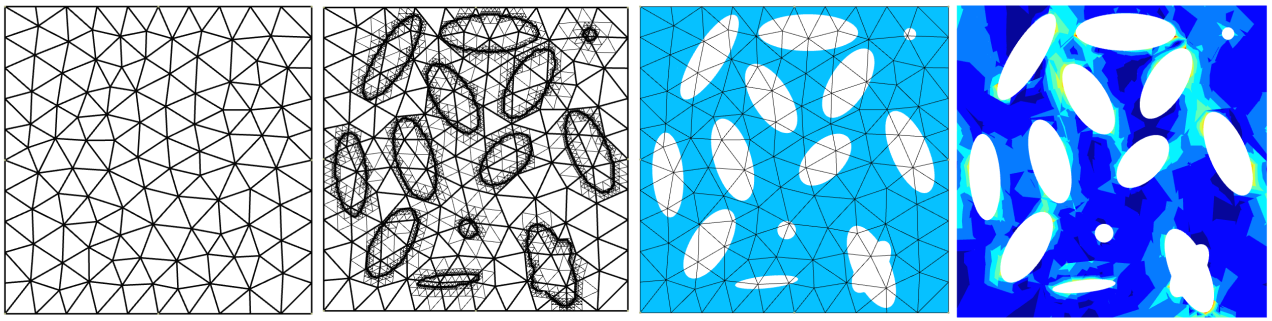


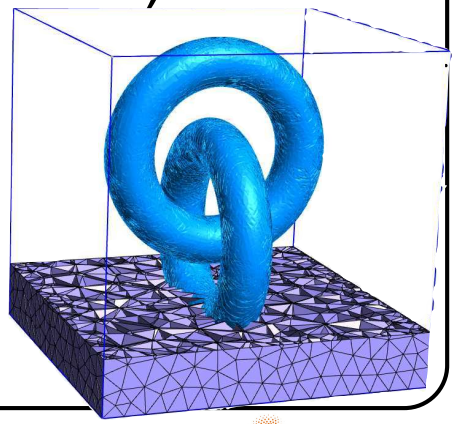


Immersed boundary method (Mittal, *et al.* 2005)
Fictitious domain (Glowinski, *et al.* 1994)
Embedded boundary method (Johansen, *et al.* 1998
Virtual boundary method (Saiki, *et al.* 1996)
Cartesian grid method (Ye, *et al.* 1999, Nadal, 2013)

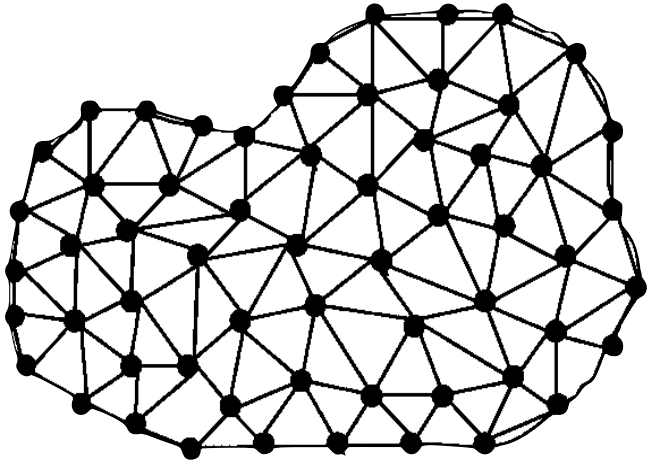


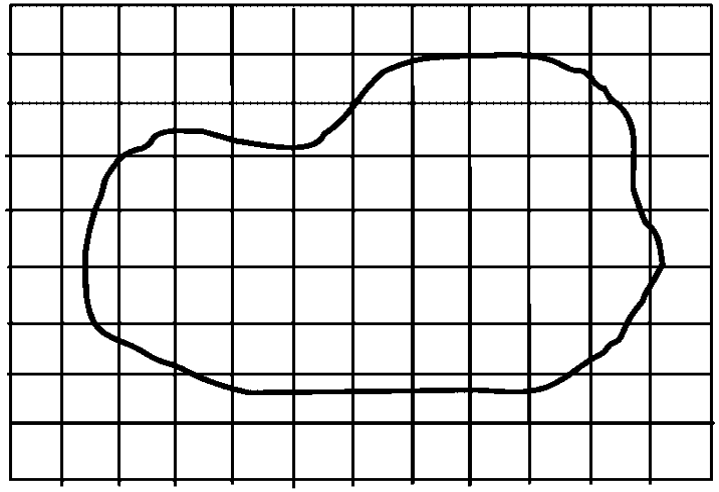
- ✓ Easy adaptive refinement + error estimation (Nadal, 2013)
- ✓ Flexibility of choosing basis functions
- • Accuracy for complicated geometries? BCs on implicit surfaces?
- ➡ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi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



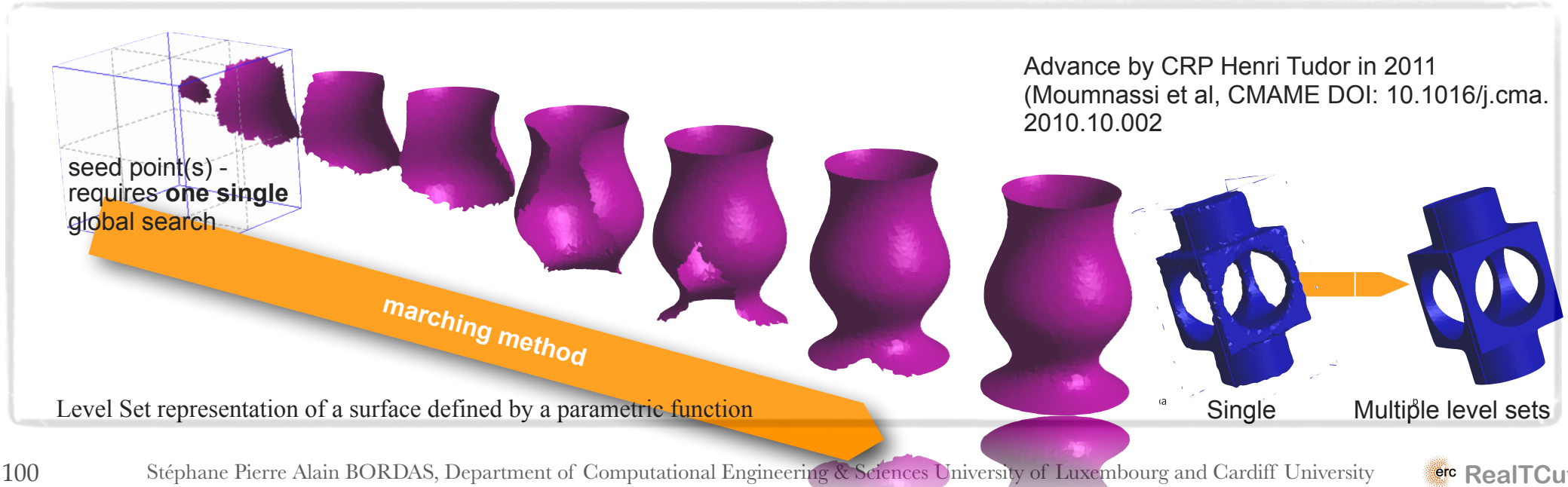


Moumnassi et al, CMAME DOI:10.1016/j.cma.2010.10.002

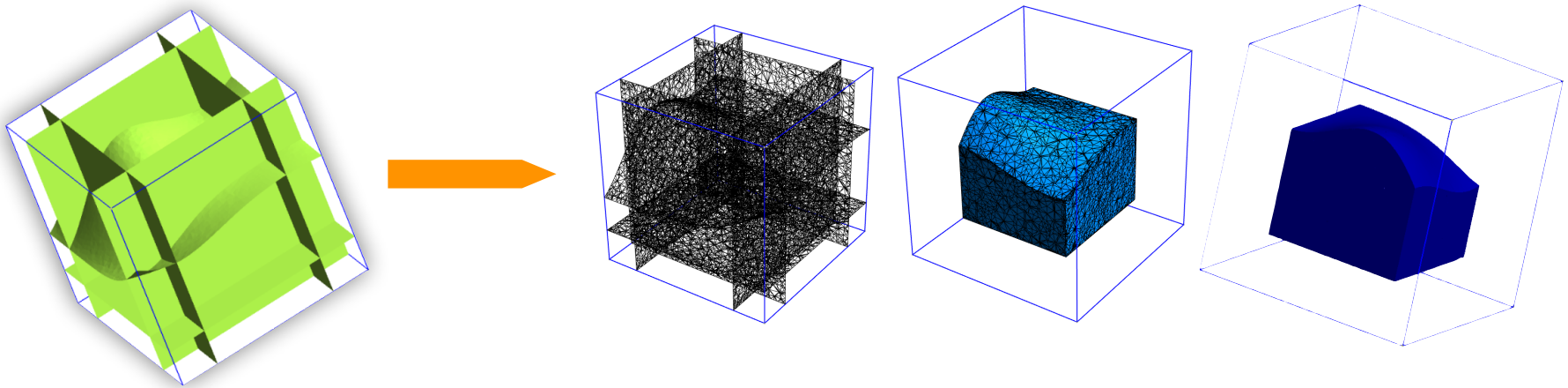


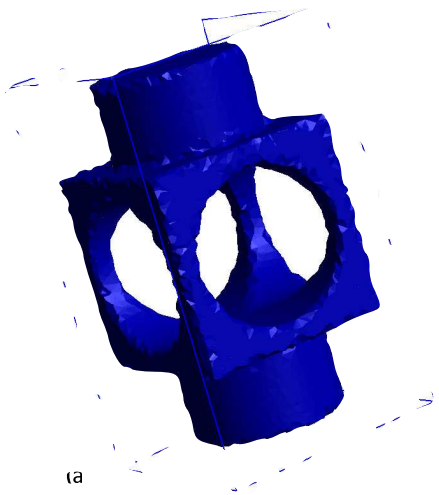


Question: How can we generate level set functions from CAD descriptions (including corners/vertices)?

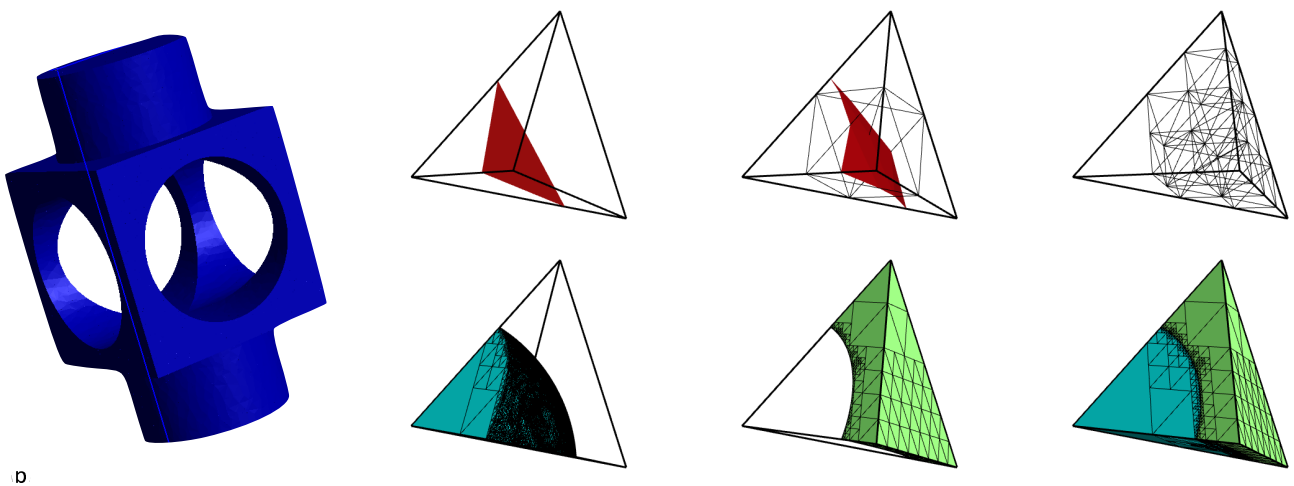


Examples



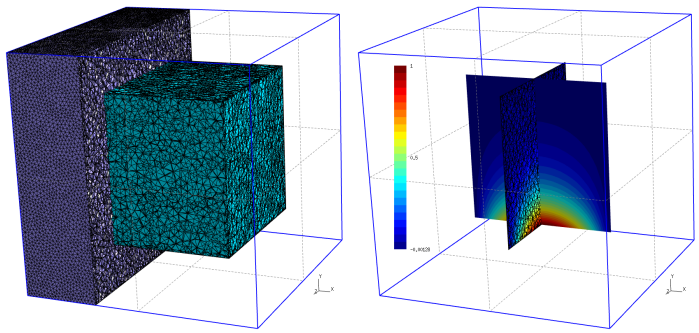


Single level set

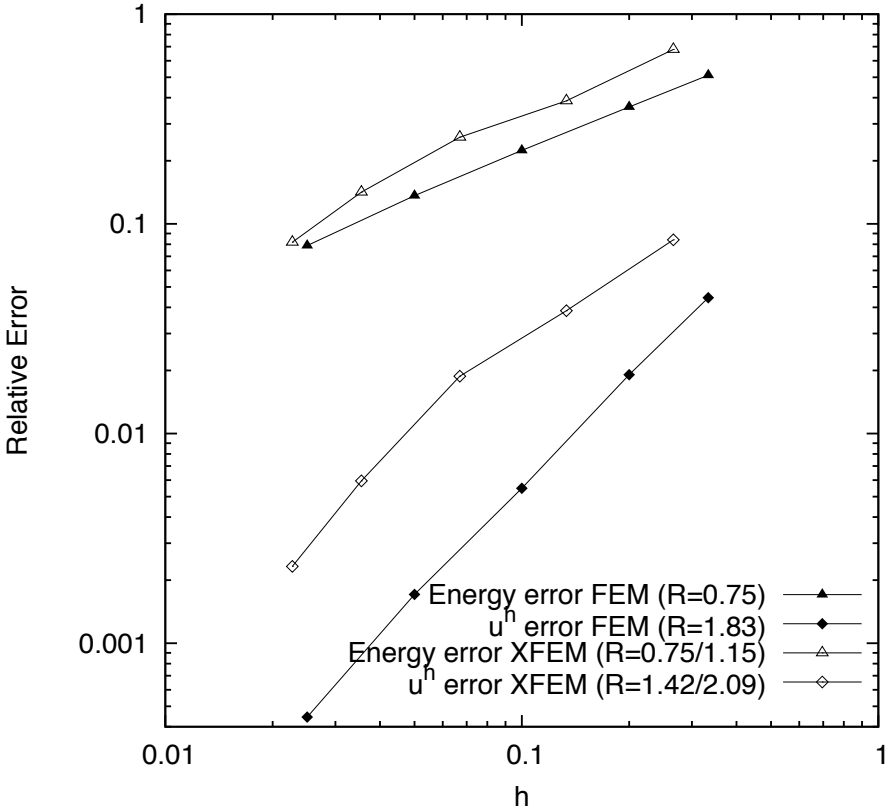


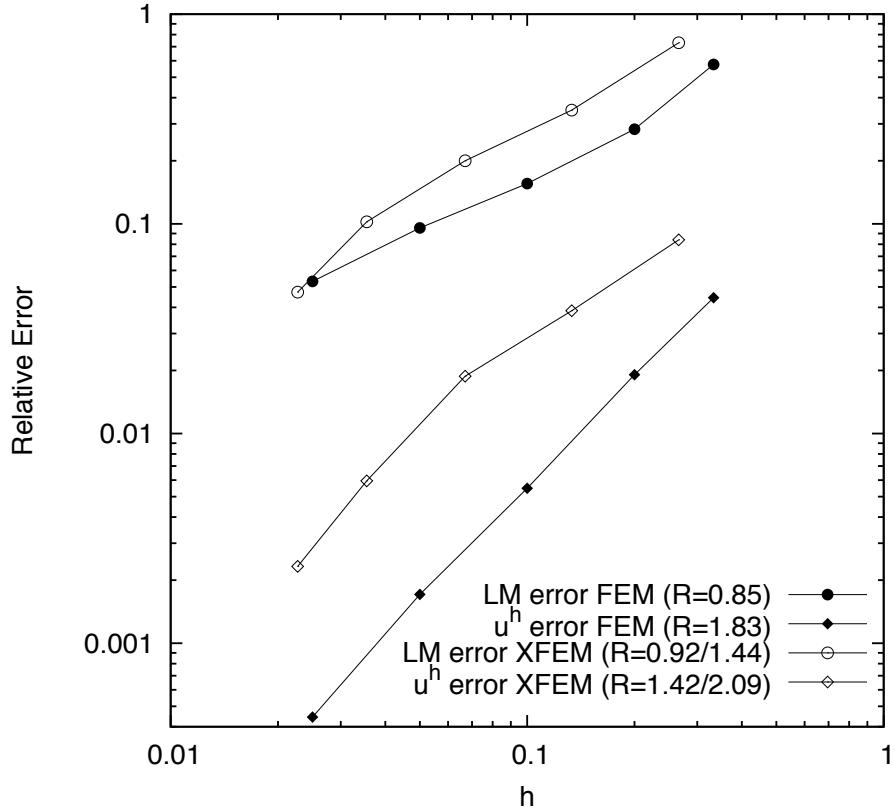
Multi level sets

Three-dimensional model problem



(a) (b)

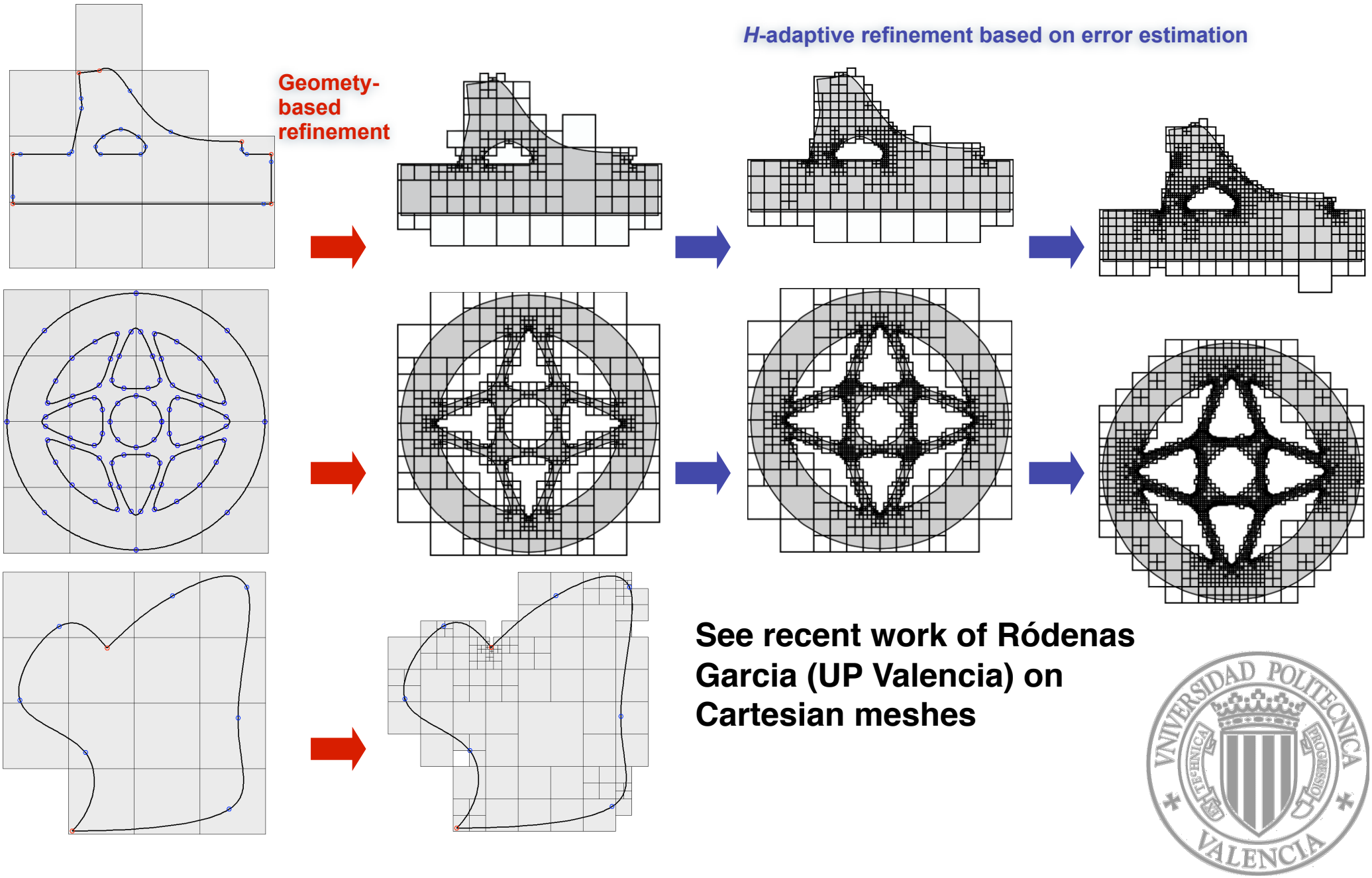




Stable boundary condition enforcement (LBB condition) - Nitsche, Augmented Lagrange

Pixel/Voxel-based FEA on Cartesian grids (Valencia)

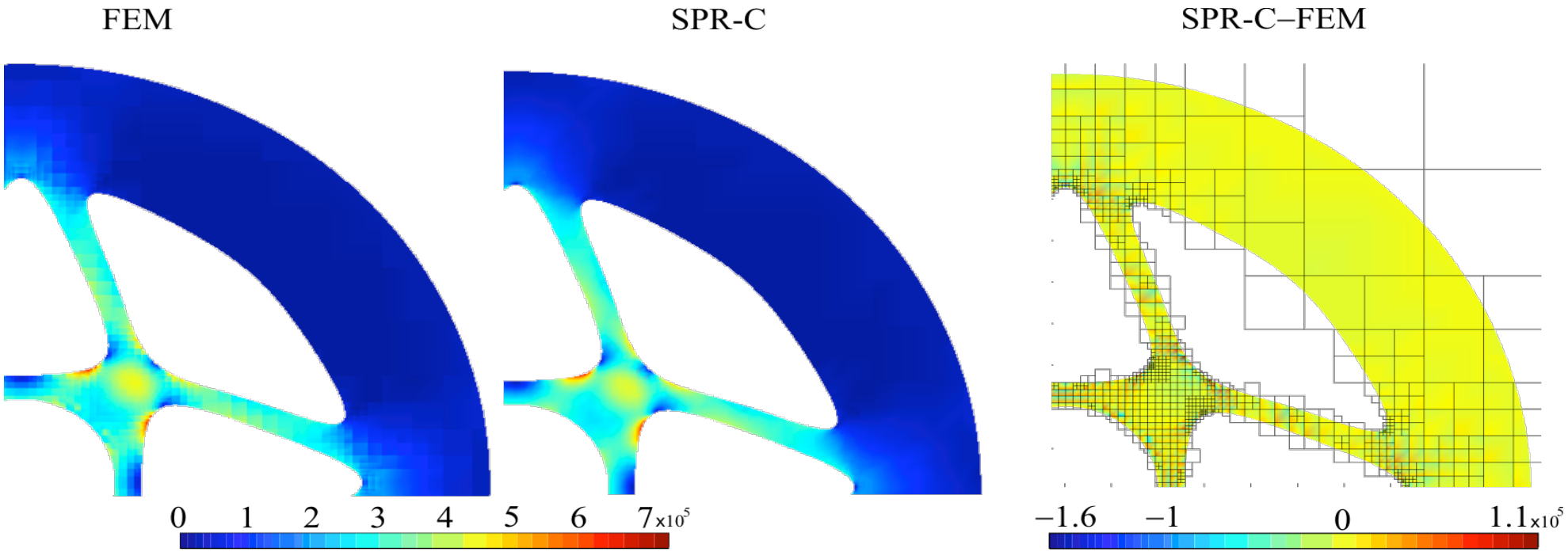
6.1.- Meshing and *h*-adaptive refinement



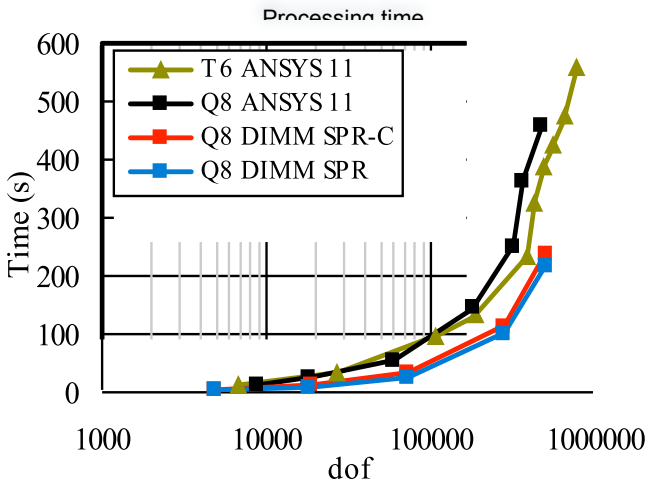
See recent work of Ródenas Garcia (UP Valencia) on Cartesian meshes

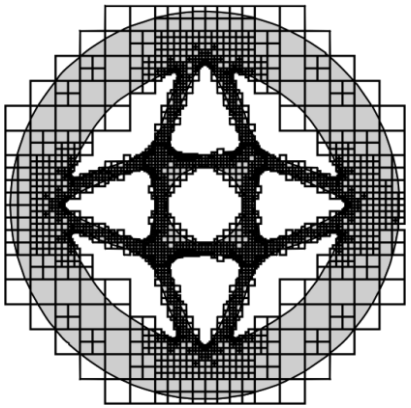
Pixel/Voxel-based FEA on Cartesian grids (Valencia)

6.1.- Meshing and *h*-adaptive refinement



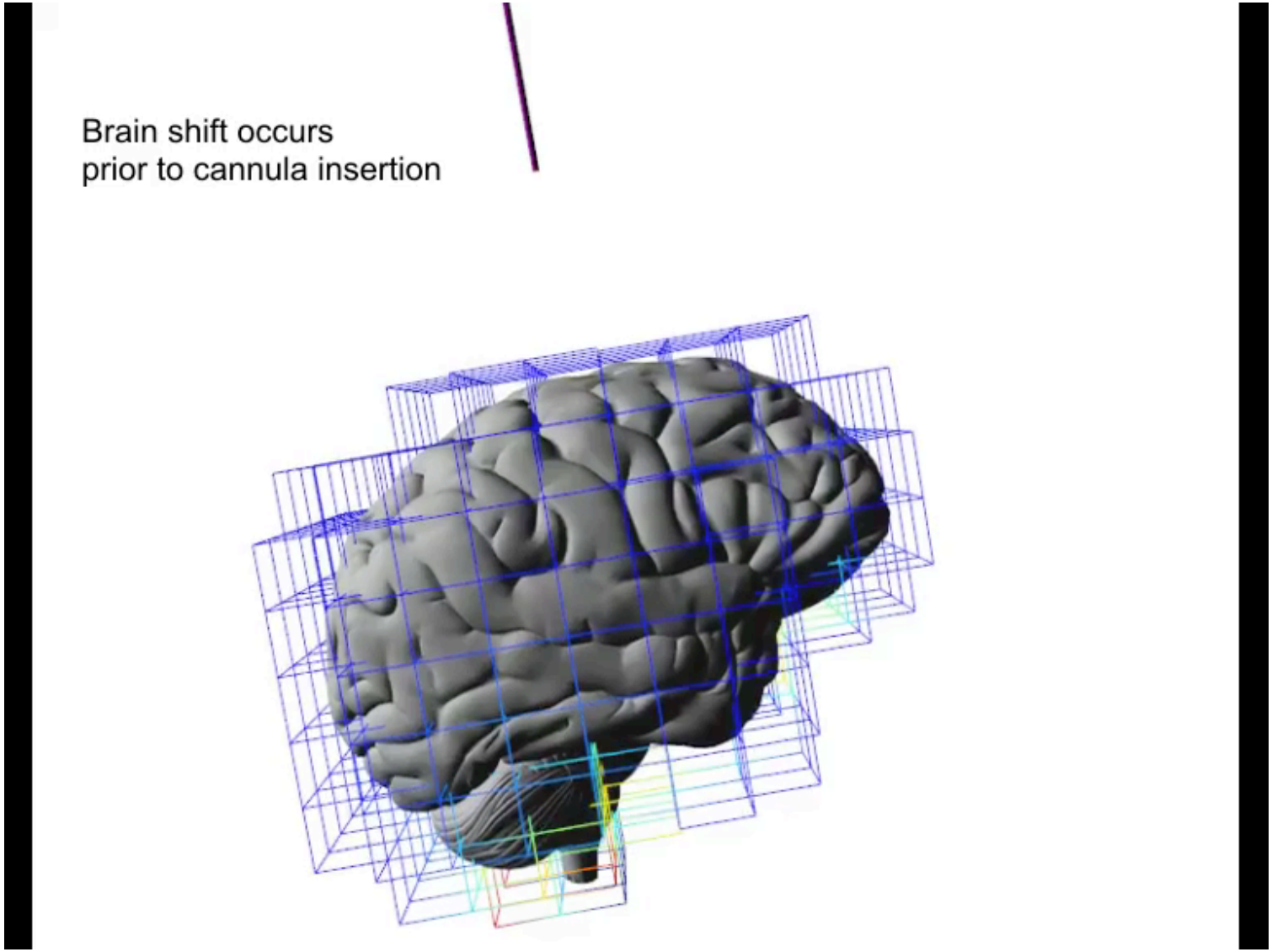
Quad8 uniform refinement





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

Real-time needle steering



Discretization of interface problems
Challenges

Evolving and complex geometries

Accurate calculations of front **velocities**

Error estimation and adaptivity

Time stepping schemes

Moving discontinuities and singularities

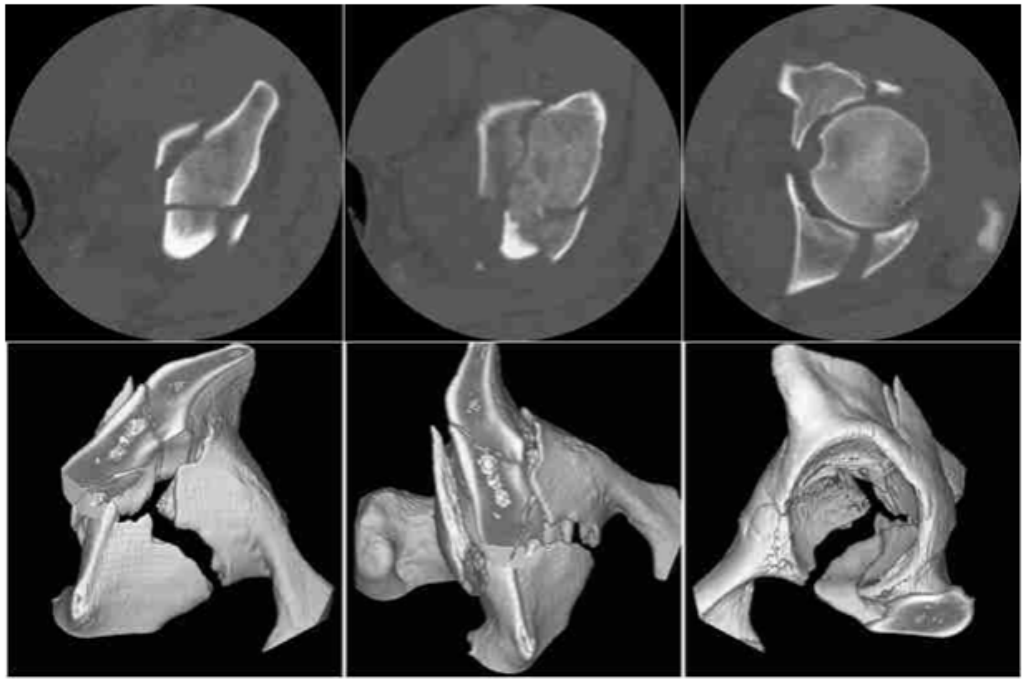
Example: fracture mechanics

Shuttle crash, 2003

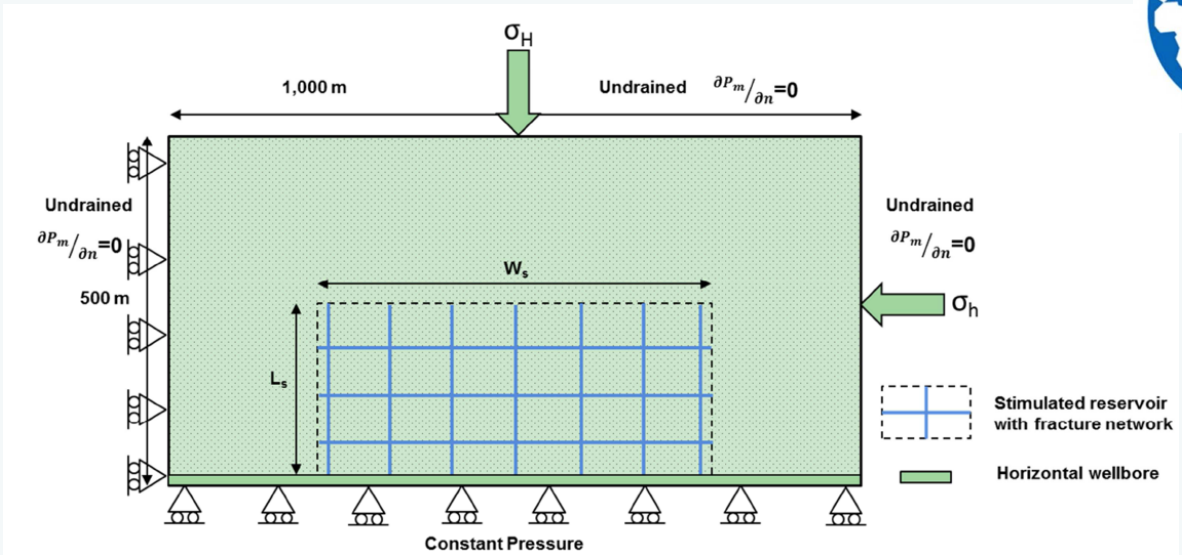
Landslide, Colorado

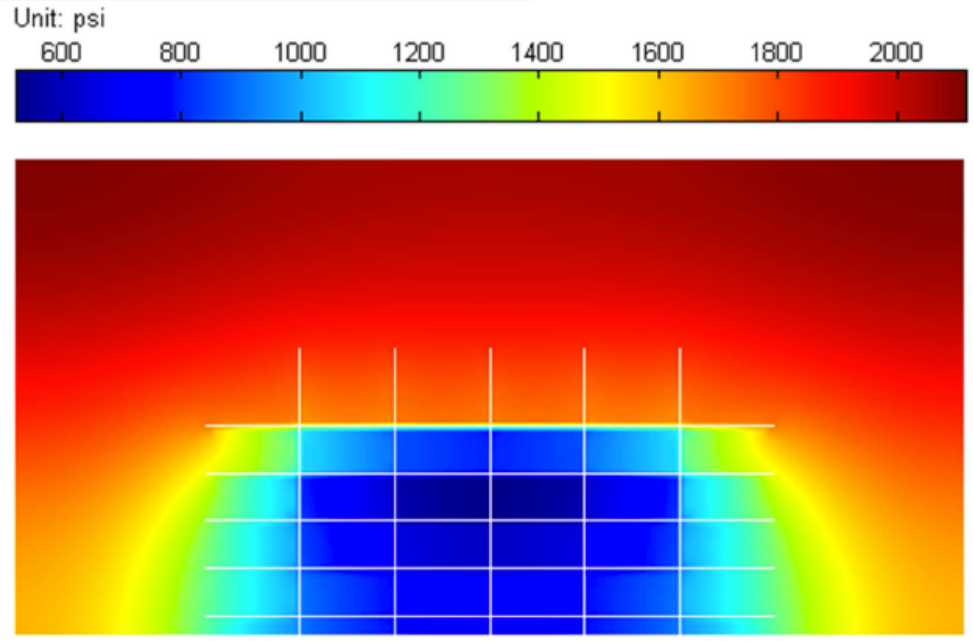
Taiwan earthquake, 2003

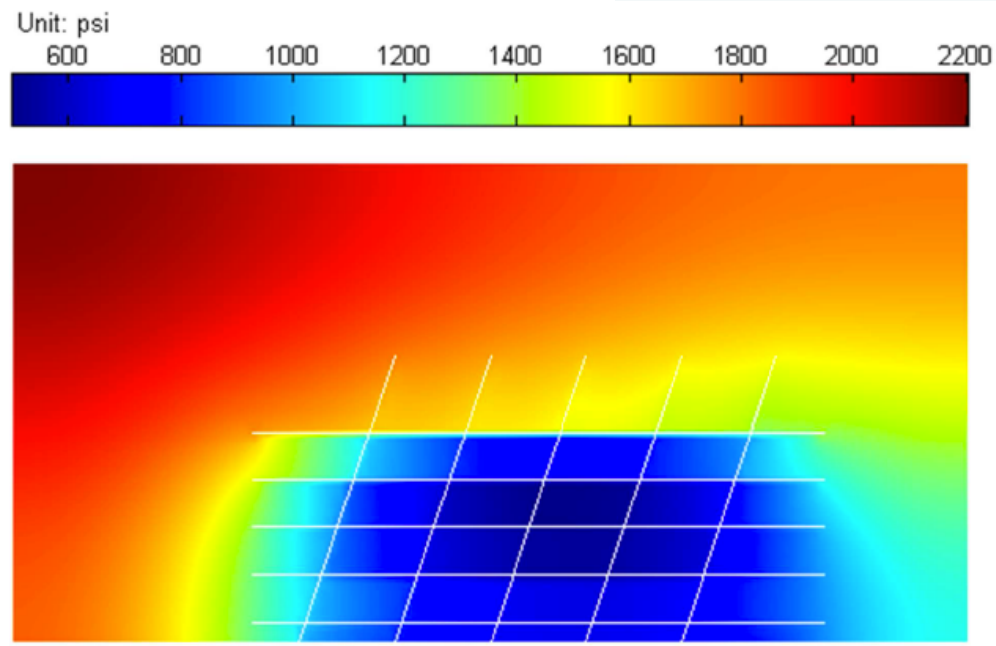
Fragmentation of concrete



Oil extraction from shale -

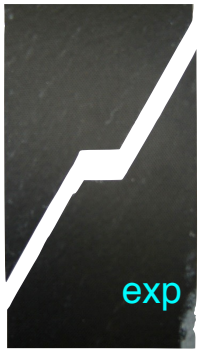






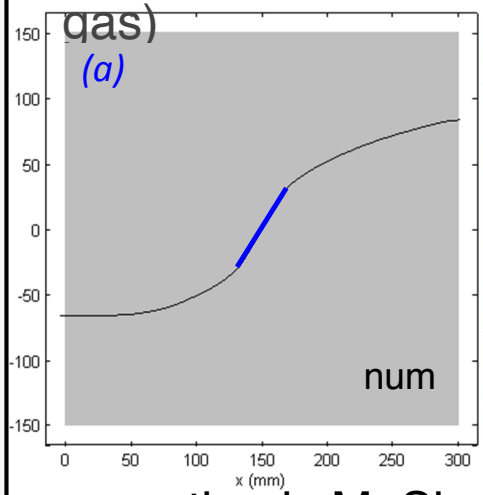
Motivation: fracture of engineering structures and materials

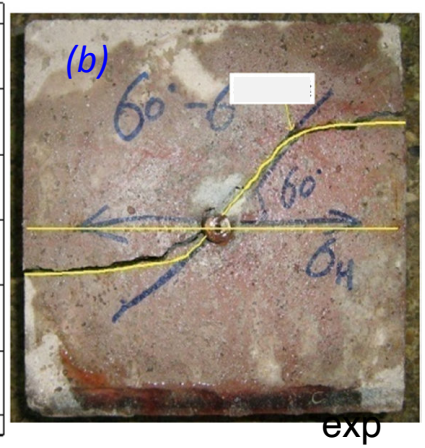
- **Limerick**: unidirectional composites



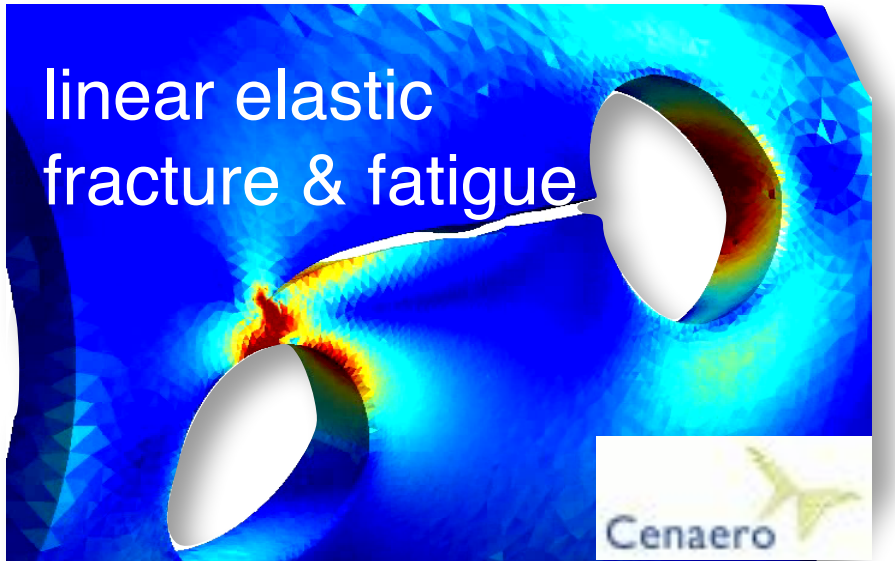
thesis L. Cahill, 2014

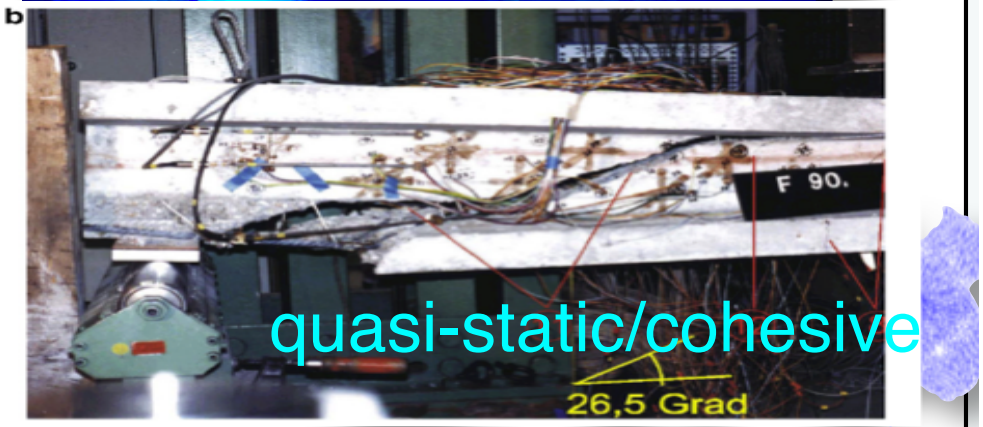
- **China/USA**: hydraulic fracturing (shale gas)



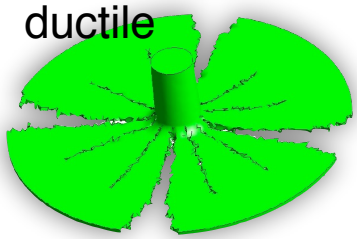


thesis M. Sheng, USA, China, 2016

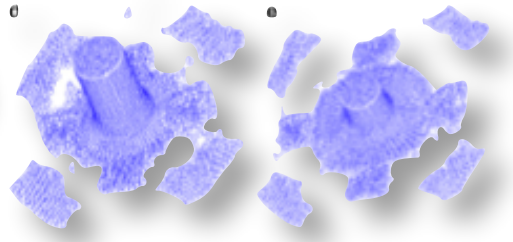




dynamics
ductile

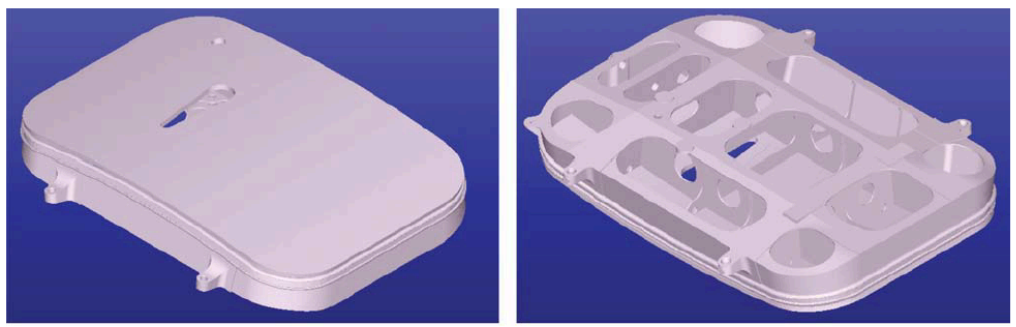


dynamics/brittle



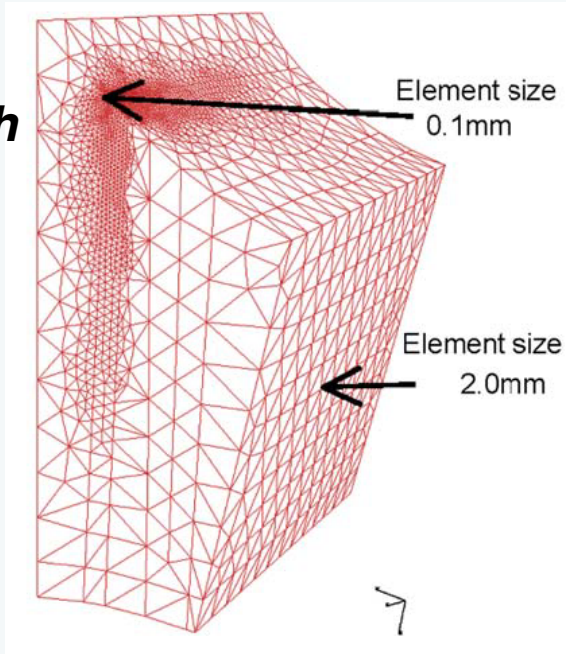
Fracture of 'homogeneous' materials

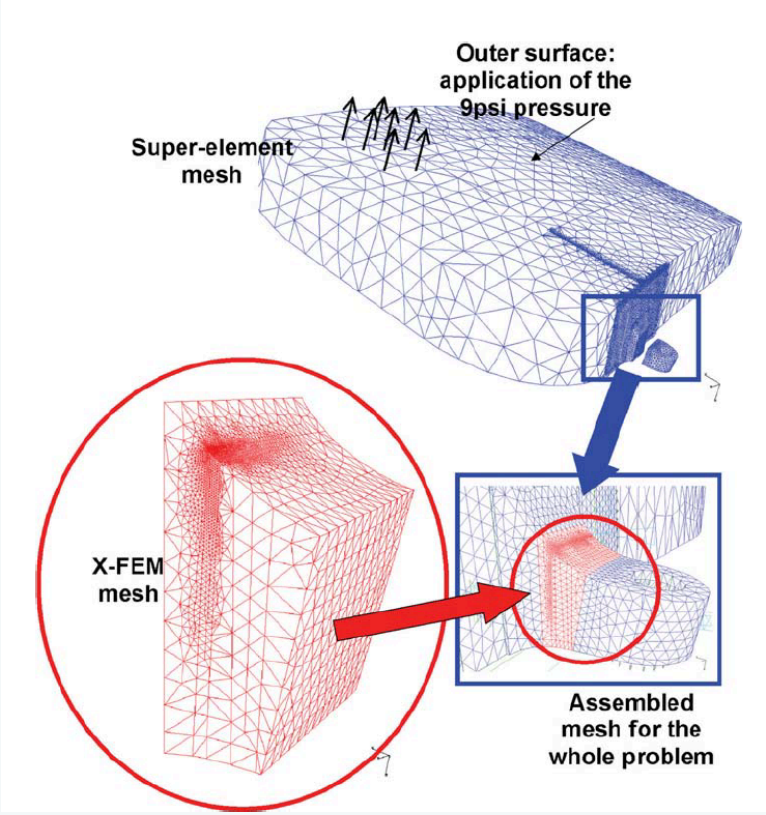
Question: when should a structure be inspected for flaws?



(a) Top view (b) Bottom view

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

Main issues in Computational Fracture

Choice of the Model

Choice of the Discretisation Scheme

Model Choice

Small scale yielding? Linear elastic fracture?

Elastic-Plastic fracture mechanics?

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

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

Discretisation Choice

Finite element method (remeshing?)

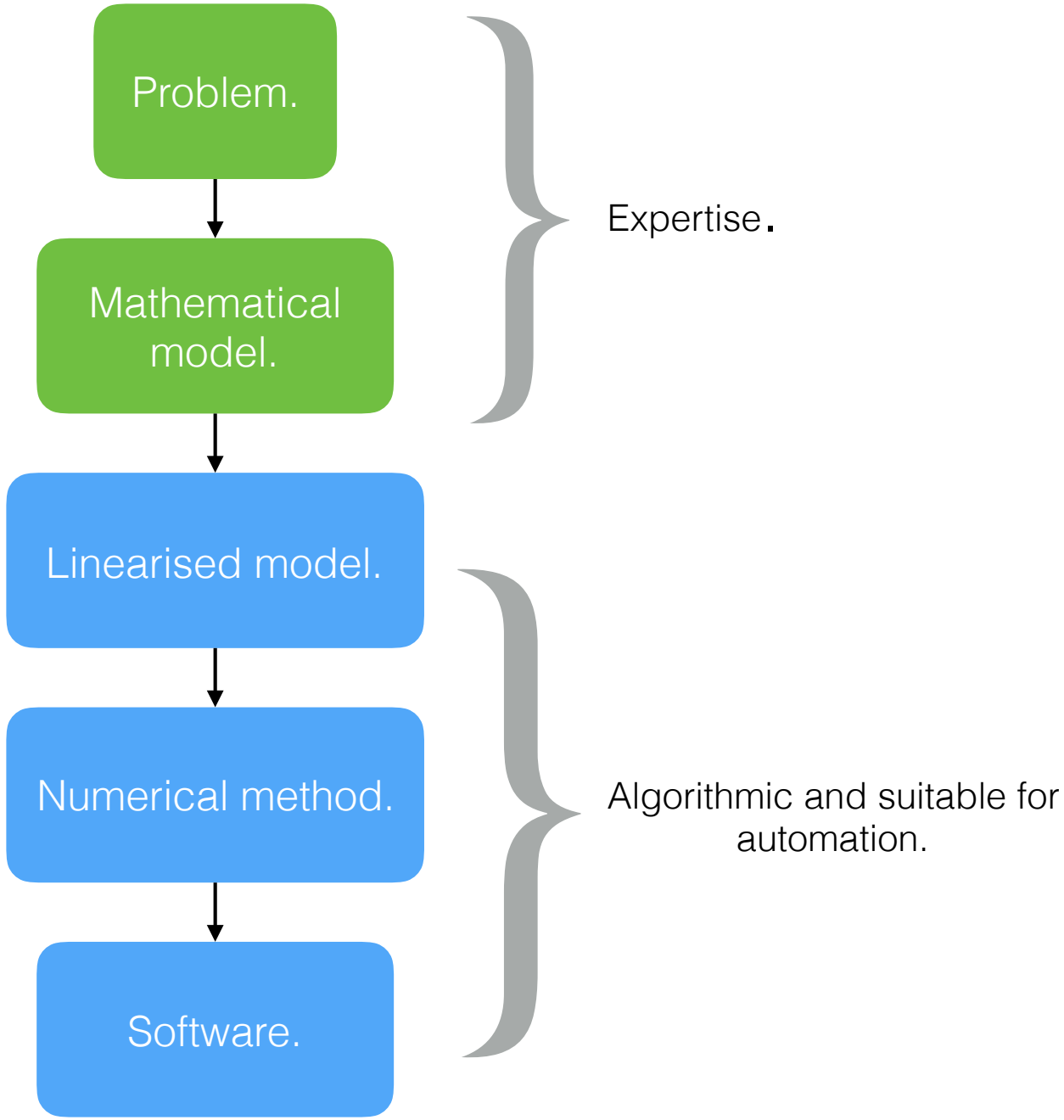
Boundary element method (non-linearities?)

Extended finite element methods (multi-crack?)

Meshfree methods (cost? stability? robustess?)

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 Top100 supercomputers.



FENICS PROJECT

Stress measure

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

```
mu = Constant(0.3)
...
S = (t**3/12)*(2.0*mu*K + \
    (2.0*mu*lmbda)/(2.0*mu + lmbda)*tr(K)*Identity(2))
```

Bending energy

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

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

FEniCS Conference 2017
University of Luxembourg
12-14 June 2017
https://fenicsproject.org

Case study I

Linear elastic fracture mechanics (LEFM)

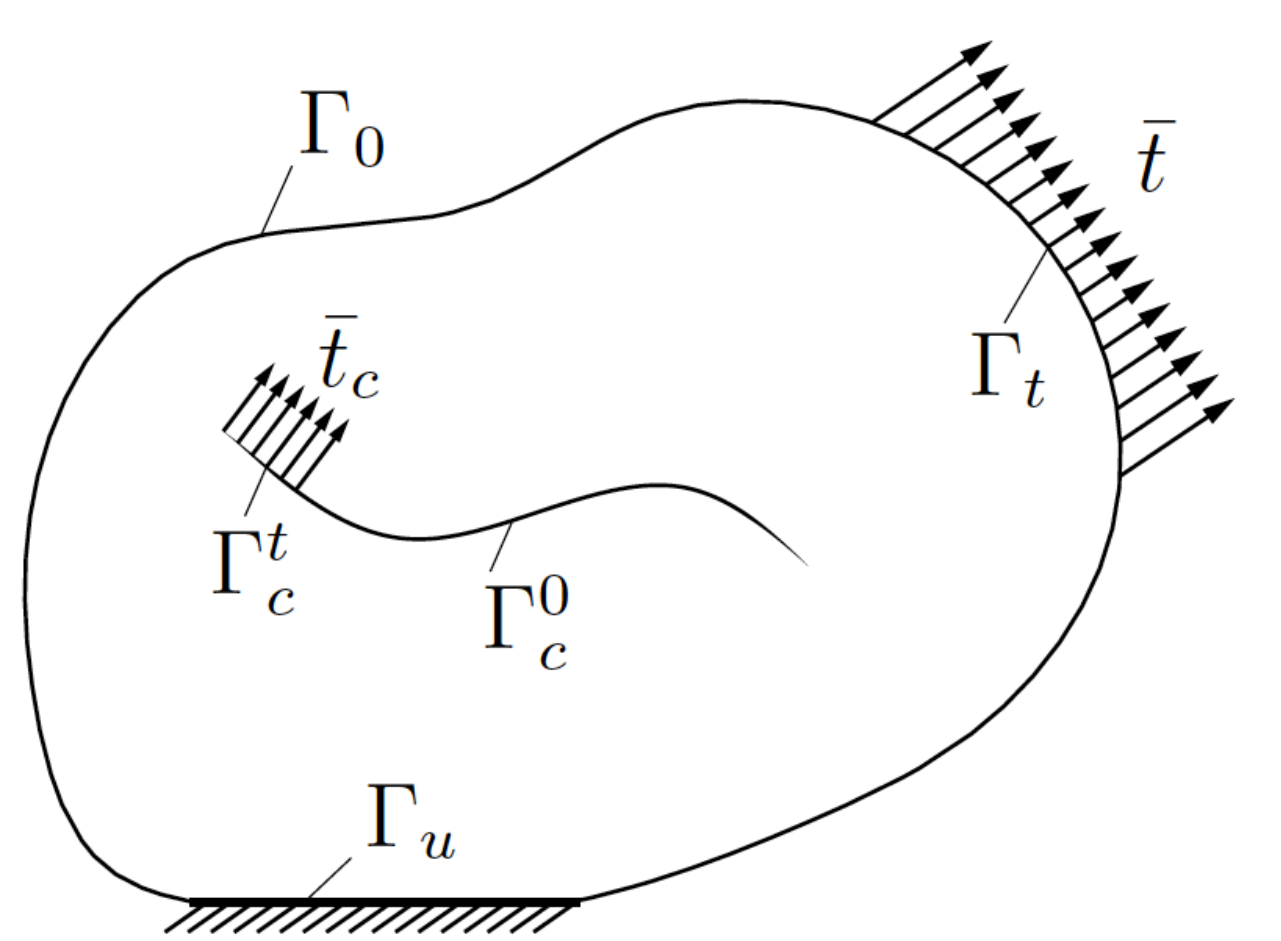
(Extended/Enriched) Finite element methods

(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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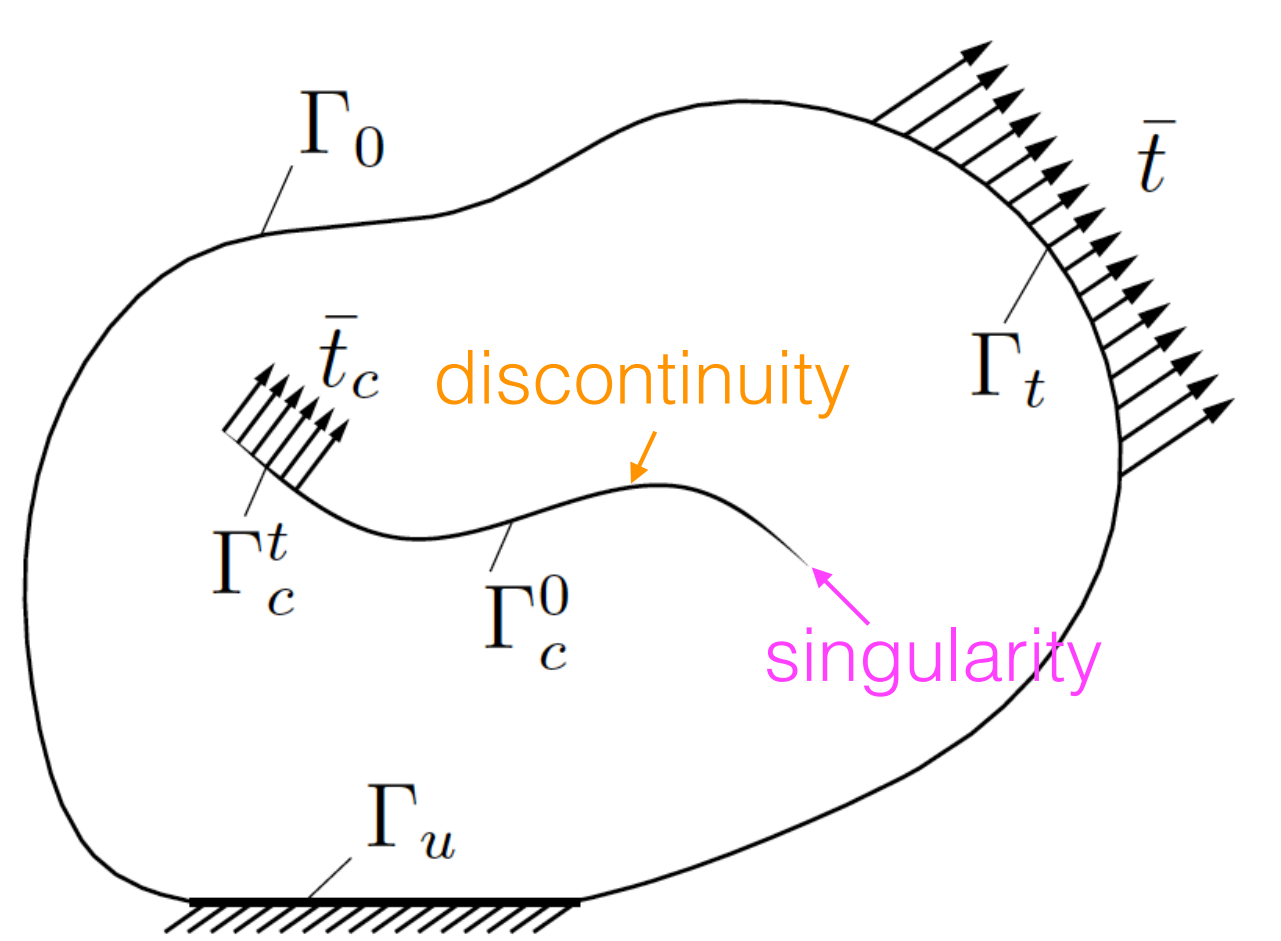
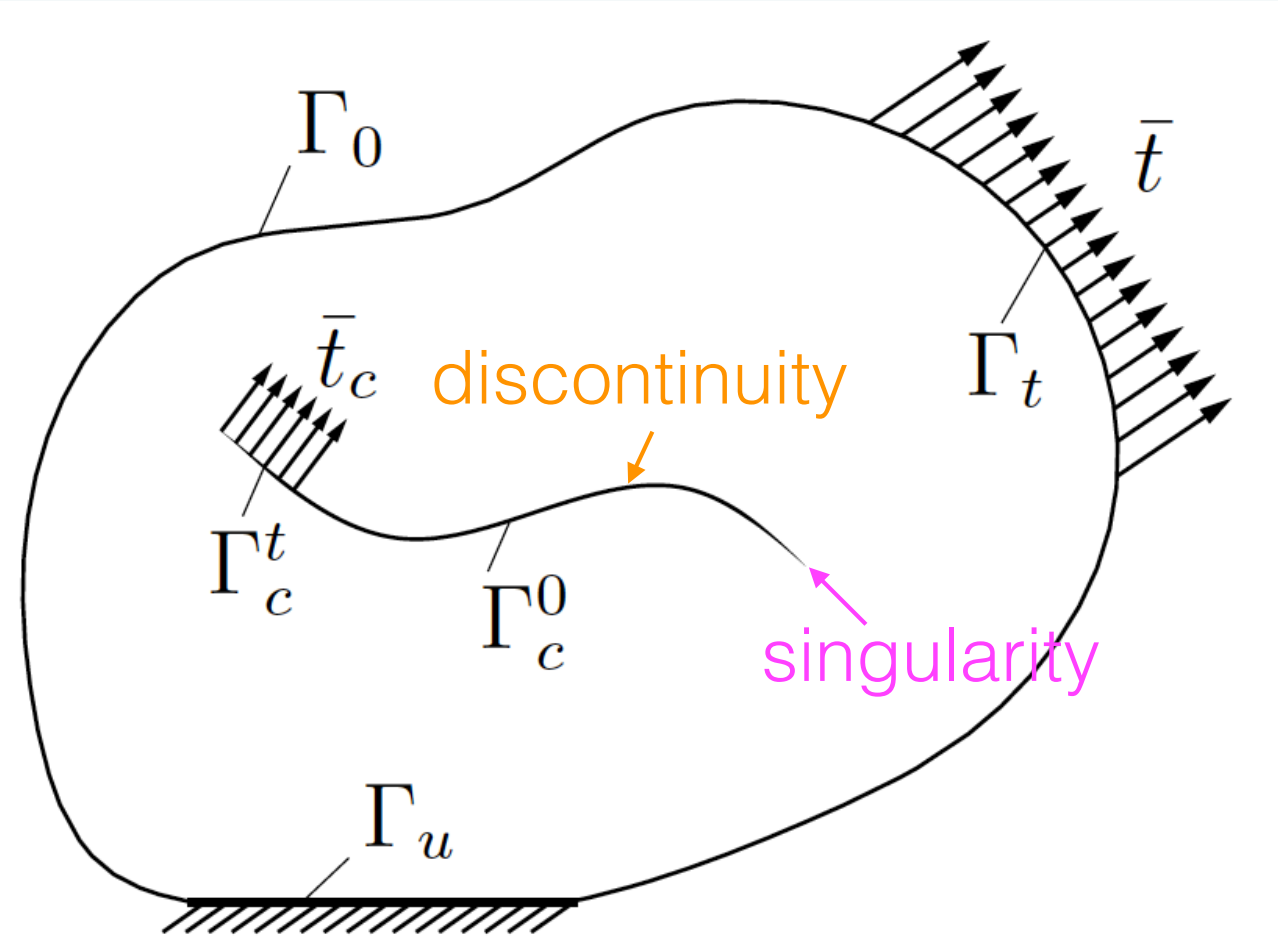
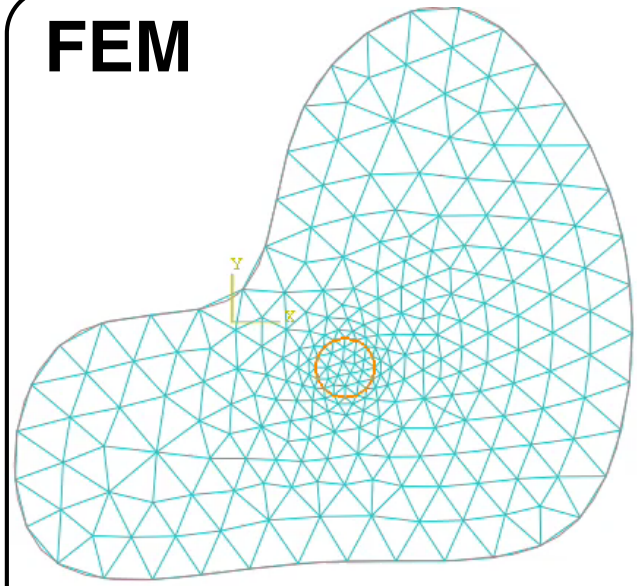


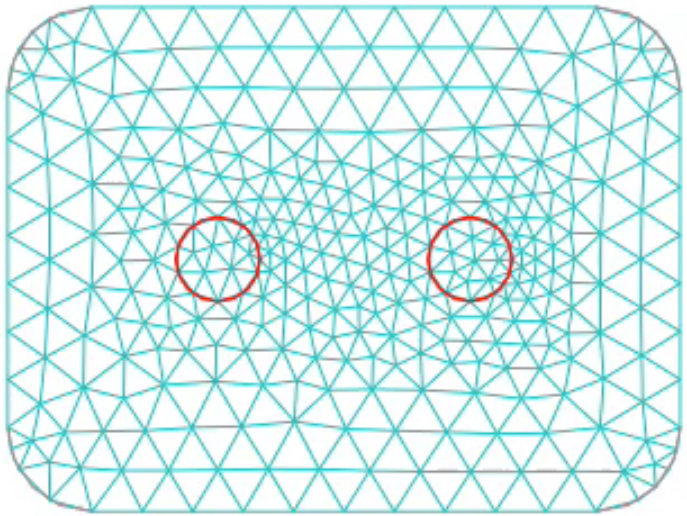
Finite elements for evolving discontinuities & singularities

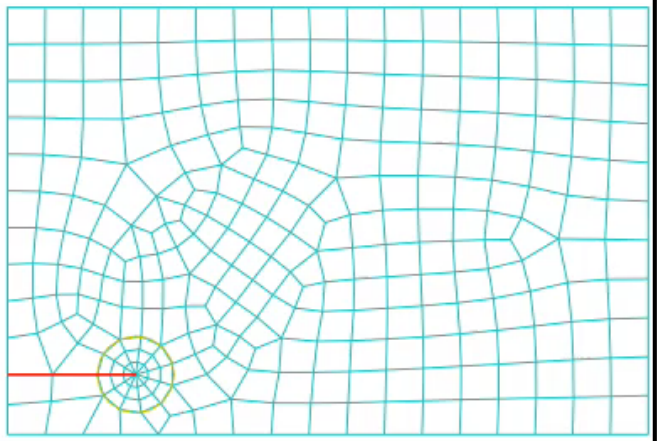


Free boundary problems

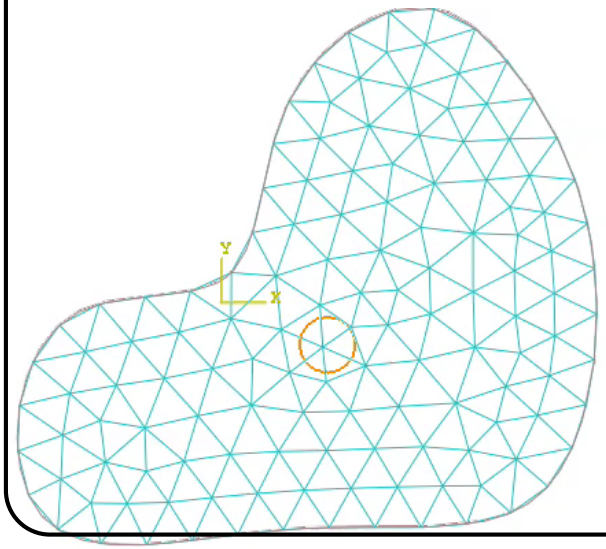
FEM

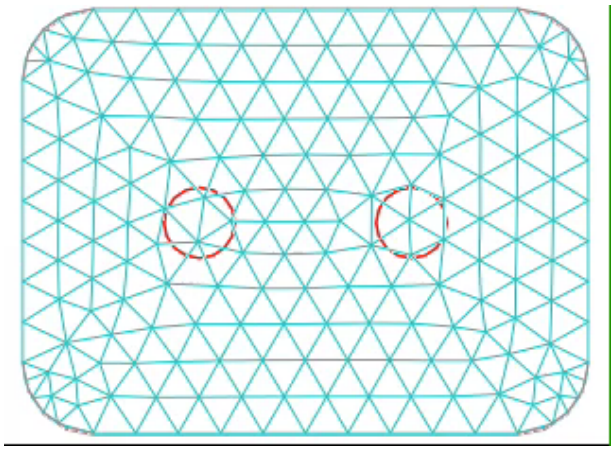


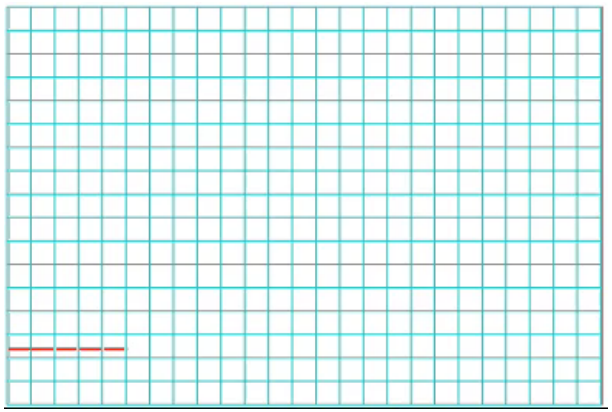




XFEM







<u>One can show</u> . if $v_h = I_h u$ Lagrange approximation of u.

Assume $u \in H^2(\Omega)$ twice weakly differentiable

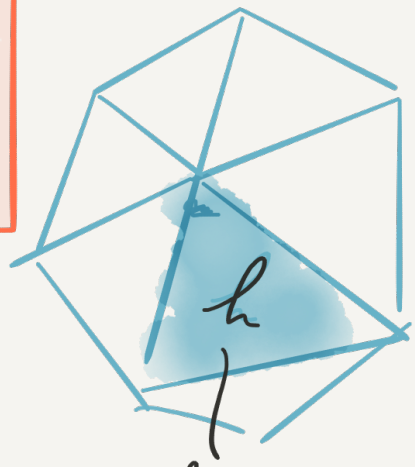
$$\|\underbrace{u-u_h}_{e_h}\|_{H^1(\Omega)} \leq \frac{1}{C} \|v - \underbrace{I_h u}_{v_h}\|_{H^1(\Omega)}$$

Cea's Constant

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

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

- <u>Depends on</u>
  - Physical Constants in Ω
  - geometry of Ω
  - Quality of elements in $\mathcal{T}_h$ (mesh)
  - Degree of polynomial approx.



largest element in $\mathcal{T}_h$

- V_h: is as good as the best approximant in V_h:

Babuška, 1994. <u>Partition of Unity</u>.
1995.

<u>One can show</u> . if $v_h = I_h u$ Lagrange approximation of u.

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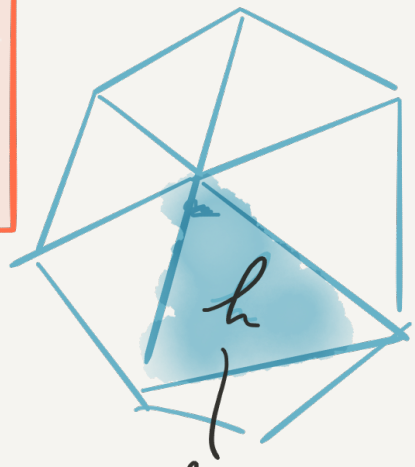
  - Degree of polynomial approx.



largest element in $\mathcal{T}_h$

- V_h: is as good as the 'best' approximant in V_h:

Babuška, 1994. <u>Partition of Unity</u>.
1995.

<u>One can show</u> . if $v_h = I_h u$ Lagrange approximation of u.

Assume $u \in H^2(\Omega)$ twice weakly differentiable

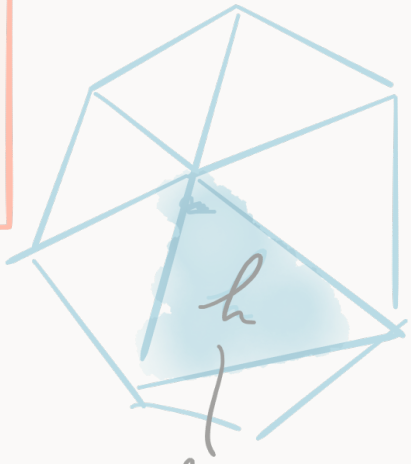
$$\|\underbrace{u-u_h}_{e_h}\|_{H^1(\Omega)} \leq \frac{1}{C} \|v - \underbrace{I_h u}_{v_h}\|_{H^1(\Omega)}$$

Cea's Constant

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

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

- <u>Depends on</u>
  - Physical Constants in Ω
  - geometry of Ω
  - Quality of elements in $\mathcal{T}_h$ (mesh)
  - Degree of polynomial approx.



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Why PUM? Babuška 1994 → 1996 ...

- A priori error estimate:

polynomial order

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

$\|e_h\|_m$: $H^m(\Omega)$ — measure of the error

C, h: see 6

r: smoothness of u

Elasticity

Fracture

$m = 1$

r : small $\Rightarrow$ u "not so smooth" $\Rightarrow$ only a "few" ∂. of u are smooth

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

LARGE.

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

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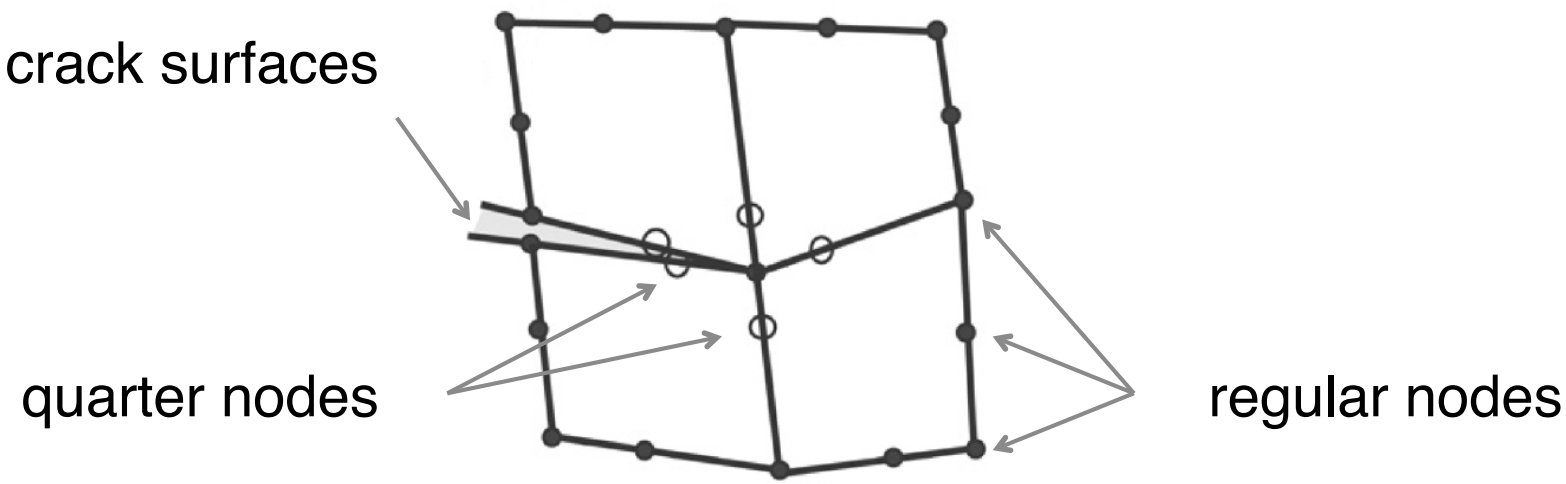
$$\leq C\, \underbrace{h}_{\text{mesh refinement}}^{\min(p,\, \underbrace{r-1}_{\text{"small"}})} \cdot \|u\|_{H^r(\Omega)}$$

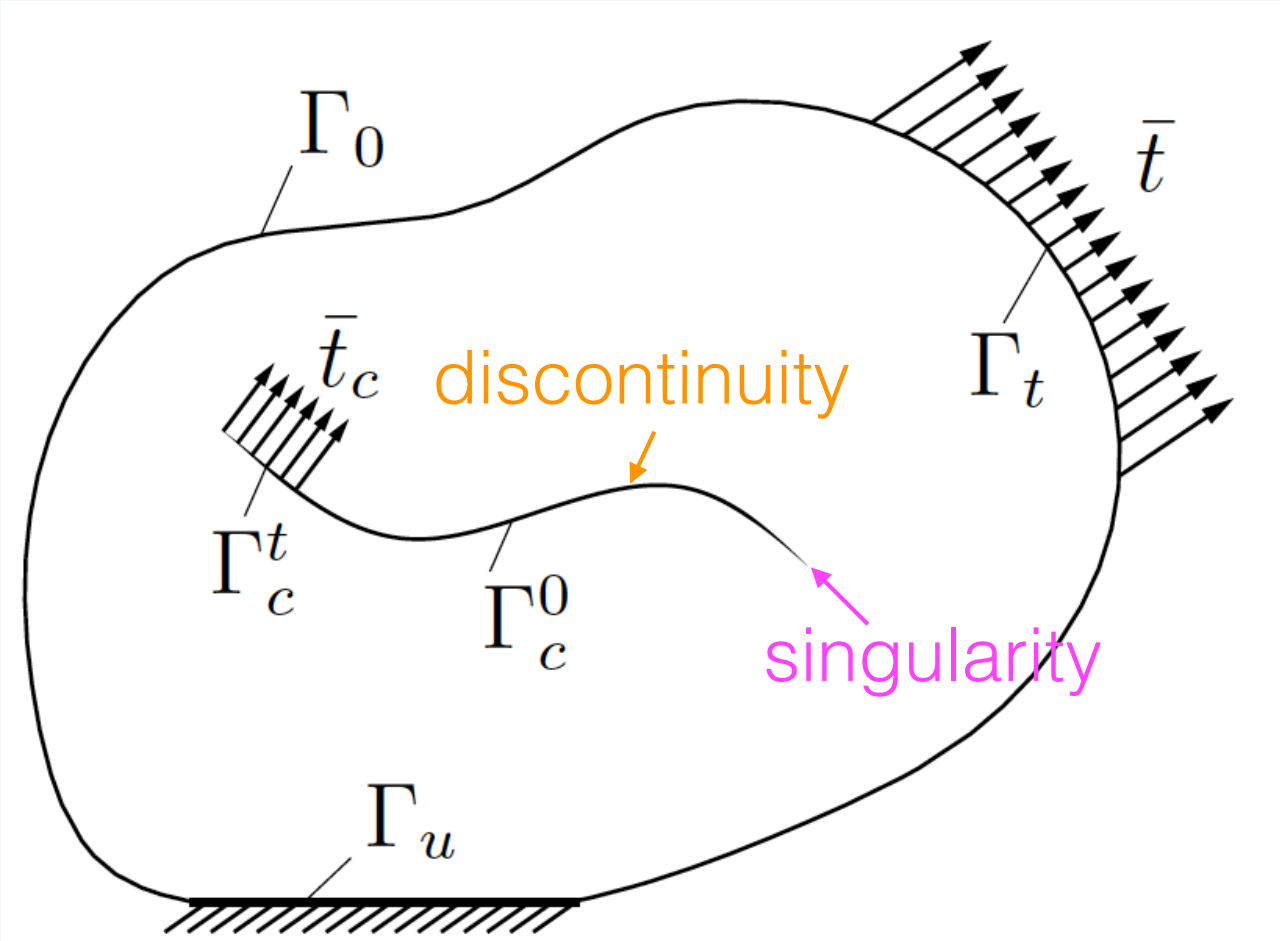
Singular elements - Barsoum 1974

For simulating the crack tip singular field in LEFM

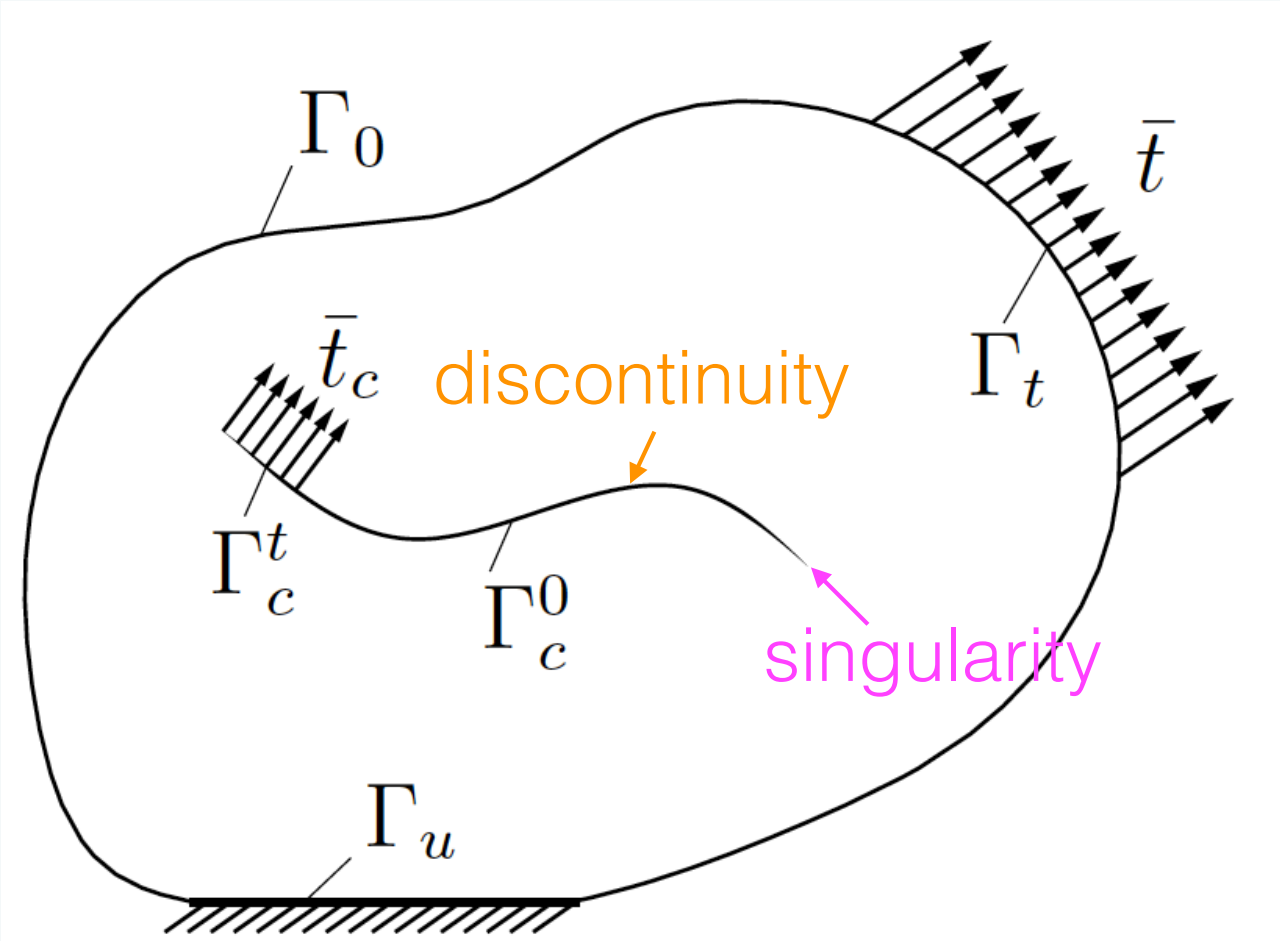
- A simple way how to introduce a singularity of $1/\sqrt{r}$ in isoperimetric finite elements is by displacing the mid-side nodes of two adjacent edges to one quarter of the element edge length from the node where the singularity is desired.



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

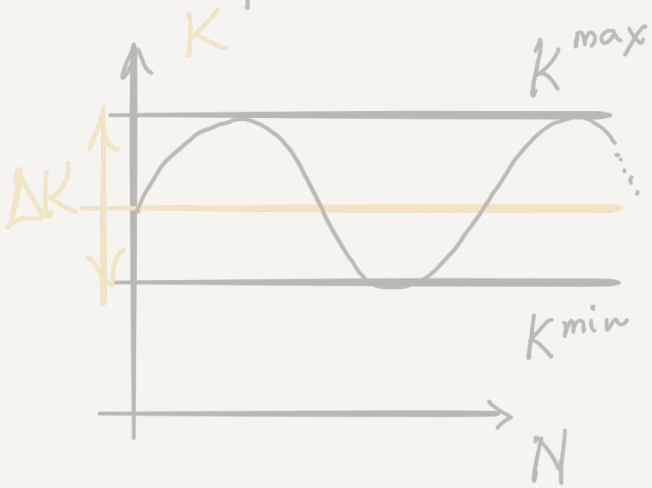


But computational fracture mechanics requires high accuracy (energy release rate)



COMPUTATIONAL FRACTURE

- Aerospace applications typically assume Linear Elastic Fracture.
- Empirical crack growth laws, e.g. Paris law & generalizations.



$$\underbrace{\Delta a}_{\text{amount of crack growth for } \Delta N \text{ cycles}} = C\,(\Delta K)^m \underbrace{\Delta N}_{\text{number of cycles}}$$

C, m are empirical coefficients

$m \in [3,5]$ typically.

ΔK: Stress Intensity factor amplitude.

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

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

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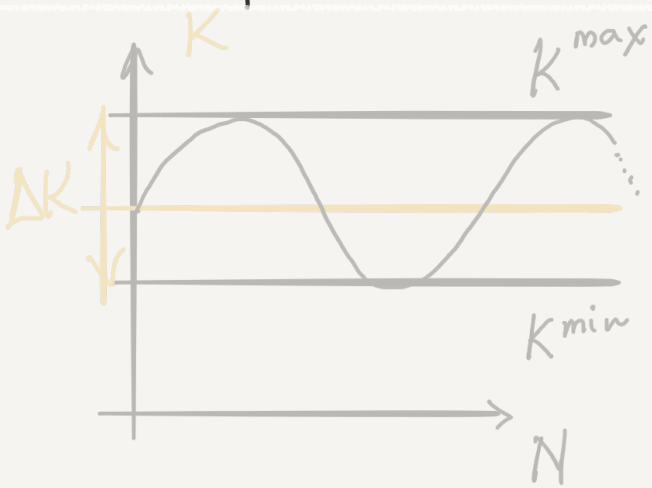

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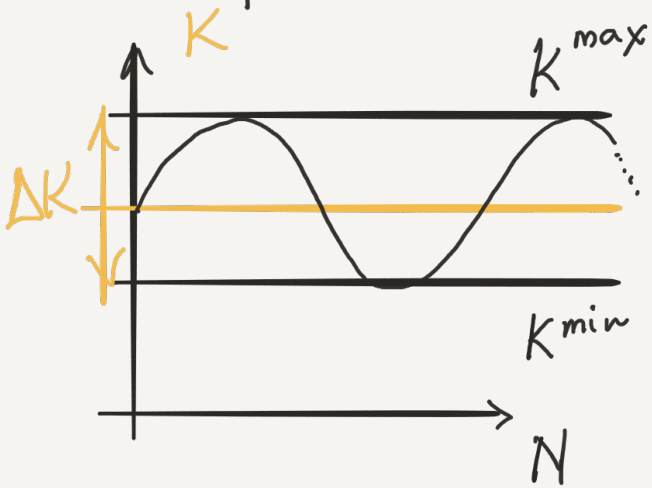

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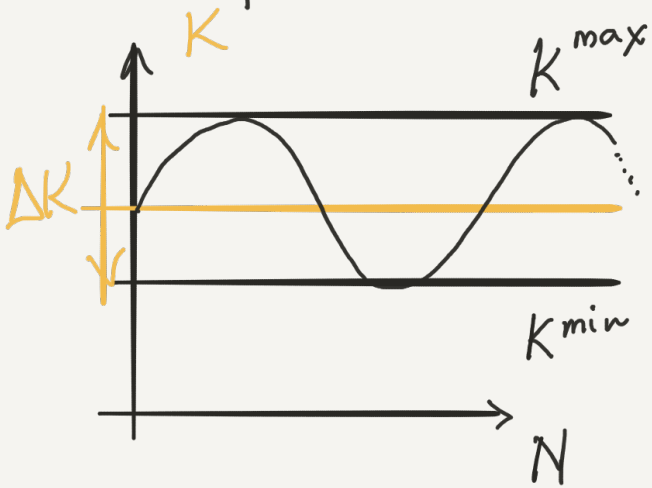

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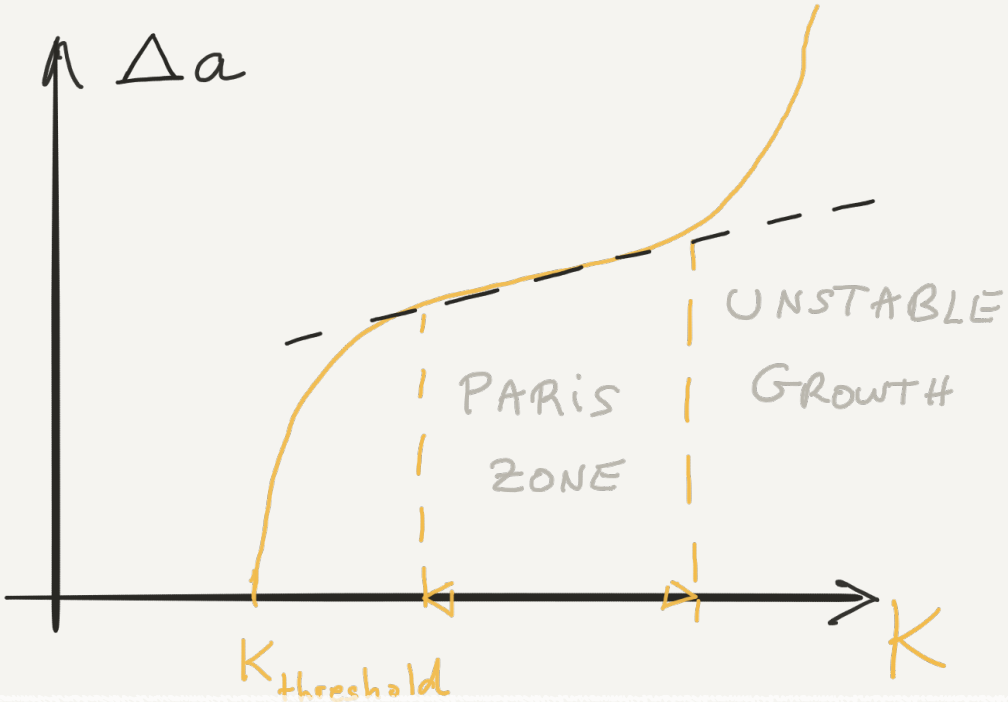


Numerically Computed

Fracture ②

$$\boxed{\Delta a = C\,(K)^m\,\Delta N}$$

$3 \leq m \leq 5$ Paris Exponent

Assume error ε_K on K

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

ε

Increment in crack advance assuming an error ε_K is committed

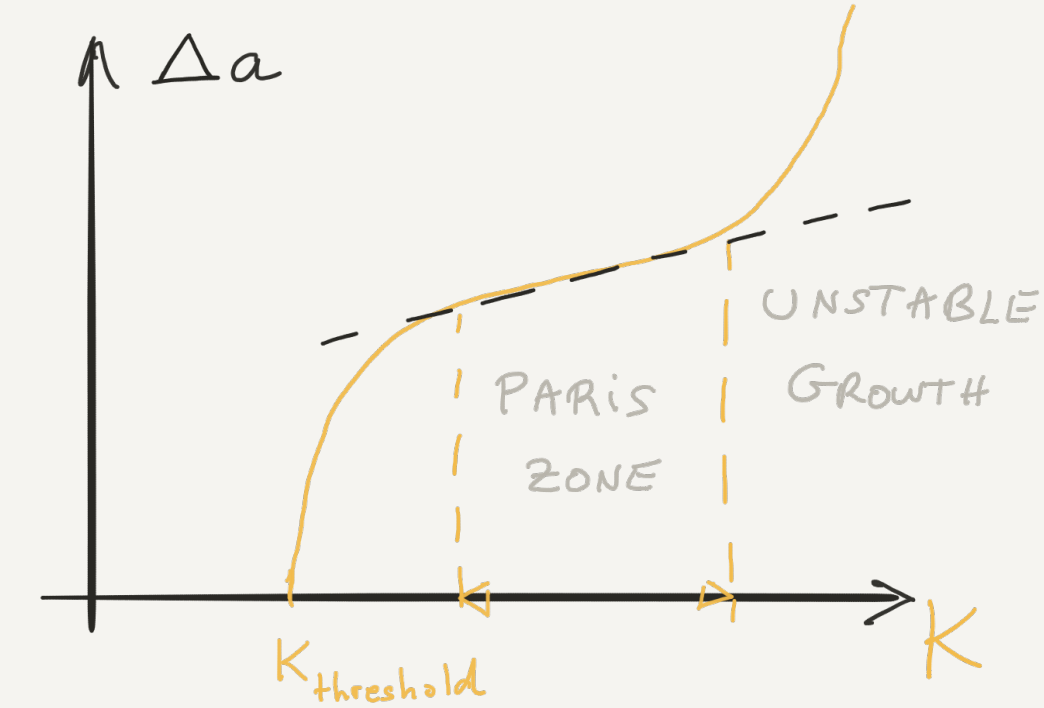
$$\boxed{\Delta a^{\varepsilon}} = C\,(K + \varepsilon_K)^m\,\Delta N$$

$$\Delta a^{\varepsilon} = C\,K\left(1 + \frac{\varepsilon_K}{K}\right)^m \Delta N$$

$$\Delta a^{\varepsilon} \simeq C\,K^m\,(1 + m\,\varepsilon)\,\Delta N$$

$$\boxed{\Delta a^{\varepsilon} \simeq \Delta a\,(1 + m\,\varepsilon)}$$

$\Rightarrow$ error of $\varepsilon\%$ on K leads to an error of $m\,\varepsilon\%$ on Δa !



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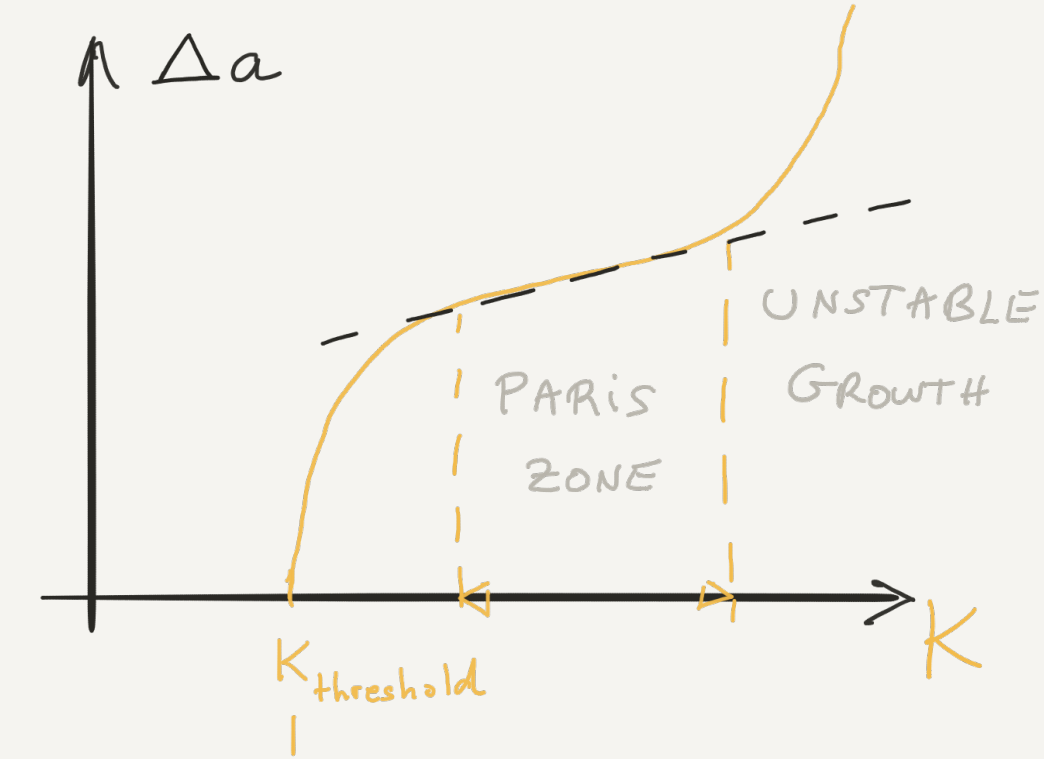

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Conclusion

It is critical to compute SIFs as accurately as possible

1. $\text{error}(\Delta a) = m\,\text{error}(K)$ $\qquad m \in [3,5]$

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

3. Fracture is history dependent.
Cracks cannot heal.
Errors cannot be corrected during growth.

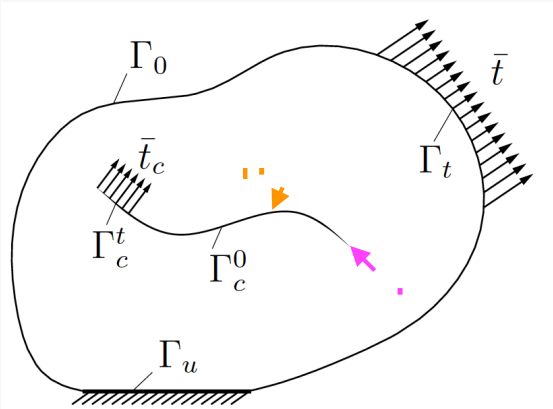
The idea of Partition of Unity Enrichment (PUFEM, GFEM, XFEM, hp clouds, enriched IGA, enriched mesfhree methods, enriched BEM…)

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

Singularities?

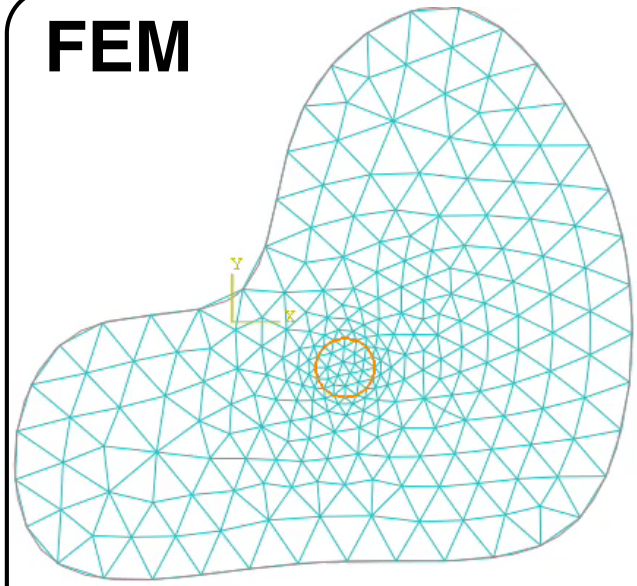
Discontinuities?

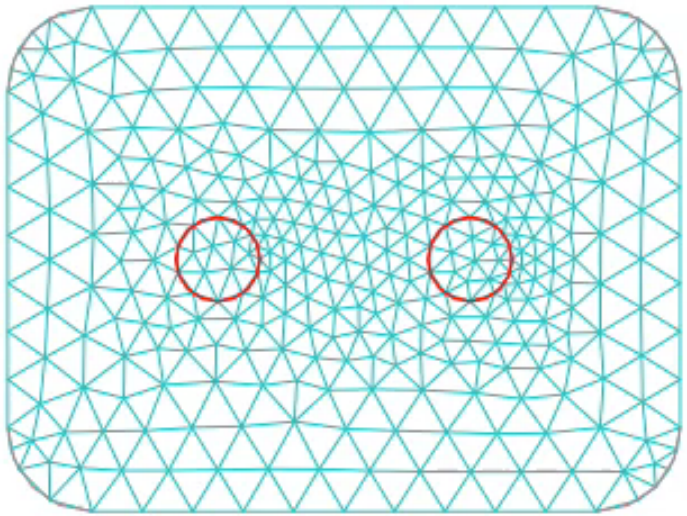
Boundary layers?

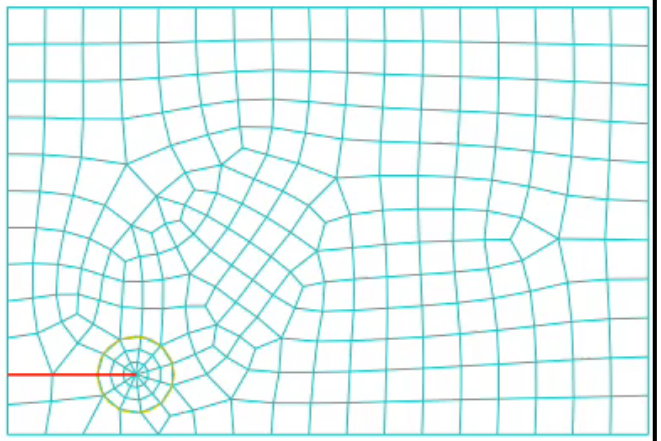


Free boundary problems

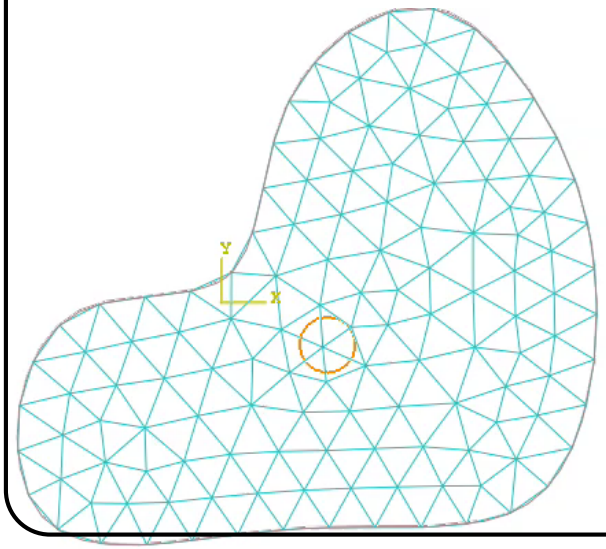
FEM

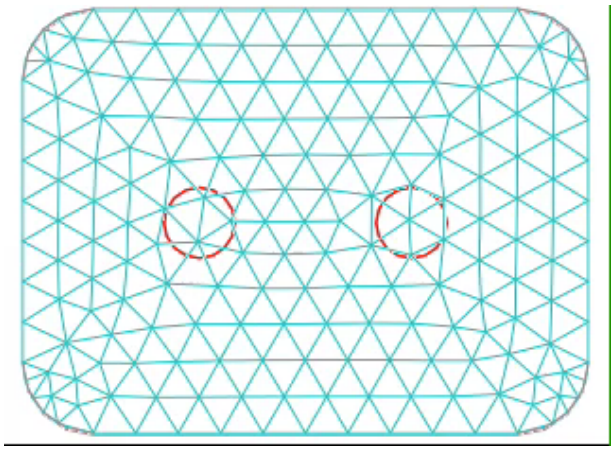


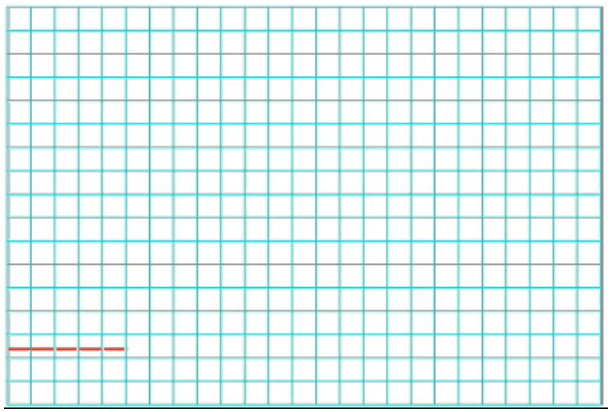




XFEM







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*

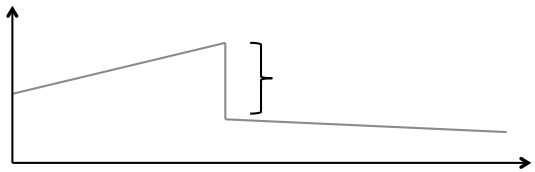
- The approximation space can be extended by introducing of an *a priori* knowledge about the sought solution, and thereby:

1. Rendering the mesh independent of any phenomena
2. reducing error of the approximation locally and globally
3. improving convergence rates

Classification of discontinuities

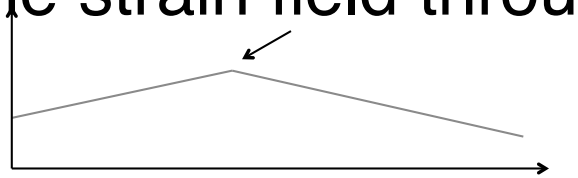
Strong discontinuities

- 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

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.

Classification of enrichments

Extrinsic enrichment

- Associated with additional degrees of freedom and additional shape functions to augment the standard approximation basis.

1.	Extended finite element method (XFEM)	- Moës et al.	(1999)
2.	Generalised finite element method (GFEM)	- Strouboulis et al.	(2000a)
3.	Enriched element free Galerkin	- Ventura et al.	(2002)
4.	*hp* – clouds (Meshless/Hybrid)	- Doarte and Oden (1996)	

Intrinsic enrichment

- Not accompanied by additional degrees of freedom. Instead, some standard functions are replaced with special (problem specific) functions.

1.	Enriched moving least squares (Meshless)	- Fleming et al.	(1997)
2.	Enriched weight function (Meshless)	- Duflot et al.	(2004b)
3.	Intrinsic partition of unity methods	- Fries, Belytschko	(2006)
4	Elements with embedded discontinuities		

Partition of Unity FEM

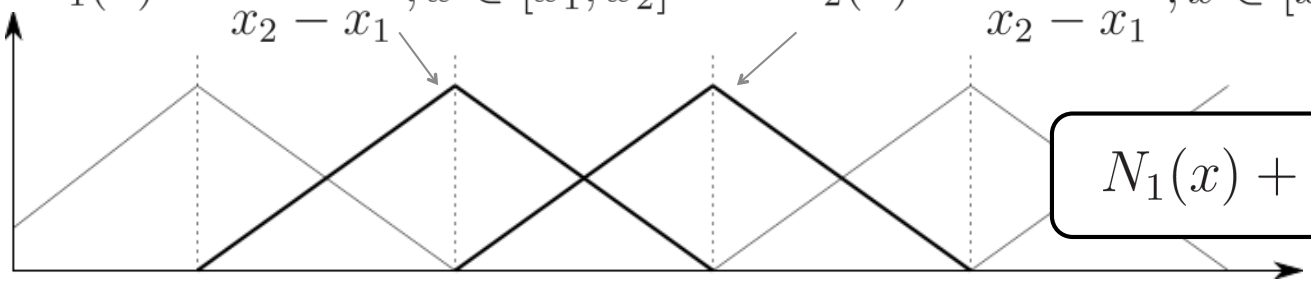
Partition of unity (PU)

- A set of functions ϕ_i whose sum at any point $\boldsymbol{x}$ inside a domain Ω 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:

$$N_1(x) = \frac{x_2 - x}{x_2 - x_1}, x \in [x_1, x_2] \qquad N_2(x) = \frac{x - x_1}{x_2 - x_1}, x \in [x_1, x_2]$$



$$N_1(x) + N_2(x) = 1$$

Partition of Unity FEM

Reproducibility of PU

- Any function $\boldsymbol{p}(\boldsymbol{x})$ 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 $\boldsymbol{q_I}$:

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

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

Partition of Unity FEM

Formulation of PUFEM (example)

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

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

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

- If we define two bilinear forms:

$$a(w, u) = \int_0^l \frac{\mathrm{d}w}{\mathrm{d}x} \frac{\mathrm{d}u}{\mathrm{d}x}\, \mathrm{d}x \qquad (w, f) = \int_0^l w f\, \mathrm{d}x$$

- 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 FEM

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:

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

$$\Downarrow$$

$$\mathbf{K}_{ij}^{se} = \int_0^l \frac{\mathrm{d}N_i}{\mathrm{d}x}\frac{\mathrm{d}(\phi_j\psi)}{\mathrm{d}x}\,\mathrm{d}x$$

$$\mathbf{K}_{ij}^{ss} = \int_0^l \frac{\mathrm{d}N_i}{\mathrm{d}x}\frac{\mathrm{d}N_j}{\mathrm{d}x}\,\mathrm{d}x$$

$$\mathbf{K}_{ij}^{es} = \int_0^l \frac{\mathrm{d}(\phi_i\psi)}{\mathrm{d}x}\frac{\mathrm{d}N_j}{\mathrm{d}x}\,\mathrm{d}x$$

$$\mathbf{K}_{ij}^{ee} = \int_0^l \frac{\mathrm{d}(\phi_i\psi)}{\mathrm{d}x}\frac{\mathrm{d}(\phi_j\psi)}{\mathrm{d}x}\,\mathrm{d}x$$

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

$$f_i^s = \int_0^l N_i f_x\,\mathrm{d}x$$

$$f_i^e = \int_0^l (\phi_i\psi) f_x\,\mathrm{d}x$$

Partition of Unity FEM

Remarks

- Allows to introduce an arbitrary function $\boldsymbol{\psi}(\boldsymbol{x})$ 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)

eXtended FEM (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)

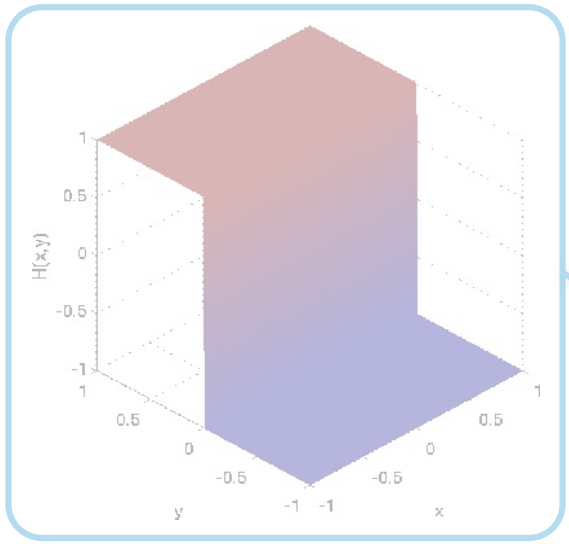
XFEM/GFEM

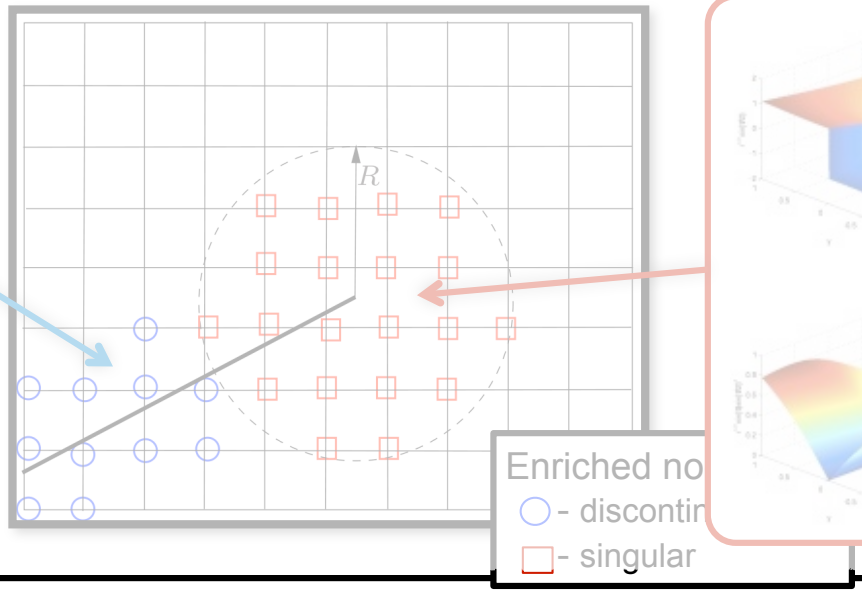
Formulation for crack growth:

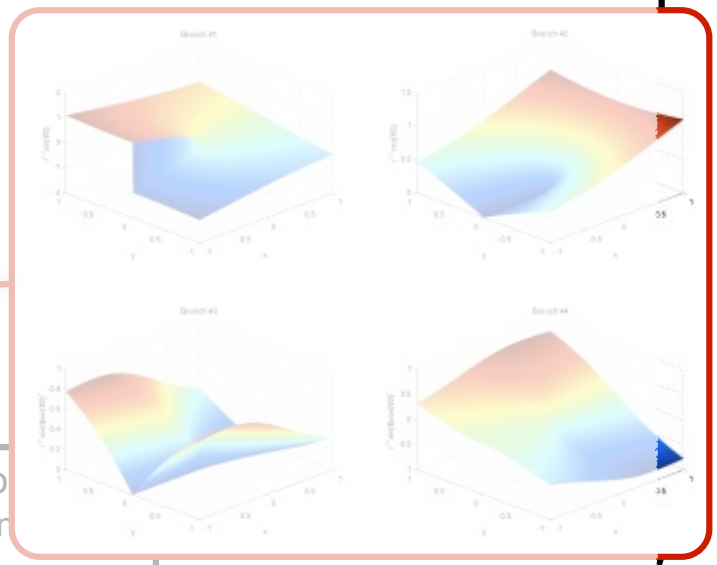
$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I\in\mathcal{N}_I} N_I(\mathbf{x})\mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J\in\mathcal{N}_J} N_J(\mathbf{x})H(\mathbf{x})\mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K\in\mathcal{N}_K} N_K(\mathbf{x})\sum_{\alpha=1}^{4}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

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

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







XFEM/GFEM

Formulation for crack growth:

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

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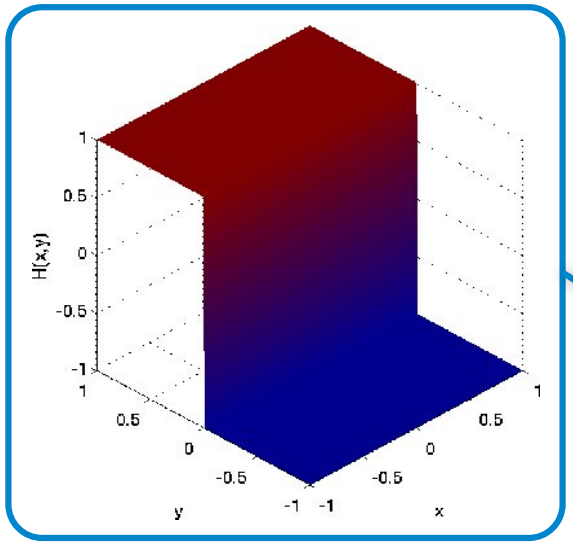
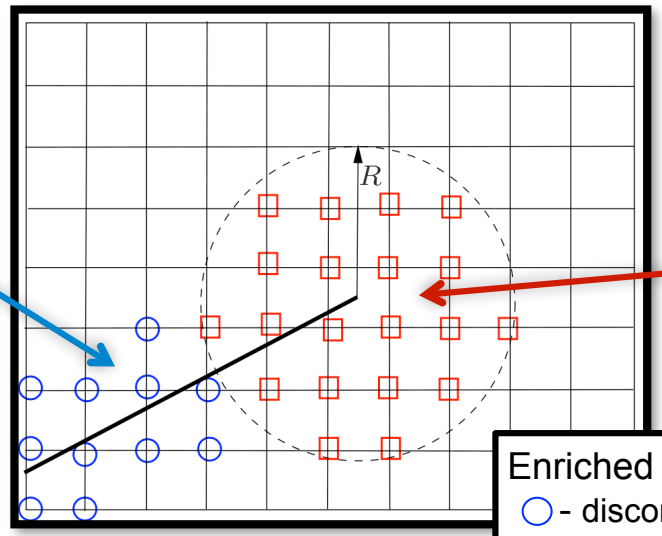
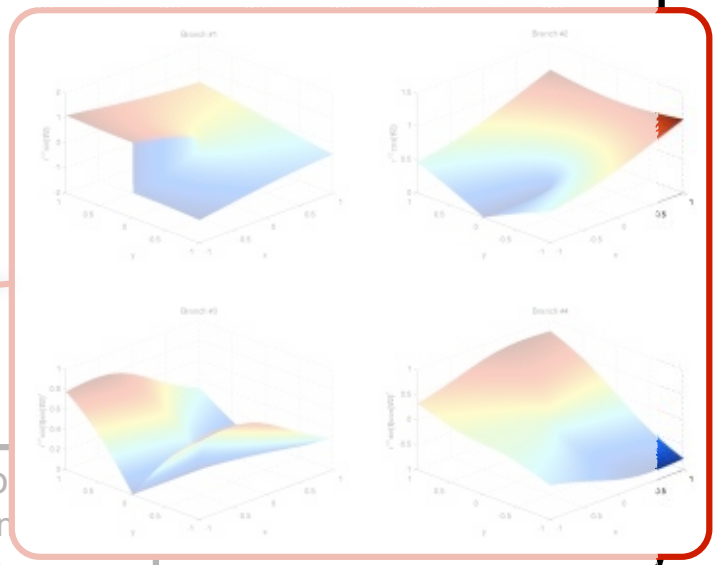
$$\{f_\alpha(r,\theta), \alpha = 1,4\} = \left\{\sqrt{r}\sin\frac{\theta}{2}, \sqrt{r}\cos\frac{\theta}{2}, \sqrt{r}\sin\frac{\theta}{2}\sin\theta, \sqrt{r}\cos\frac{\theta}{2}\sin\theta\right\}$$





Enriched no
- discontin
- singular



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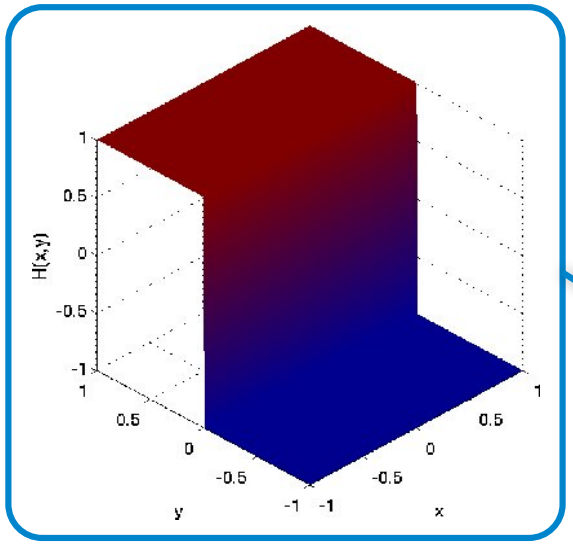
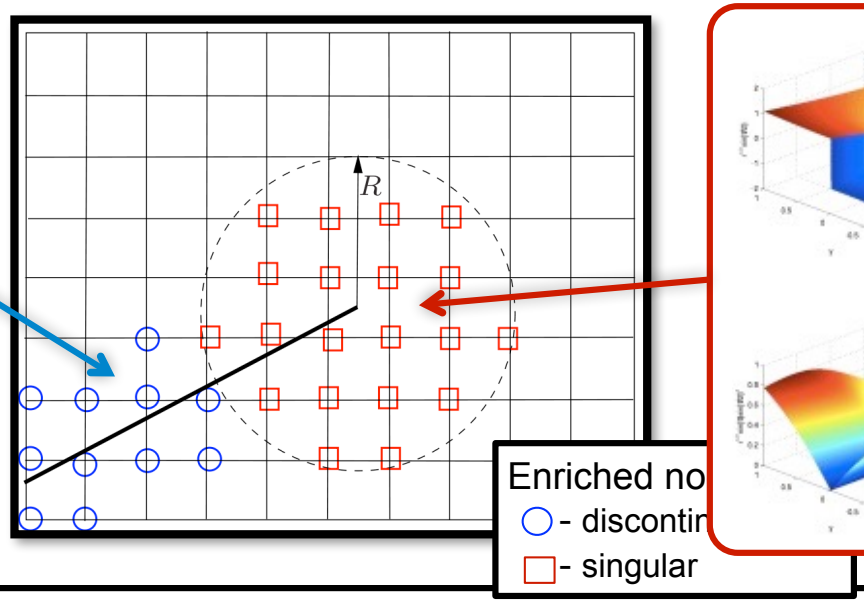
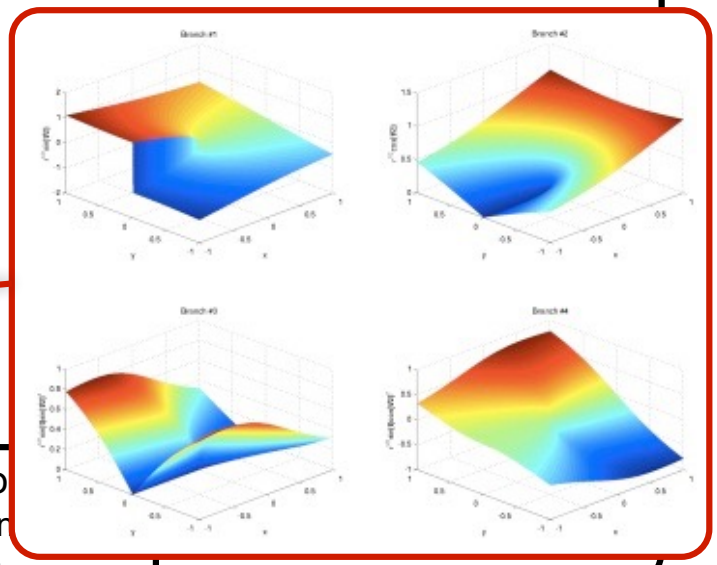
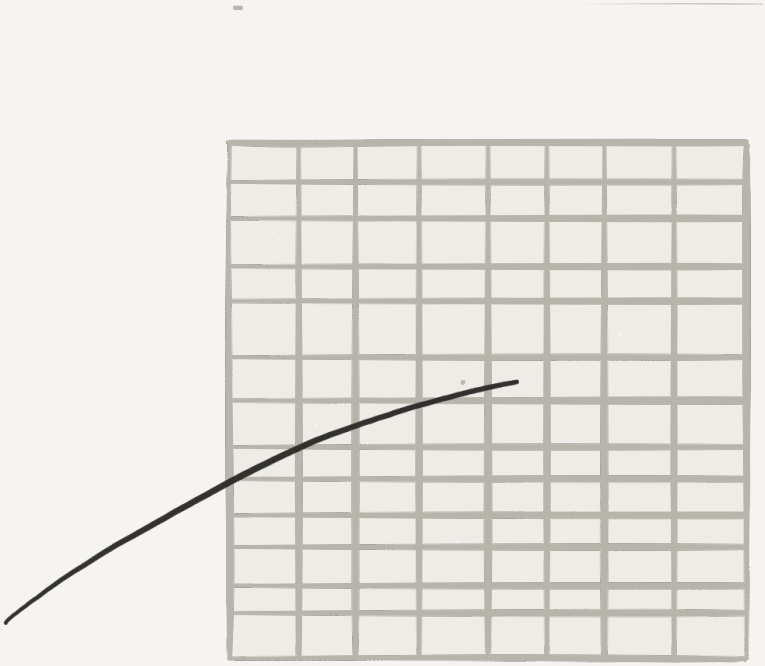
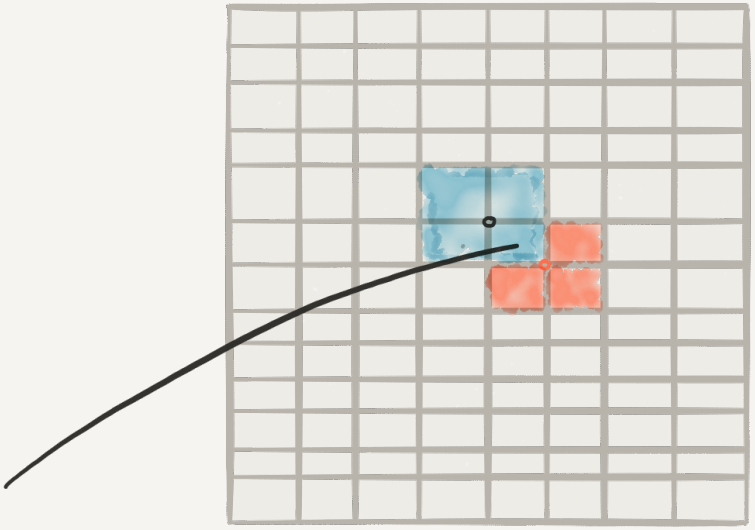
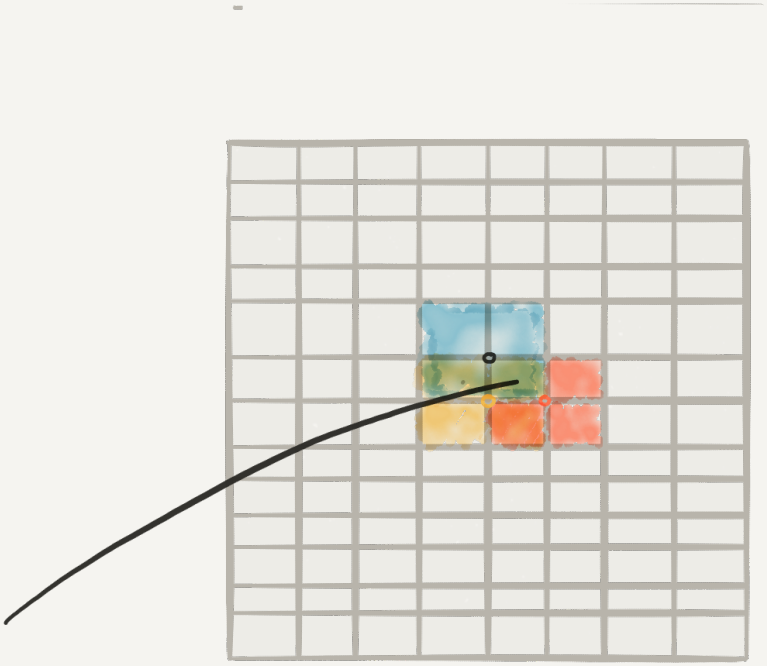


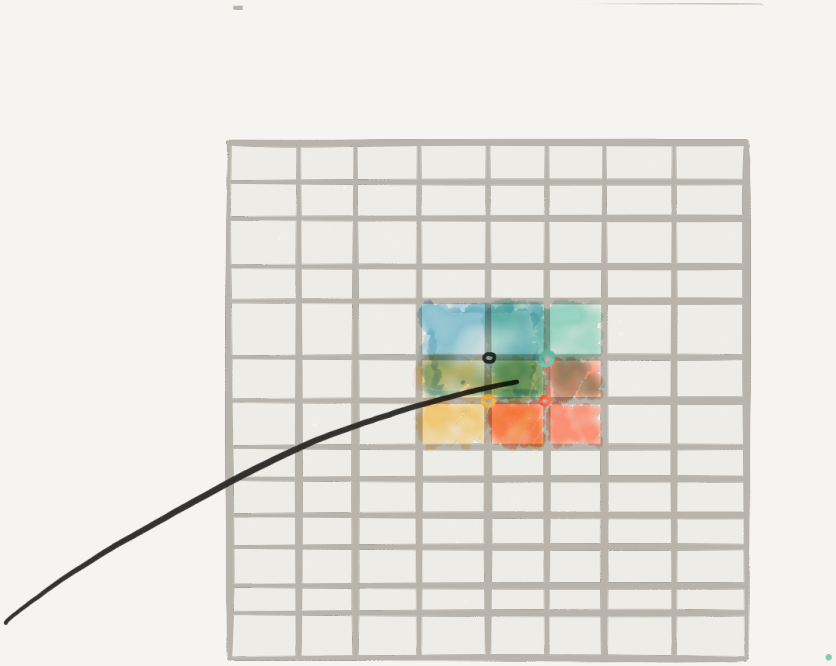


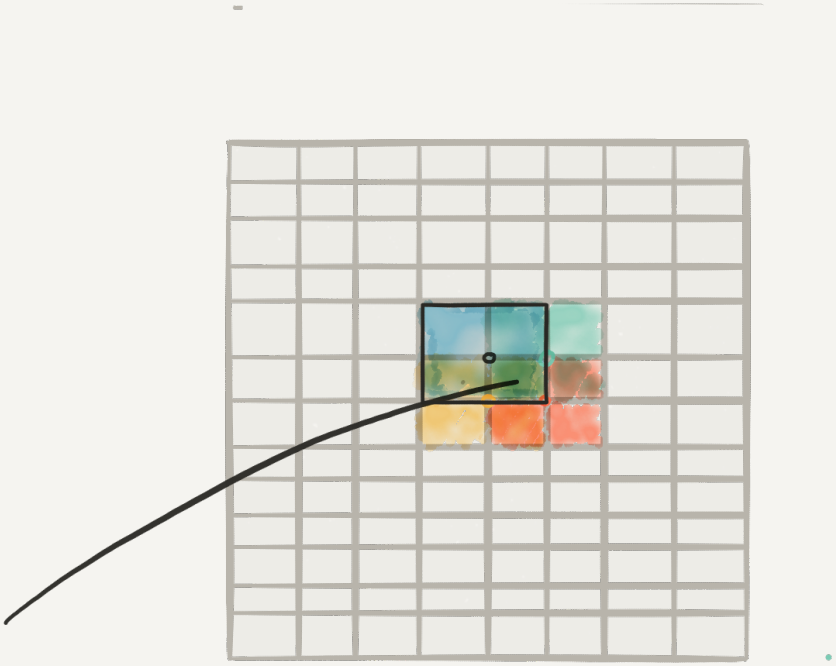


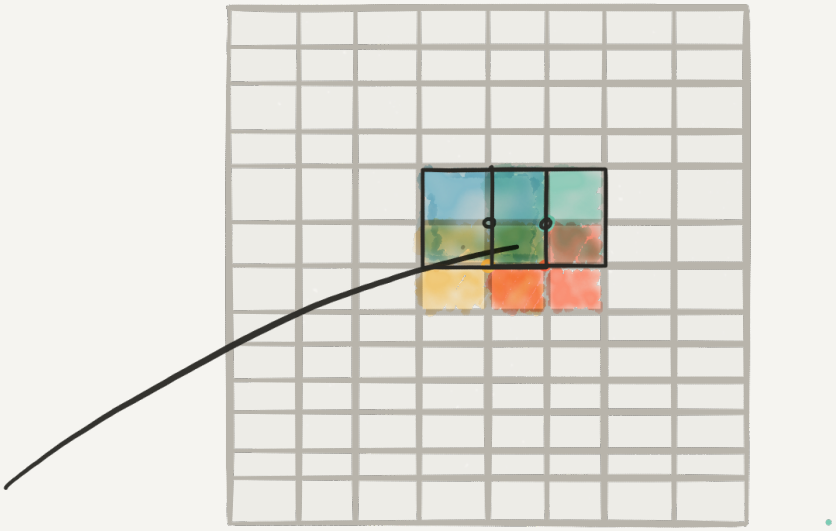


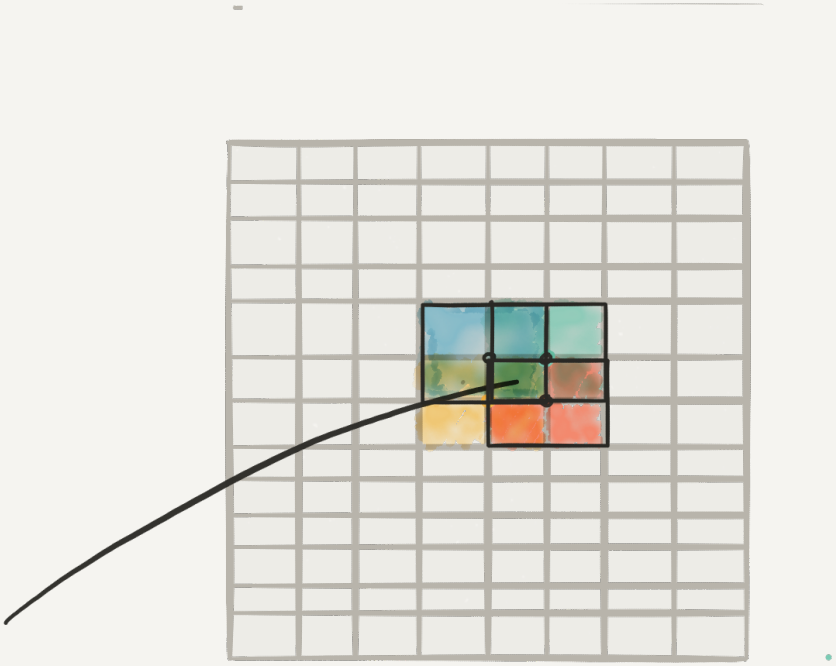


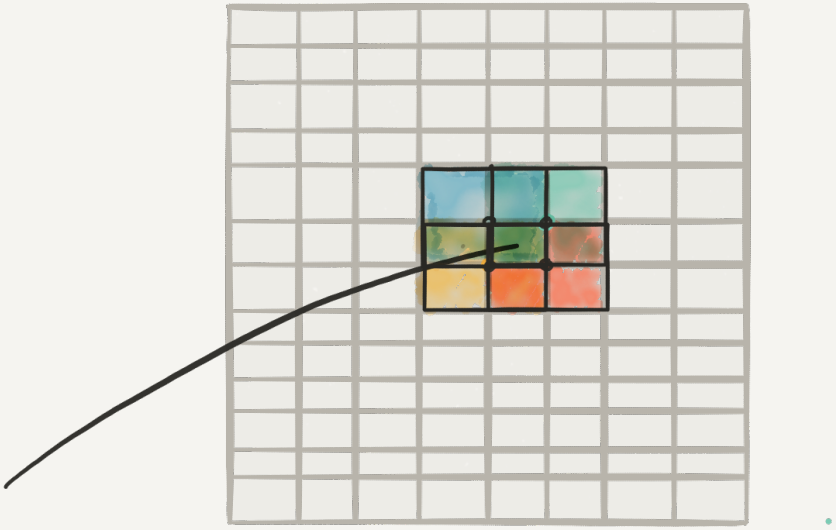


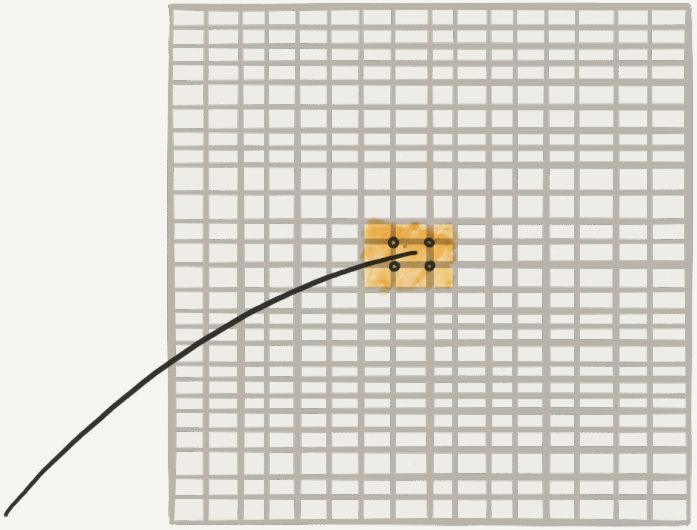


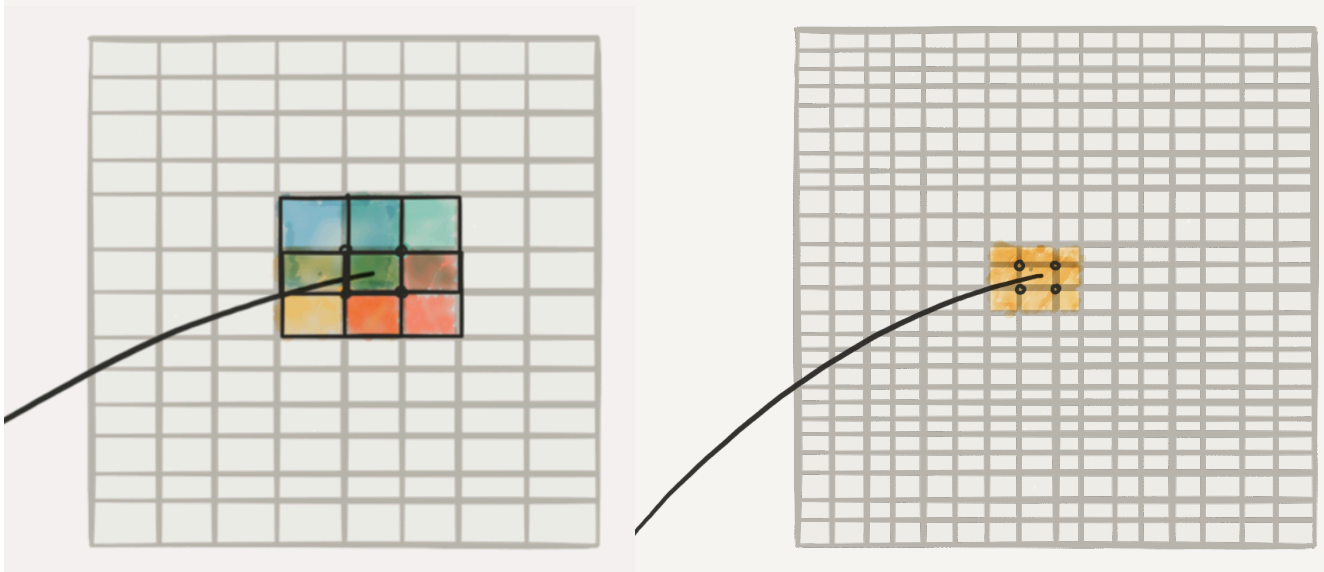






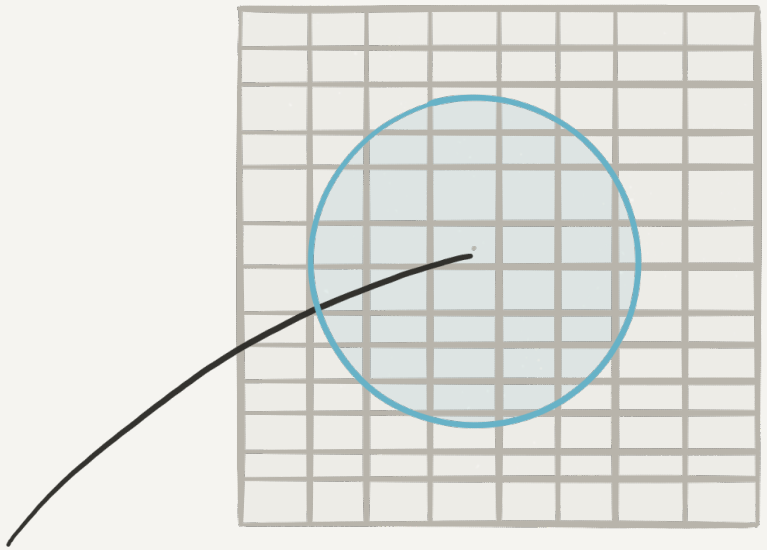




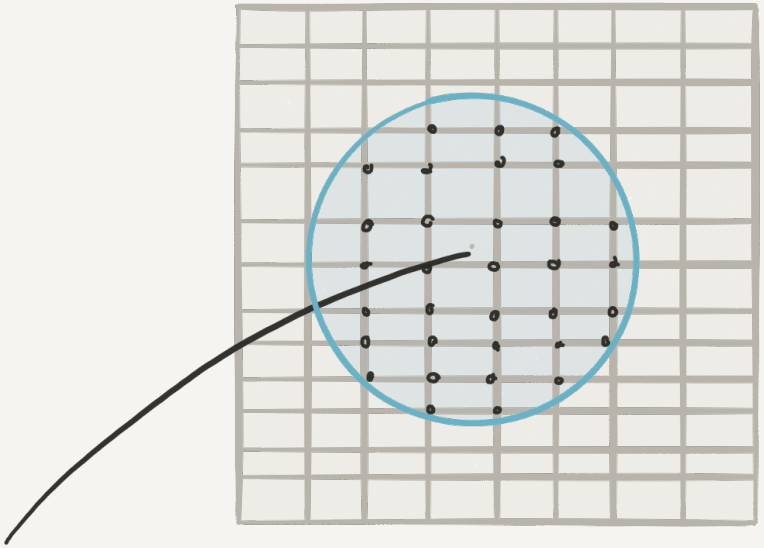


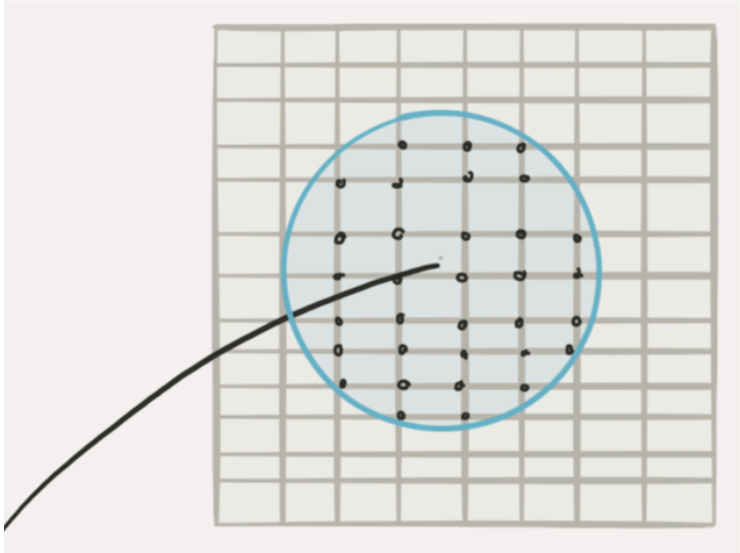
By refining the mesh, the influence of the enrichment zone on the convergence of the method tends to zero

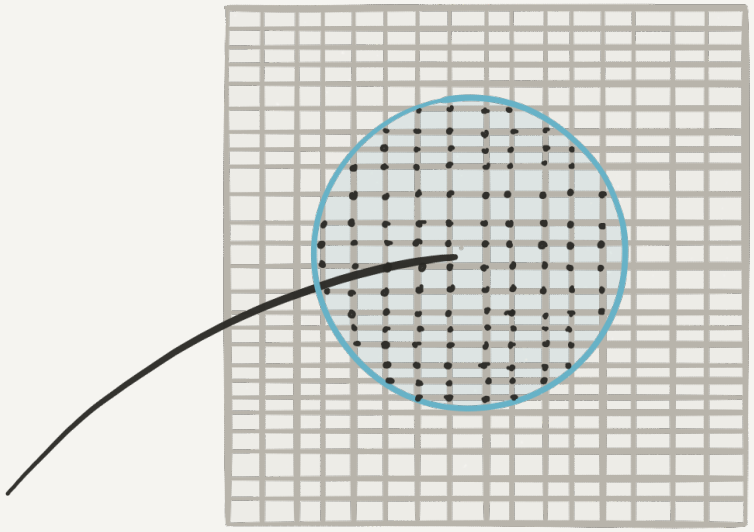
<u>We lose the benefit of enrichment</u>



Enriching an area independent of the mesh size



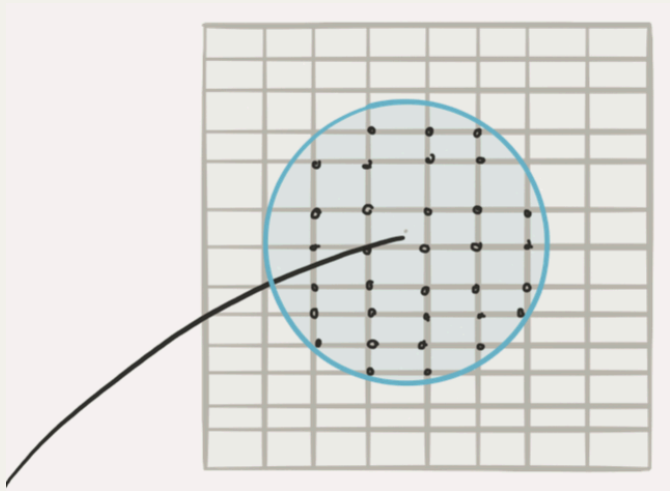


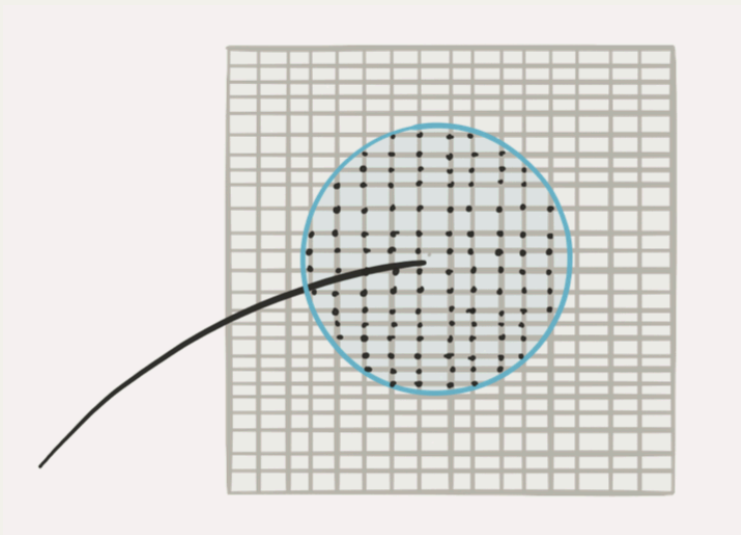


ensures that as the mesh is refined, more and more nodes become enriched

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)

Summary

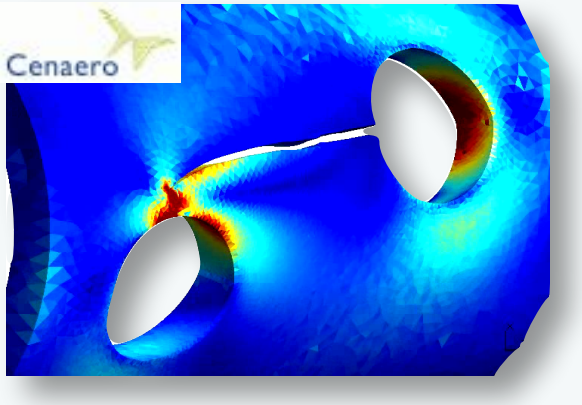
Fracture of homogeneous materials

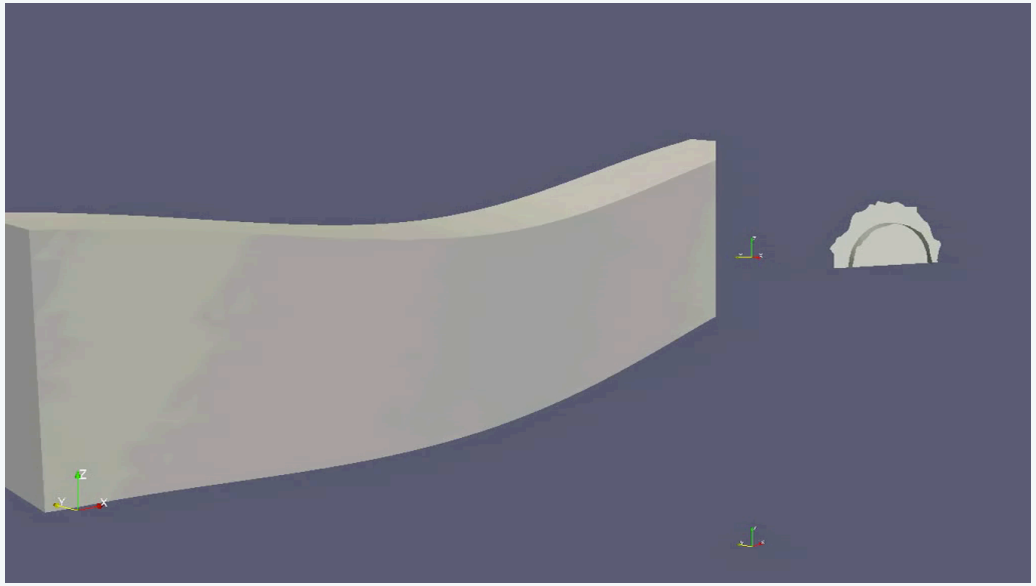
Question: How to control accuracy and simplify/avoid meshing?

- 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 ~ (Error on SIF)^4
  - ☐ Standard enrichment => oscillations along the front

Fracture of homogeneous materials

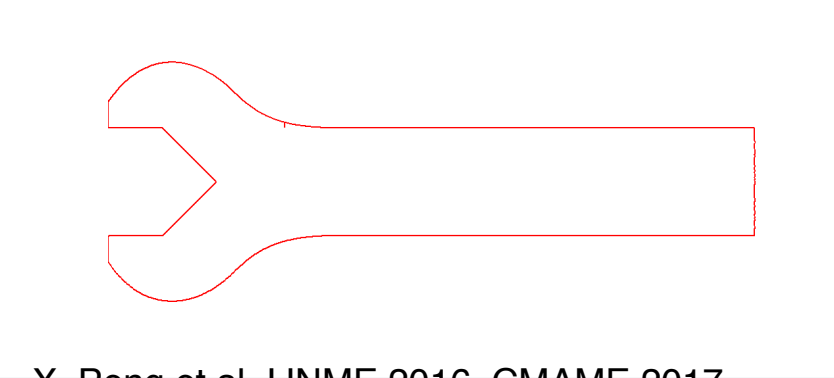
Question: How to control accuracy and simplify/avoid meshing?





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.

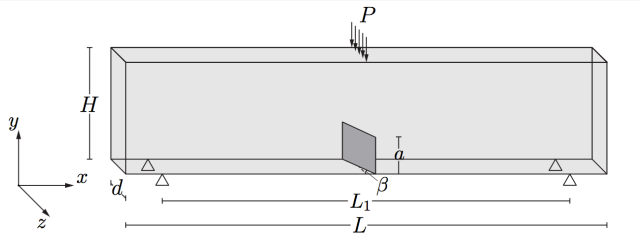
Agathos K, Chatzi E, Bordas S, Talaslidis D. A well−conditioned and optimally convergent XFEM for 3D linear elastic fracture. International Journal for Numerical Methods in Engineering. 2016 Mar 2;105(9):643-77.

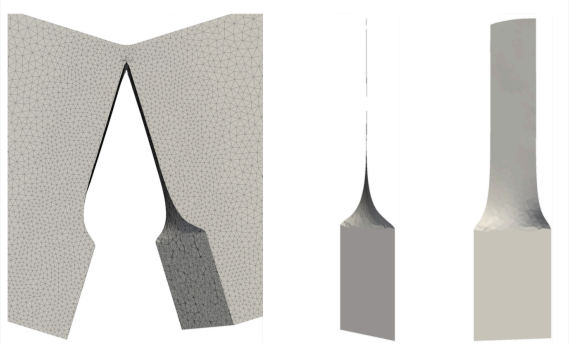
Agathos, K., E. Chatzi, and SPA Bordas. "Stable 3D extended finite elements with higher order enrichment for accurate non planar fracture." *Computer Methods in Applied Mechanics and Engineering* 306 (2016): 19-46.

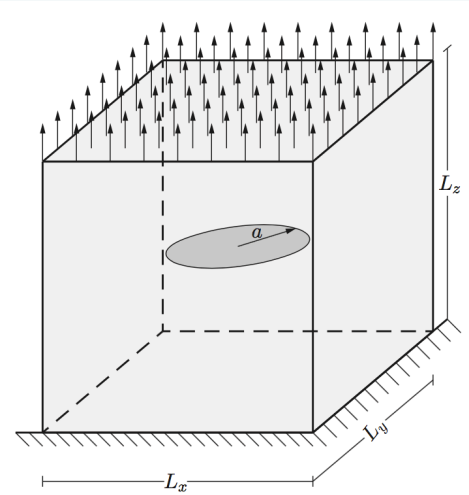
https://orbilu.uni.lu/bitstream/10993/22331/2/paper.pdf

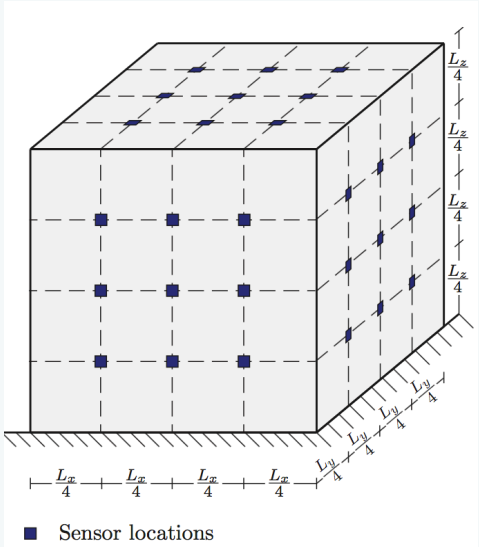
http://orbilu.uni.lu/bitstream/10993/22420/1/presentation.pdf

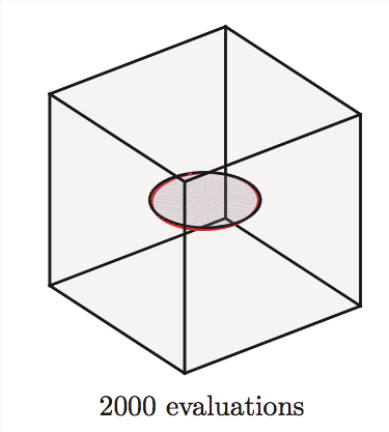
Conclusions









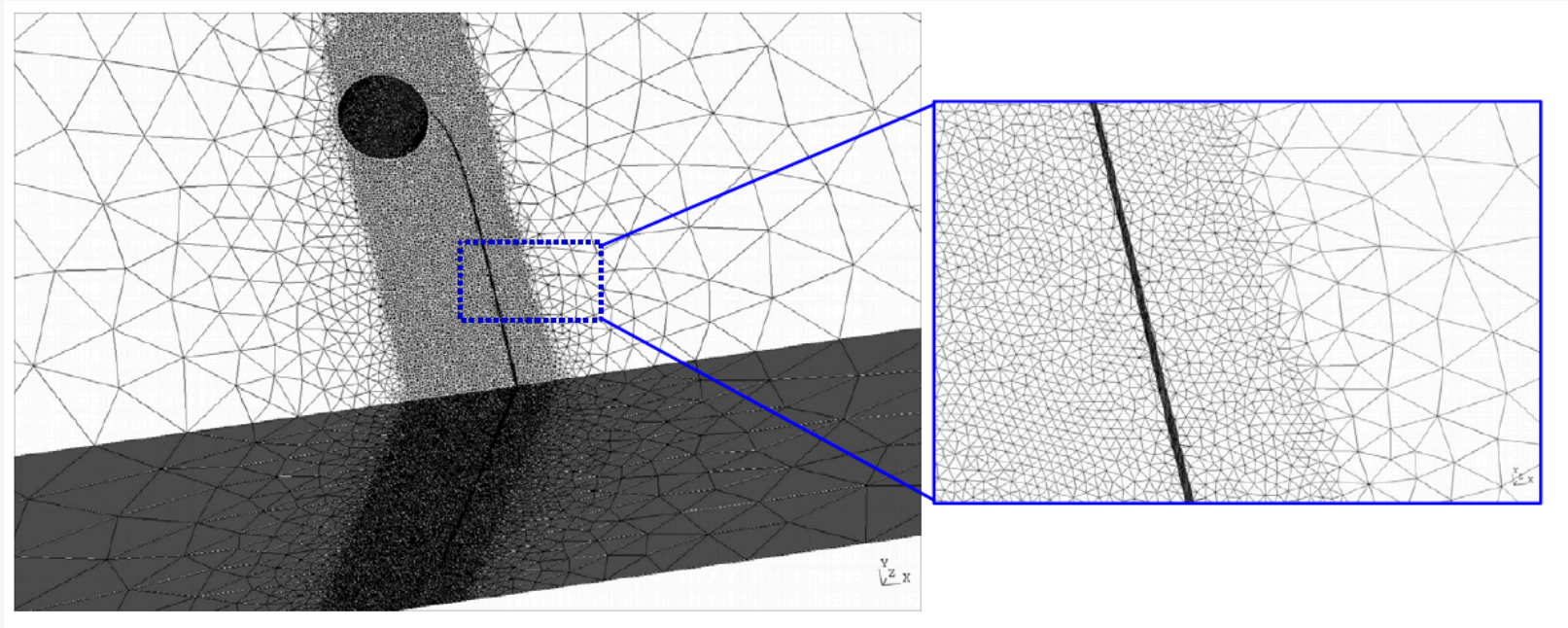


- ☑ Introduces a novel form of enrichment.
- ☑ Provides improved conditioning.
- ☑ Enables the use of geometrical enrichment.
- ☑ Enables the use of higher order terms in fracture mechanics
- ☑ Was combined to vector level sets to solve crack propagation problems.
- ☑ Was applied to inverse problems.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

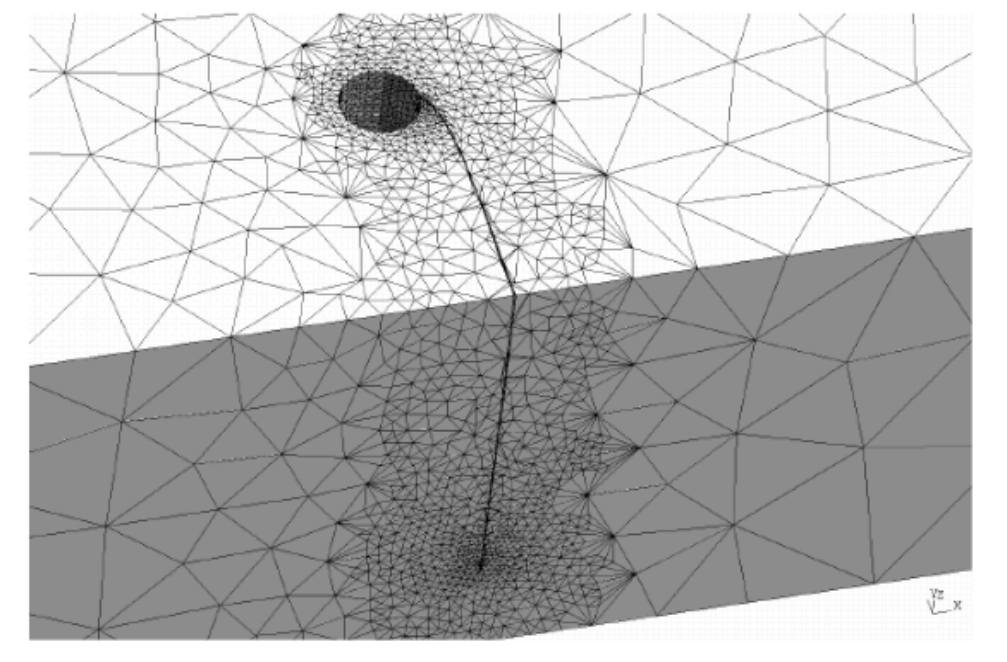


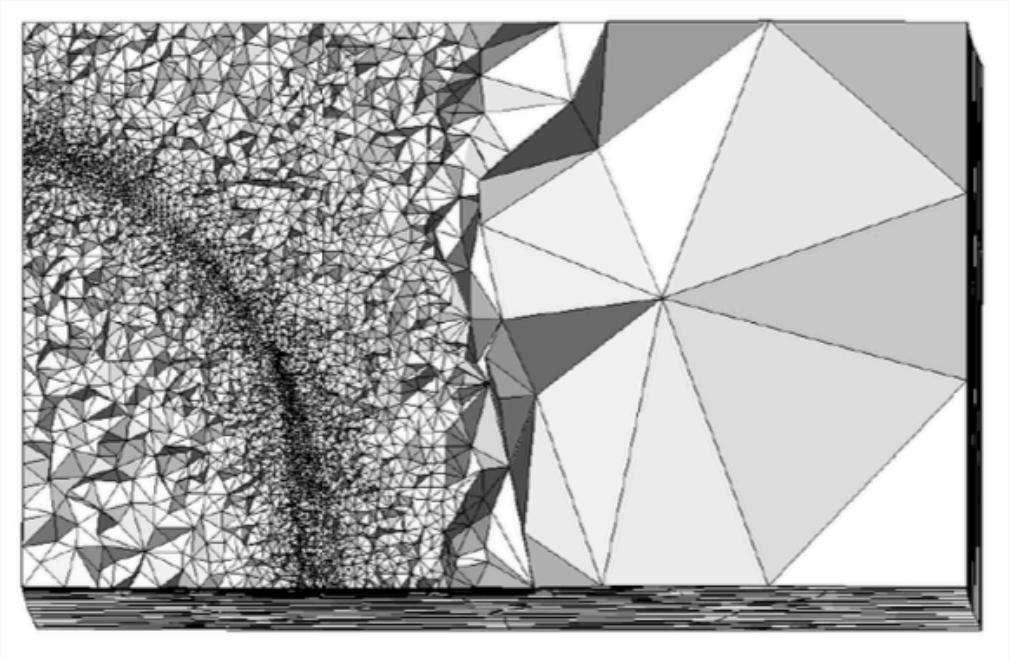
Before: mesh “finely” in the region where the crack is “expected” to propagate

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 alIJNME 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.

Motivation

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.

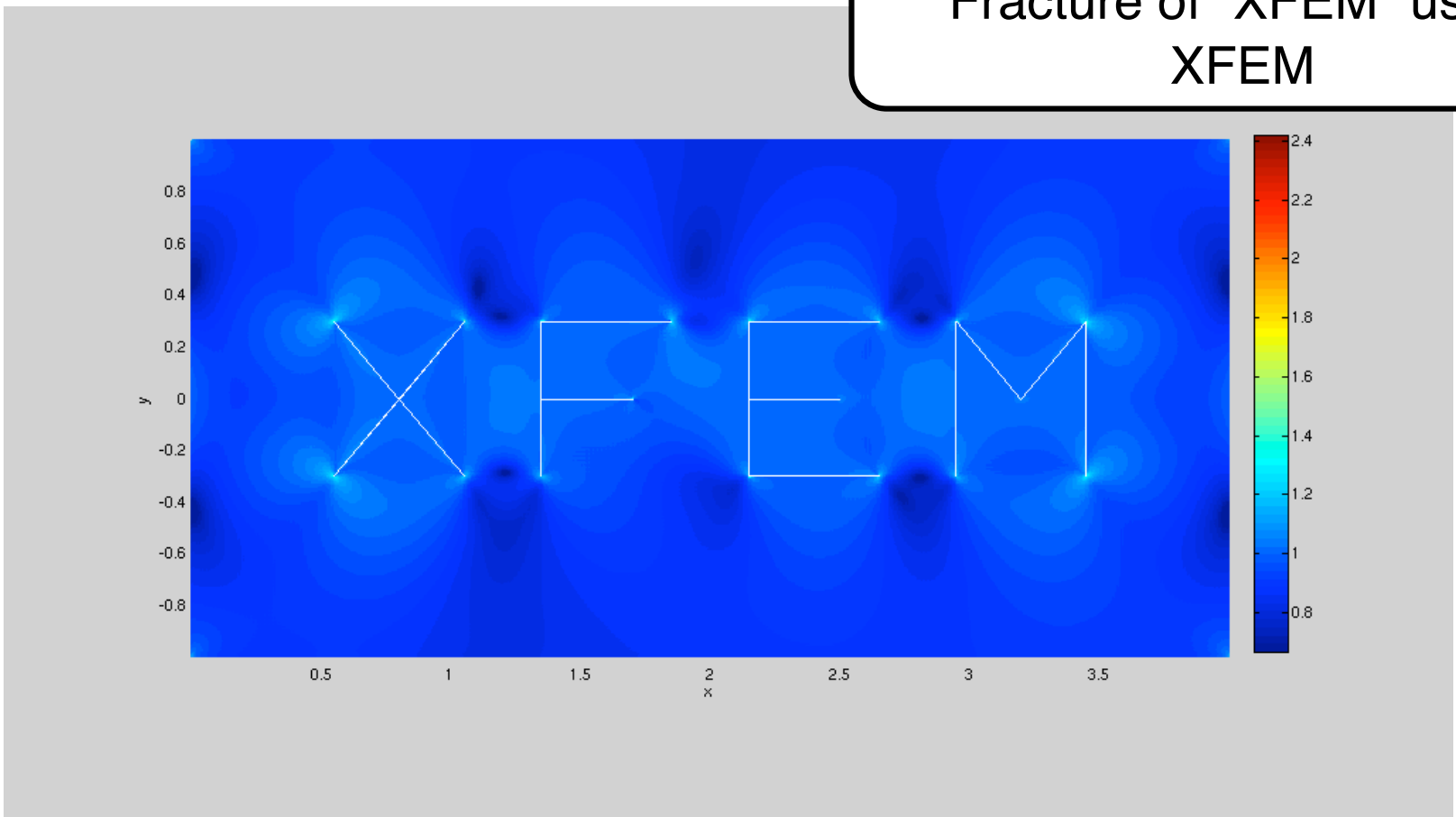
Partial Conclusions

- 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….

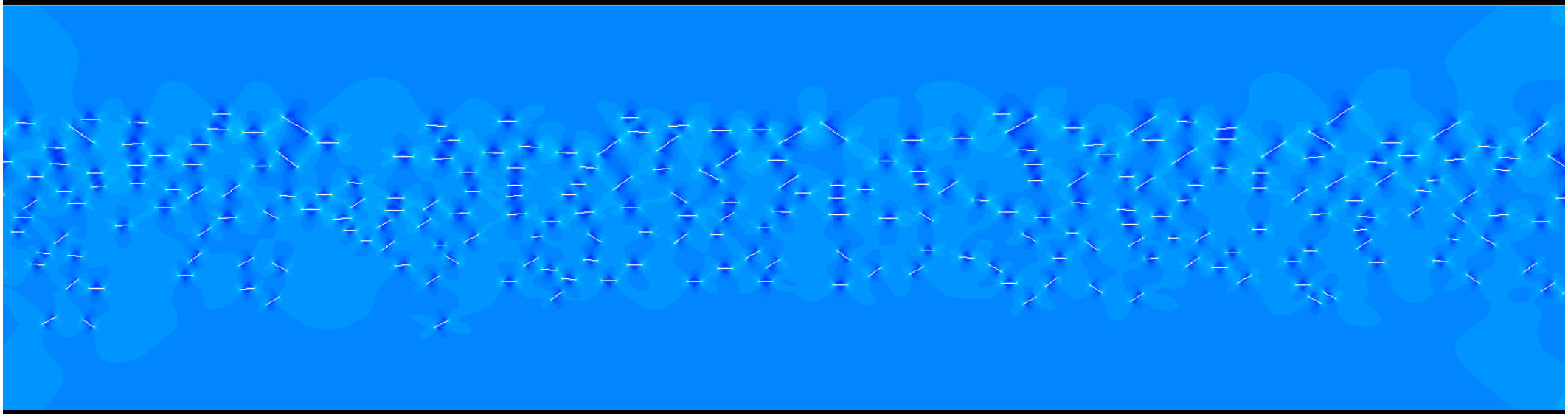
Extended Finite Element Method (XFEM)

Fracture of “XFEM” using XFEM



Case study II. Plate with 300 cracks vertical extension BCs

Energy-minimal crack growth using XFEM

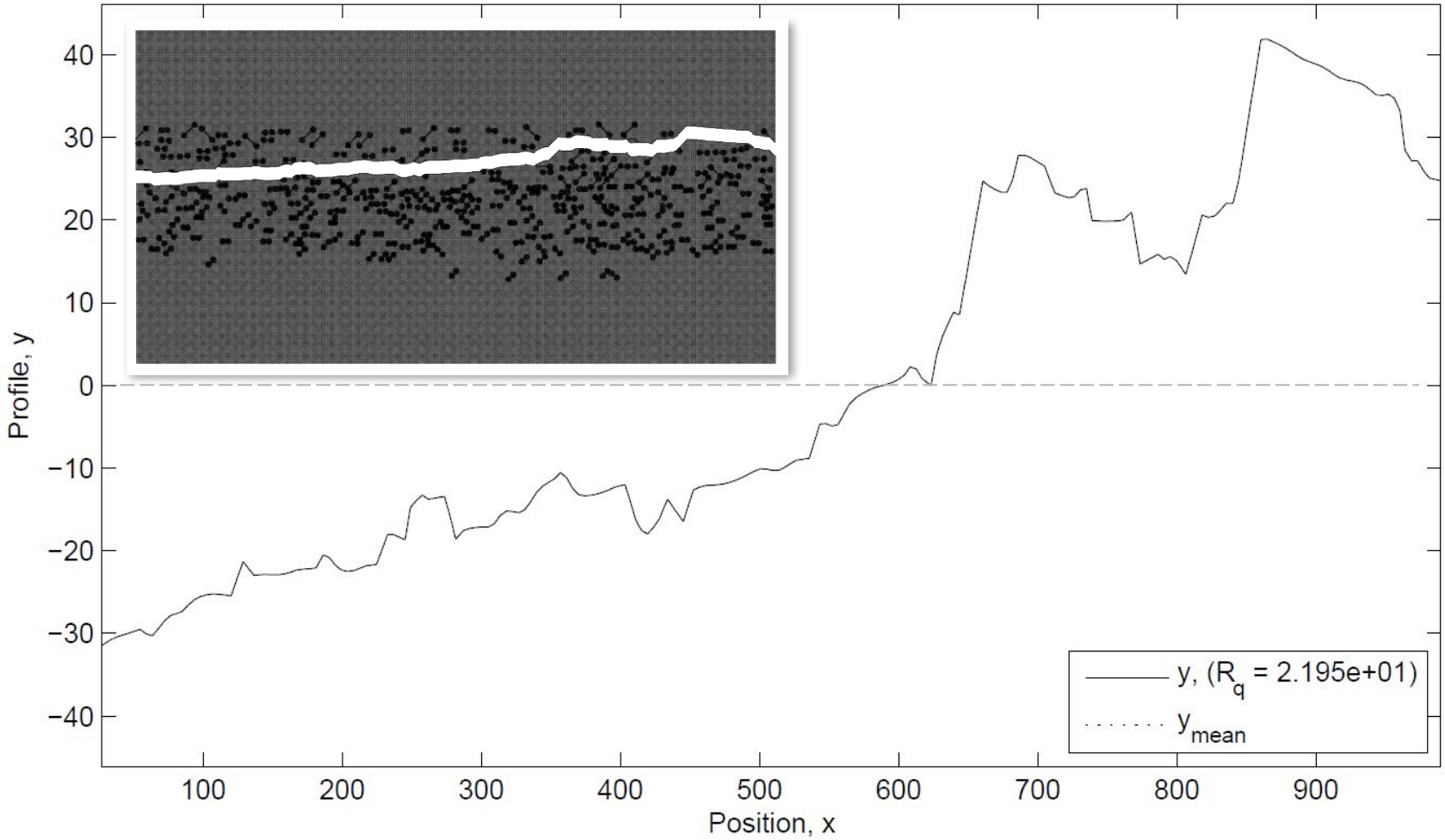


Sutula et al. Preprint of three part EFM paper at
http://hdl.handle.net/10993/29414

Example #1

Vertical extension of a plate with 300 cracks

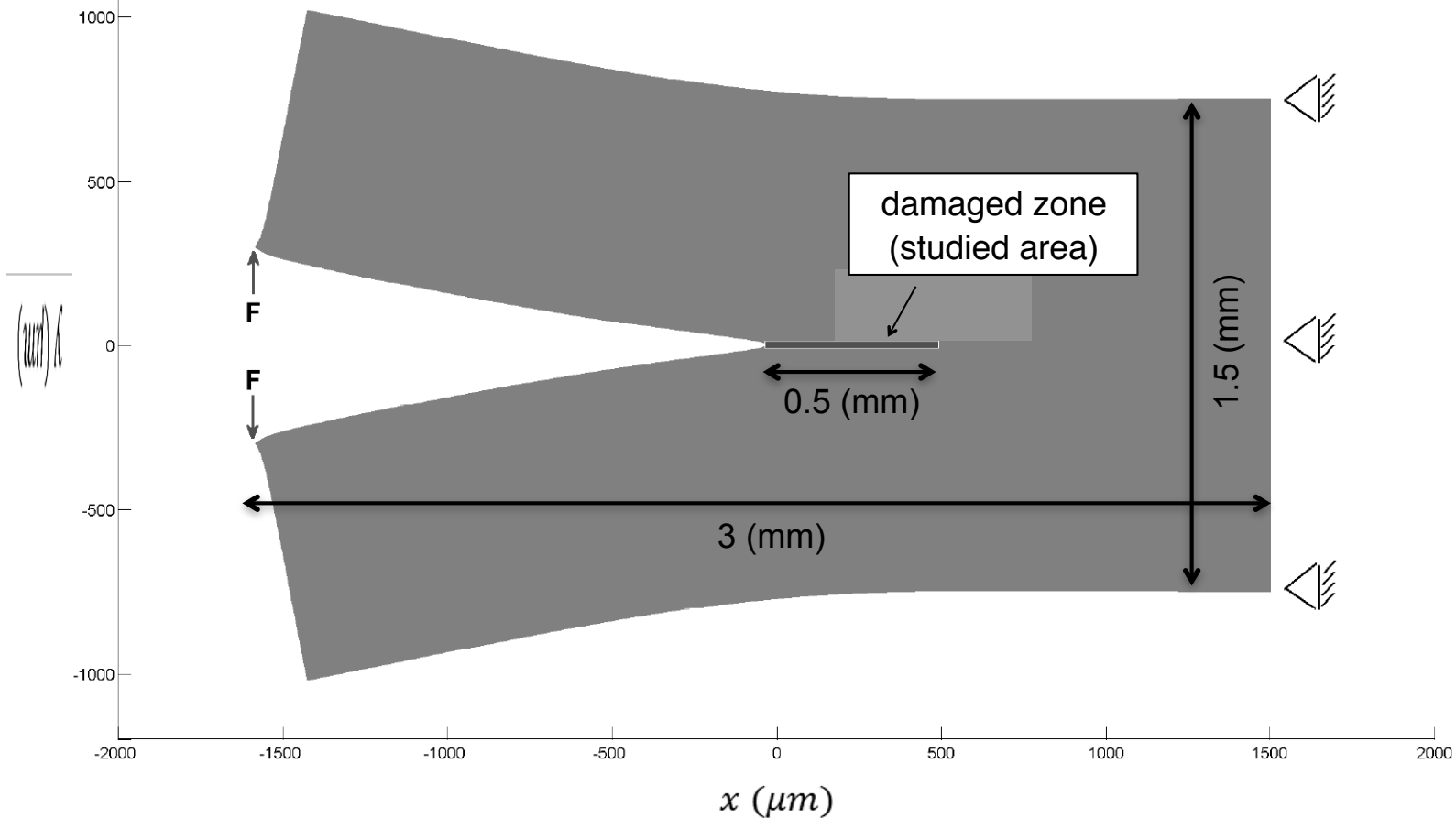
Post-split roughness



Example #2

Mechanical splitting of a wafer sample

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



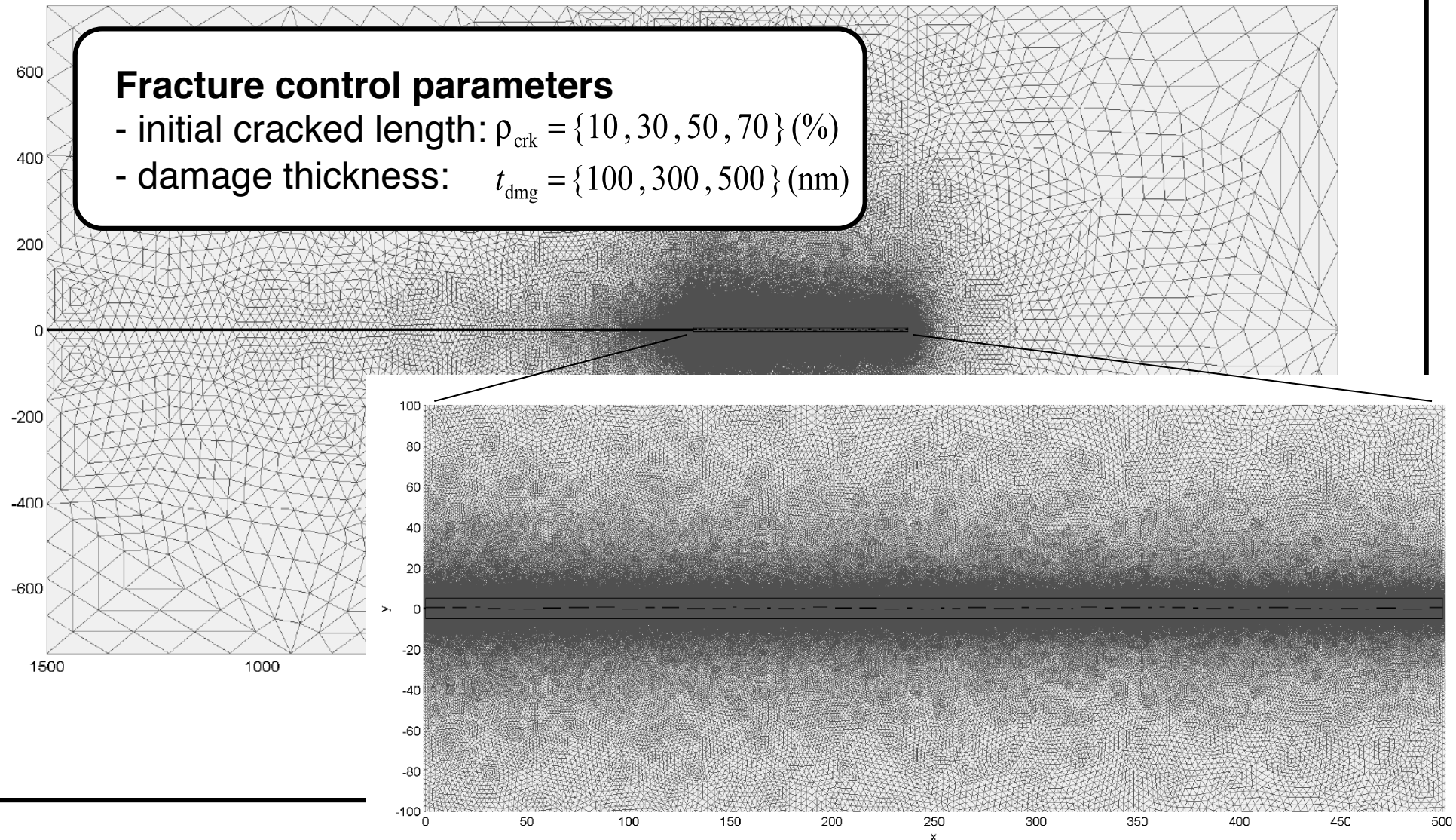
Example #2

Mechanical splitting of a wafer sample

- Discretisation (≈1mln. DOF, h_e = 150 nm)

Fracture control parameters

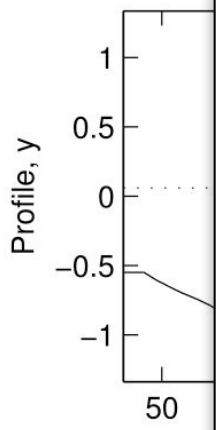
- initial cracked length: $\rho_{crk} = \{10, 30, 50, 70\}$ (%)
- damage thickness: $t_{dmg} = \{100, 300, 500\}$ (nm)



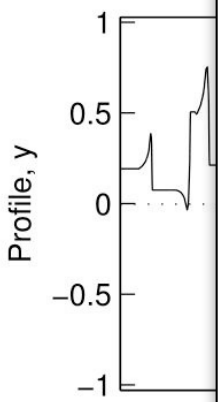
Example #2

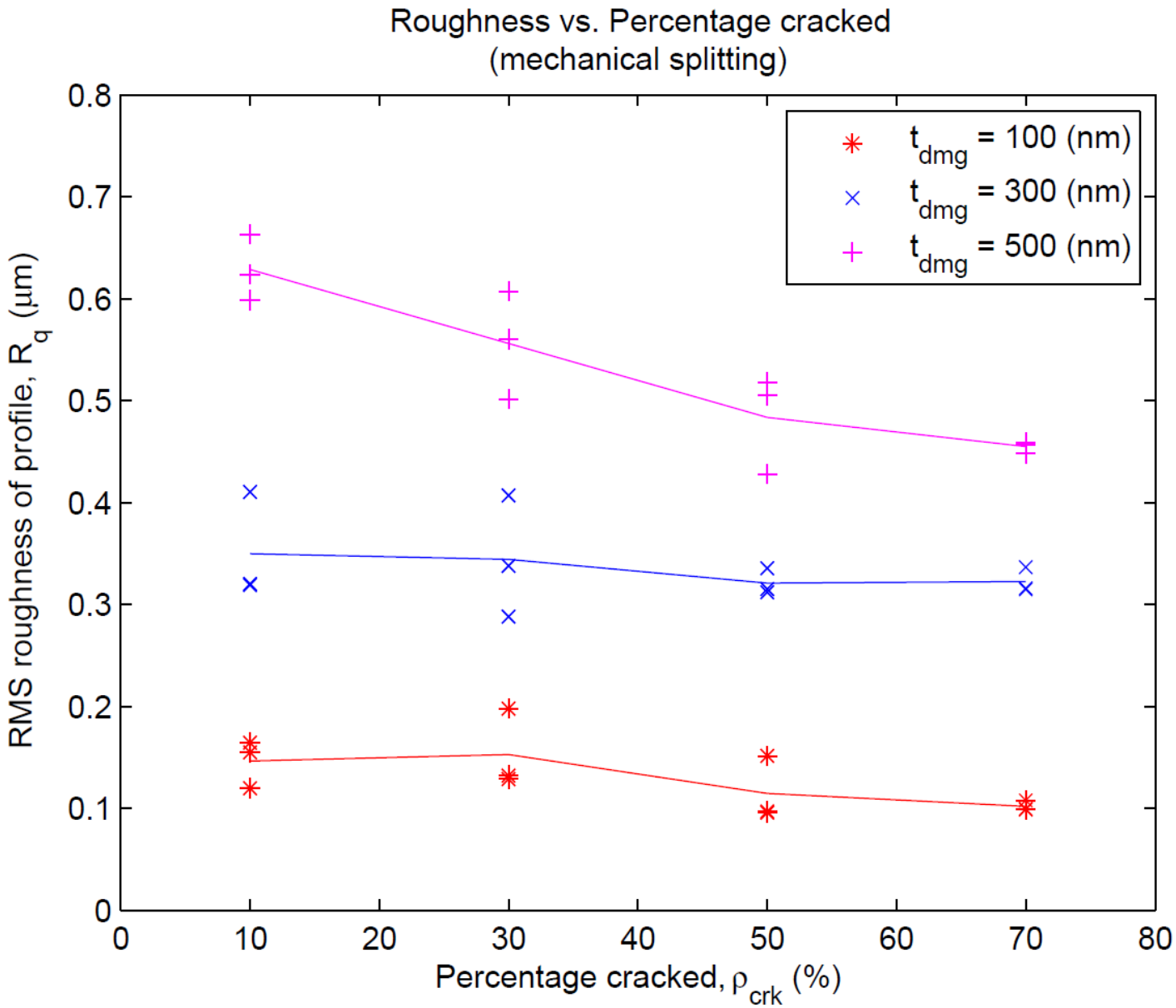
Fracture r

- Case ex



- Case ex





Summary

LEFM model

- Assuming mechanical interactions dominate during micro crack growth

Crack growth

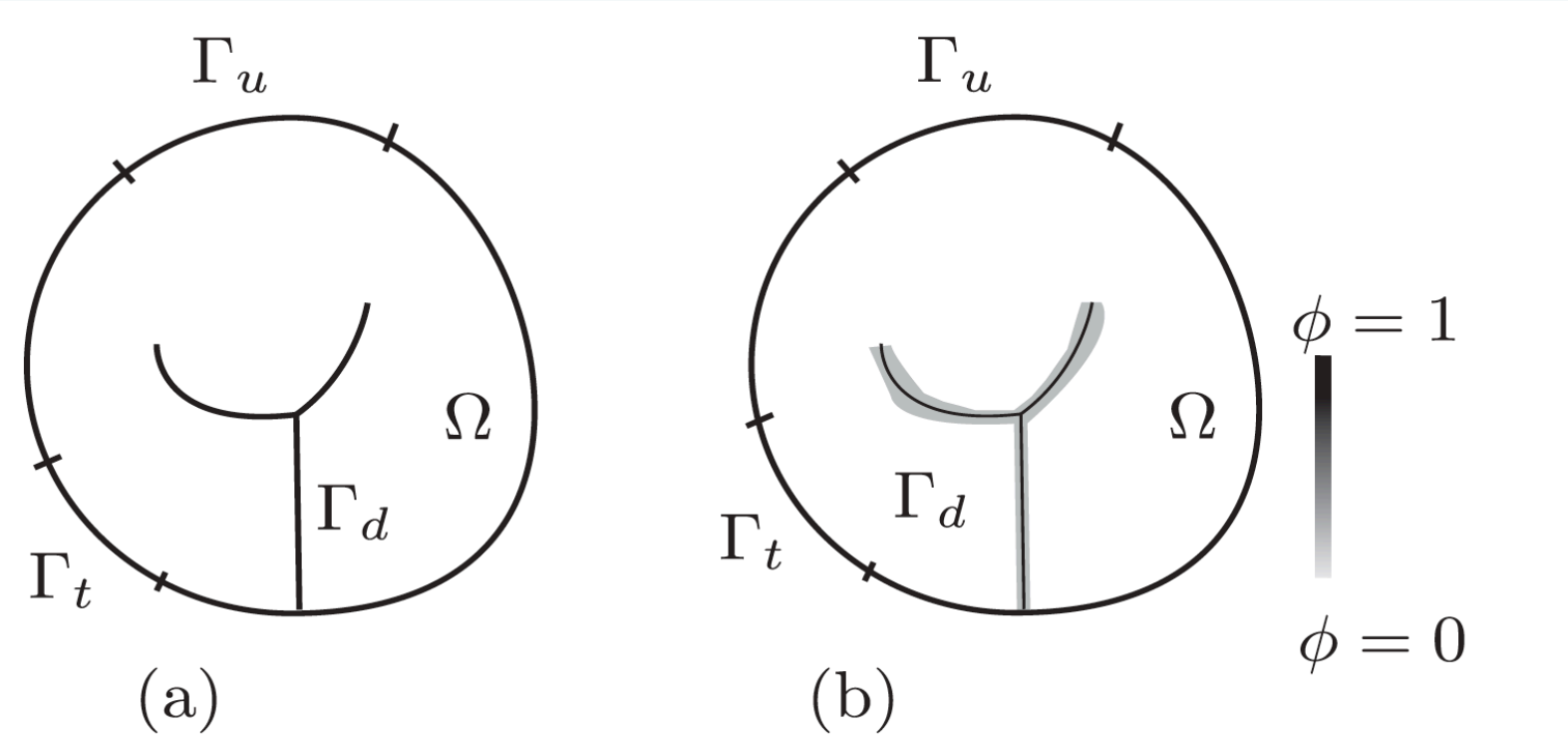
- crack tip with max SIF in direction of max hoop stress

Discretization

- XFEM for efficient multiple fracture modeling

More cracks?… 3D? …

Phase field/thick level sets



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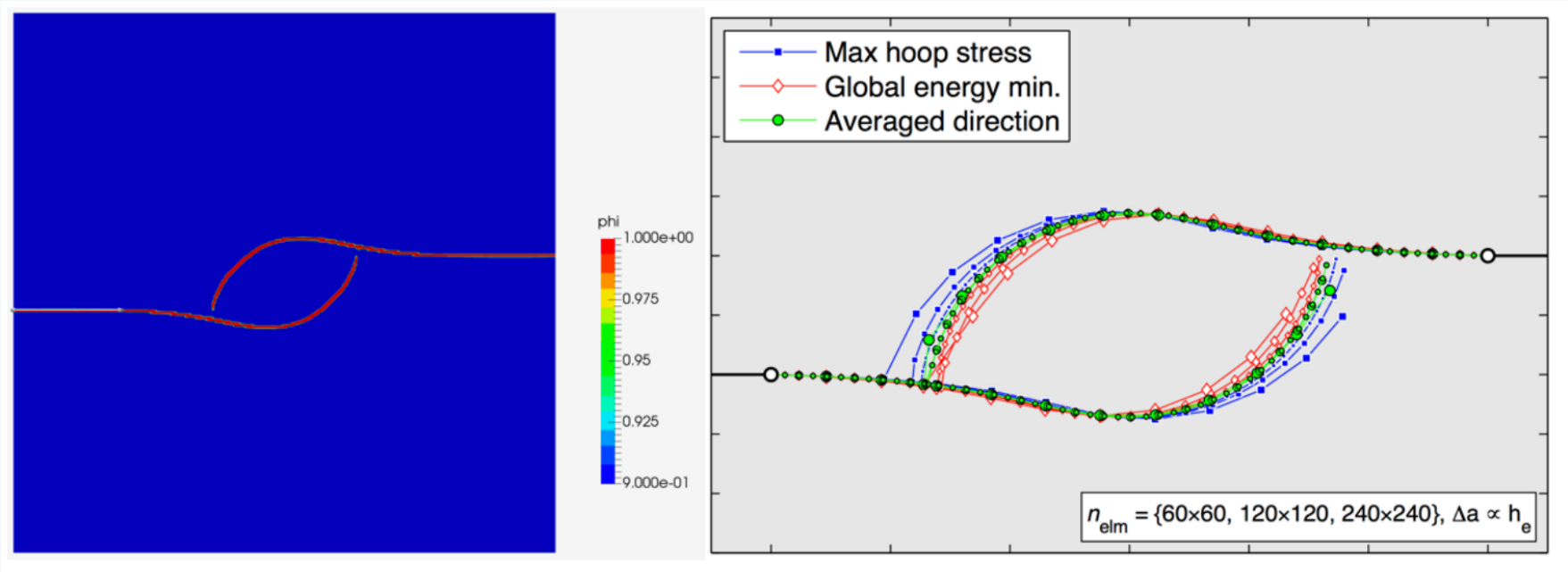
27 - 29 November 2017
phu.nguyen@monash.edu

Energy minimal XFEM vs. Phase field



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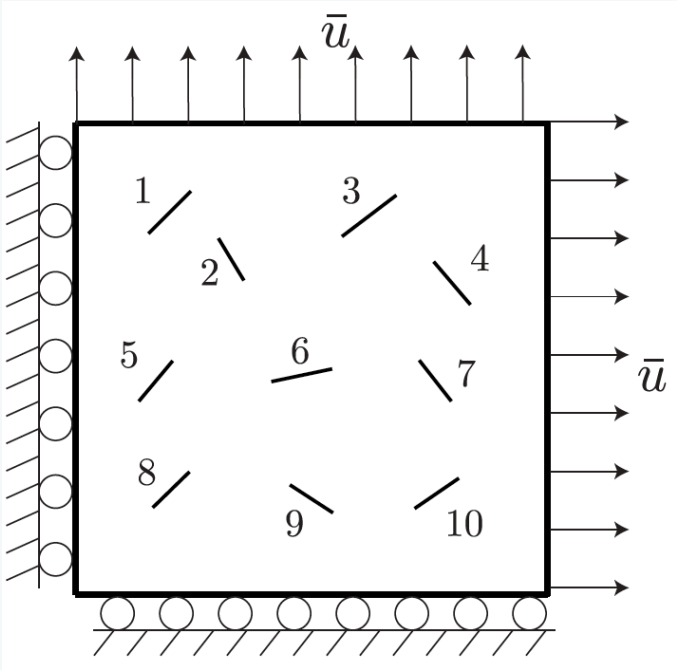
$\bar{u}$
1
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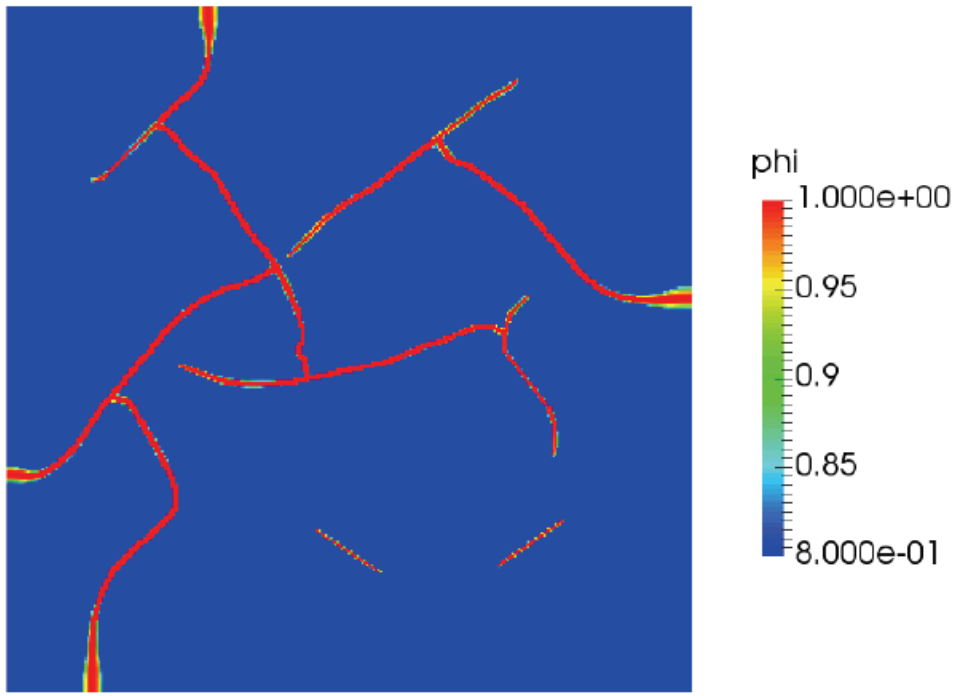
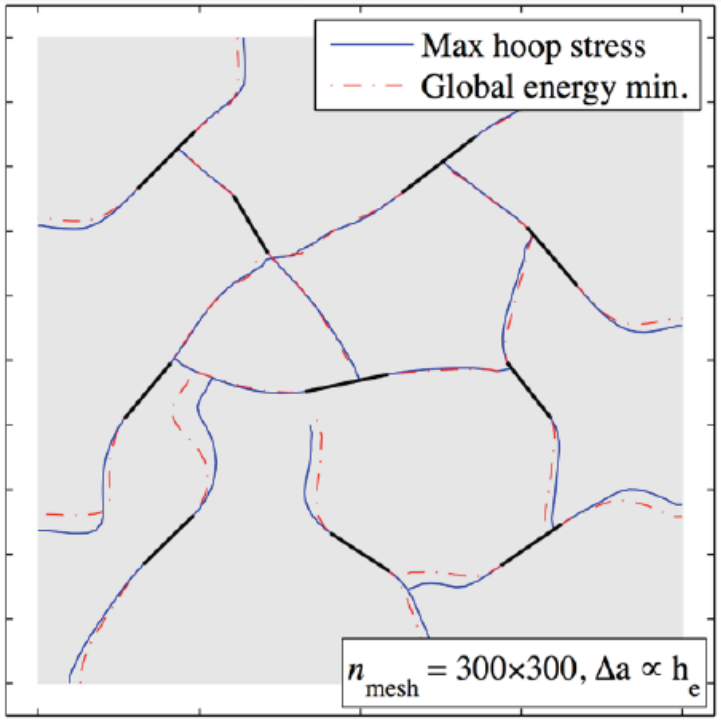
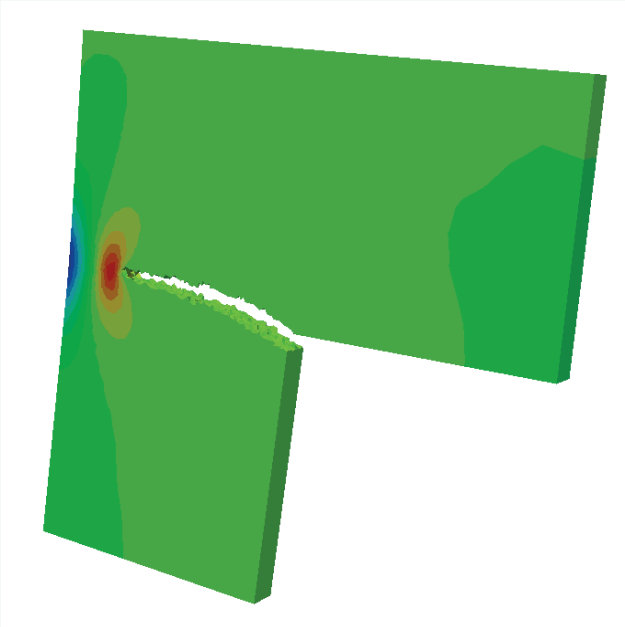
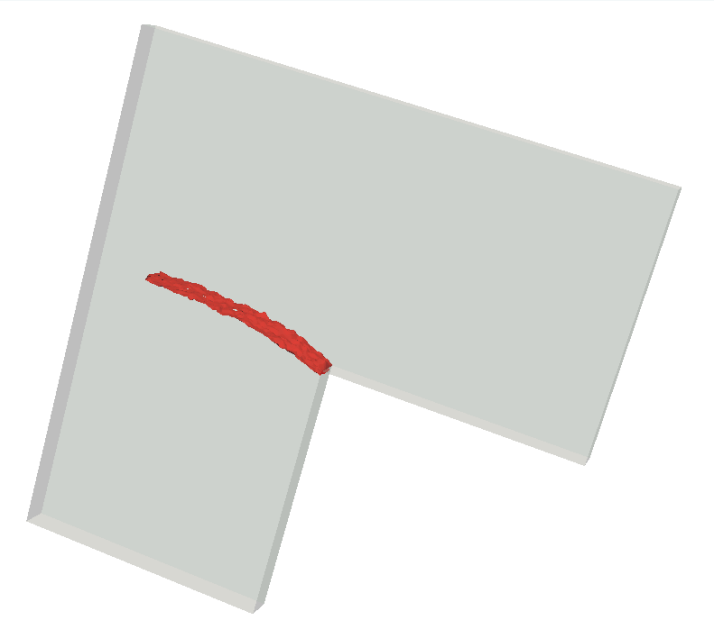
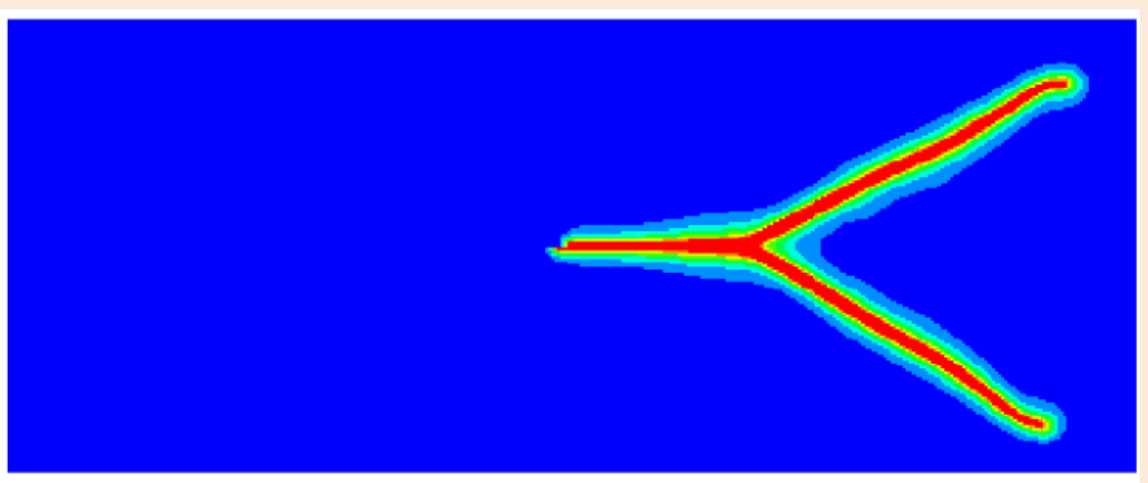

phi
1.000e+00
0.95
0.9
0.85
8.000e-01


Max hoop stress
Global energy min.
n_{mesh} = 300×300, Δa ∝ h_e







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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,

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

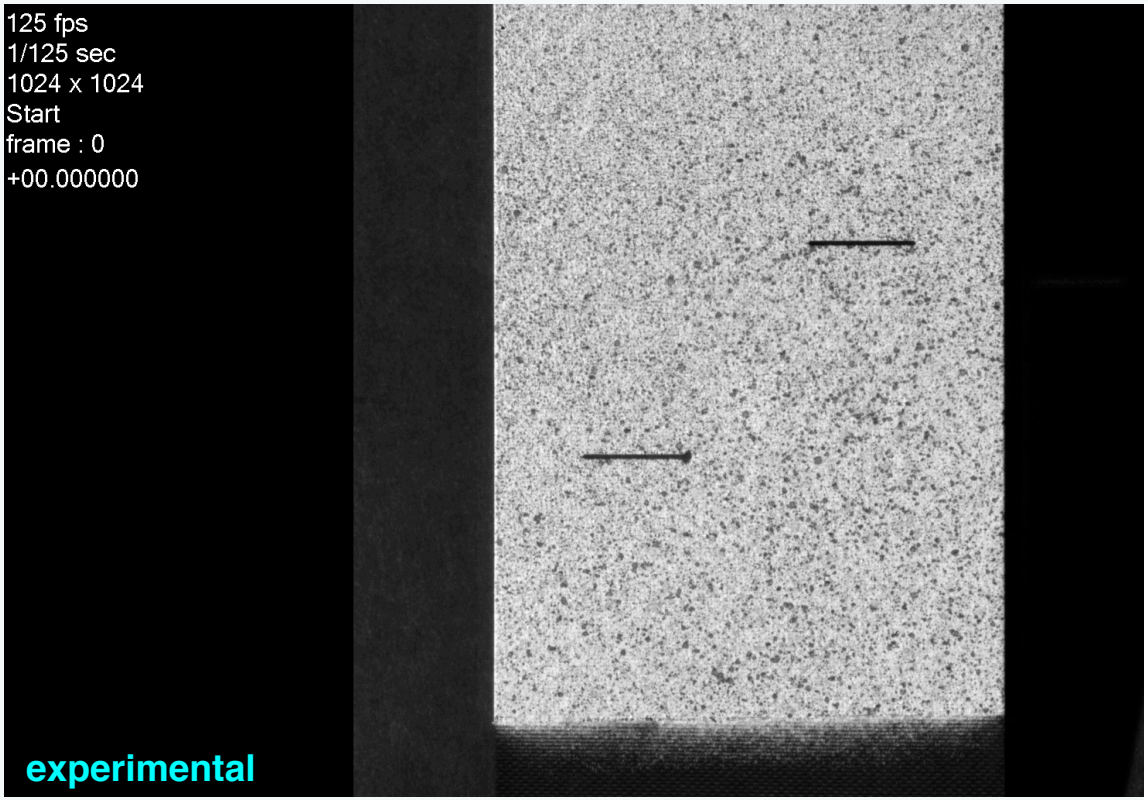
Case study III: Fracture of heterogeneous materials

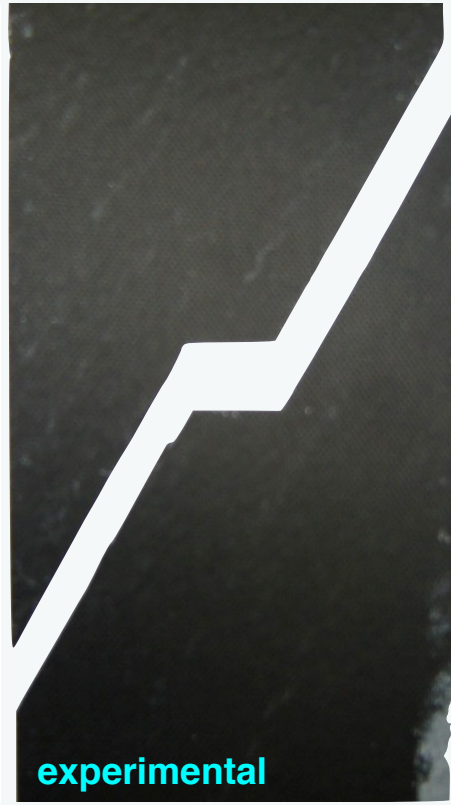
Partial conclusions on fracture of homogeneous materials using enriched FEM

- Adaptivity for enriched approximations using error estimates
    - Adapt enrichment radius
    - Adapt the choice of enrichment
    - Locally h-adapt the mesh
- 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)
- Next step: heterogeneities

Mild heterogeneities/anisotropy
Homogenized models are sufficient

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



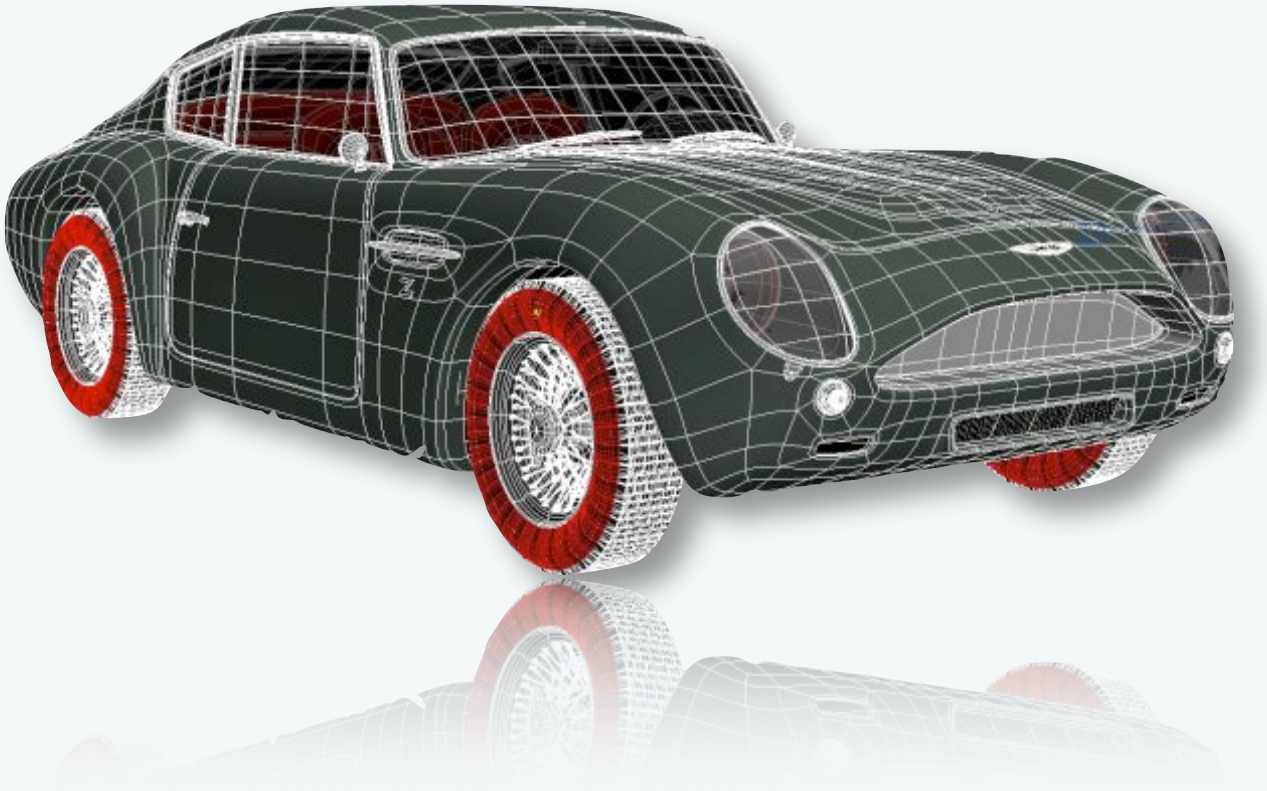


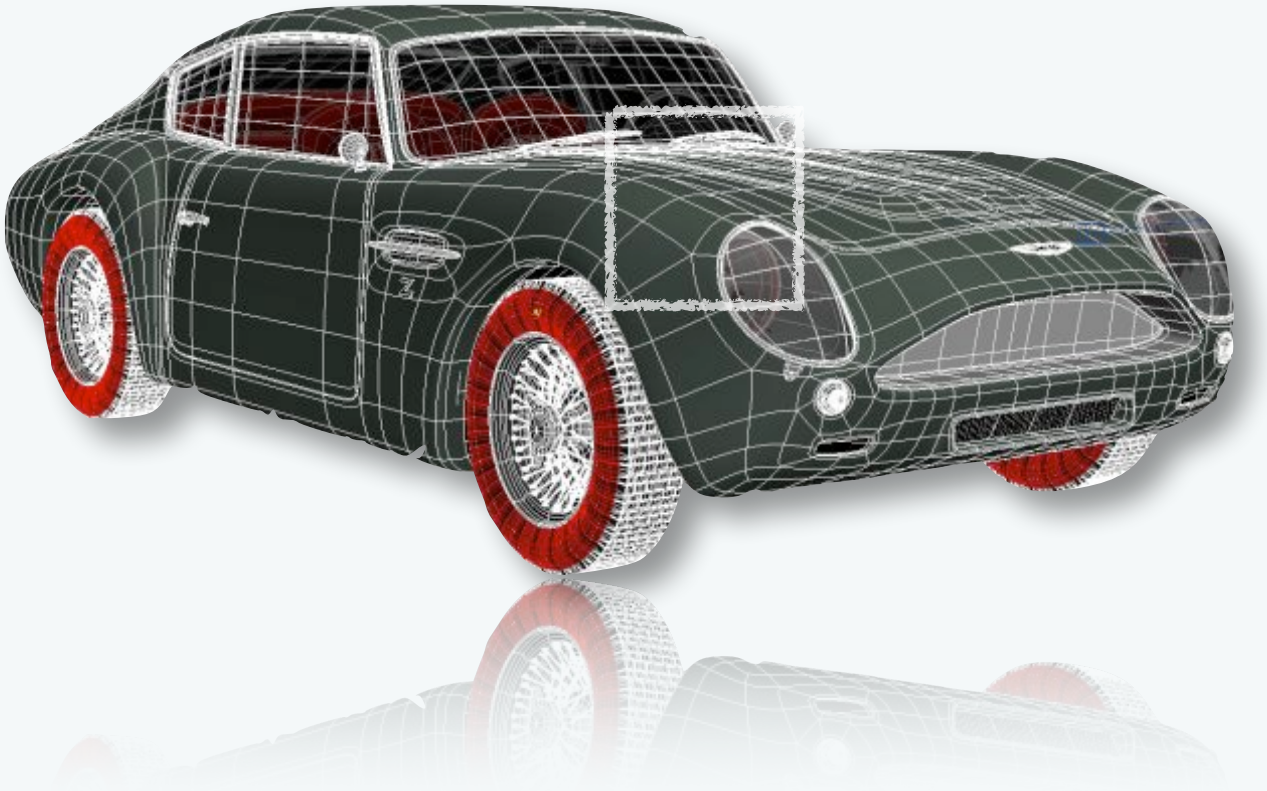
L. Cahill et al. Composite Structures, 2014

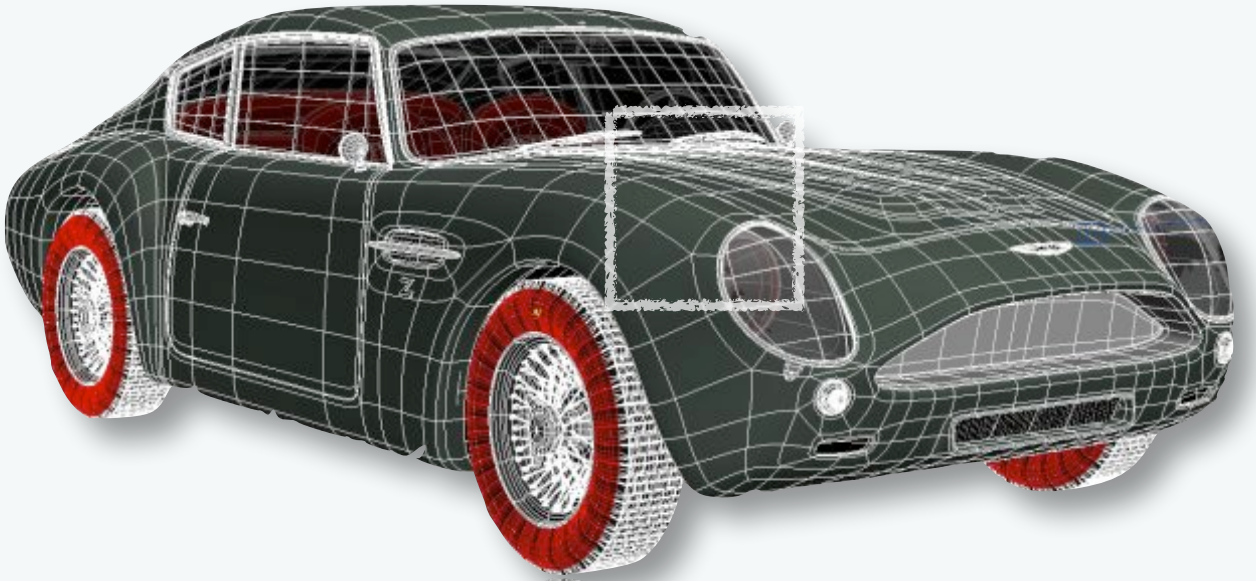
Experimental/Numerical approach to determining the driving force for fracture in composites

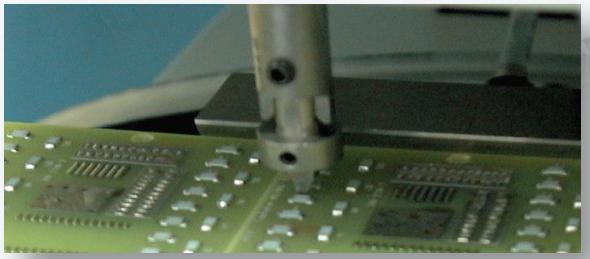
XFEM can effectively deal with orthotropic fracture

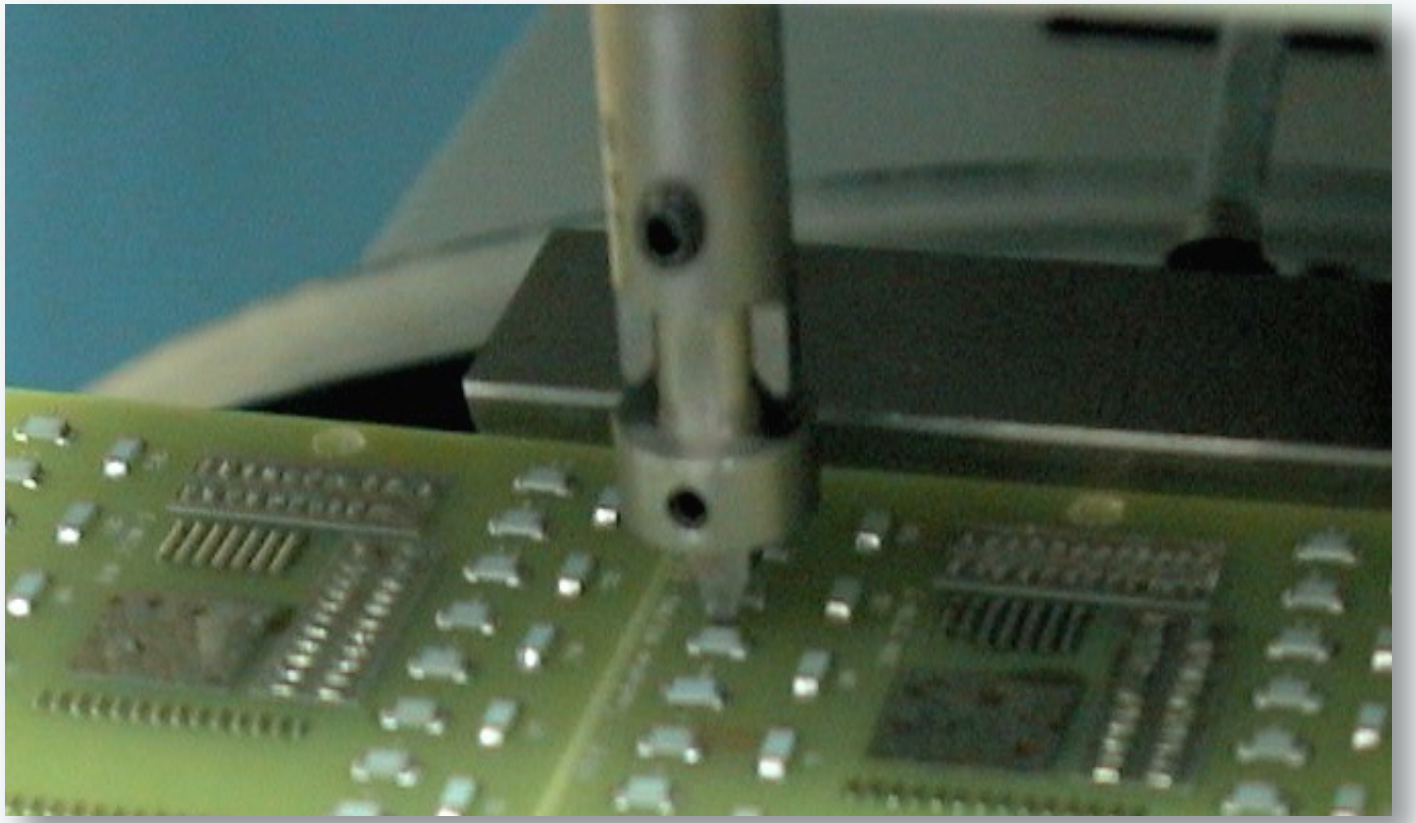
Strong heterogeneities
Homogenized models are insufficient

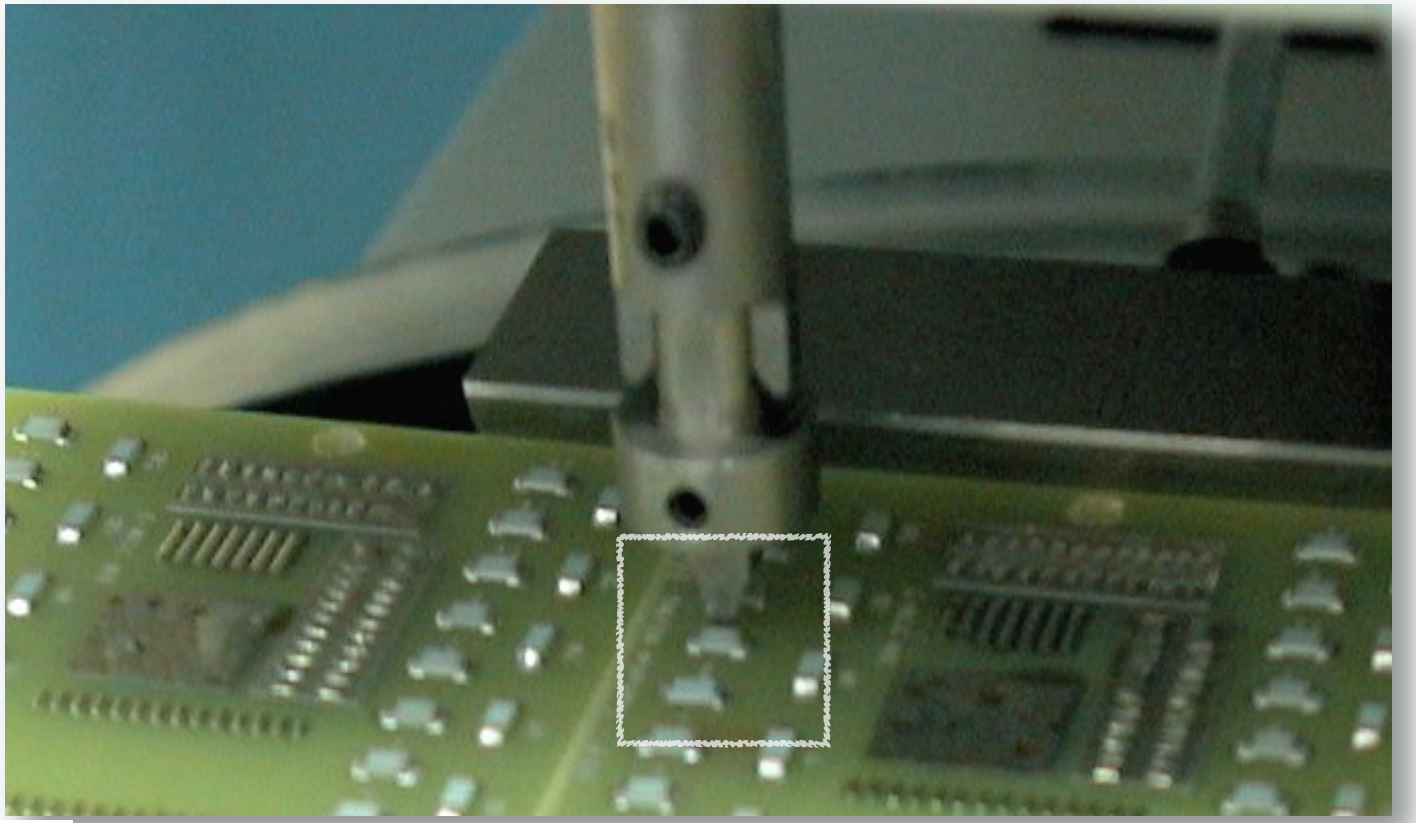


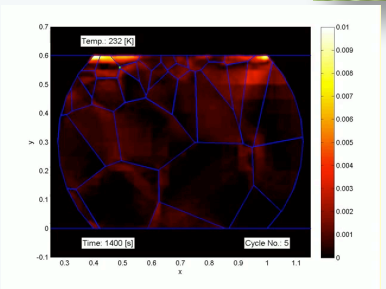








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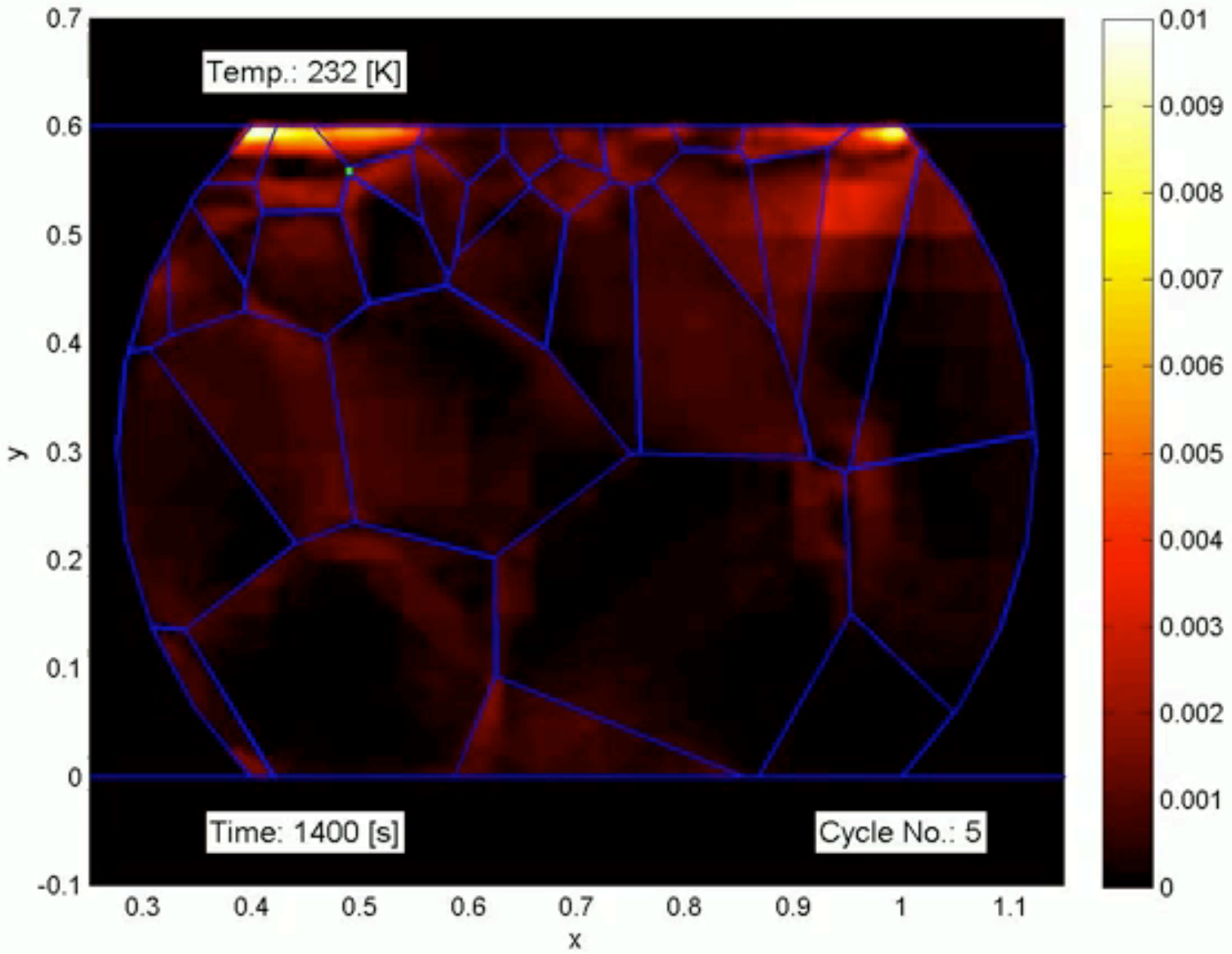
Cycle No.: 5
x
y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Time: 1400 [s]
Cycle No.: 5
y
x
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0.9
1
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0.01
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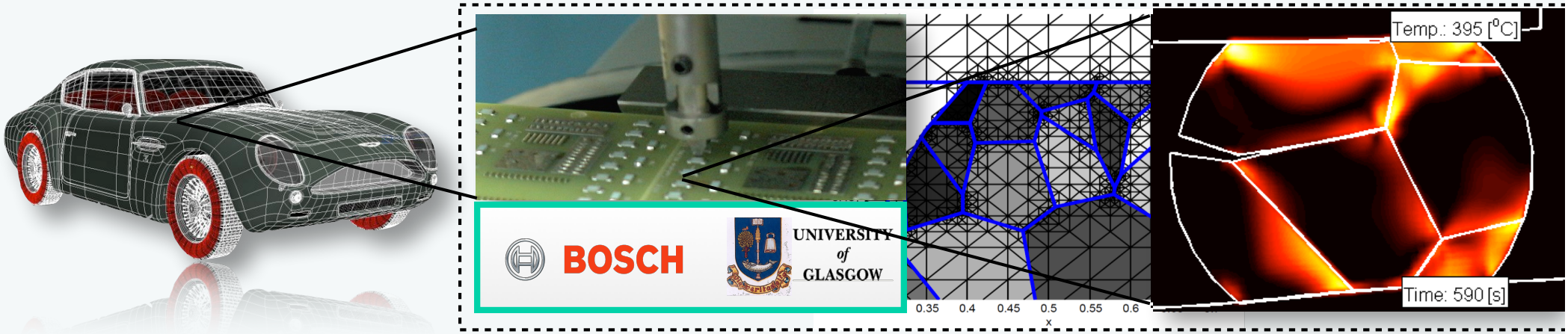
0

Fracture over the scales

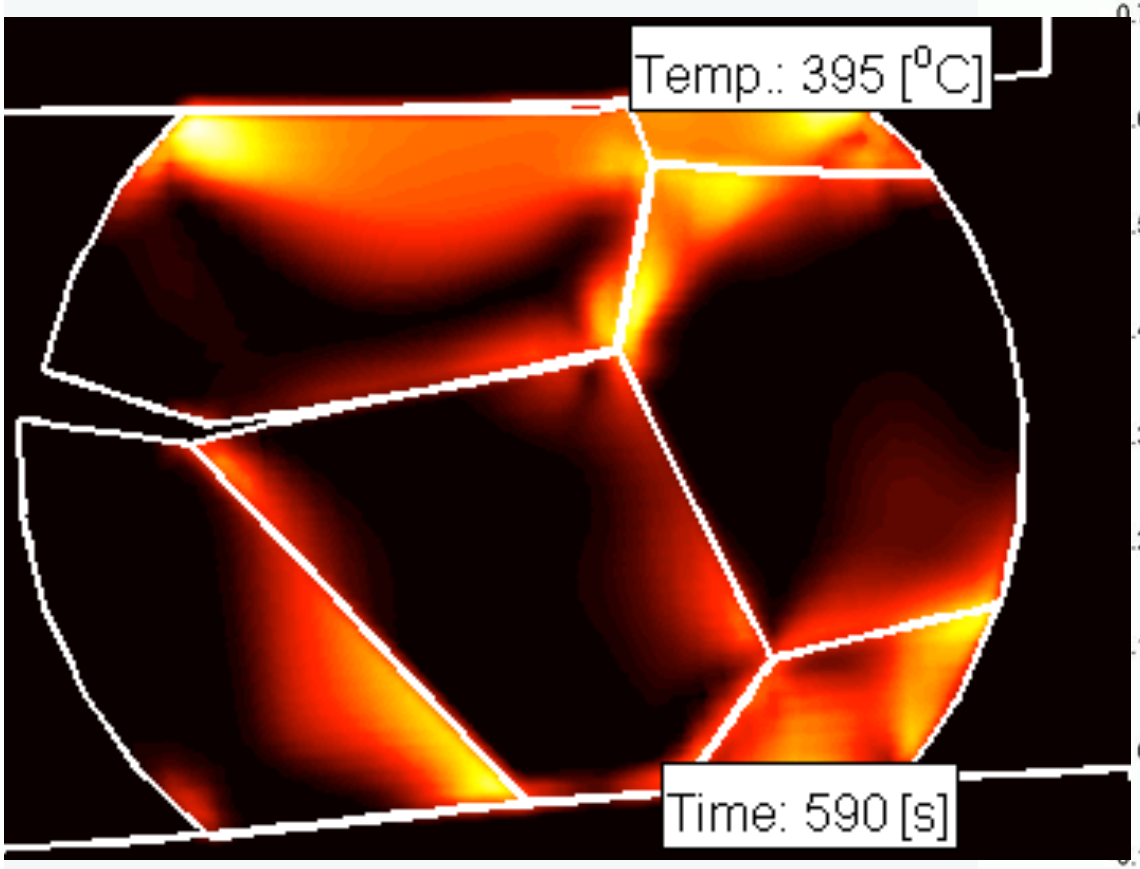
Solder joint durability (microelectronics), Bosch GmbH

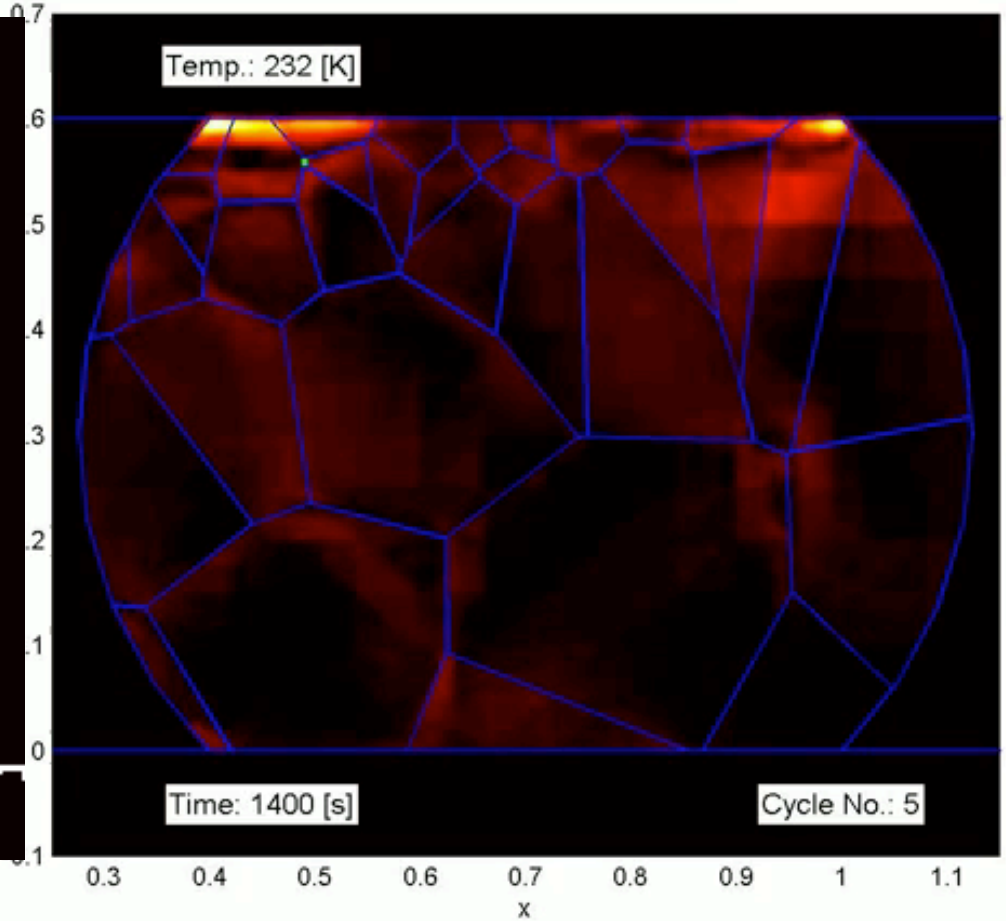


Question: what is the role of Pb in thermo-mechanical reliability of solder joints?

A. Menk and SPAB, IJNME 2011, Comp. Mat. Sci. 2012
XFEM Preconditioning and application to polycrystalline fracture

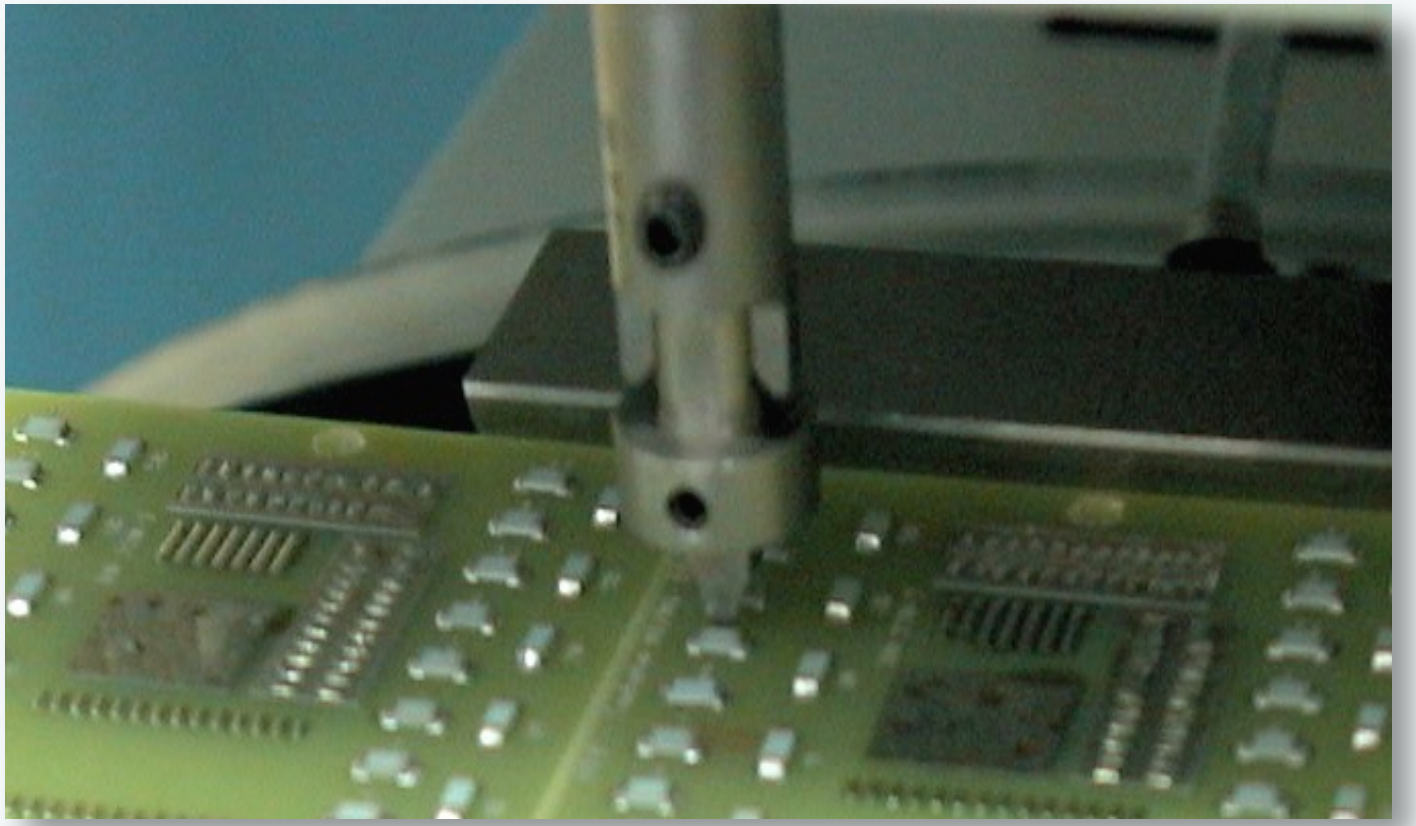
D. A. Paladim et al. Int. J. Numer. Meth. Engng 2017; 110:103–132
P. Kerfriden et al. Int. J. Numer. Meth. Engng 2014; 97:395–422
P. Kerfriden et al. Int. J. Numer. Meth. Engng 2012; 89:154–179
P. Kerfriden et al. Comput. Methods Appl. Mech. Engrg. 200 (2011) 850–866
K. C. Hoang et al. Num Meth PDEs DOI 10.1002/num.21932



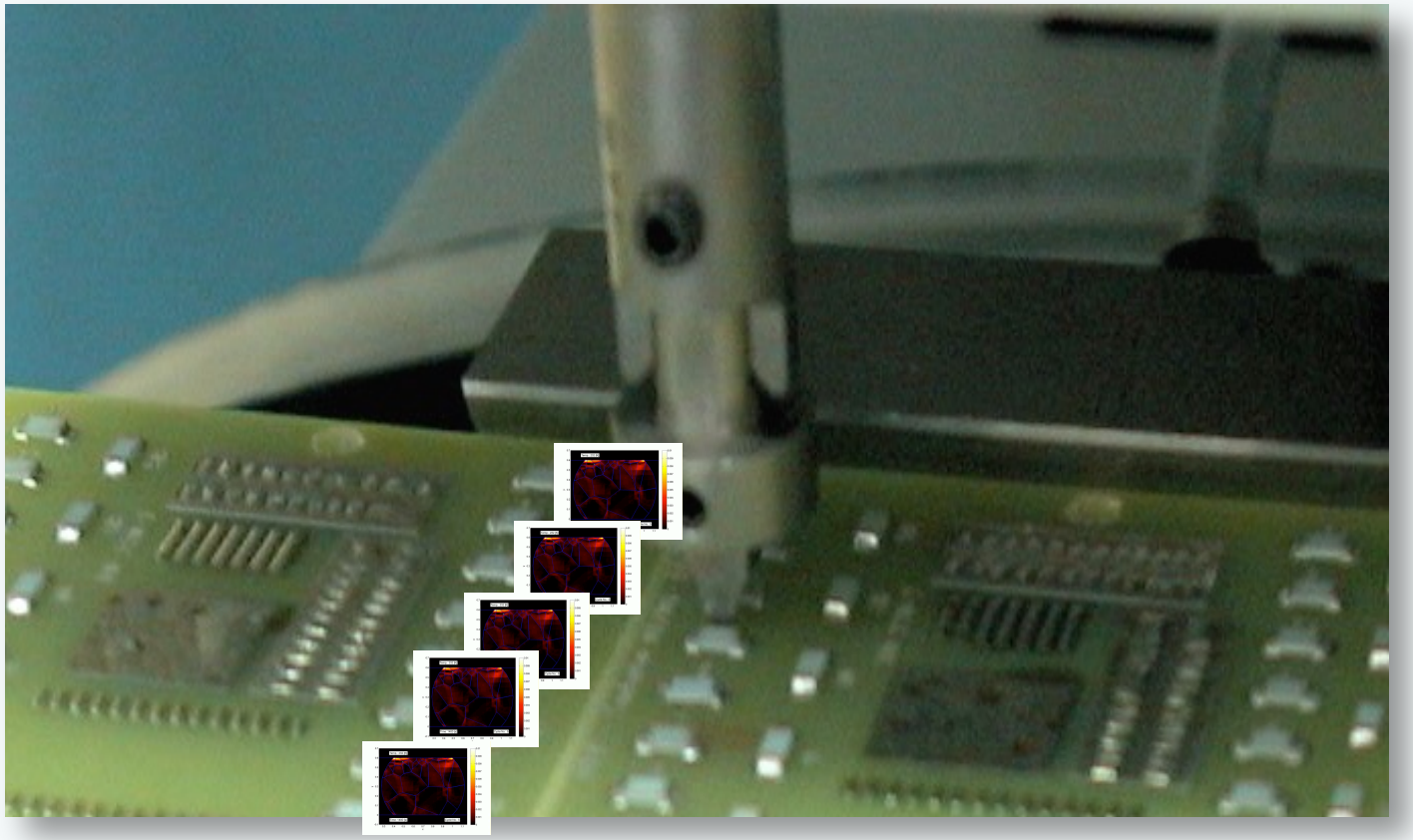


Microstructure plays a major role in thermomechanical durability in Pb-free solders

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



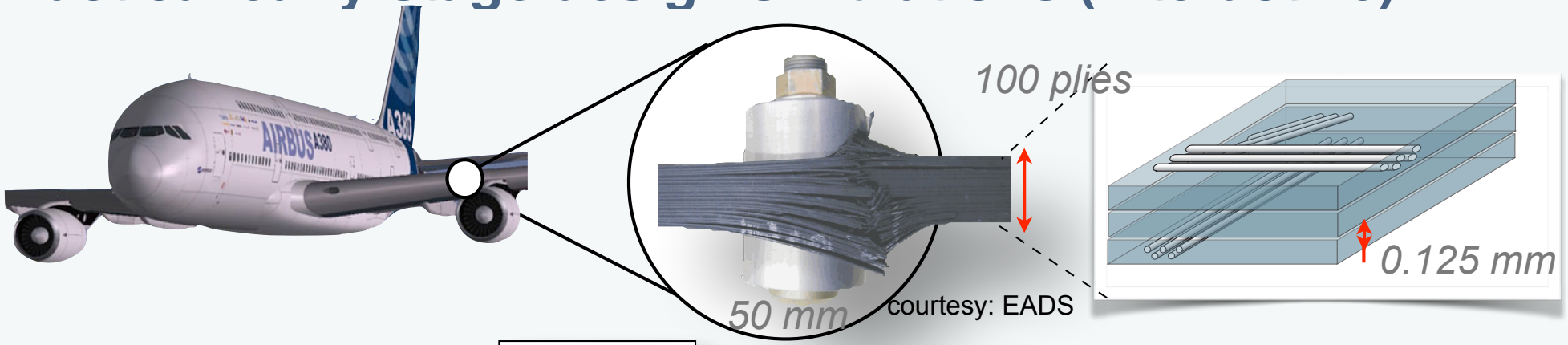
What can be done to account for microstructures for structures of engineering relevance?



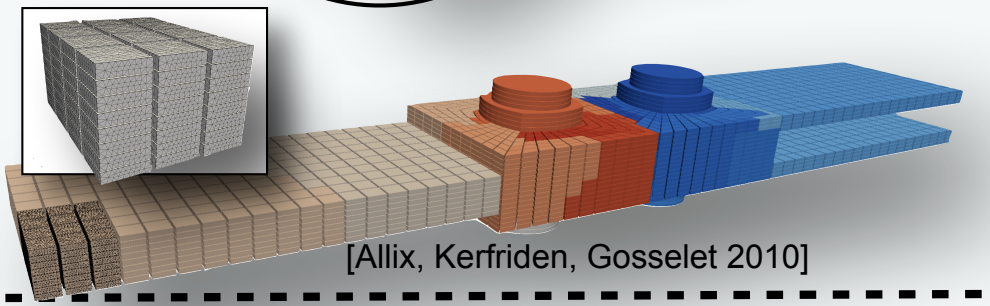
All is fine as long as the microstructures simulations are localised or few in number

Interfaces in engineering and biomechanics

Practical early-stage design simulations (interactive)

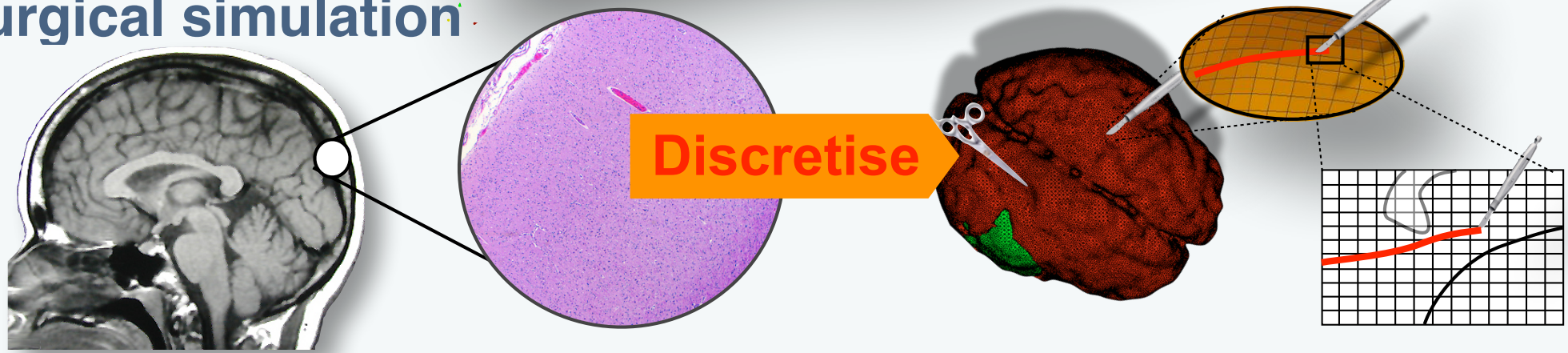


Discretise



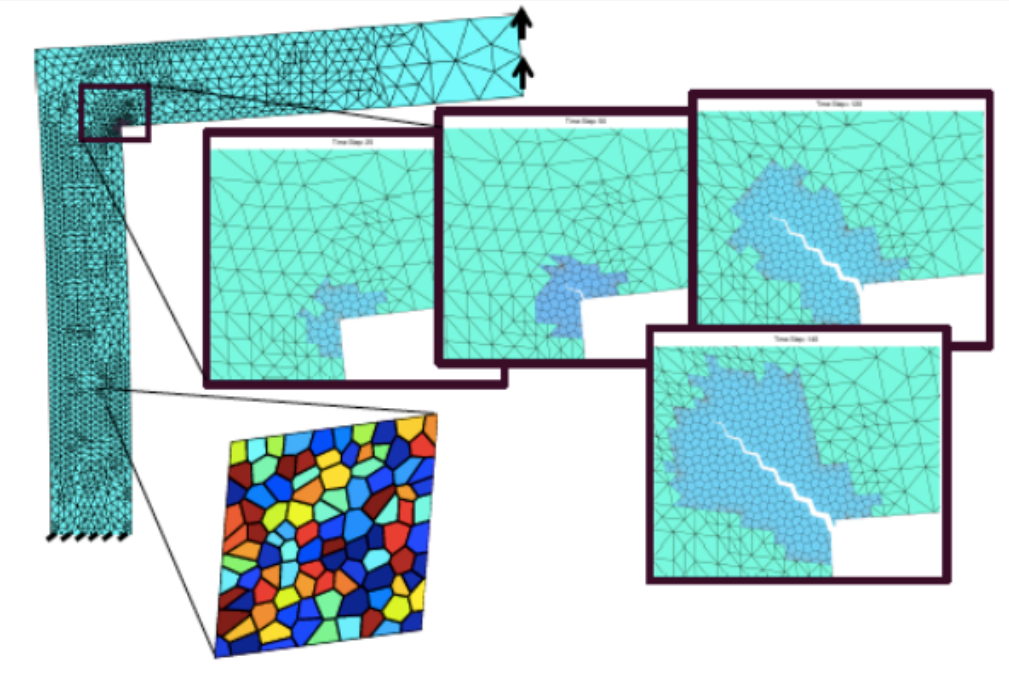
[Allix, Kerfriden, Gosselet 2010]

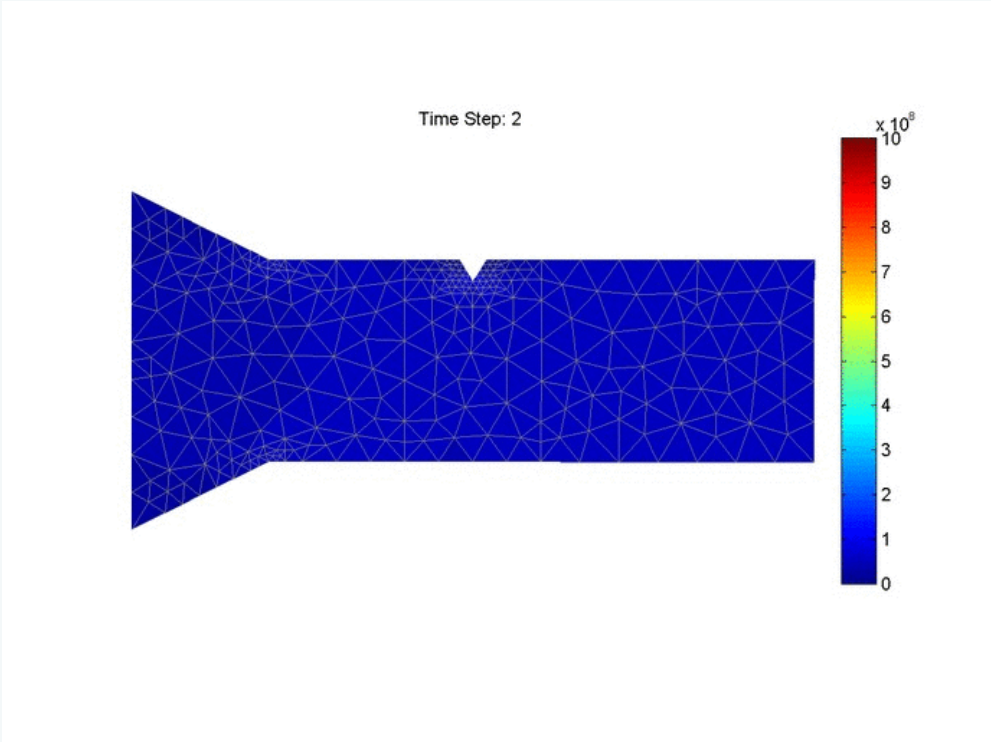
Surgical simulation



- 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

Partial conclusions on fracture of heterogeneous materials

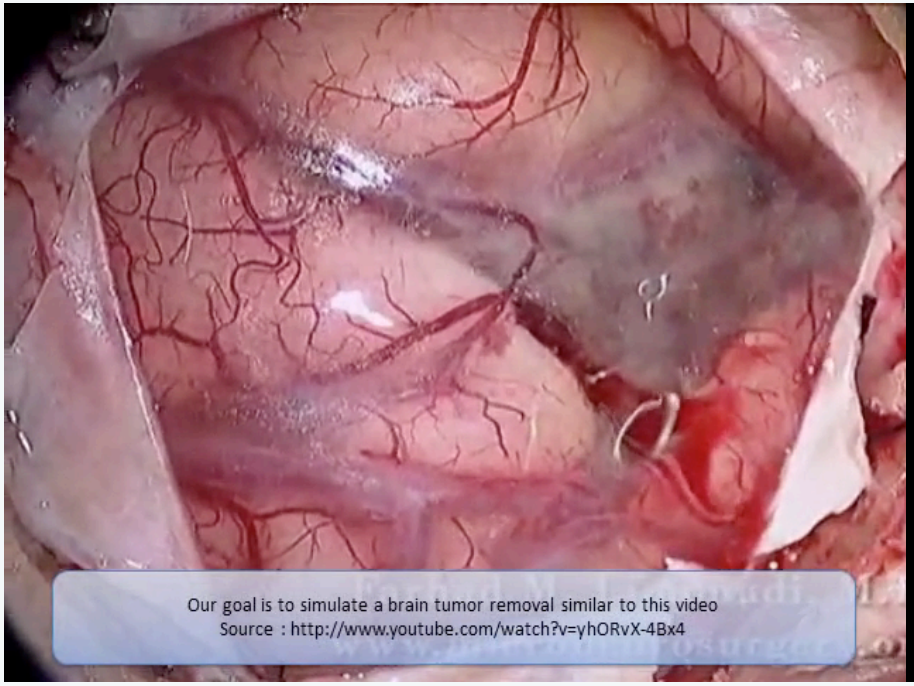
- Model + mesh adaptivity for adaptive fracture mechanics simulations: expensive + implementation must be done carefully
- Model order reduction, e.g. POD, PGD are ineffective for problems lacking separation of scales (see Kerfriden, Goury and others)
    - Domain-wise model selection
    - Adaptive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

Partial conclusions on fracture of heterogeneous materials

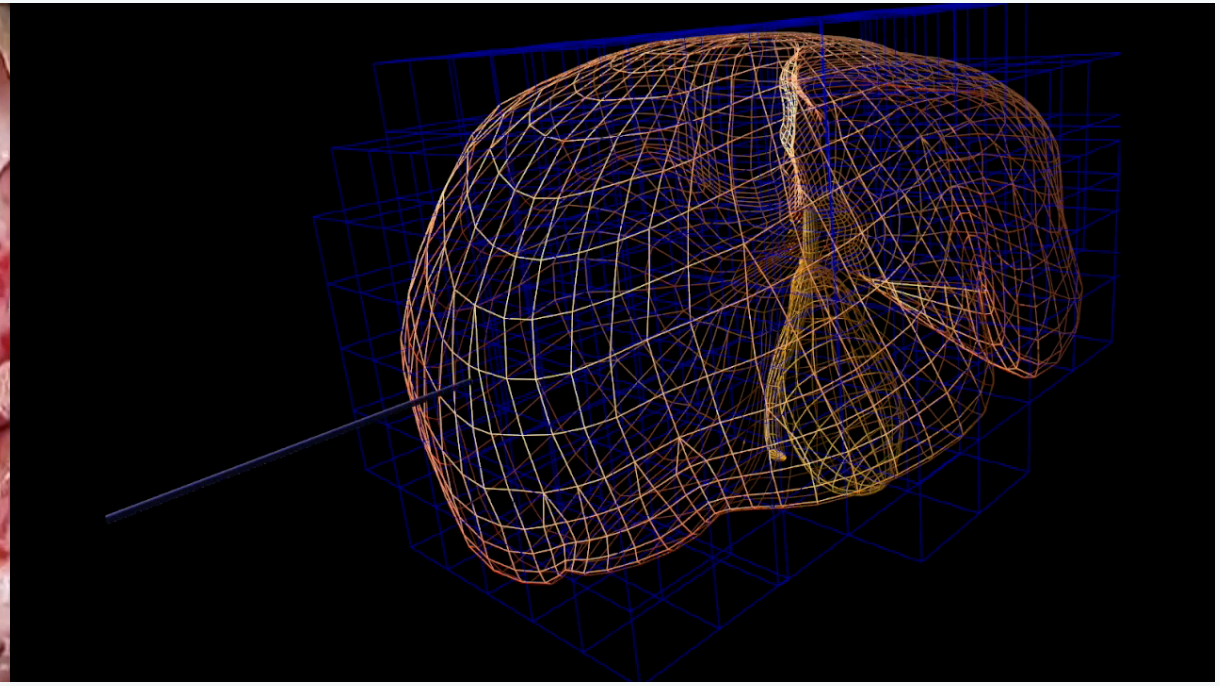
- Simple methods can deal with fracture in unidirectional composites
- Model + mesh adaptivity for adaptive fracture mechanics simulations: expensive + implementation must be done carefully
- Model order reduction is ineffective for problems lacking separation of scales
    - Domain-wise model selection
    - Adaptive model selection
    - Machine learning…
- Next step: biomechanics/real-time

Topological changes in surgical simulation

Cutting and Needle Insertion



H. Courtecuisse et al. Medical Image Analysis, 2014



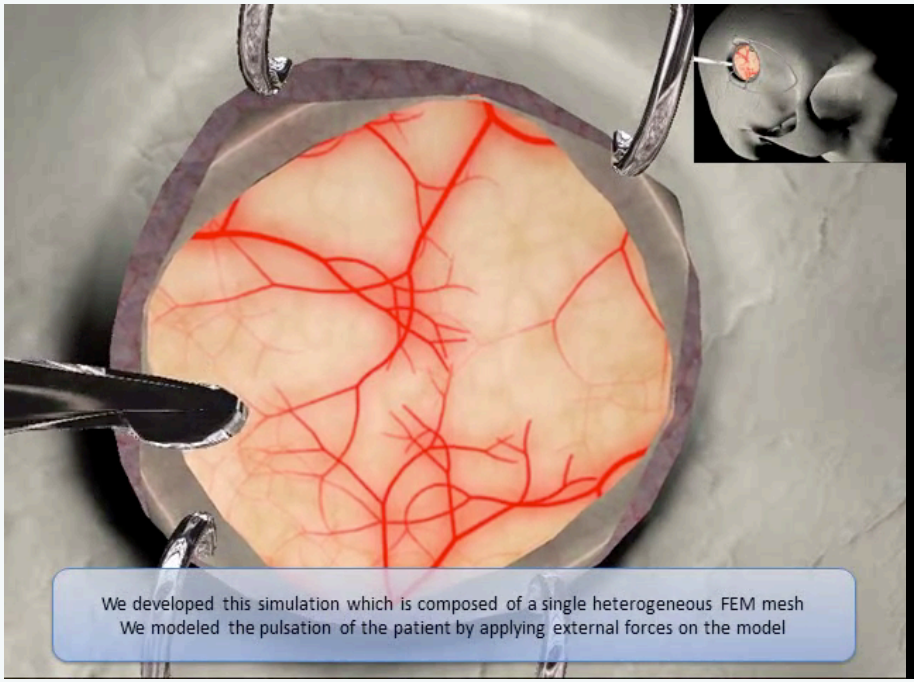
P.H. Bui et al. IEEE T. Biomed Eng. 2017 & Frontiers in Surgery, 2017

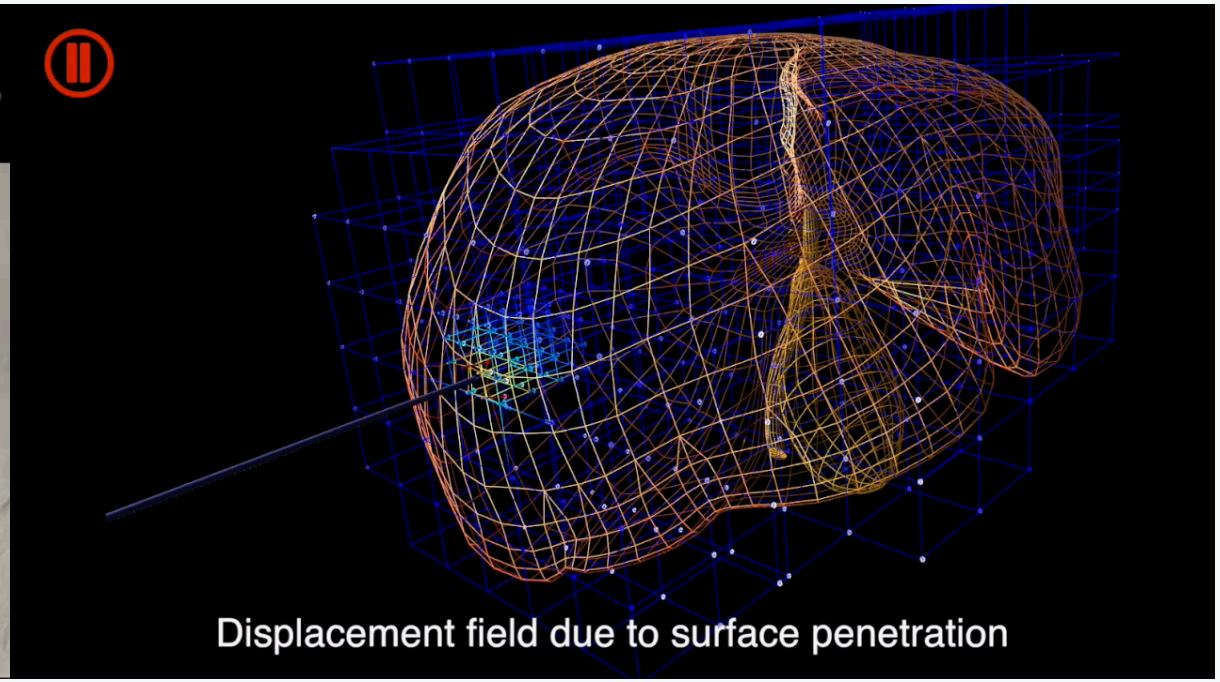
http://orbilu.uni.lu/handle/10993/30937

http://orbilu.uni.lu/handle/10993/29846

Topological changes in surgical simulation

Cutting and Needle Insertion





H. Courtecuisse et al. Medical Image Analysis, 2014

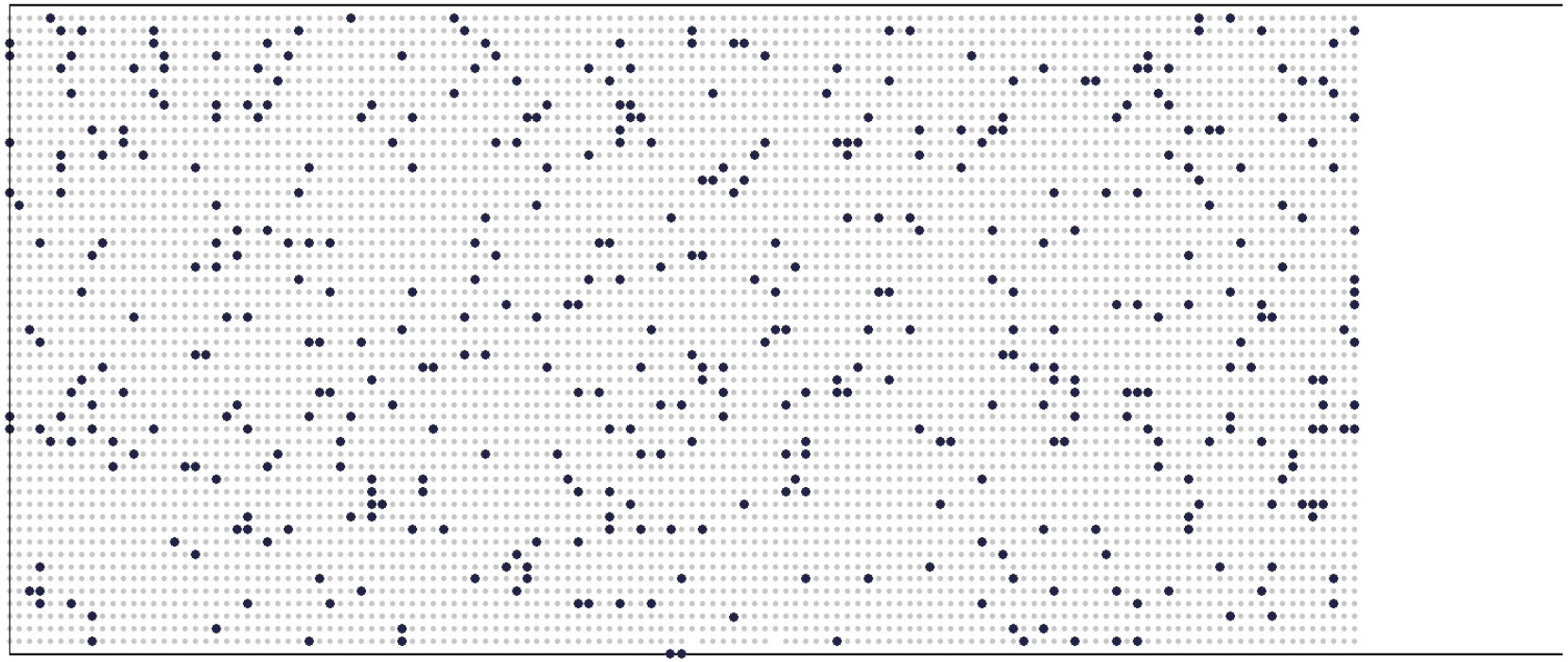
Question: how can we simulate cutting/fracture in real time using implicit time stepping?

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?

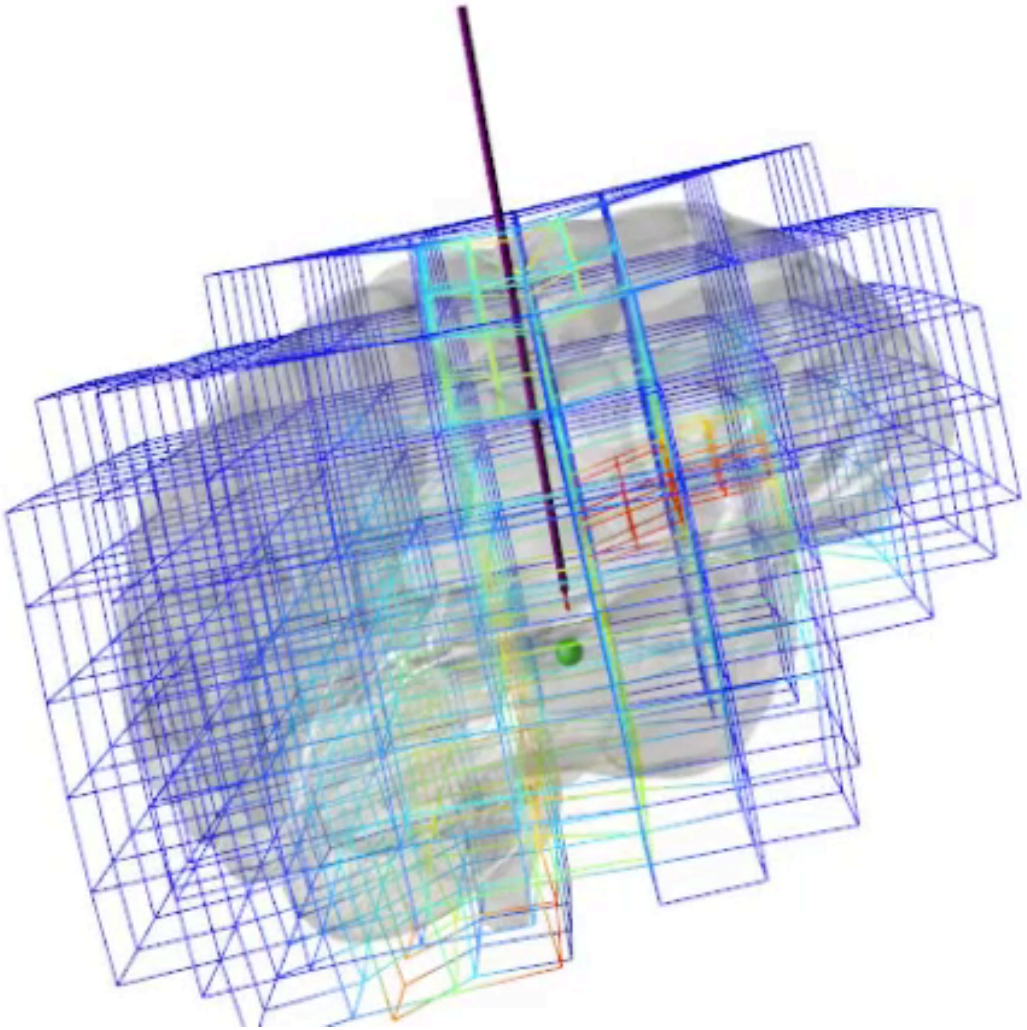
http://orbilu.uni.lu/handle/10993/30937 http://orbilu.uni.lu/handle/10993/29846

Thrombus formation in an artery



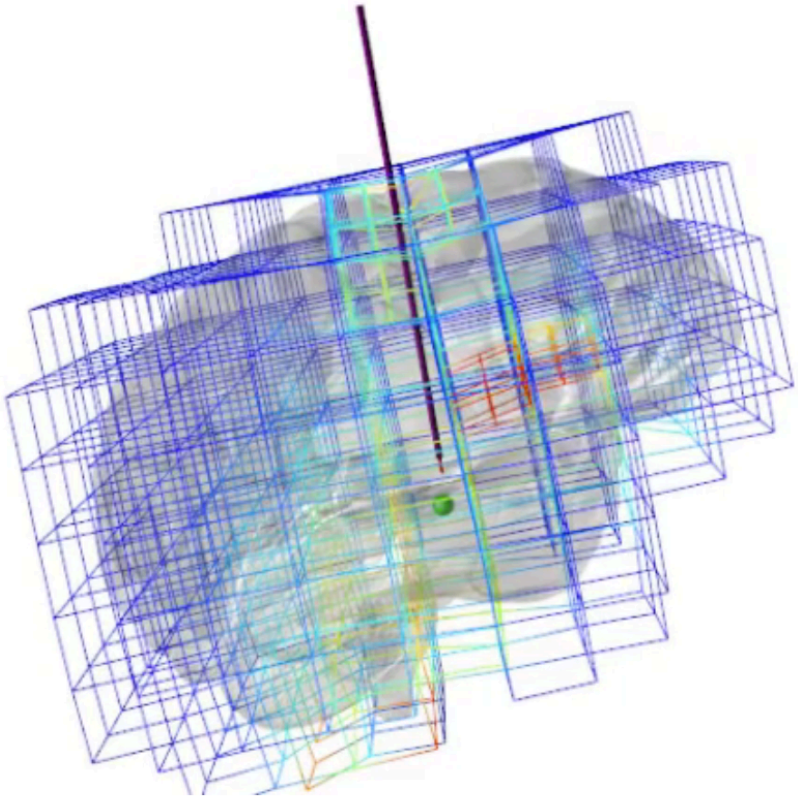
IJNMBE2017 Moh

Cannula insertion

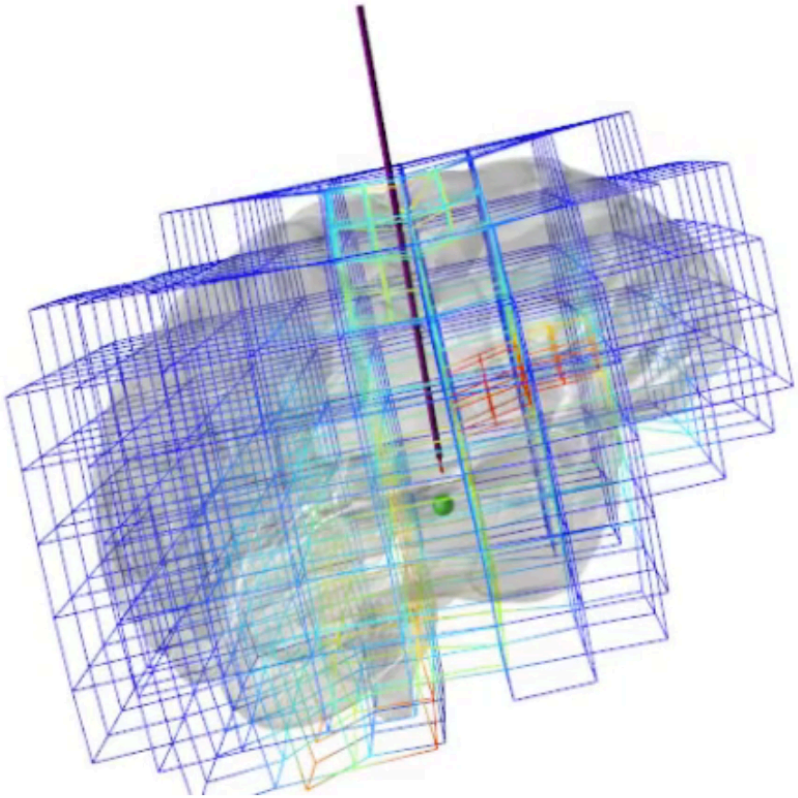


Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg

CHALLENGE: everything happens close to the needle… focus the



CHALLENGE: everything happens close to the needle… focus the



But HOW can we decide where and what the element size should be?

QUESTIONS

Local mesh refinement is necessary, but where? how?

What else is missing?

Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg

Model of contractile tissue

$$\min_{\mathbf{u}\in\mathbf{V}} \frac{1}{2}\int_\Omega \boldsymbol{\sigma}(\mathbf{u},\beta) : \boldsymbol{\varepsilon}(\mathbf{u})\, d\mathbf{x} - \int_\Omega \mathbf{g}\cdot\mathbf{u}\, d\mathbf{x}$$

with $\boldsymbol{\sigma}(\mathbf{u},\beta) = \underbrace{\boldsymbol{\sigma}_P(\mathbf{u})}_{\text{passive material}} + \underbrace{\boldsymbol{\sigma}_A(\beta)}_{\text{muscular activation}}$

$$\begin{cases} \boldsymbol{\sigma}_A(\beta) = \beta T e_A \otimes e_A \\ e_A : \text{ fiber direction} \\ T : \text{ tension} \\ \beta : \text{ activation} \end{cases}$$

where

Cowin & Humphrey 2001

Payan & Ohayon 2017

Biomechanics of Living Organs : Hyperelastic Constitutive Laws for Finite Element Modeling.

Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg

a posteriori error estimates

$$\mathbf{u} \in \mathbf{V} \; : \; a(\mathbf{u}, \mathbf{v}) = l(\beta, \mathbf{v}) \quad \forall \, \mathbf{v} \in \mathbf{V}$$

$$a(\mathbf{u}, \mathbf{v}) = \int_\Omega \boldsymbol{\sigma}_P(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, d\mathbf{x} \qquad l(\beta, \mathbf{v}) = \int_\Omega \boldsymbol{\sigma}_A(\beta) : \boldsymbol{\varepsilon}(\mathbf{v}) \, d\mathbf{x} + \int_\Omega \mathbf{g} \cdot \mathbf{v} \, d\mathbf{x}$$

Prediction of a quantity of interest (e.g., local strain or stress) :

$$J : \mathbf{V} \ni \mathbf{u} \mapsto J(\mathbf{u}) \in \mathbb{R}.$$

(Goal-oriented) discretization error : $|J(\mathbf{u}) - J(\mathbf{u}_h)|$?

Exact solution : $\mathbf{u} \in \mathbf{V}$
MEF approximation : $\mathbf{u}_h \in \mathbf{V}_h$

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Dual Weighted Residuals (DWR)

$$J(\mathbf{u}) - J(\mathbf{u}_h) = a(\mathbf{u},\mathbf{z}) - a(\mathbf{u}_h,\mathbf{z}) = \underbrace{l(\mathbf{z}) - a(\mathbf{u}_h,\mathbf{z})}_{\text{residual}} =: \eta_h(\mathbf{z})$$

where $\mathbf{z} \in \mathbf{V}$ s.t. $a(\mathbf{v},\mathbf{z}) = J(\mathbf{v}) \qquad \forall\, \mathbf{v} \in \mathbf{V}$ (dual problem)

➥ **global estimator** : η_h

Local representation

$$\begin{aligned} J(\mathbf{u}) - J(\mathbf{u}_h) &= \sum_{K\in\mathcal{K}_h} \langle R_K, \mathbf{z} - \pi_h\mathbf{z}\rangle_K + \langle R_{\partial K}, \mathbf{z} - \pi_h\mathbf{z}\rangle_{\partial K} \\ &=: \sum_{K\in\mathcal{K}_h} \eta_K(z - \pi_h z) \end{aligned}$$

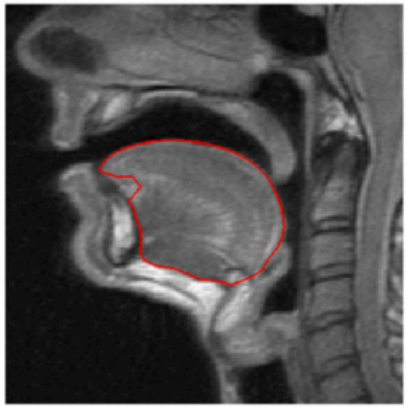
local estimator

$\pi_h\mathbf{z}$: interpolant of dual solution
R_K / $R_{\partial K}$: residual contributions on K / ∂K

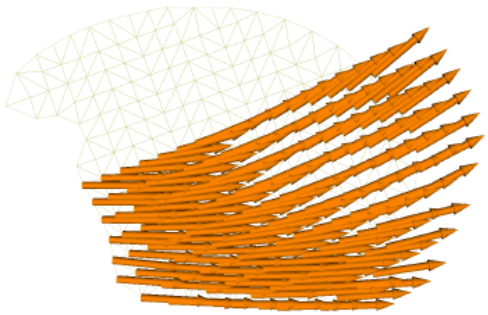
➥ **local estimators** : η_K

Becker & Rannacher 1997, 2001
Rognes & Logg 2013 (FEniCS)

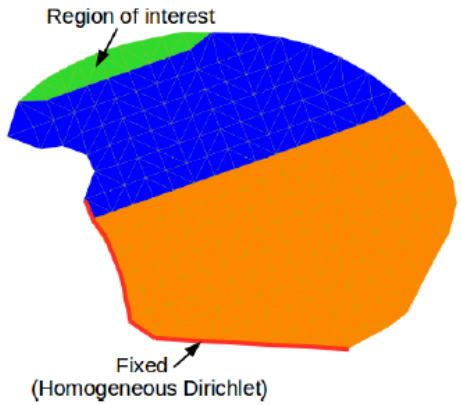
Genioglossus activation



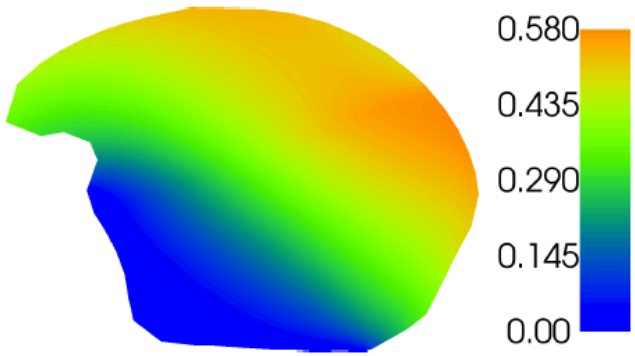
Bijar, Rohan, Perrier & Payan 2015



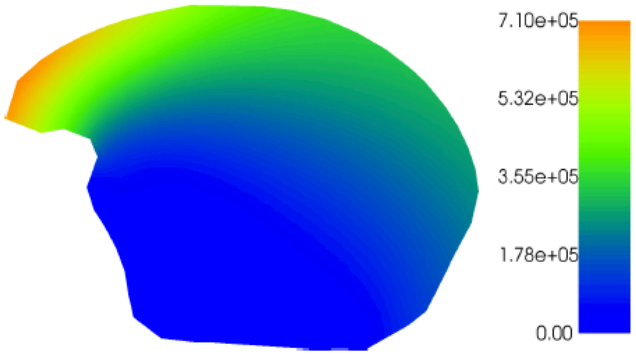
fibers (genioglossus)



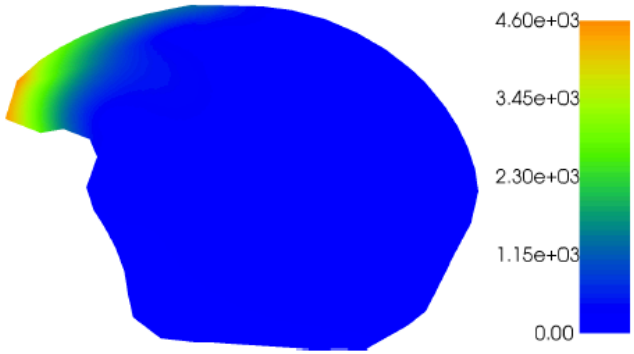
region of interest ω (green)



$\mathbf{u}$



$\mathbf{z} \,/\, J_1$

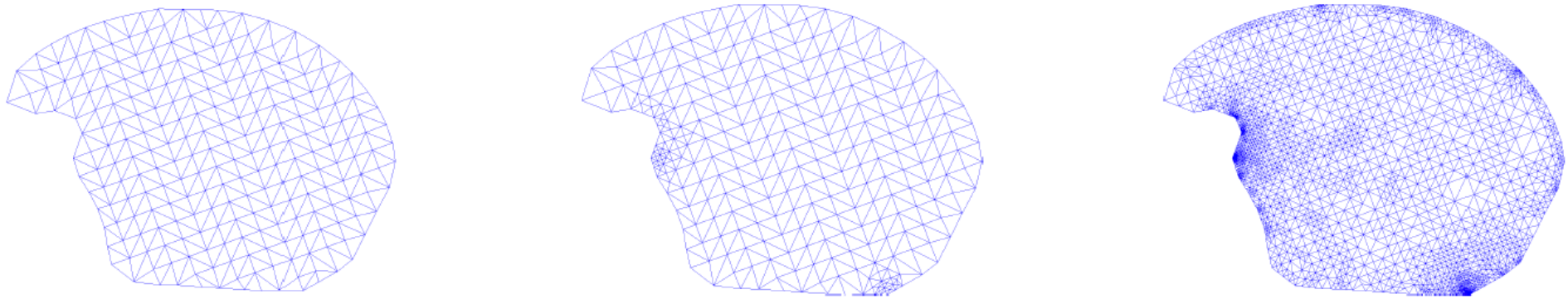


$\mathbf{z} \,/\, J_2$

$$J_1(\mathbf{u}) := \int_\omega (u_x + u_y)\, d\mathbf{x} \qquad J_2(\mathbf{u}) := \int_\omega \operatorname{div} \mathbf{u}\, d\mathbf{x}$$

Genioglossus activation

J_1 :

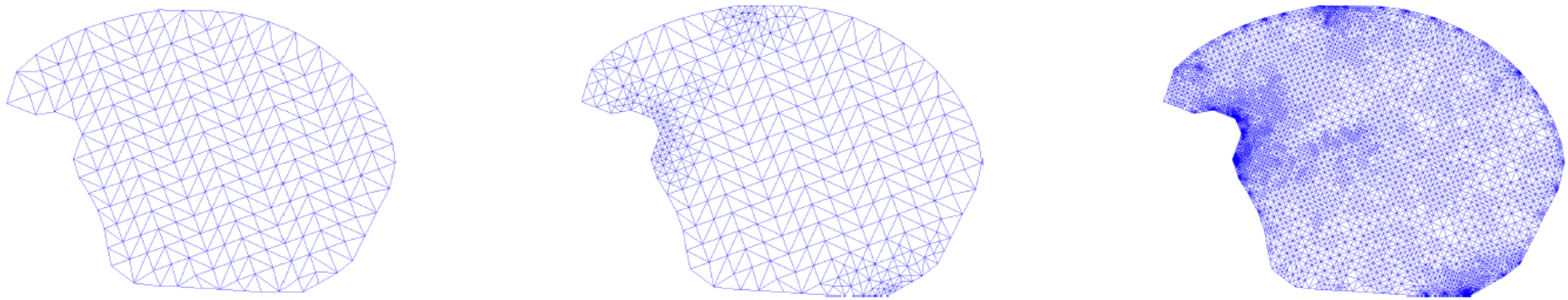


init
(N=426, $\varepsilon = 1.10^{-2}$)

2nd iteration
(N=523, $\varepsilon = 3.10^{-3}$)

8th iteration
(N=5143, $\varepsilon = 4.10^{-5}$)

J_2 :

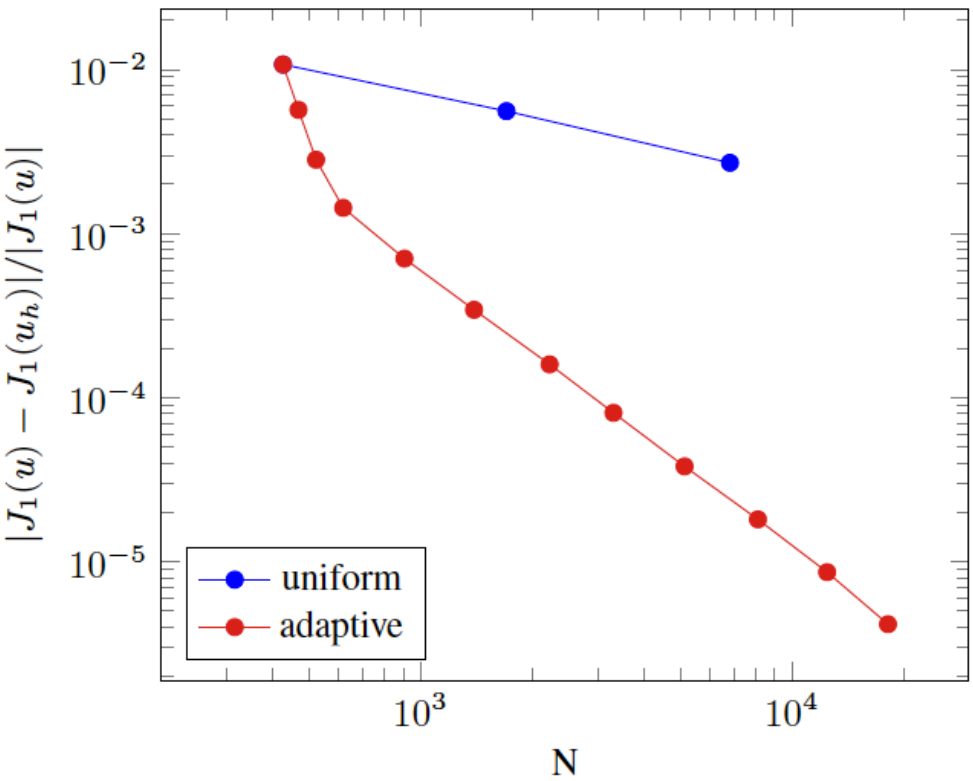


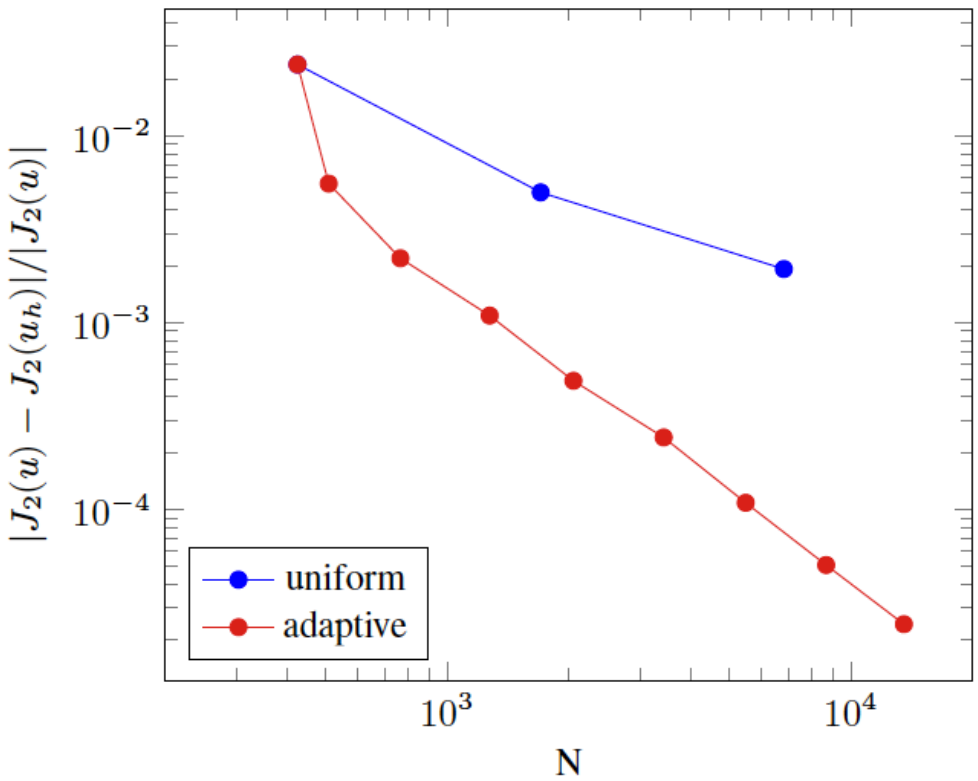
init
(N=426, $\varepsilon = 3.10^{-2}$)

2nd iteration
(N=766, $\varepsilon = 2.10^{-3}$)

8th iteration
(N=13513, $\varepsilon = 2.10^{-5}$)

Effect of adaptive refinement





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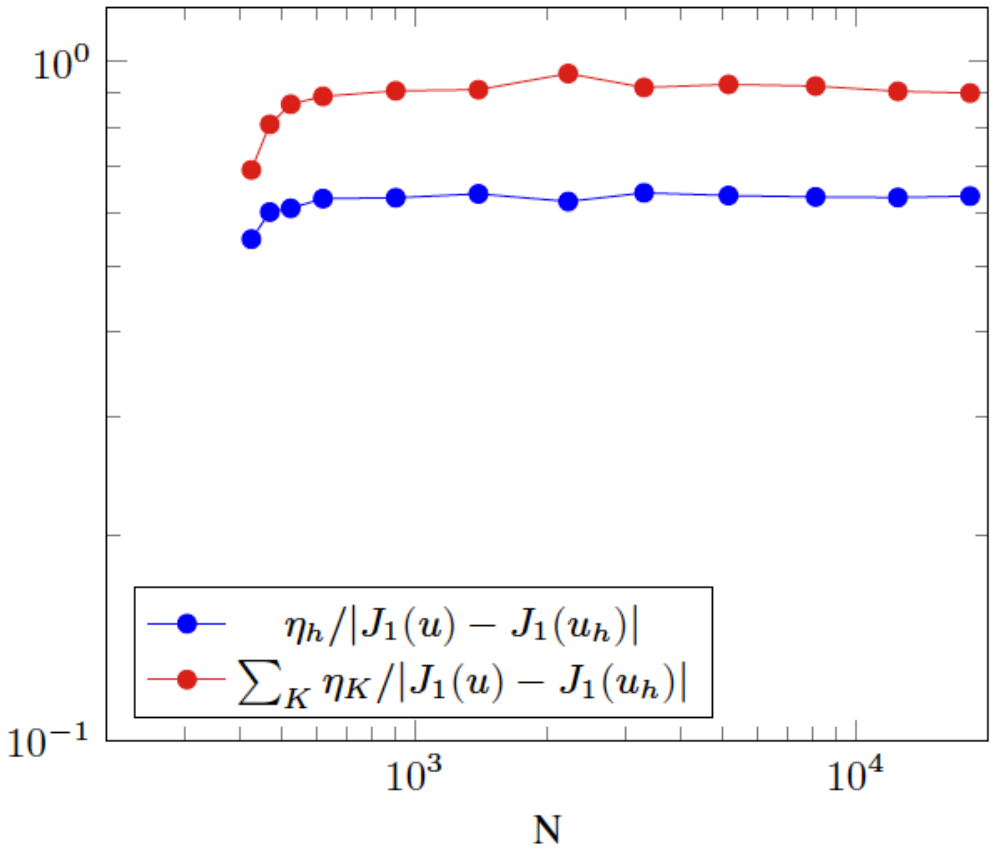
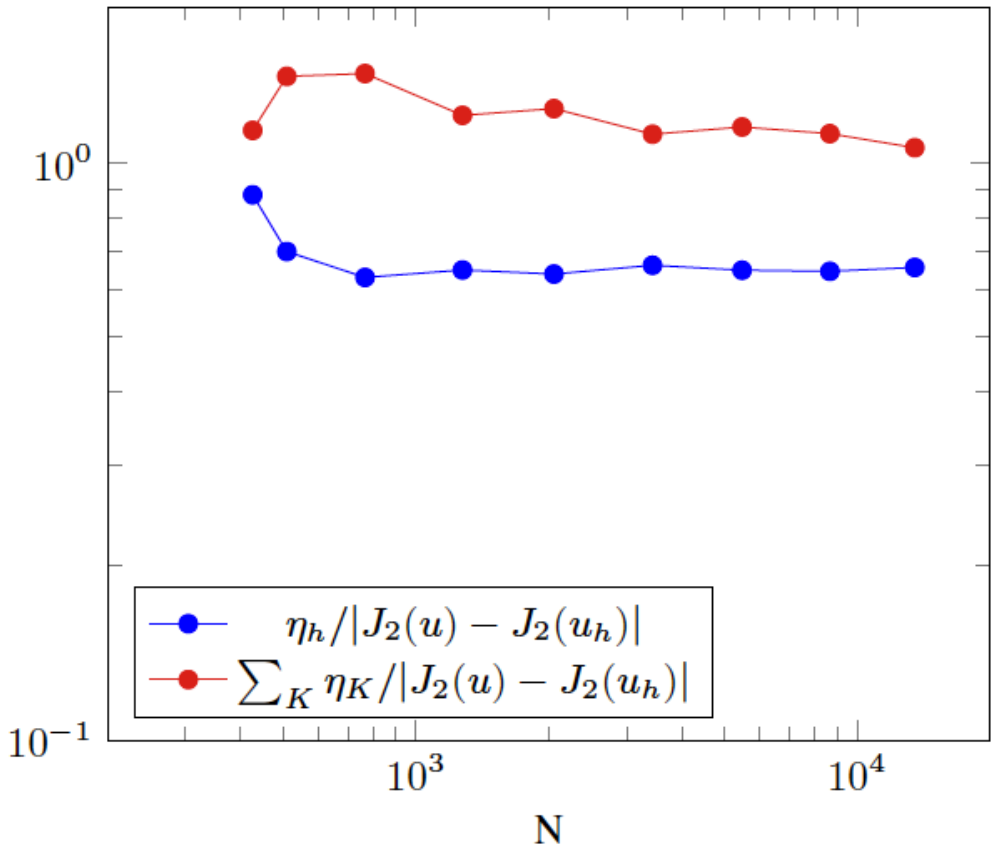
Effectivity of the error indicator





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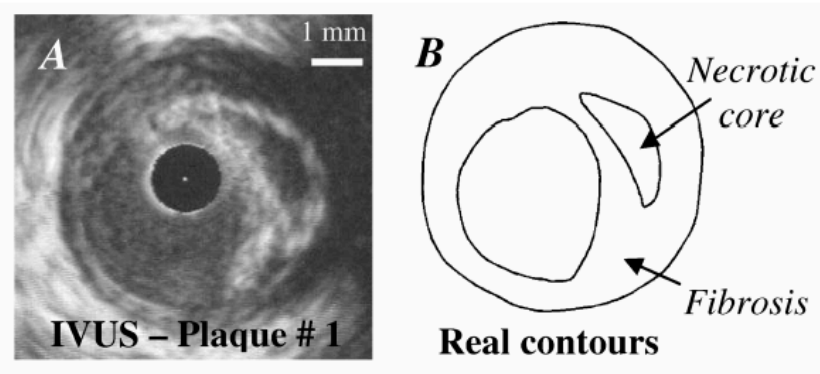
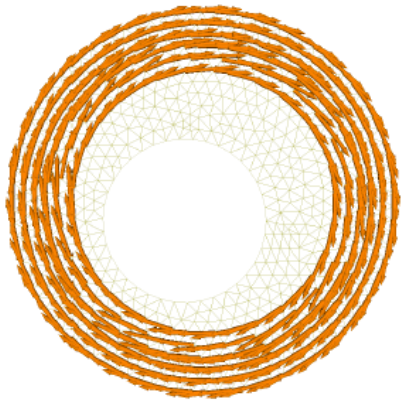
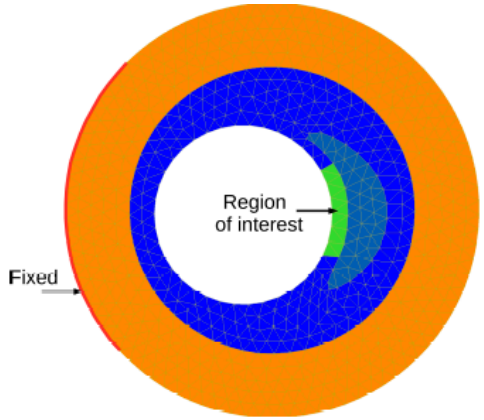
Arterial wall activation



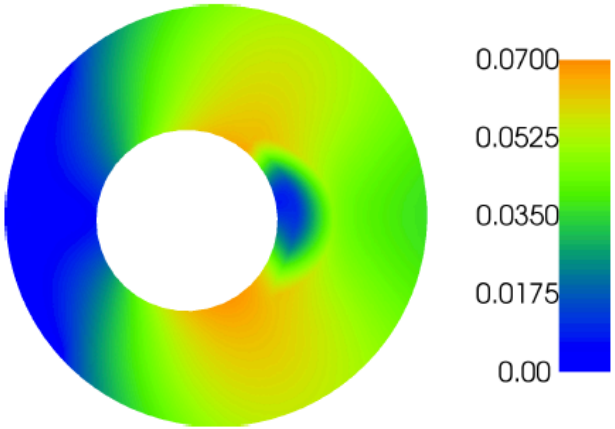
Le Floc'h et.al 2008



media



region of interest ω (green)



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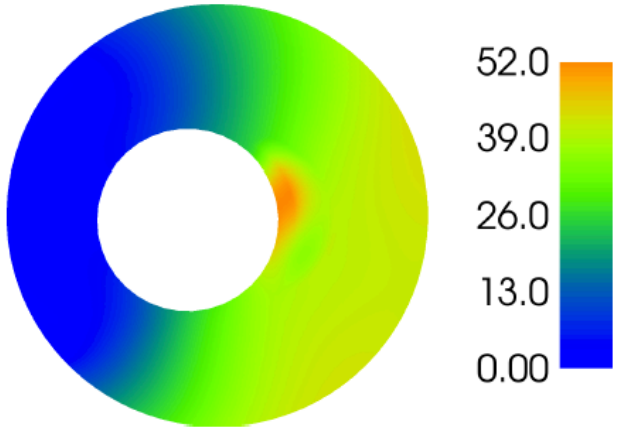
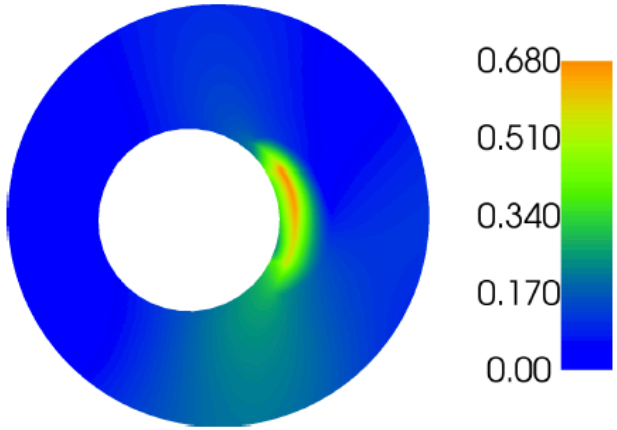


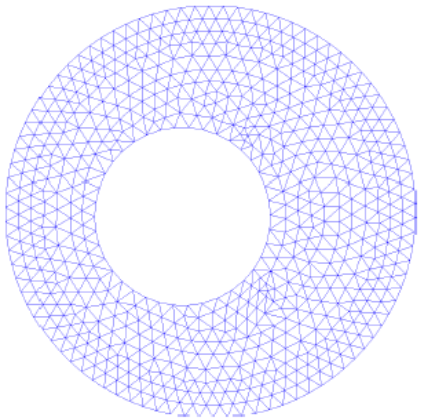
$\mathbf{z} \,/\, J_1$



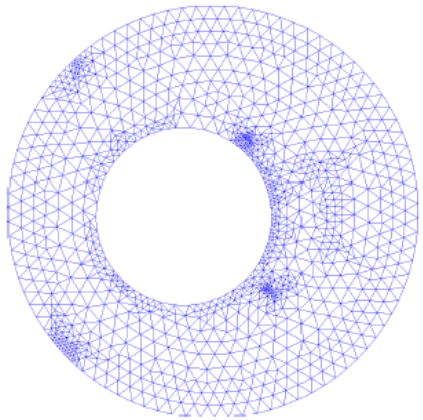
$\mathbf{z} \,/\, J_2$

$$J_1(\mathbf{u}) := \int_\omega (u_x + u_y)\, d\mathbf{x} \qquad J_2(\mathbf{u}) := \int_\omega \operatorname{div} \mathbf{u}\, d\mathbf{x}$$

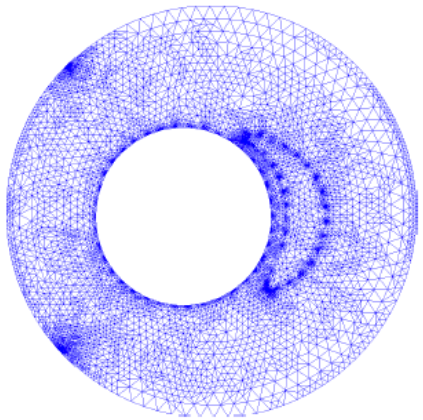
J_1 :



init
(N=1242, $\varepsilon = 0.4$)



2nd iteration
(N=2079, $\varepsilon = 0.05$)



6th iteration
(N=15028, $\varepsilon = 3.10^{-3}$)

J_2 : similar results.

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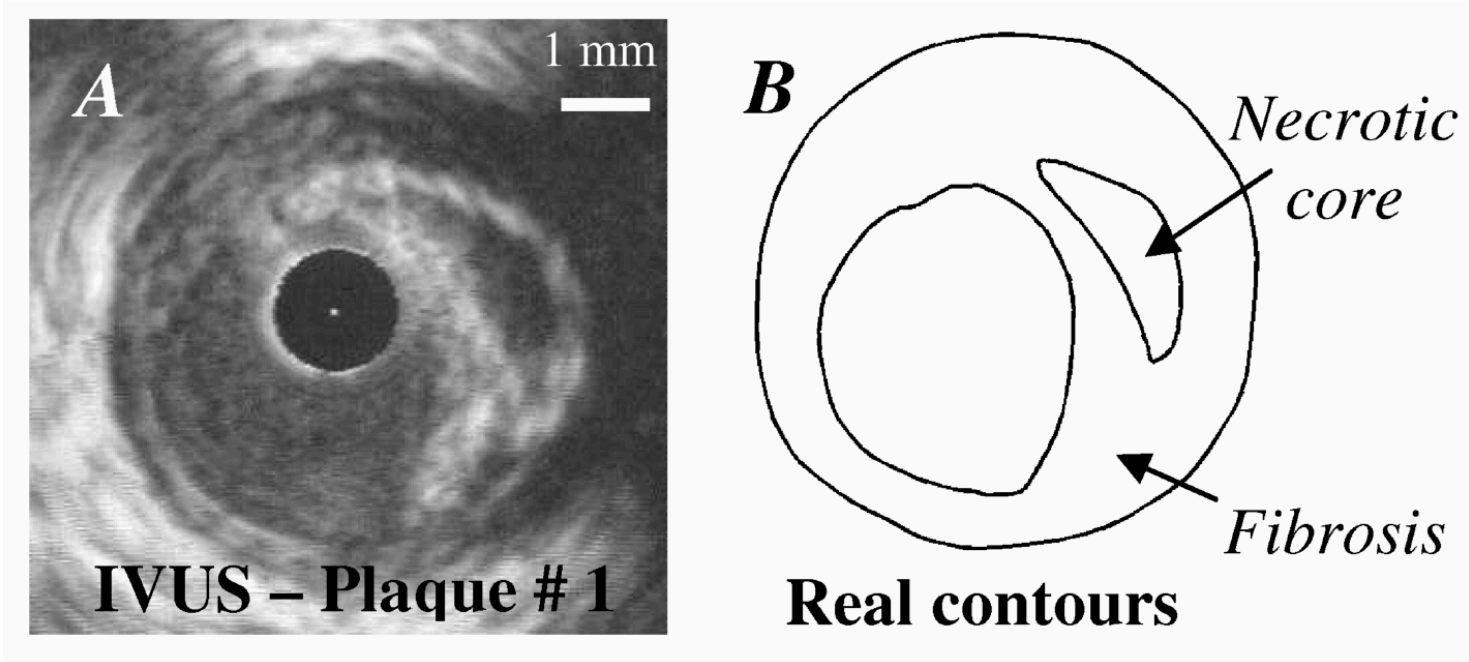
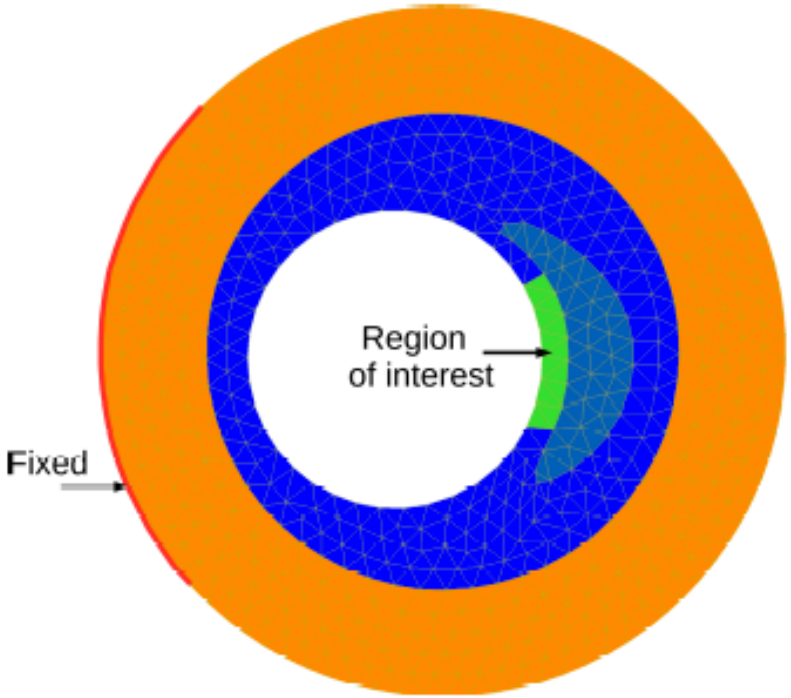
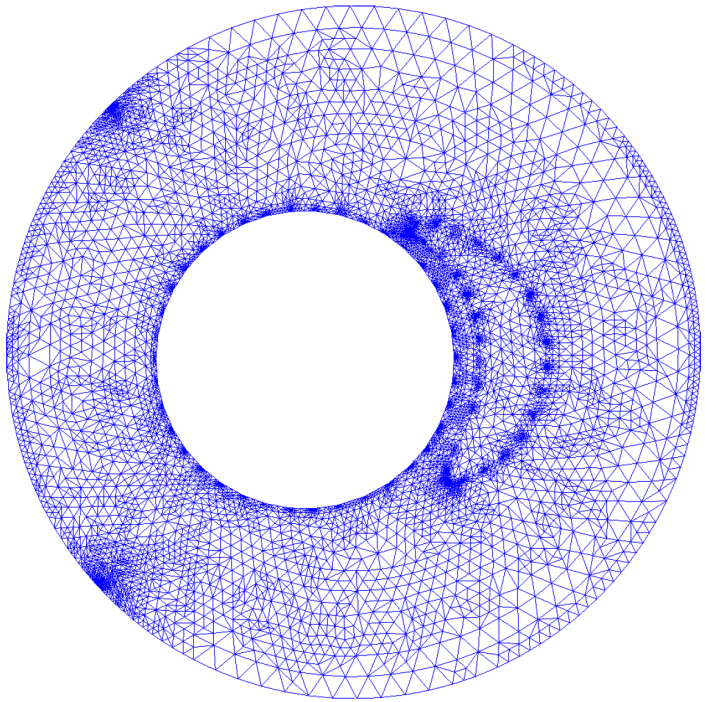
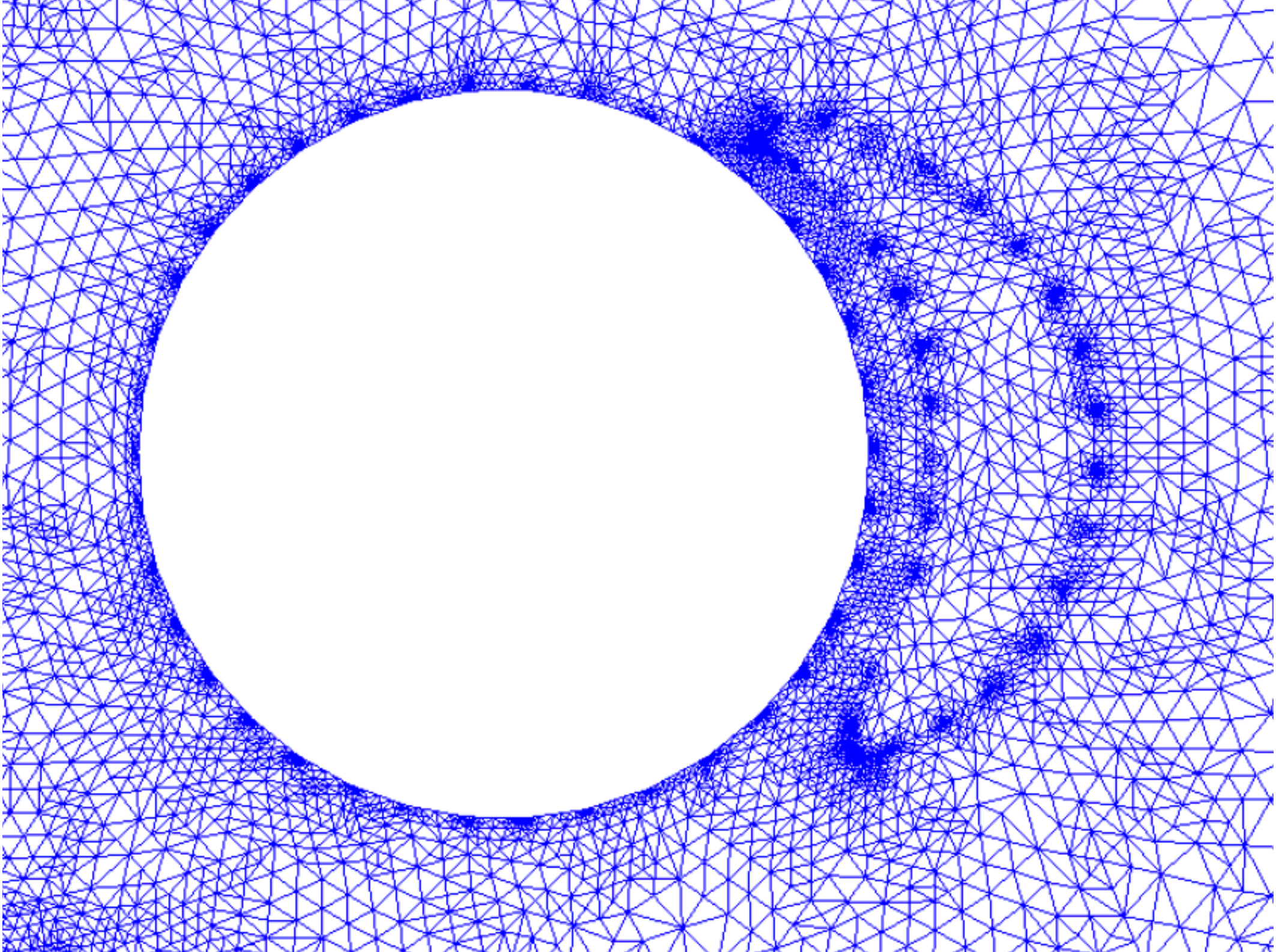
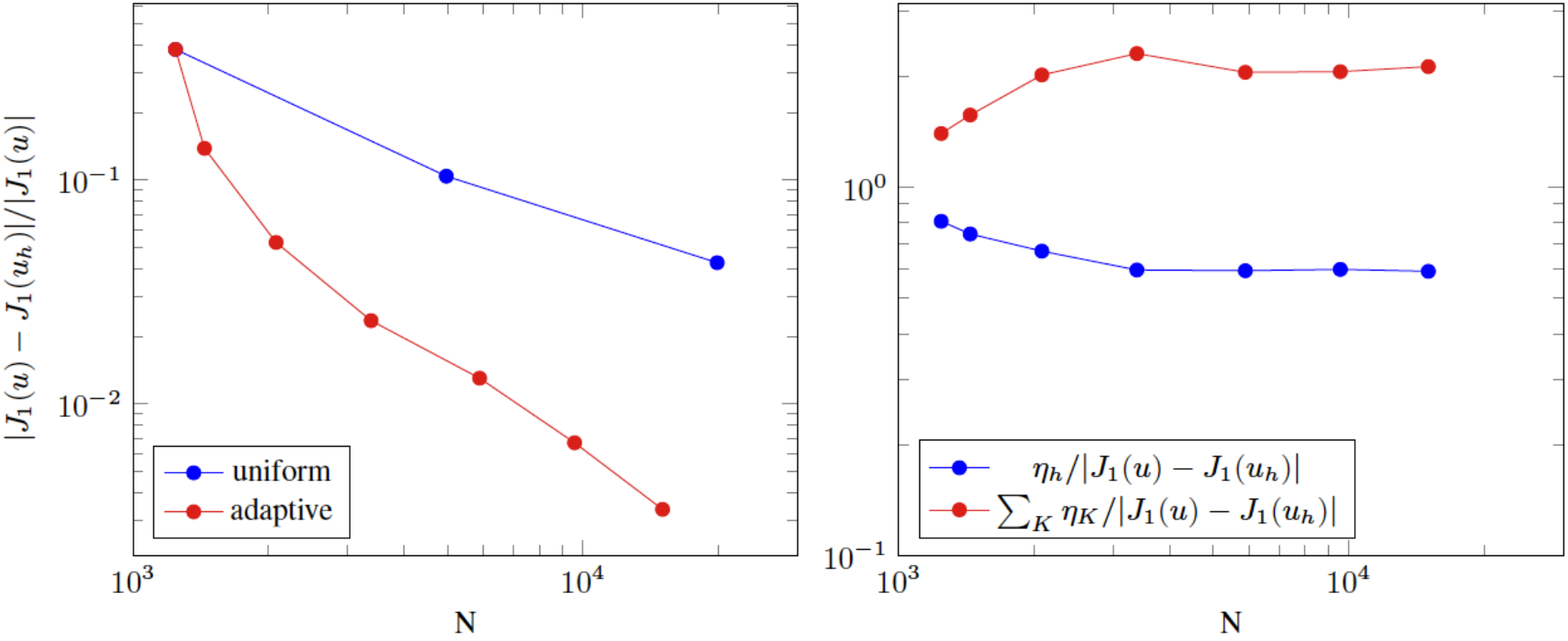

A
1 mm
IVUS – Plaque # 1
B
Necrotic core
Fibrosis
Real contours


Region of interest
Fixed





Effectivity



uniform vs. adaptive (left) / efficiency (right)

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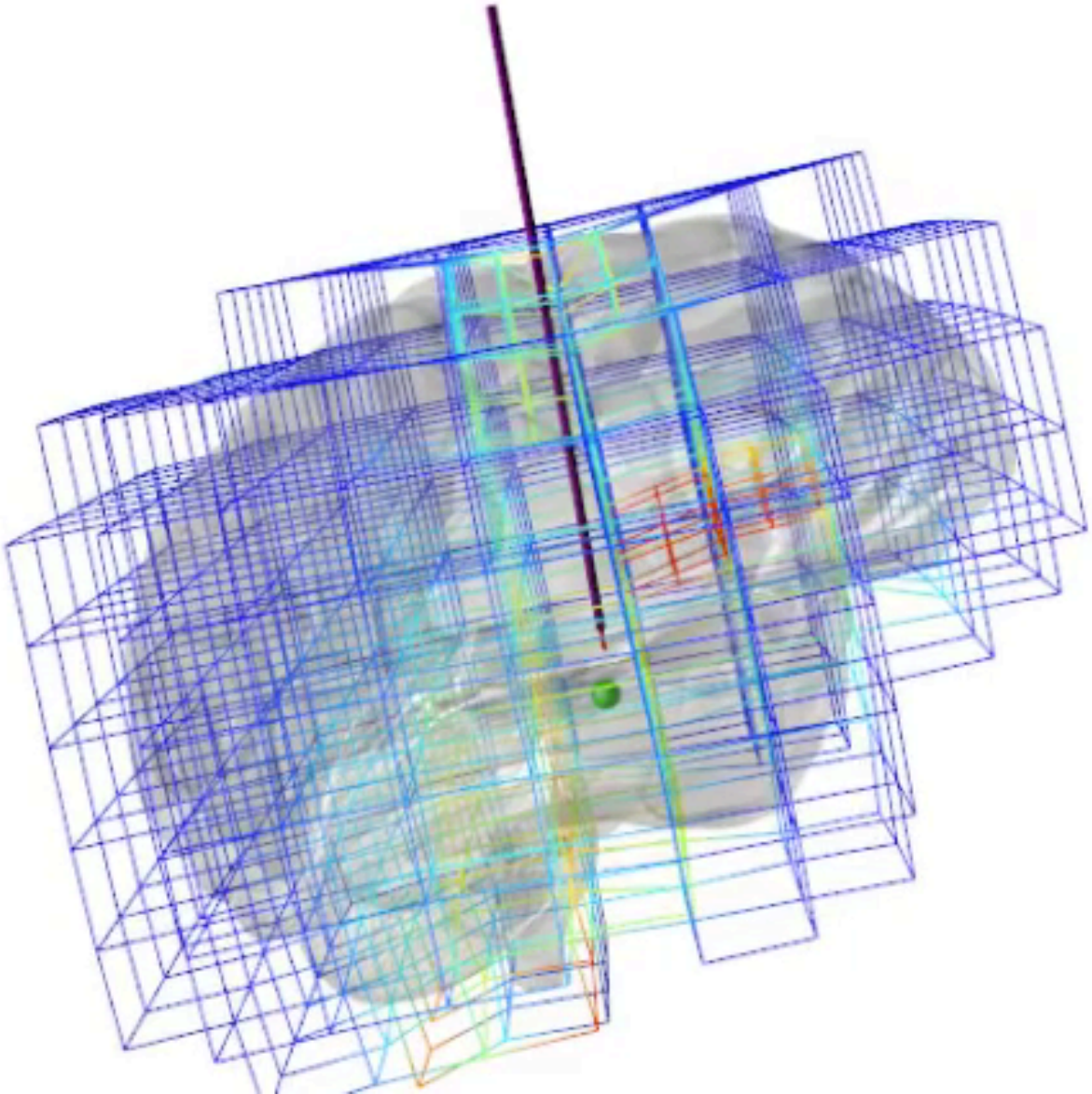
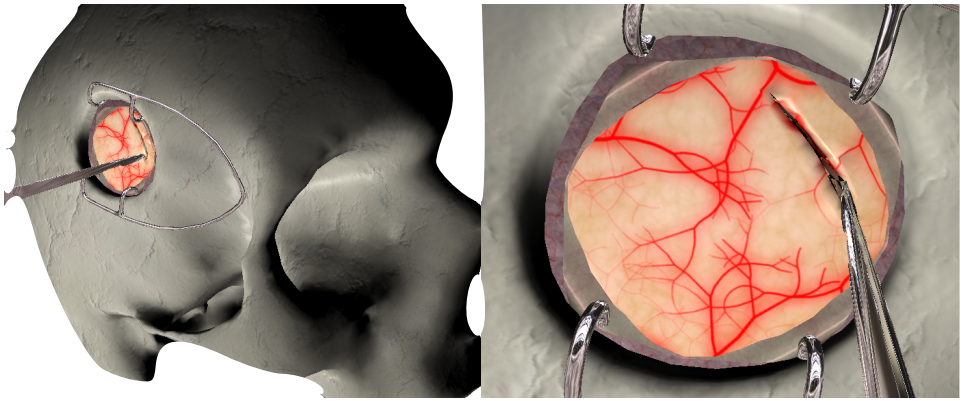
Cannula insertion



NEXT CHALLENGES

ERC RealTCut
Train surgeons safely on simulators

- Generic material models: *a priori.*
- Errors in quantities of interest for cuts in linear materials.
- Interactive simulations (solution in ms).

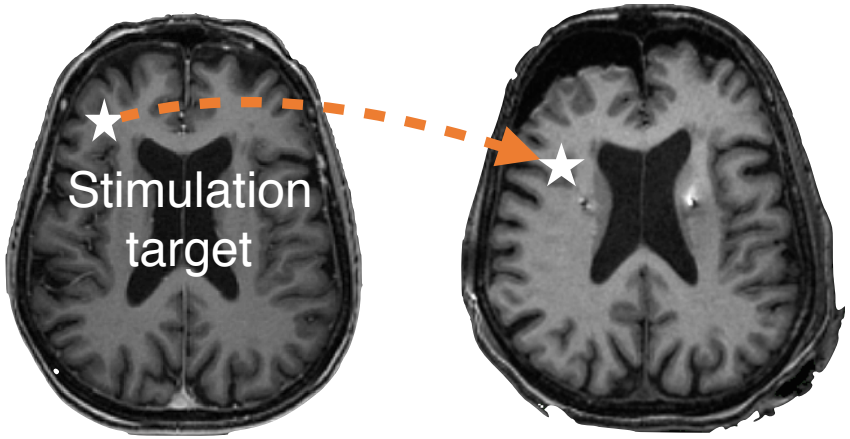


Courtecuisse, 2014, Implicit method for cutting in real-time. MEDIA

A generic organ is sufficient.

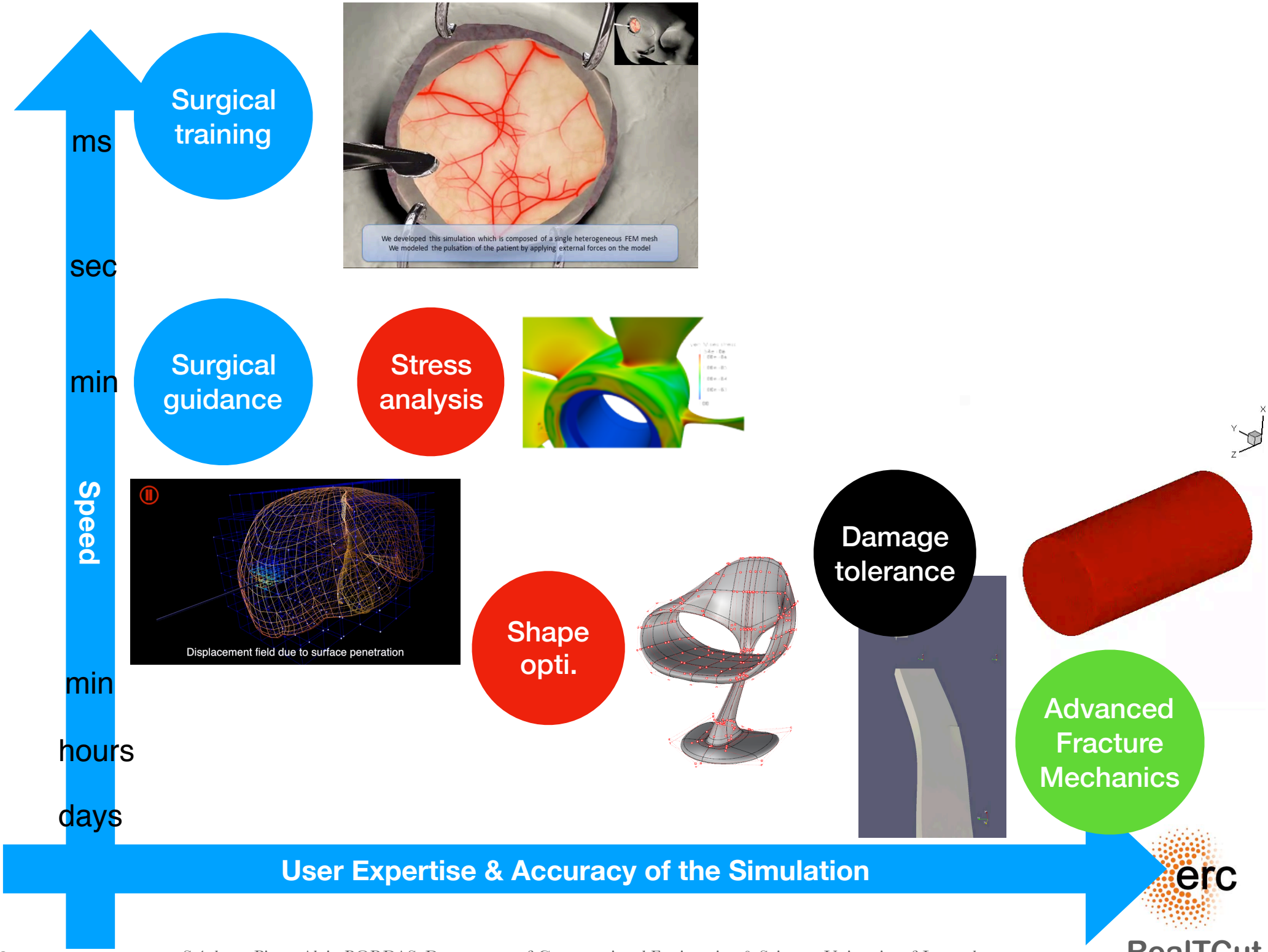
Future
Surgical assistance and planning

- Data-driven material models (real-time).
- Error control in quantities of interest for strong non-linearities, multi-field…
- Clinical time scales (solution in minutes).



Predict shift of brain target.

Patient specificity is



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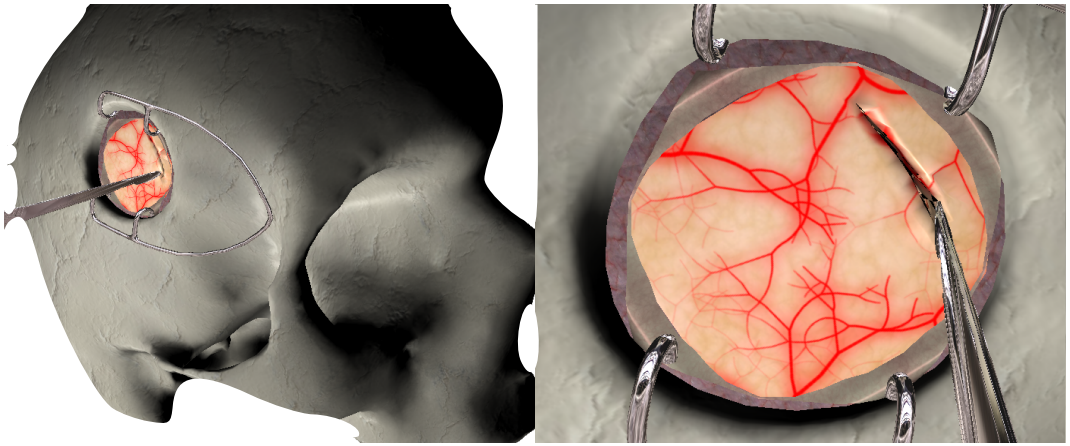
Surgical simulation: train surgeons safely on simulators



ERC RealTCut Bordas, 2014, First implicit method for cutting in real-time (25 frames/second): ***error control***

Current standing after RealTCut

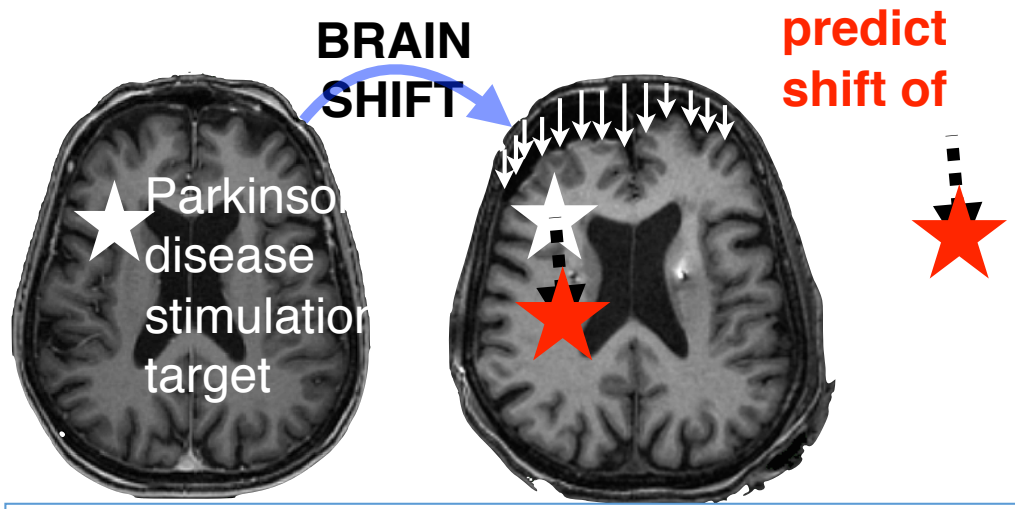
- Interactive cutting
- Multi-organ contact
- Generic material models
- Errors on quantities of interest for cuts in linear materials

erc

RealTCut

A generic organ is sufficient

inCERT: Surgical assistance and planning: guide with limited data



Non-rigid registration: *With Dr Frank Hertel, neurosurgeon, Luxembourg*

Beyond current capabilities

- Patient specific geometry & materials
- Error control for
  - contact
  - non-linear materials and multi-field
- Clinical time scales

Patient specificity is essential

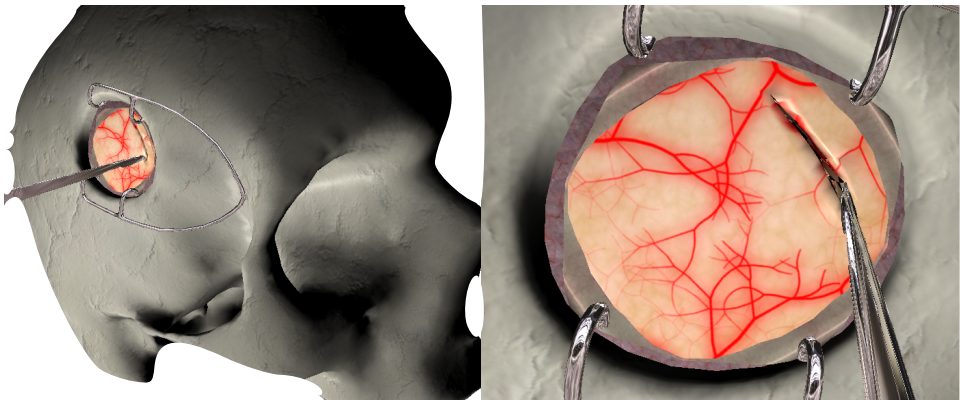
Today RealTCut, train surgeons safely on simulators

Current standing

- Generic
  - Material models,
  - Organ geometry.
- Errors in quantities of interest for cuts in linear materials.

RealTCut

A generic organ is sufficient.



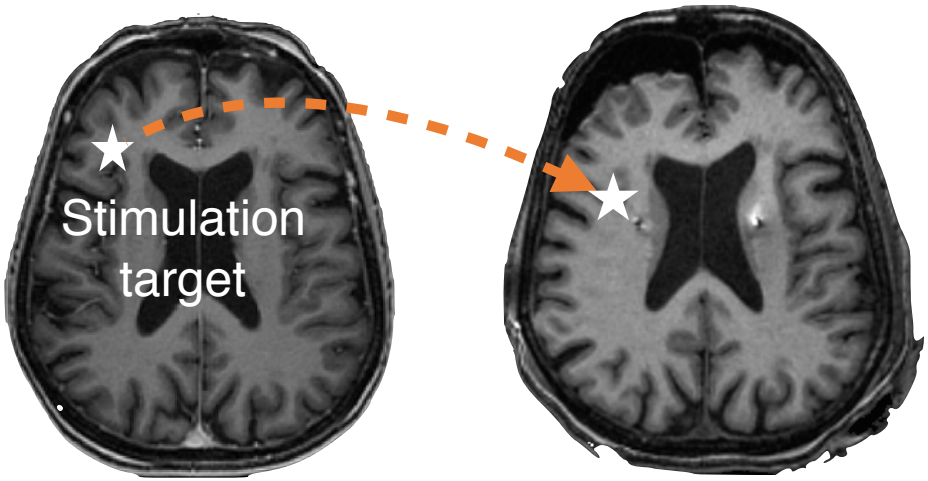
Bordas, 2014, First implicit method for cutting in real-time.

Tomorrow inCERT: Surgical assistance and planning: guide with limited data

Beyond current capabilities

- Patient-specific
  - Material models,
  - Organ geometry.
- Error control in quantities of interest for
  - contact,
  - non-linear materials and multi-field.

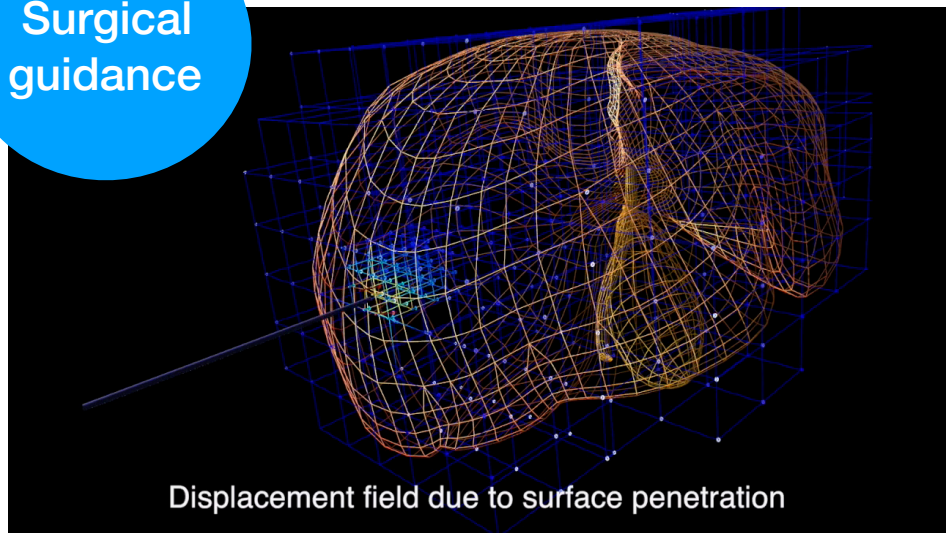
Patient specificity is



Predict shift of brain target.

From surgical training to surgical planning and assistance

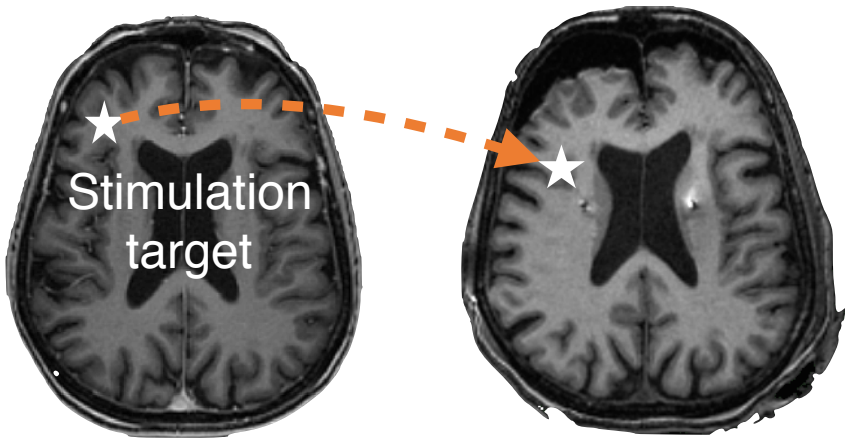
Surgical guidance



QUESTION: What (material) model should be used for a given patient?

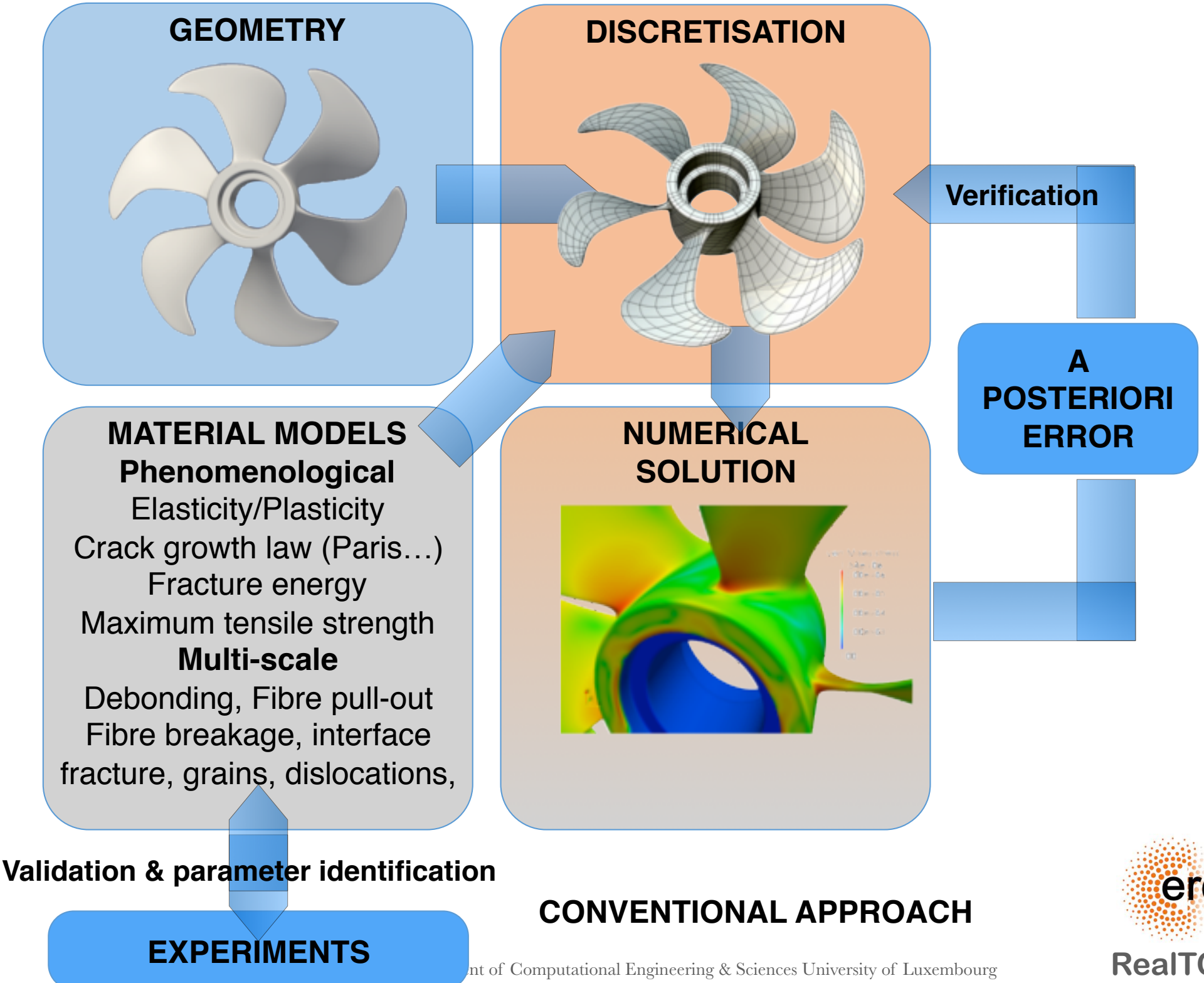
Future
Surgical assistance and planning

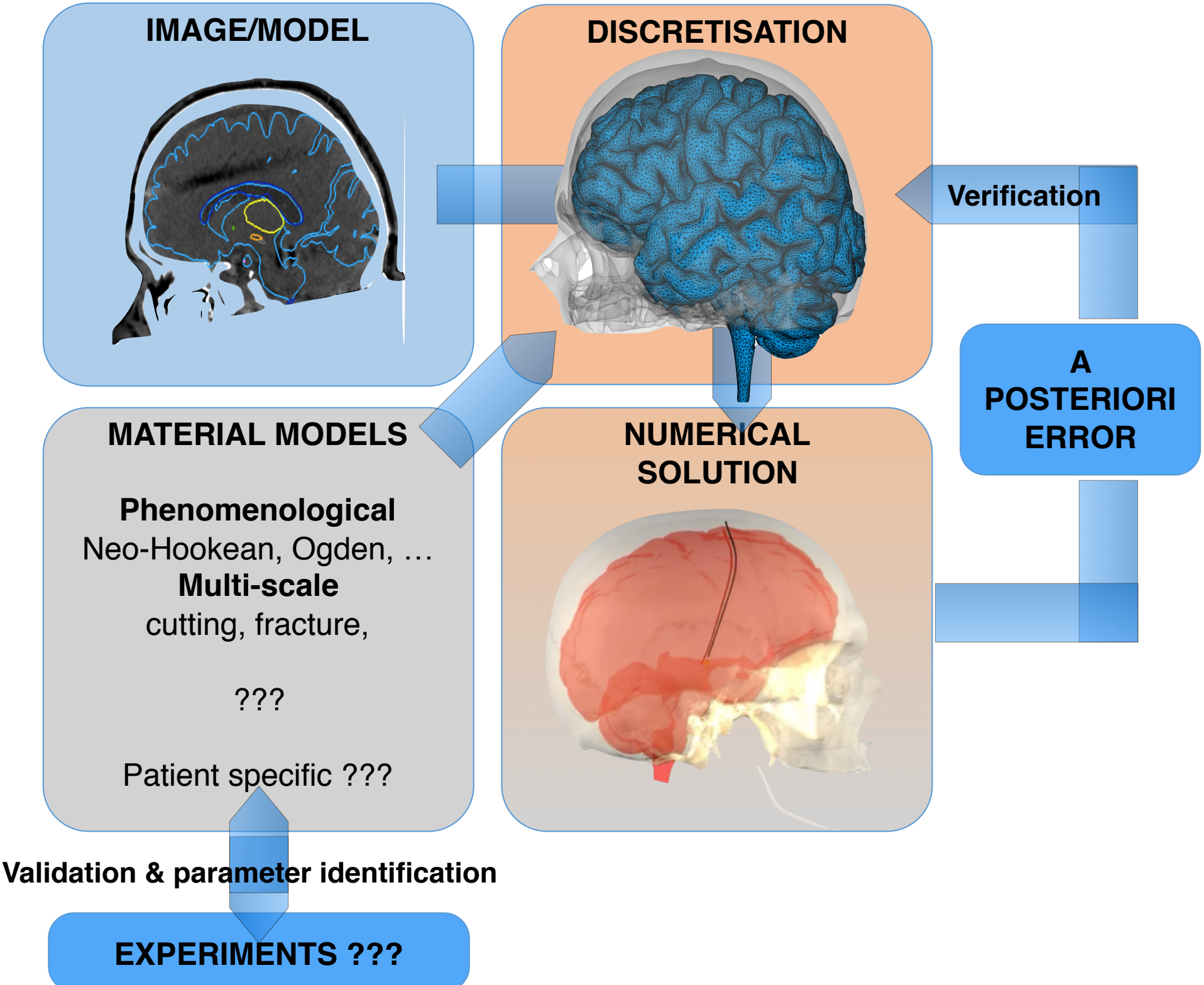
- Data-driven material models (real-time).
- Error control in quantities of interest for strong non-linearities, multi-field…
- Clinical time scales (solution in minutes).



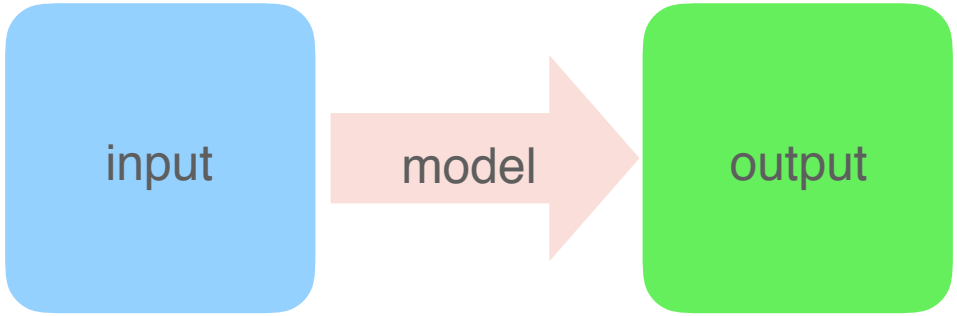
Predict shift of brain target.

Patient specificity is


GEOMETRY
DISCRETISATION
Verification
A POSTERIORI ERROR
MATERIAL MODELS
Phenomenological
Elasticity/Plasticity
Crack growth law (Paris…)
Fracture energy
Maximum tensile strength
Multi-scale
Debonding, Fibre pull-out
Fibre breakage, interface
fracture, grains, dislocations,
NUMERICAL SOLUTION
Validation & parameter identification
EXPERIMENTS
CONVENTIONAL APPROACH
erc
RealTCut


IMAGE/MODEL
DISCRETISATION
Verification
A POSTERIORI ERROR
MATERIAL MODELS
Phenomenological
Neo-Hookean, Ogden, …
Multi-scale
cutting, fracture,
???
Patient specific ???
NUMERICAL SOLUTION
Validation & parameter identification
EXPERIMENTS ???

Data-driven Modelling



$$f : \mathbf{x} \rightarrow \mathbf{y}$$

The structure of f is known but its parameters are not.

There is no a priori knowledge about the function f available.

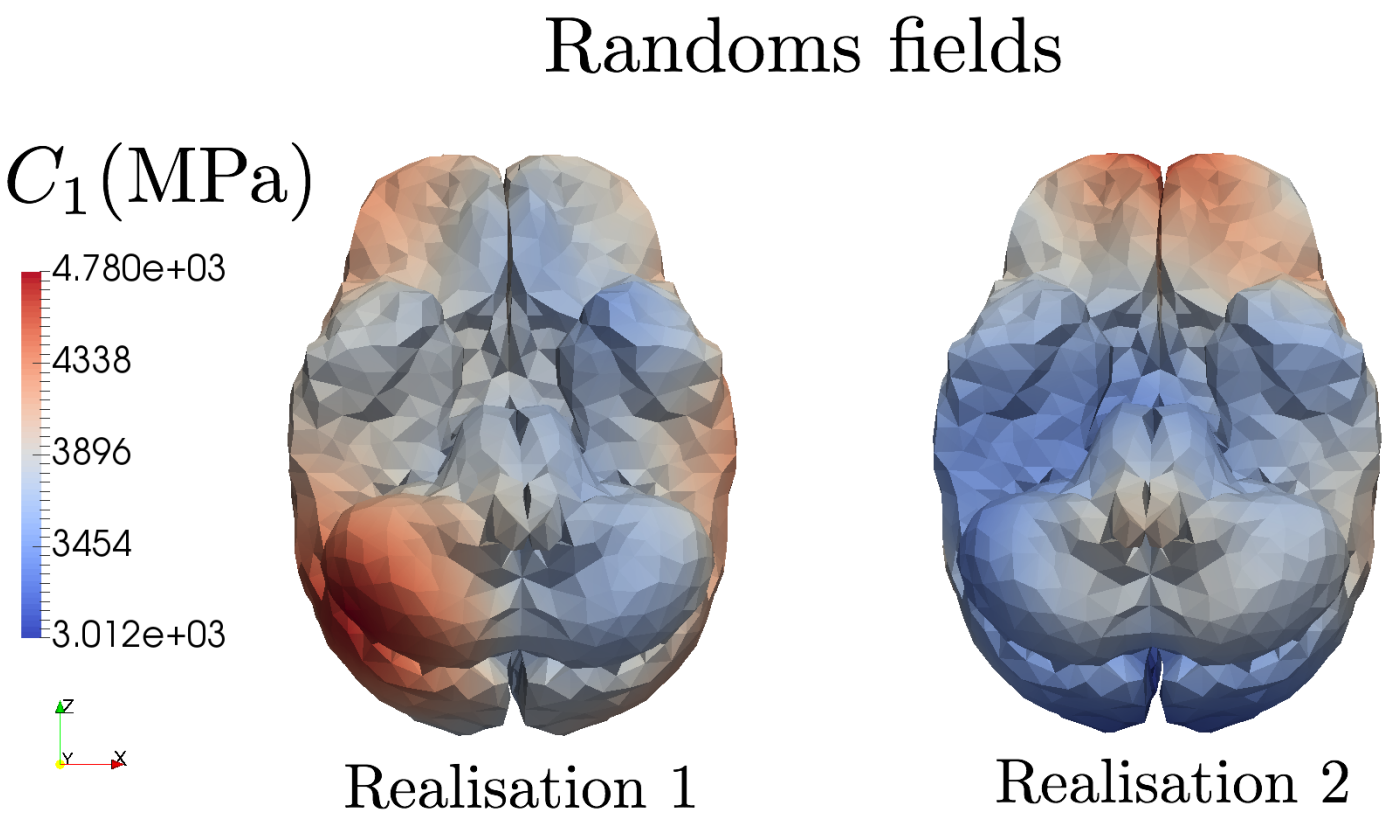
model calibration

model identification

Embrace the conceptual shift from *"model through data abstraction"* to *"data is the model"*.

Assuming the material model is representative, what is the influence of each parameter in the model?

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



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

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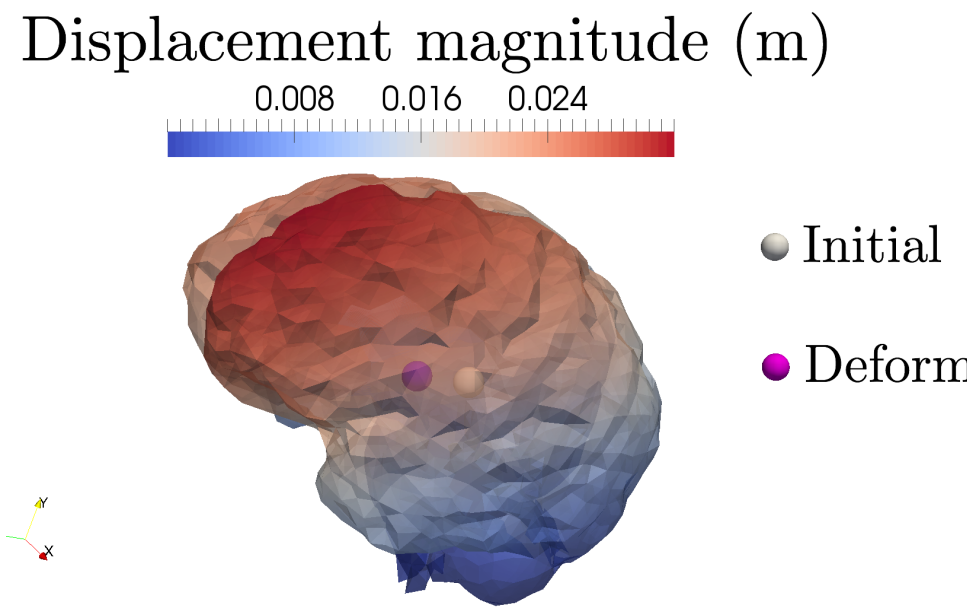
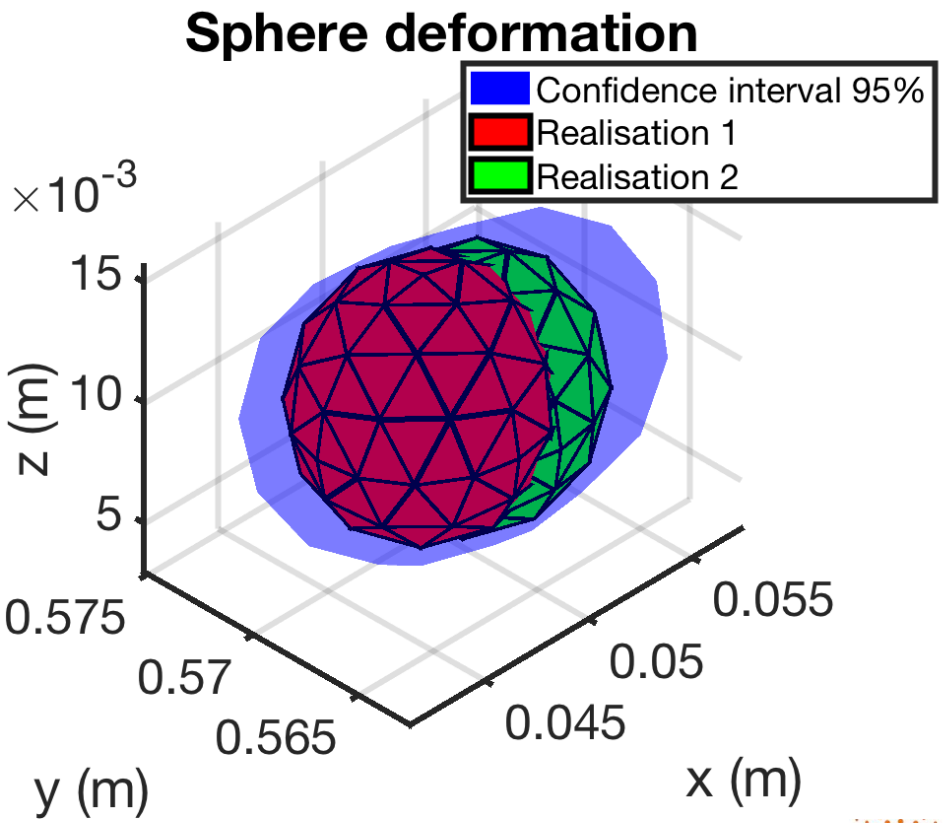
Confidence level in predicting the target location

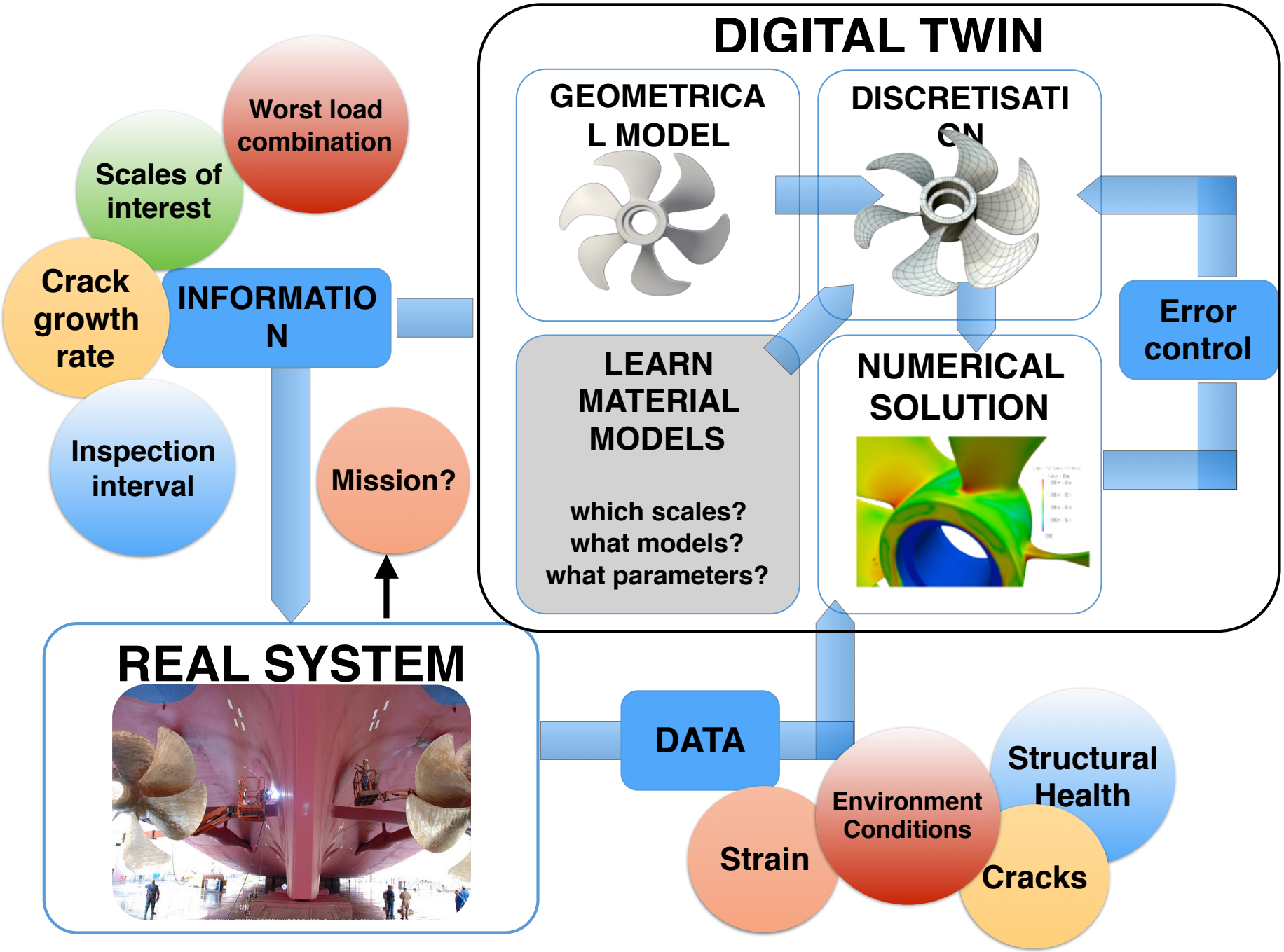


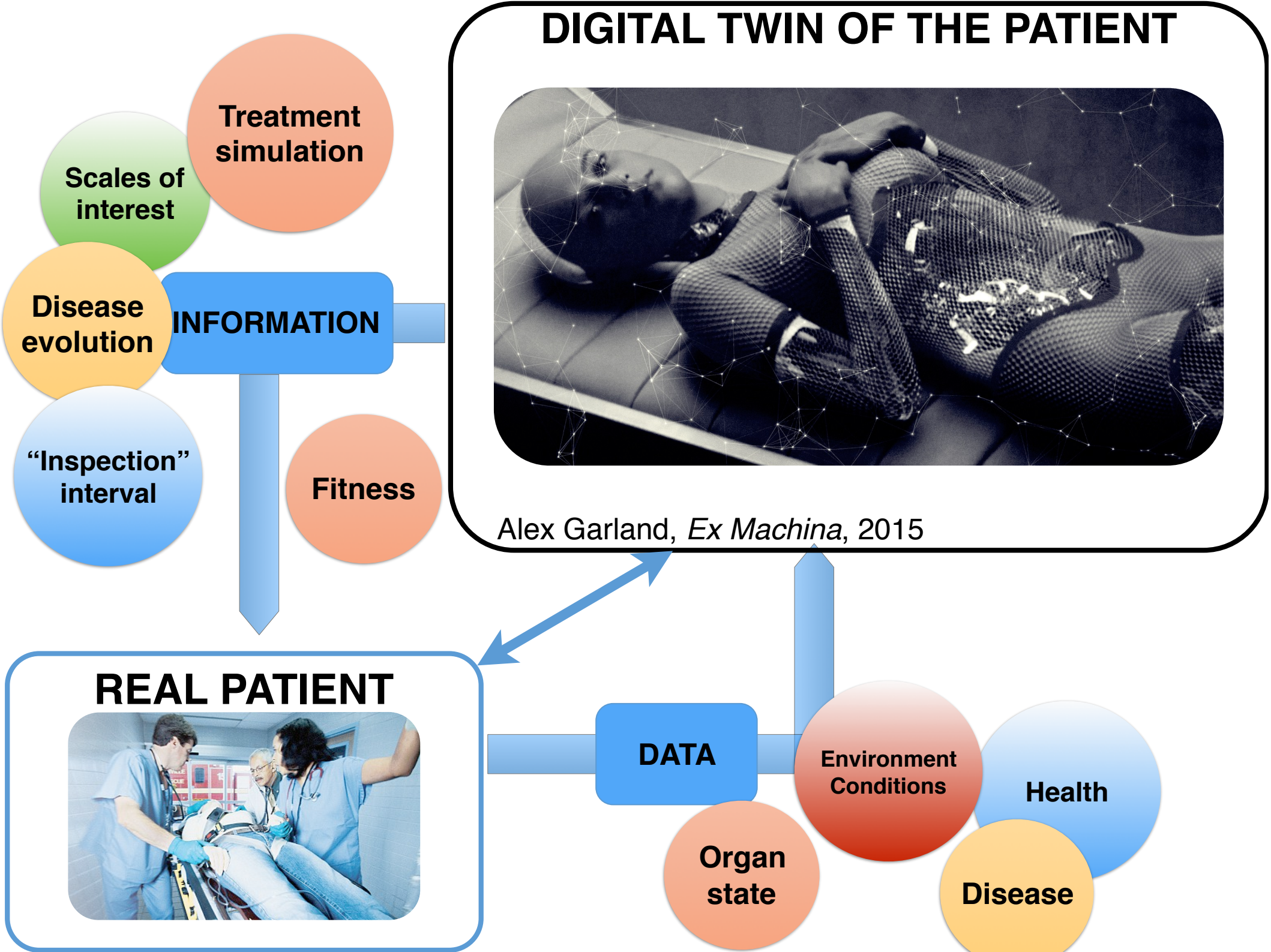


What is the influence of material parameters on computed quantities of interest?

Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg

Possible approach




DIGITAL TWIN OF THE PATIENT
Alex Garland, *Ex Machina*, 2015
Treatment simulation
Scales of interest
Disease evolution
INFORMATION
"Inspection" interval
Fitness
REAL PATIENT
DATA
Environment Conditions
Health
Organ state
Disease

Prior Knowledge

Prior Knowledge

Hypothesis

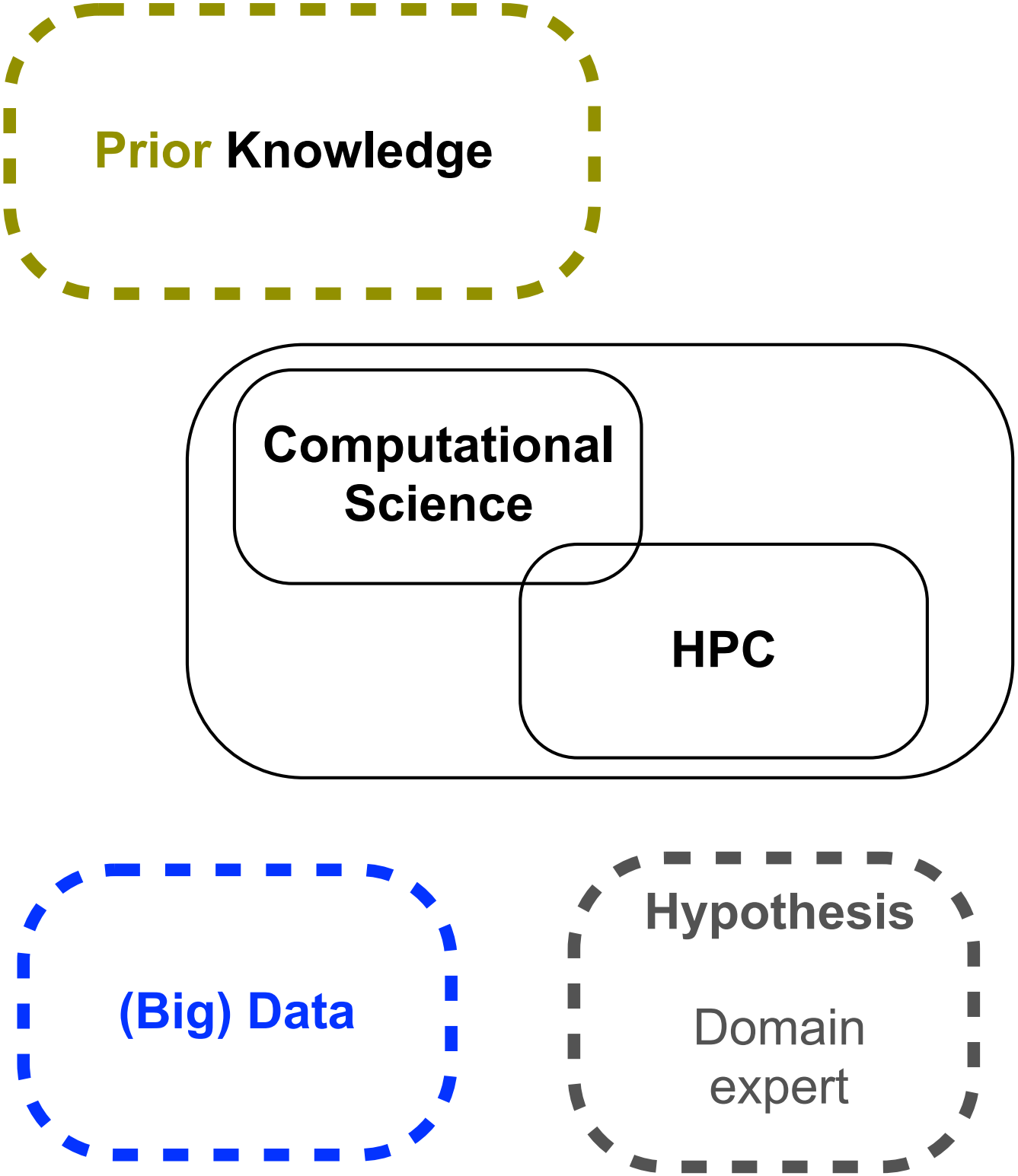
Domain expert

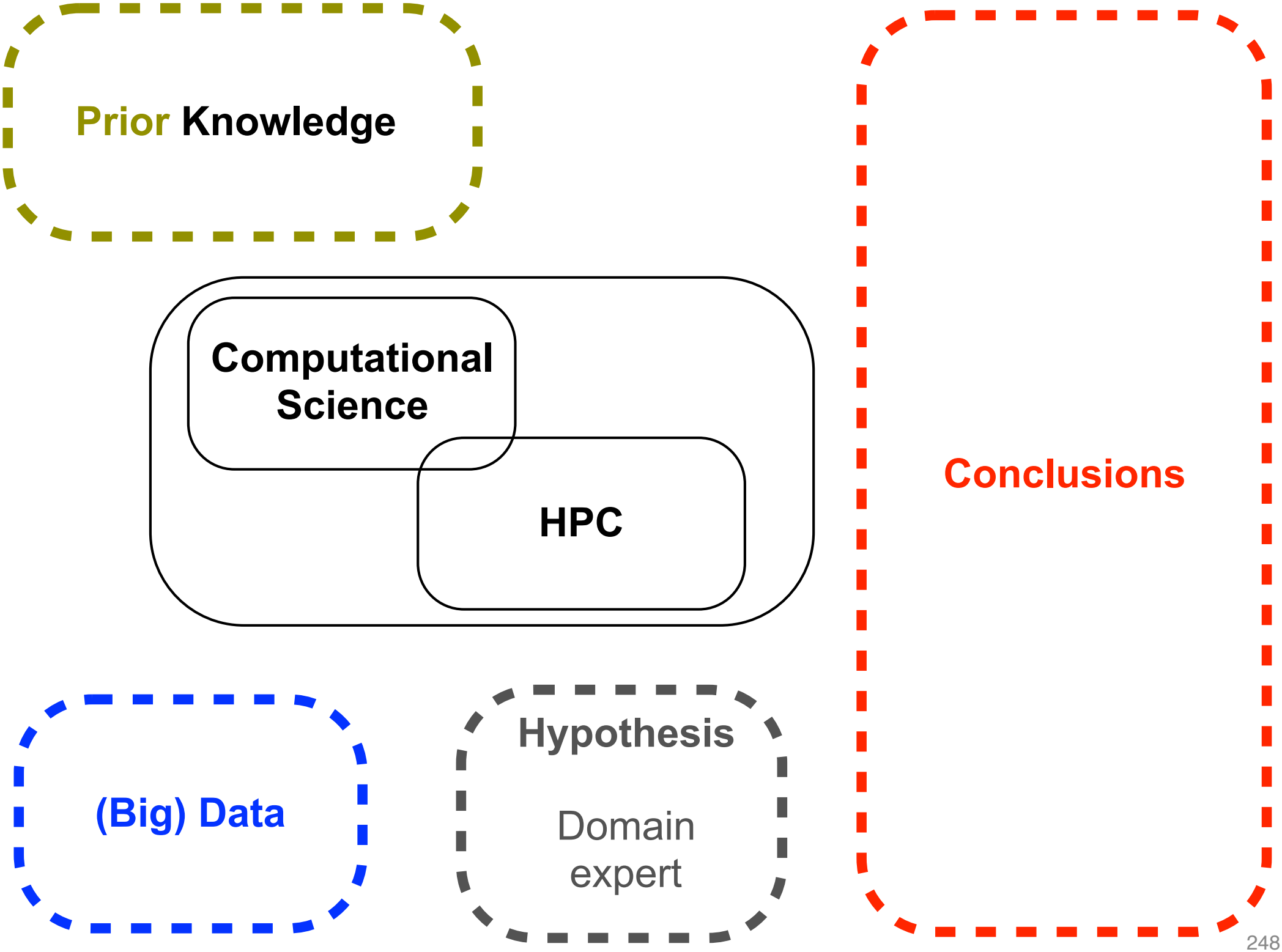
Prior Knowledge

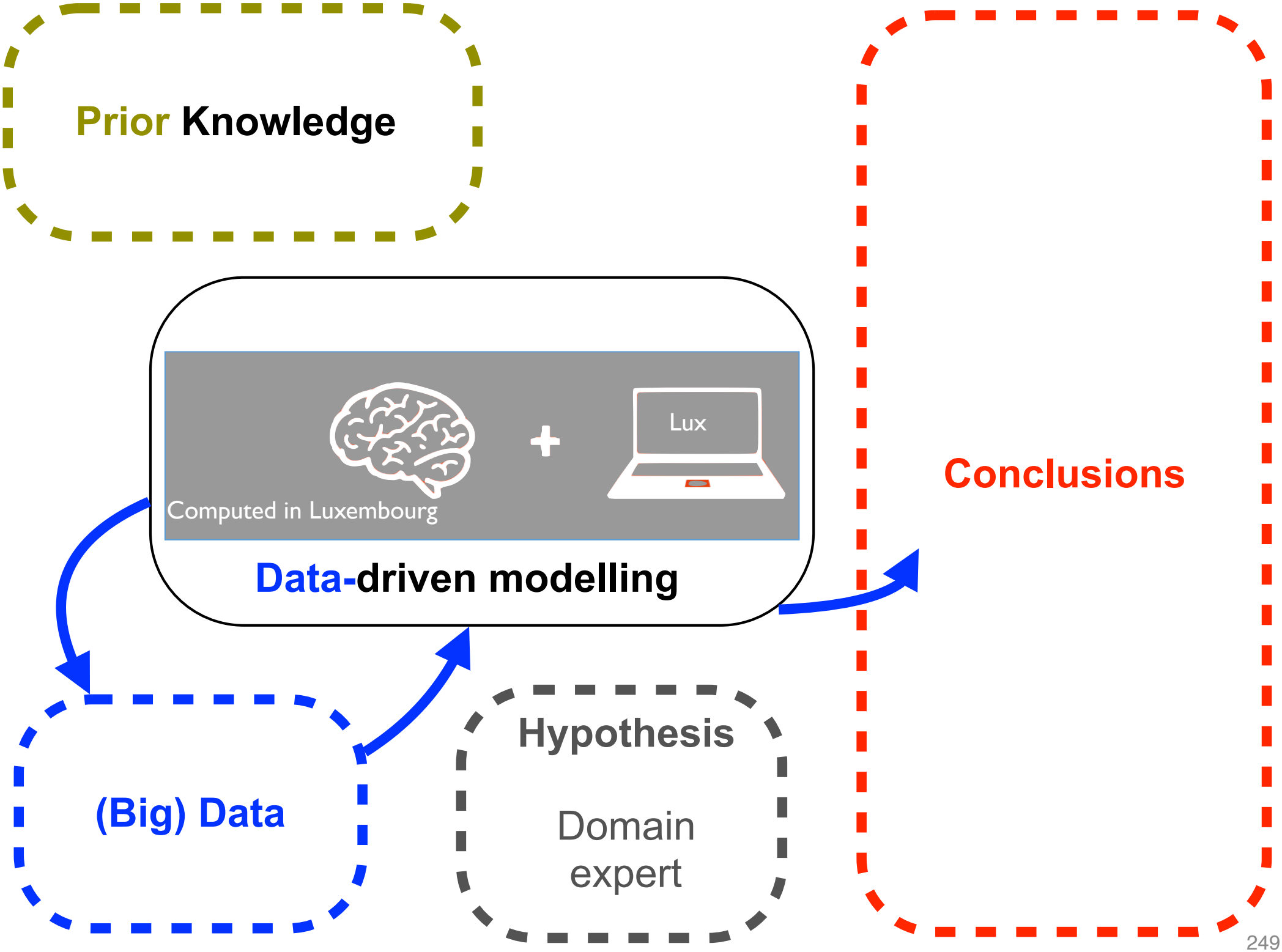
(Big) Data

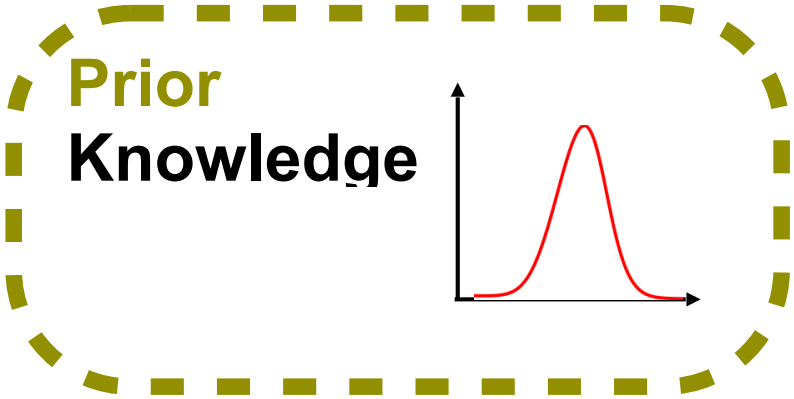
Hypothesis

Domain expert


Prior Knowledge
Computational Science
HPC
(Big) Data
Hypothesis
Domain expert


Prior Knowledge
Computational Science
HPC
Conclusions
(Big) Data
Hypothesis
Domain expert


Prior Knowledge
Lux
Computed in Luxembourg
Data-driven modelling
Conclusions
(Big) Data
Hypothesis
Domain expert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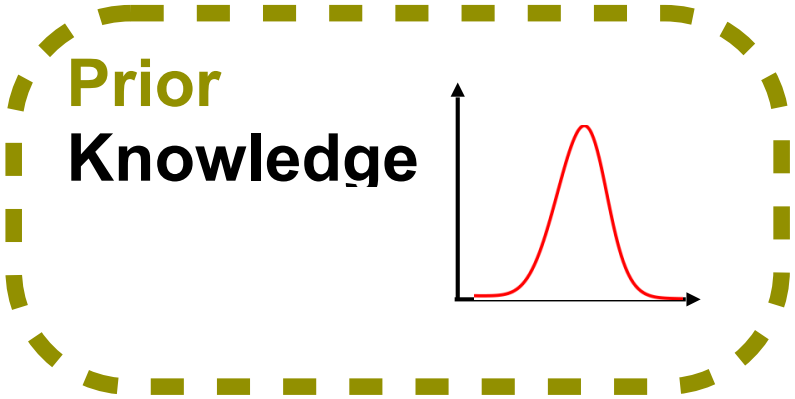
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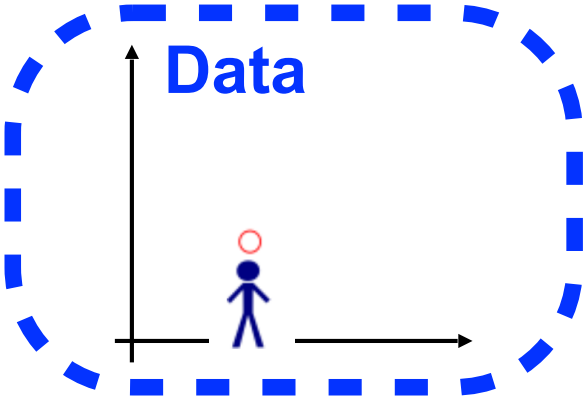
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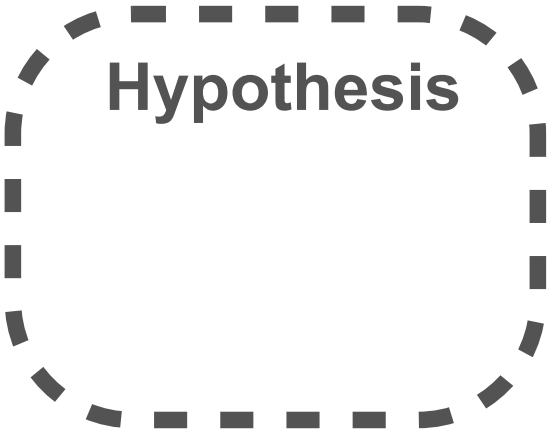
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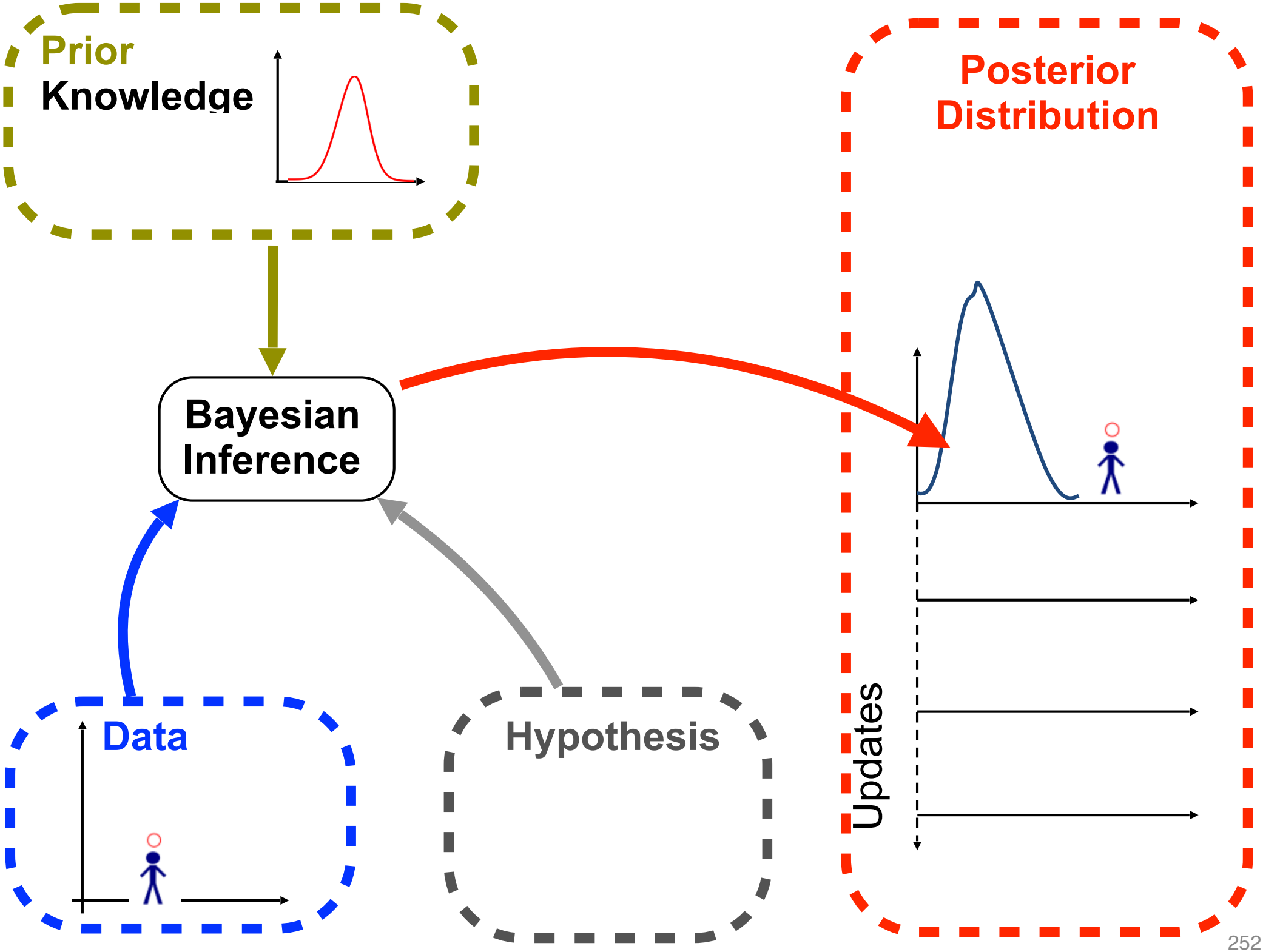
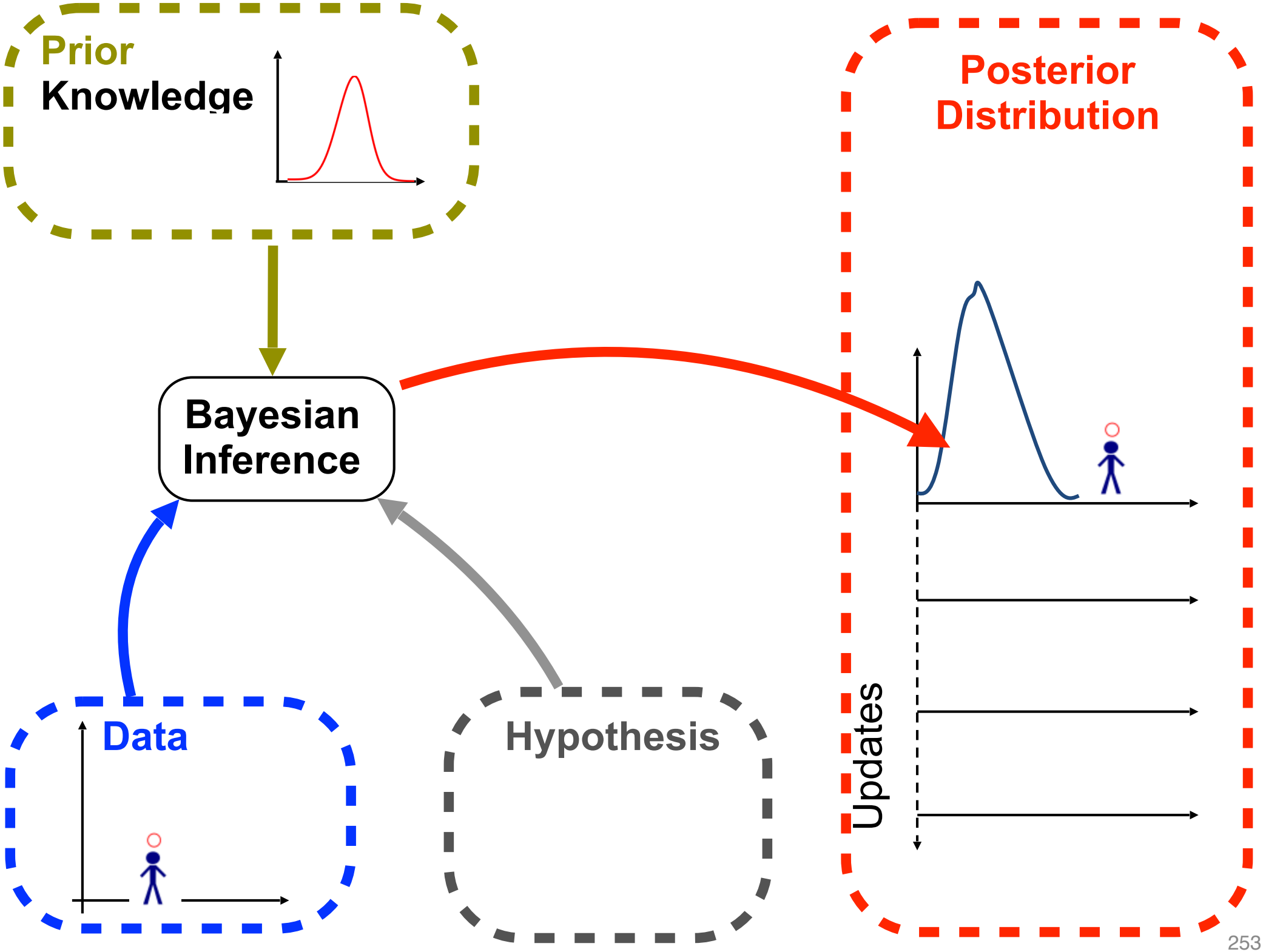

Prior
Knowledge
Posterior
Distribution
Bayesian
Inference
Updates
Data
Hypothesis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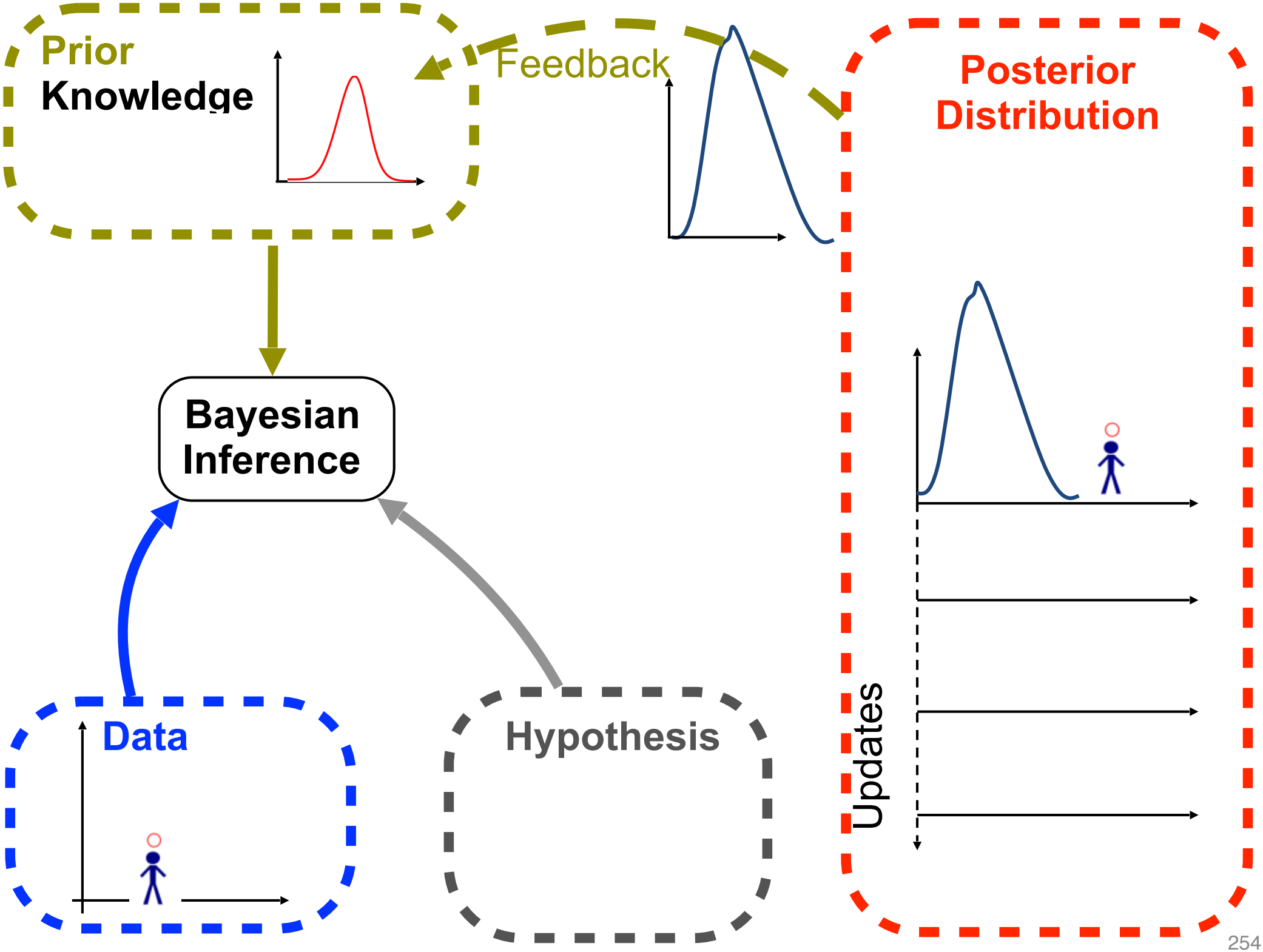
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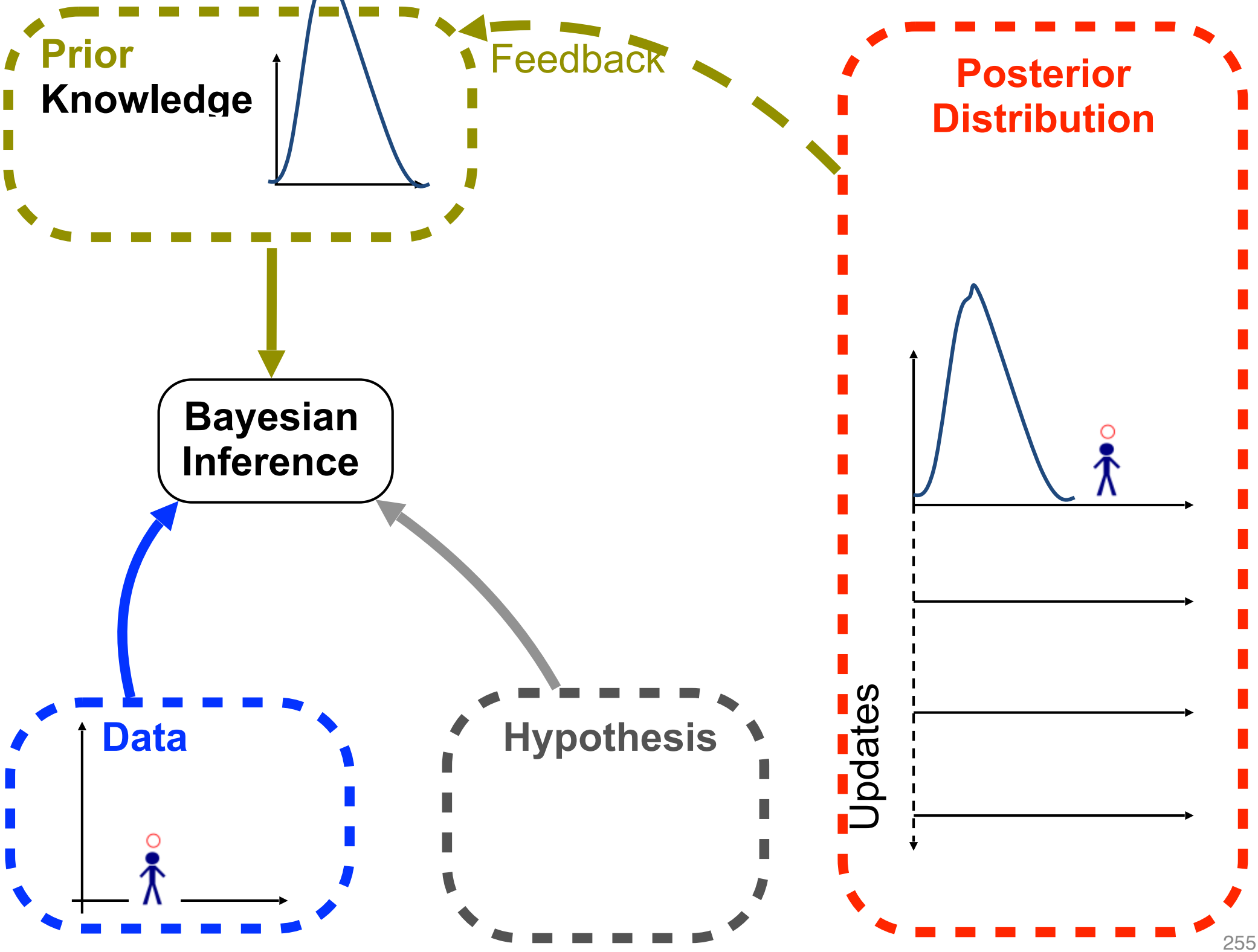
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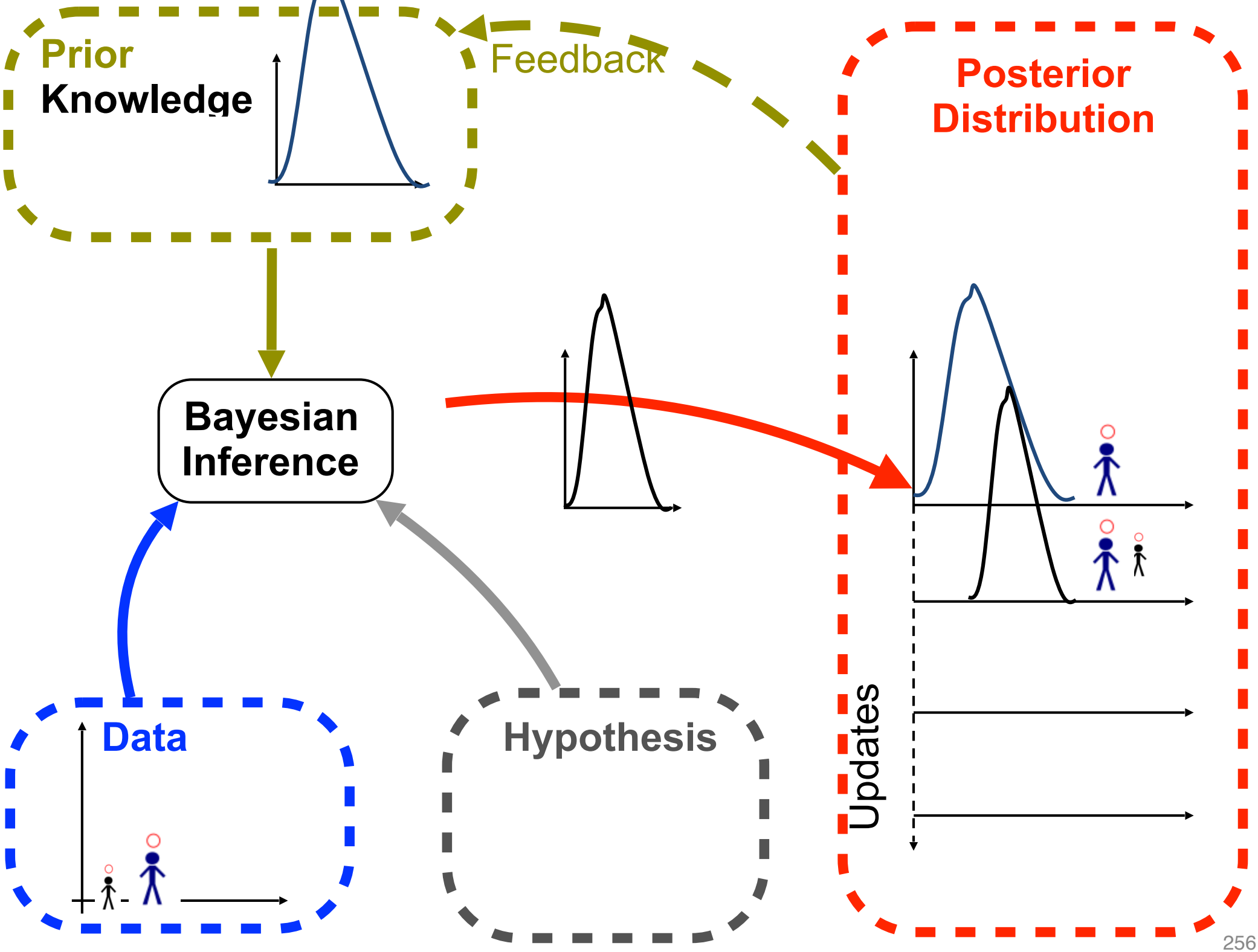
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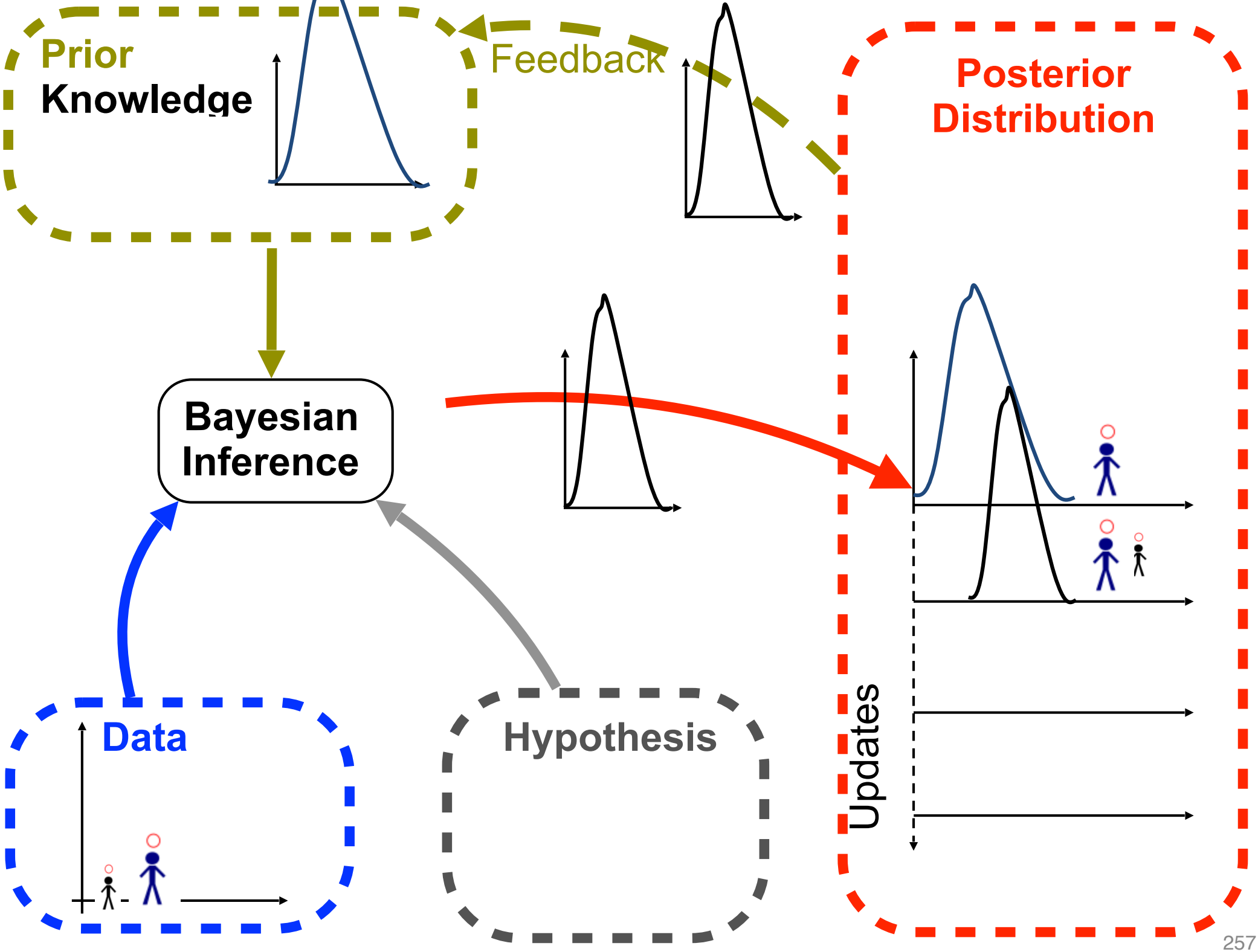
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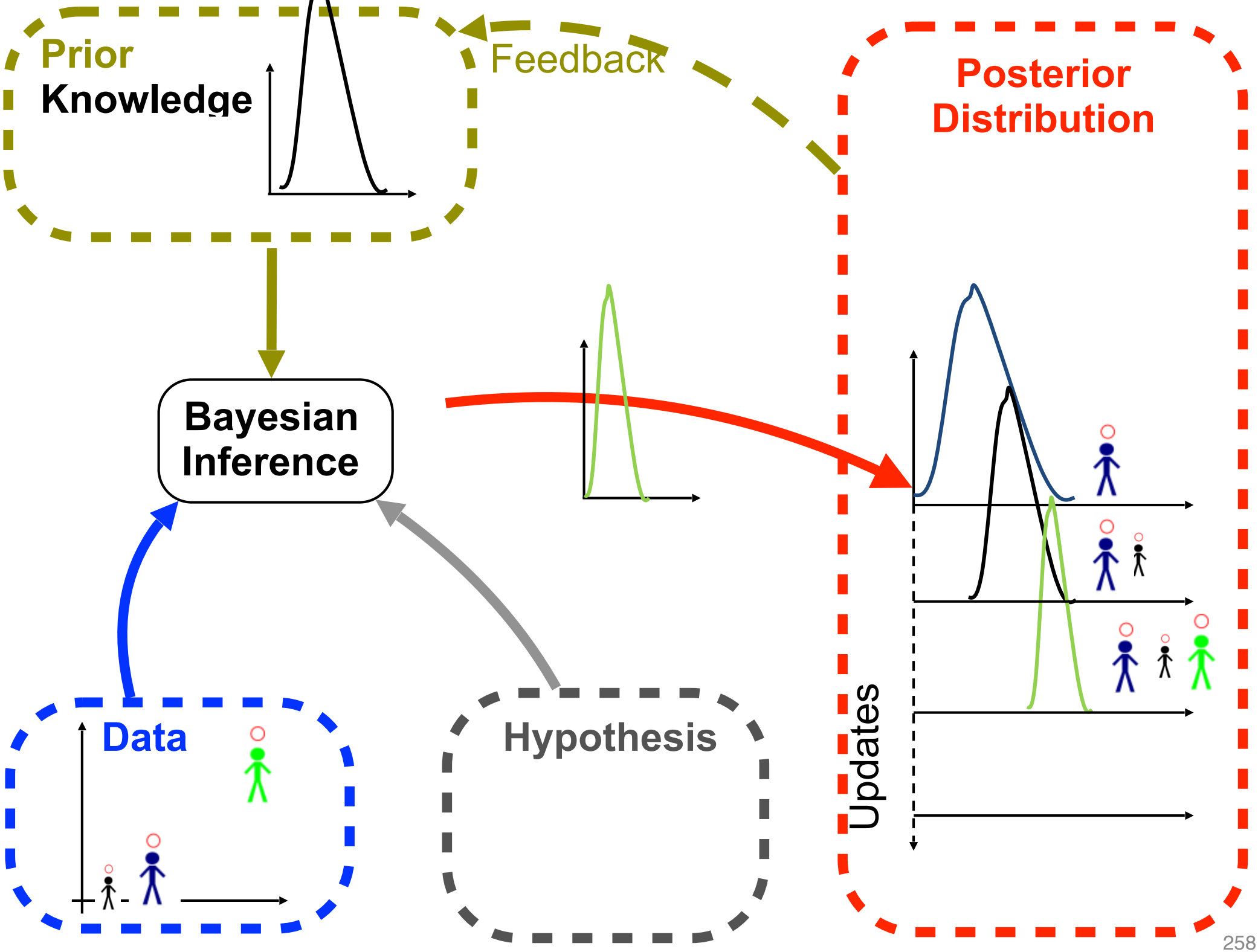
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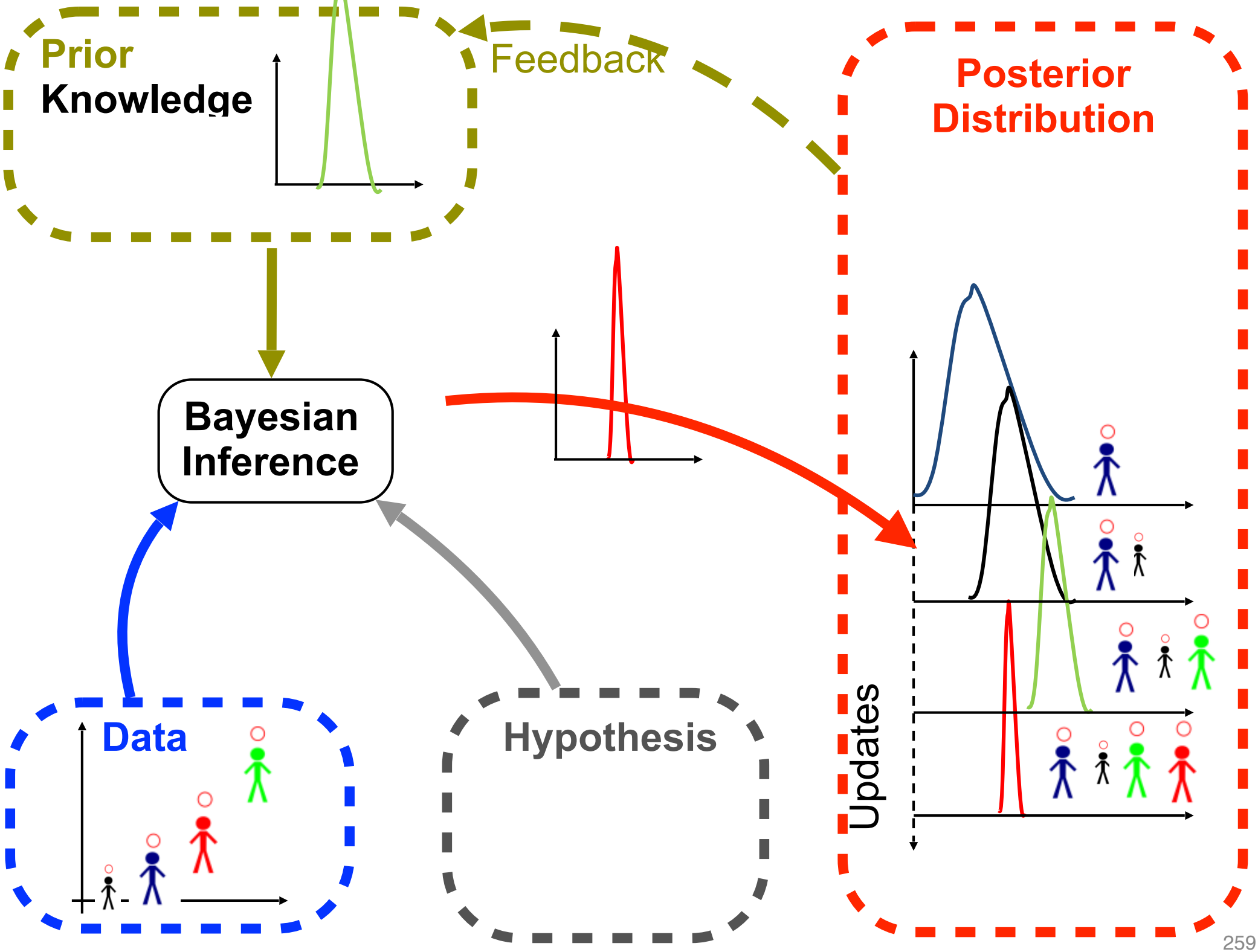
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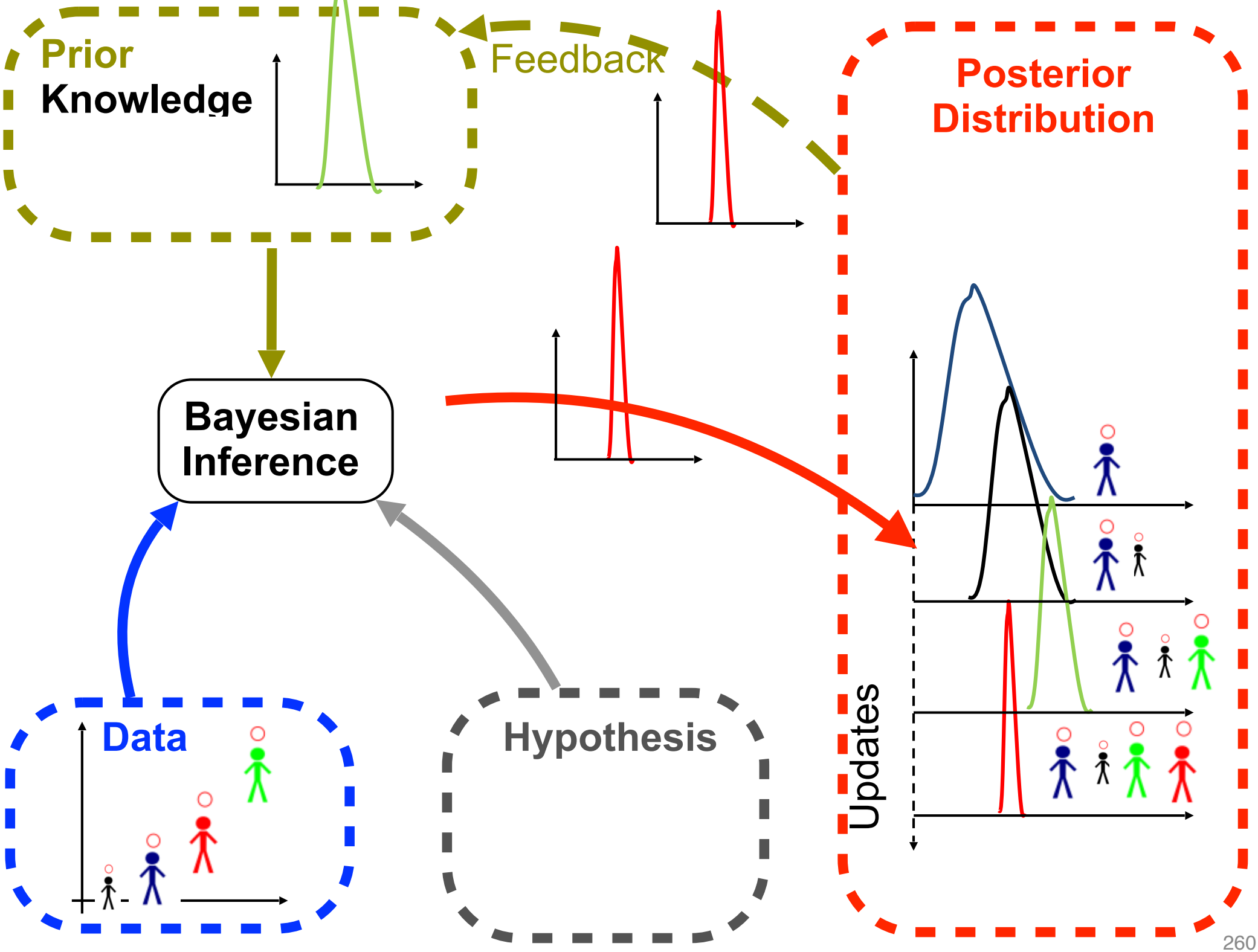
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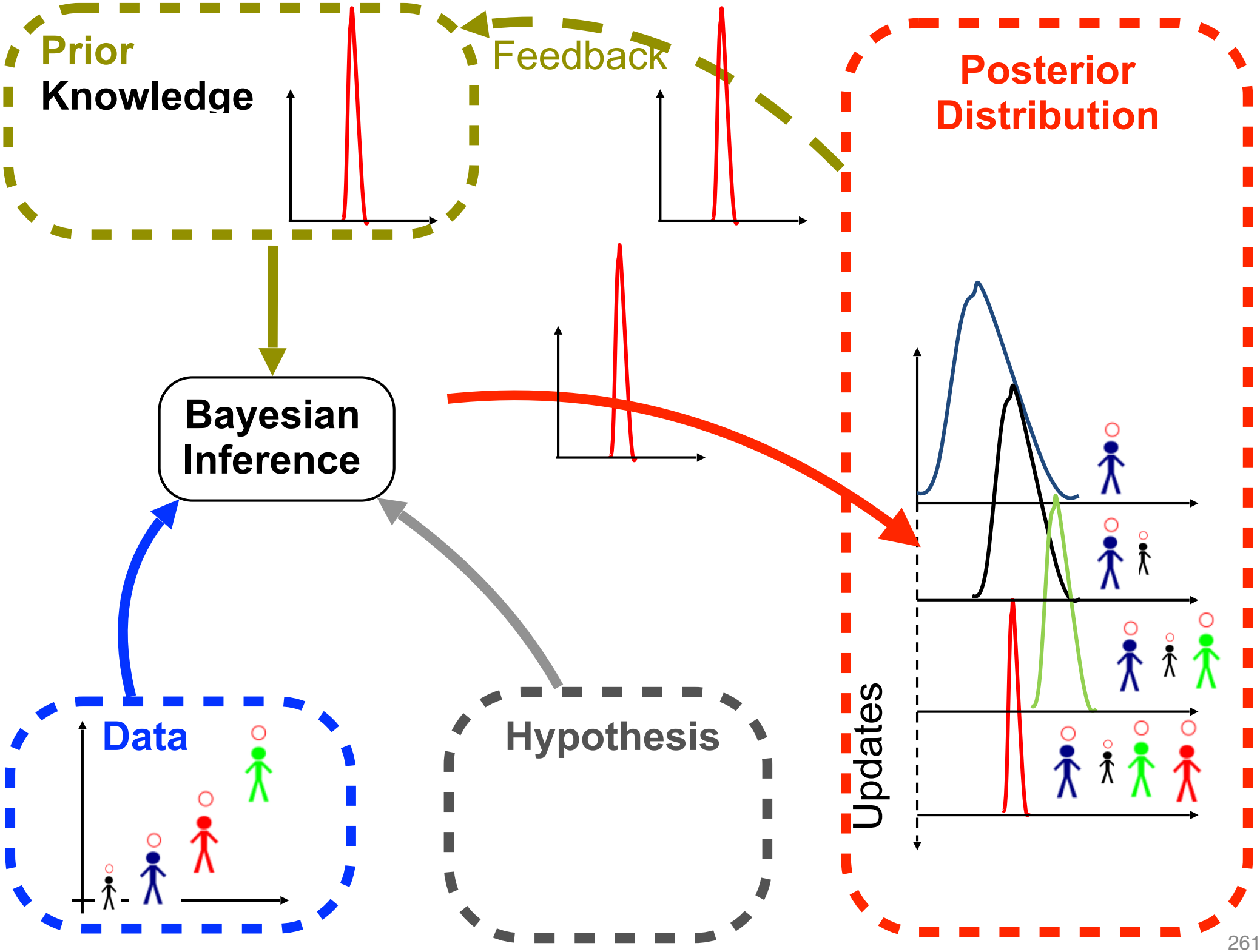
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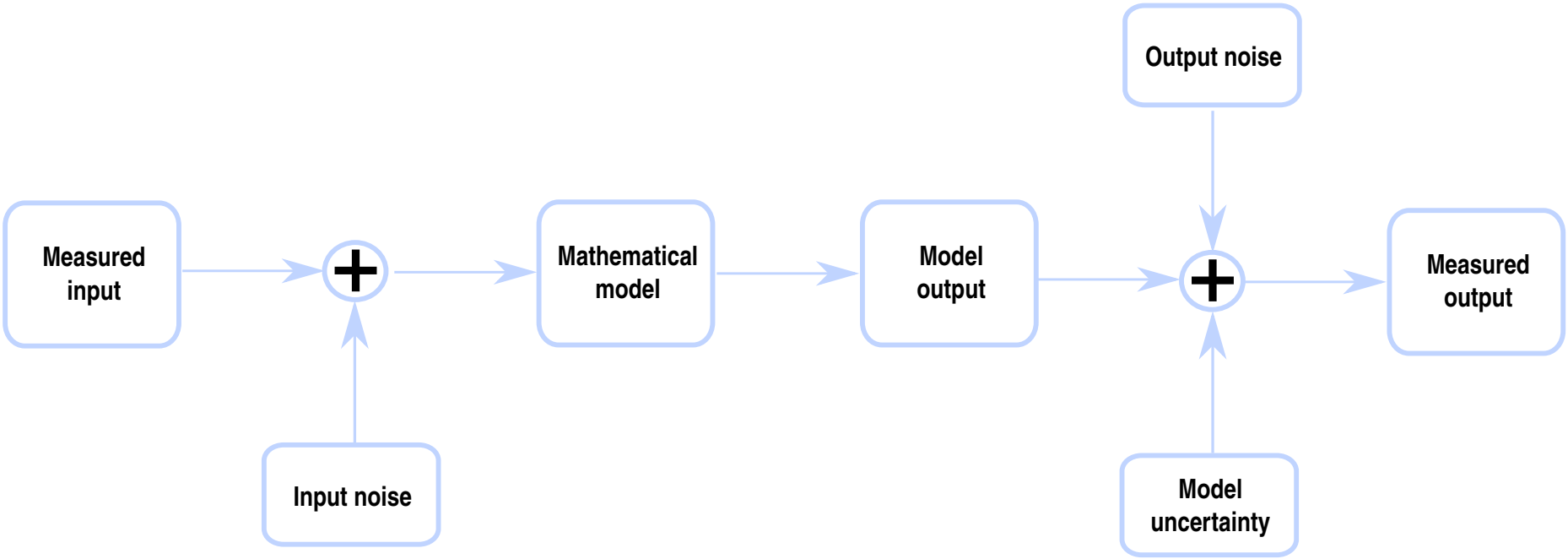
Updates

Uncertainties and errors in parameter identification



Uncertainties and errors in parameter identification

Uncertainty in Observations only

$$y = F(x, \theta) + \omega_{\text{obs}}$$

Model uncertainty and uncertainty in observation only

$$\begin{cases} y = y_{\text{true}} + \omega_{\text{obs}} \\ y_{\text{true}} = F(x, \theta) + \delta(x) \end{cases}$$

Model uncertainty and uncertainty in both observation and input

$$\begin{cases} y = y_{\text{true}} + \omega_{\text{obs}} \\ y_{\text{true}} = F(x, \theta) + \delta(x) \\ x^* = x + \omega_{\text{input}} \end{cases}$$

Note: We only have "y" and "x*" from our experiments.

Conclusions

❖Different sources of uncertainty can be considered in an identification problem (here we have considered the uncertainties in the output, input and model response).

Incorporating the model uncertainty as well as the error in the input increases the chance that resulting distribution (so-called posterior) includes the true value of the parameter of interest.

❖ Incorporating these uncertainty sources furthermore, result to wider prediction intervals which therefore contain more measurements.

❖ If the difference between the true response, and the response of the material model increases incorporating the model uncertainty improves the data coverage for interpolation. However, this **is not** necessarily the case for extrapolation.

❖In the case above the added value of incorporating the input error as well reduces substantially.

See Hussein Rappel, Lars Beex, Jack Hale, SPAB 2017, 2018

Conclusions

- **Understanding and optimisation of fracture of heterogeneous materials**
  - multi-scale methods are being developed
  - these methods are expensive
  - model selection remains an open problem
  - variability of the material properties exacerbate these difficulties
  - taking into account realistic situations remains elusive
  - coupling with sensing systems may be the future

... mechanical twinning

real-time simulations could also help engineers gain insight into complex non-intuitive phenomena by allowing to probe, quickly, the parameter space and design space