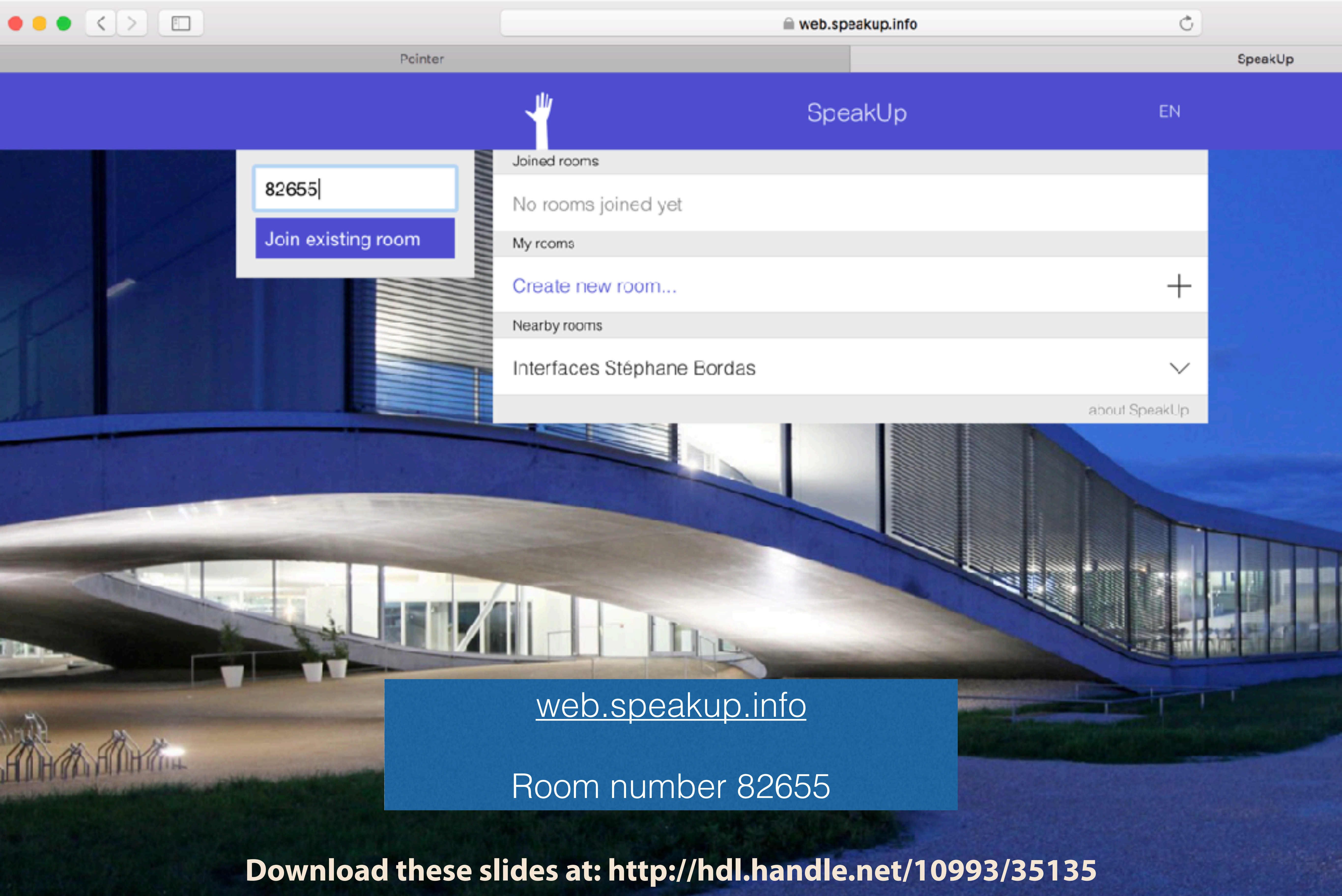
Numerical methods for free boundary problems

and data-driven modelling

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

Oxford Engineering Mechanics Seminar 2018 03 05



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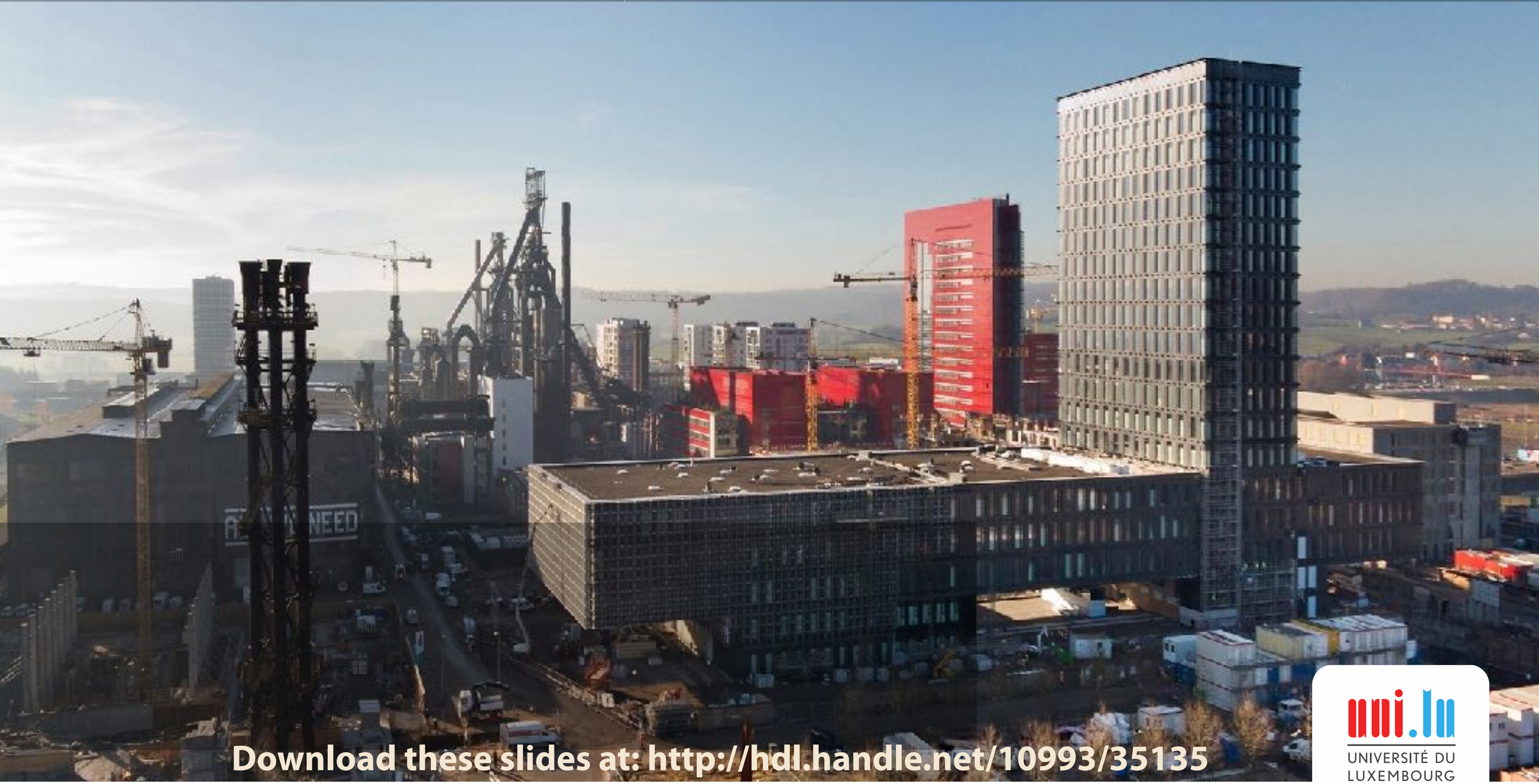
Computational Sciences Luxembourg



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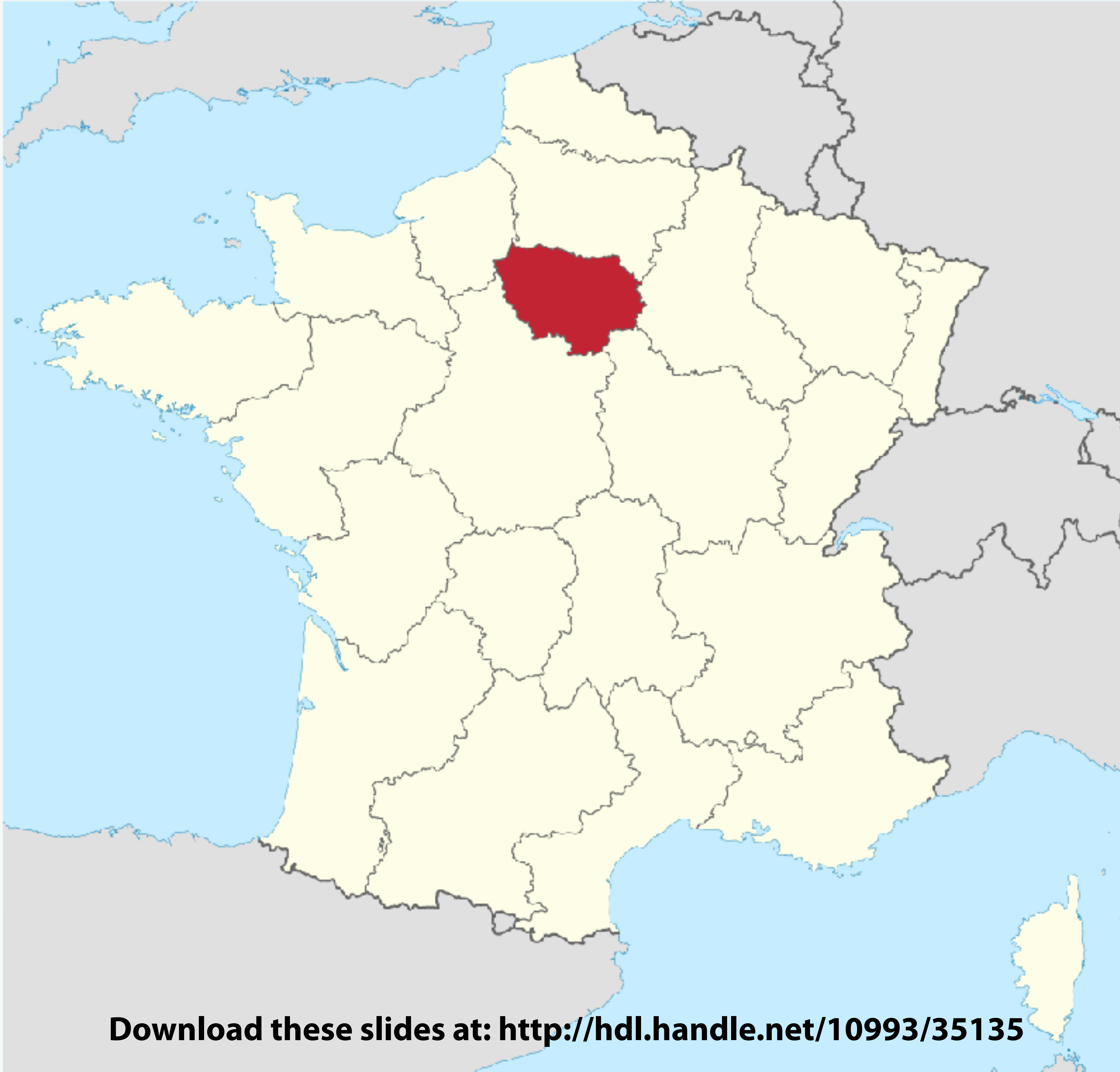

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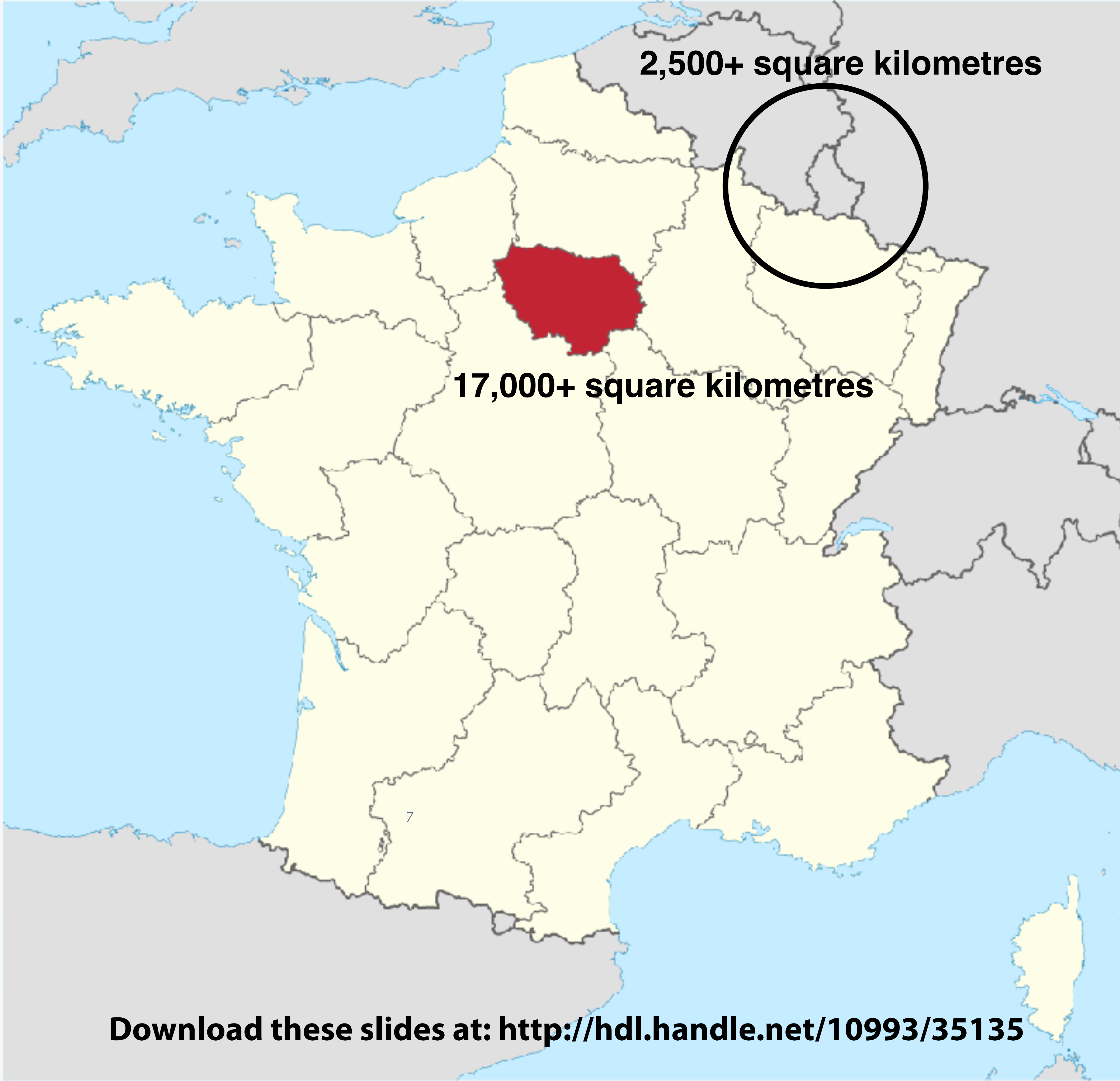

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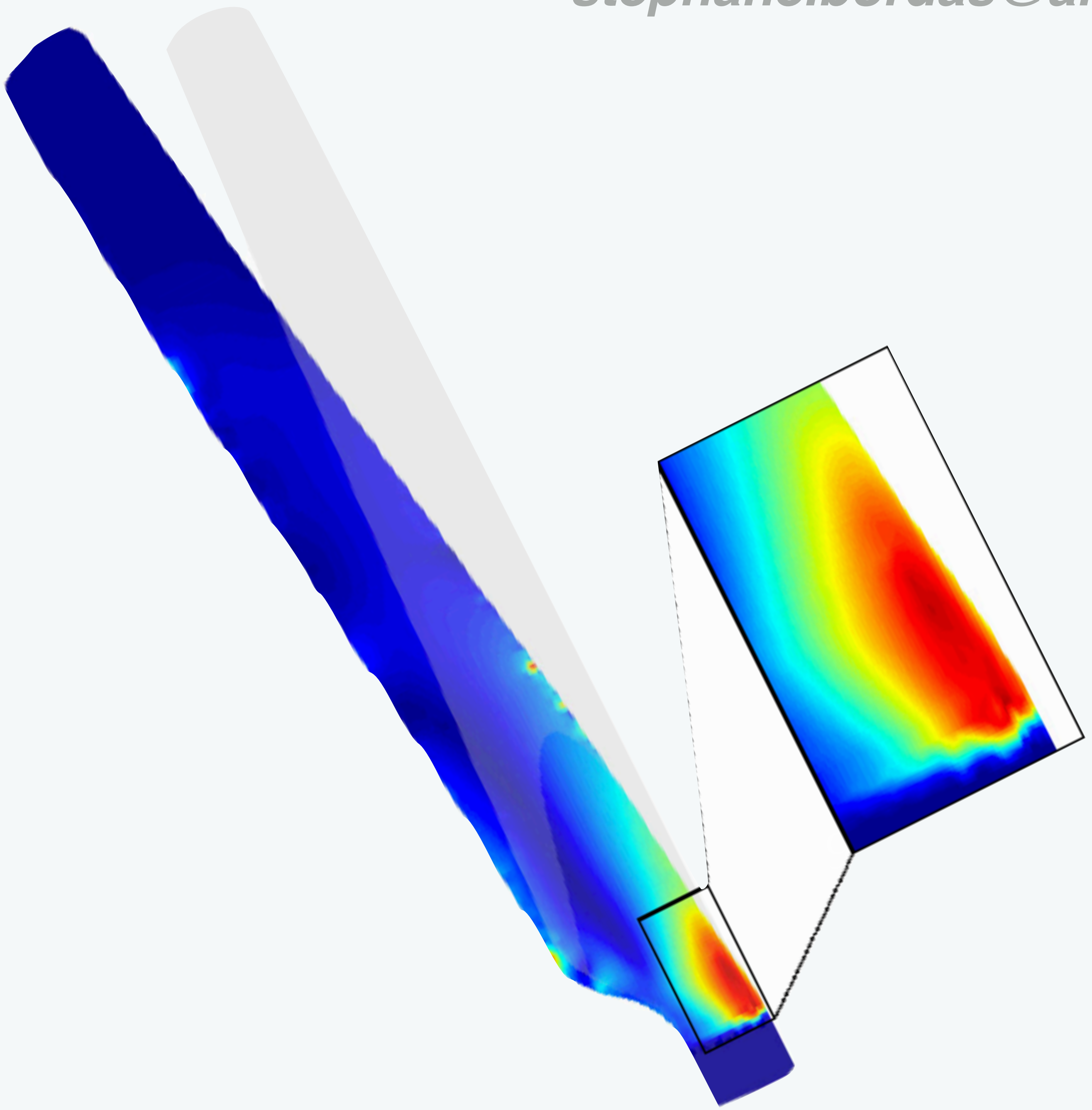
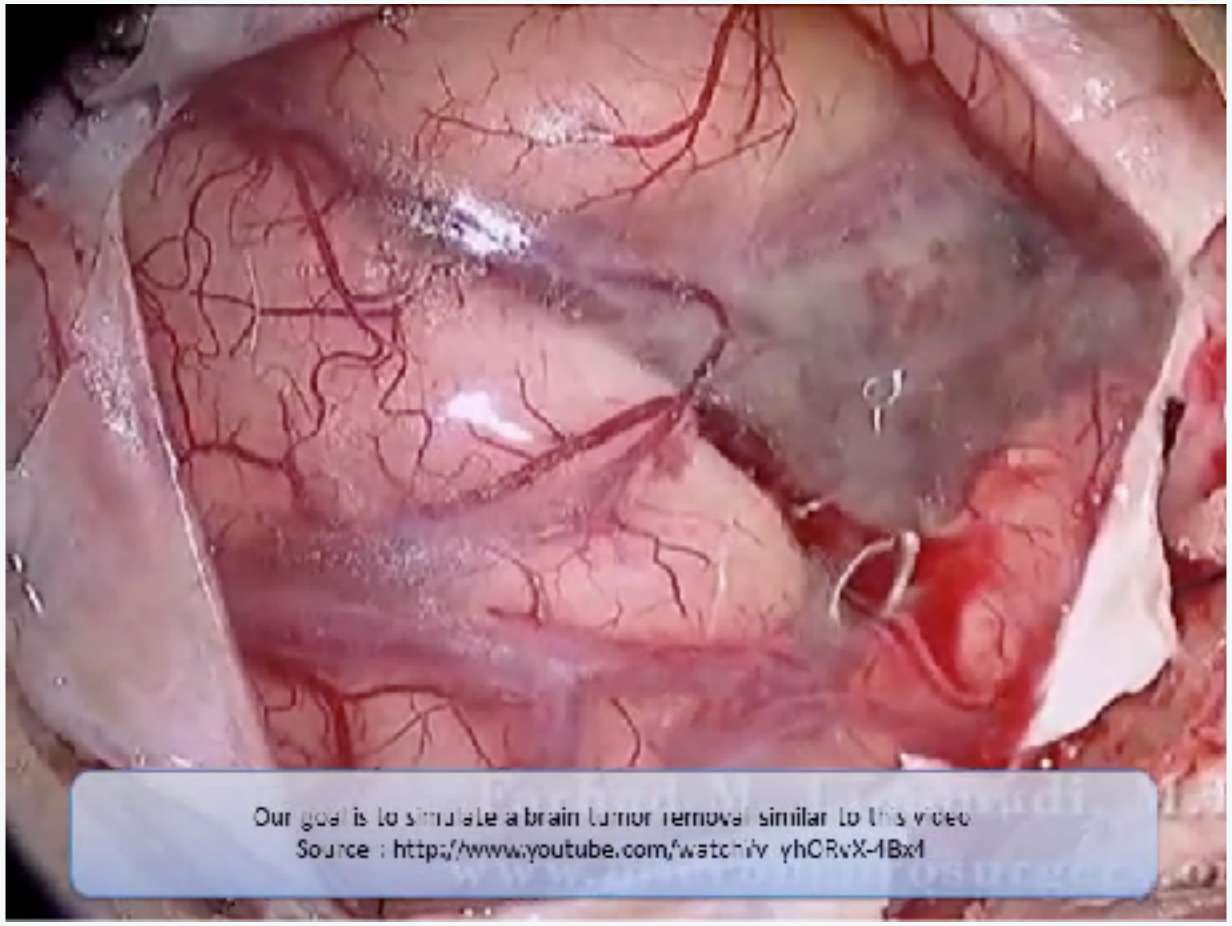
Numerical Methods for Free Boundary Problems

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”

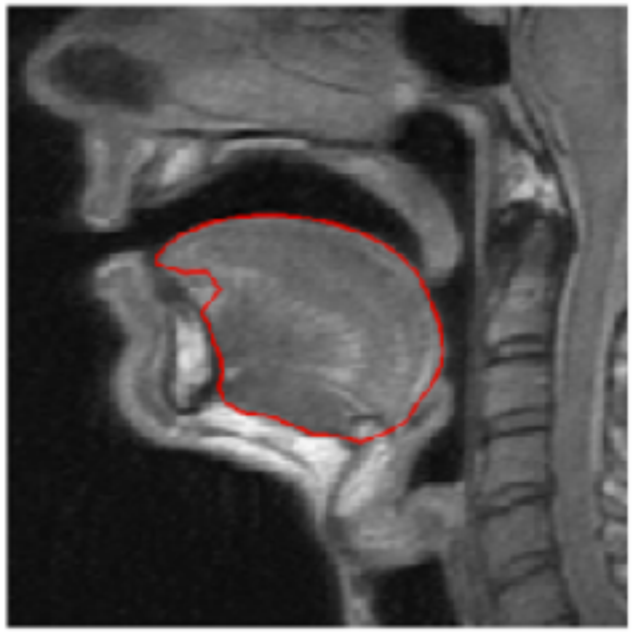
Avner Friedman (Friedman, 2000).

Mathematical Modelling

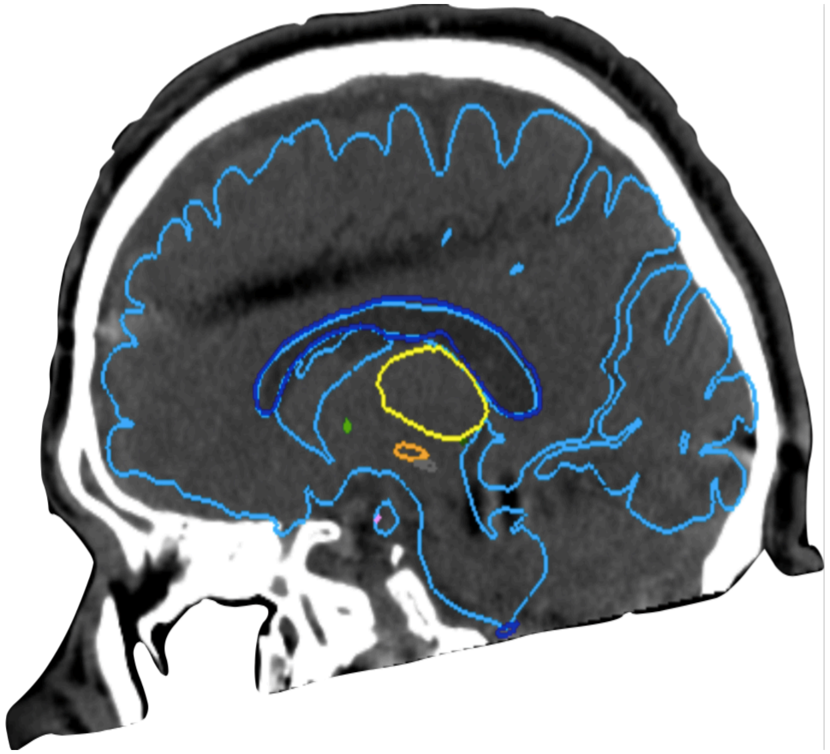
Continuous Problem

Mathematical Modelling

Continuous Problem



Bijar, Rohan, Perrier & Payan 2015



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Mathematical Modelling

Continuous Problem

↓

Mathematical Model

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

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

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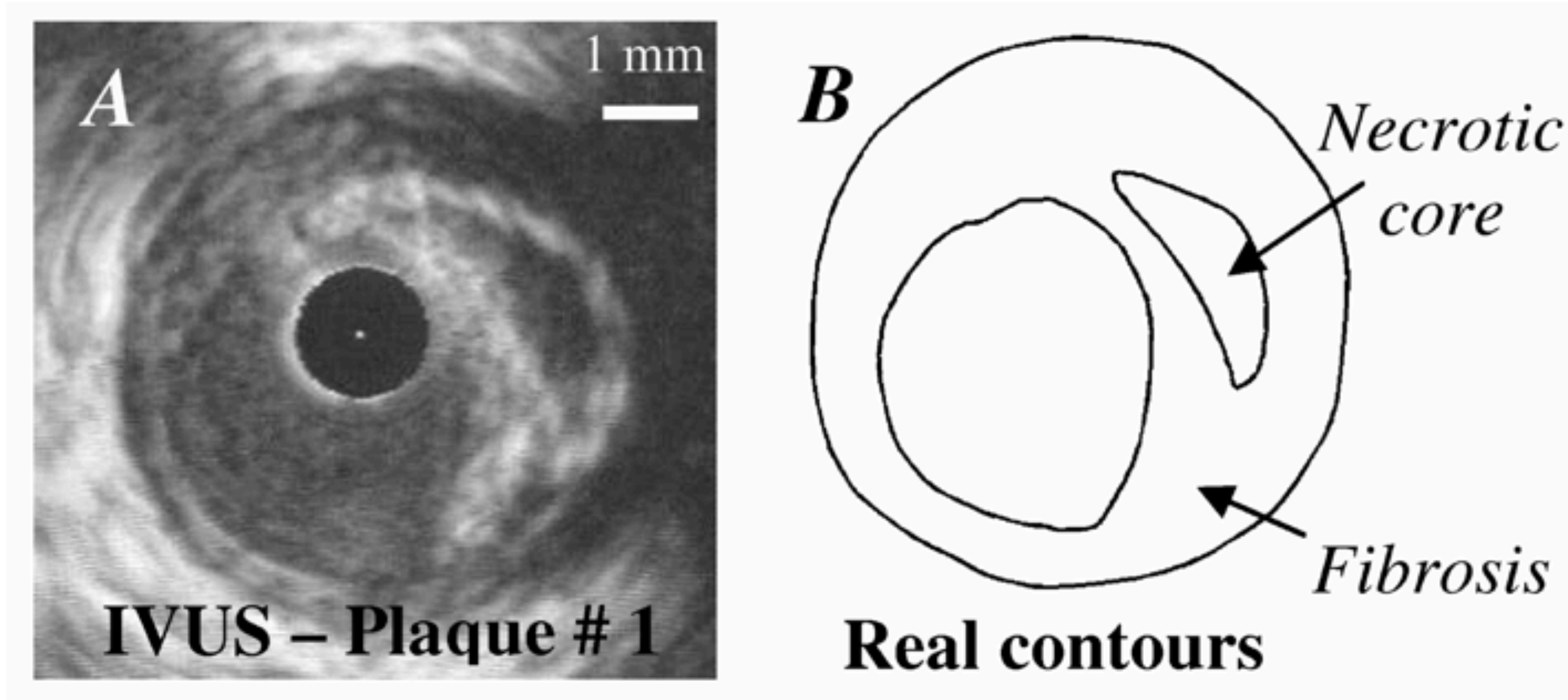
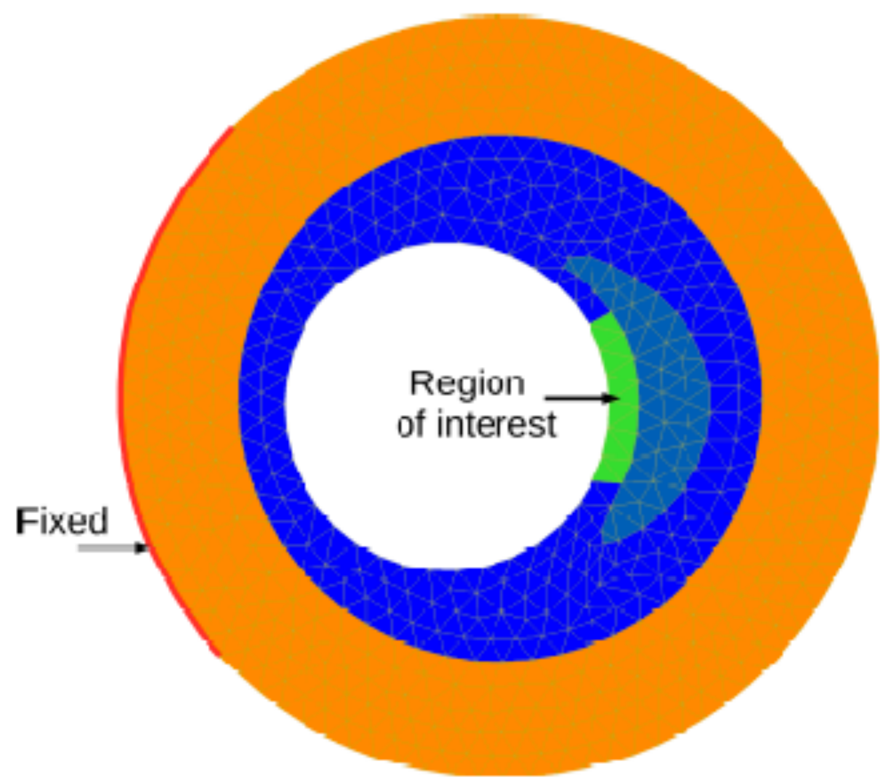
Mathematical Modelling

Continuous Problem

↓

Mathematical Model





Mathematical Modelling

Continuous Problem

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Mathematical Model

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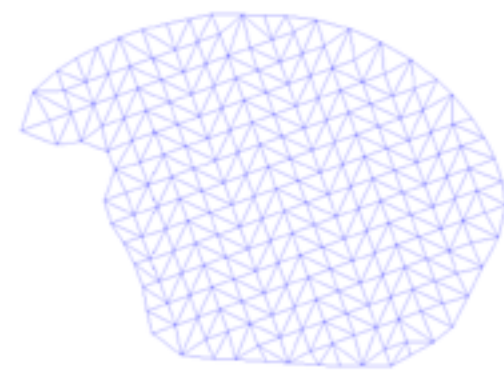
Discrete Problem

Mathematical Modelling

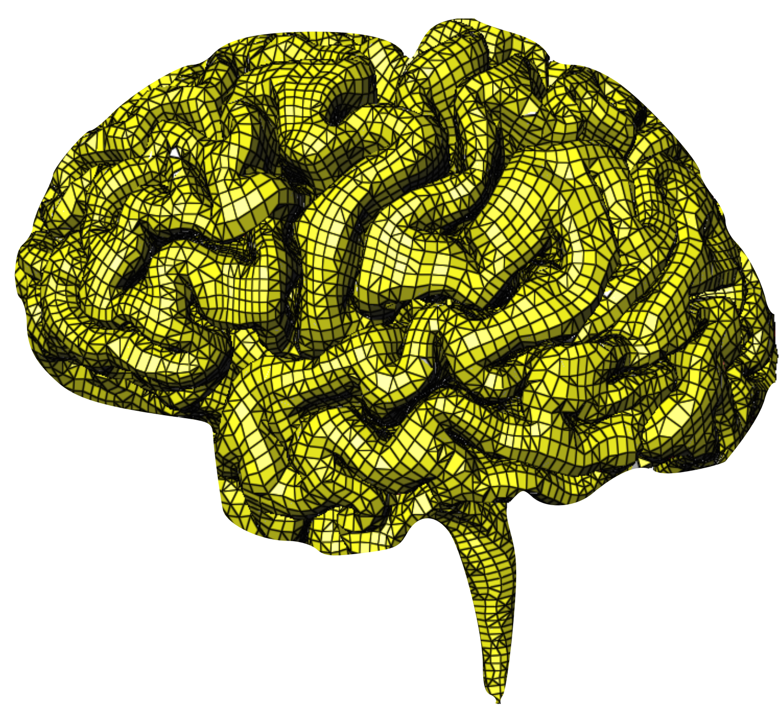
Continuous Problem

Mathematical Model

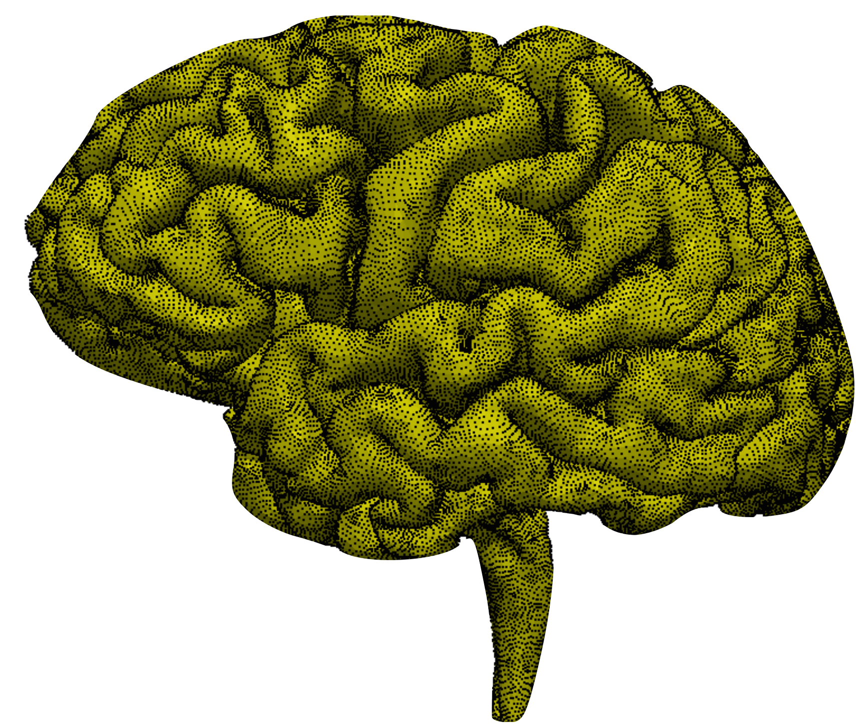
Discrete Problem



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

↓

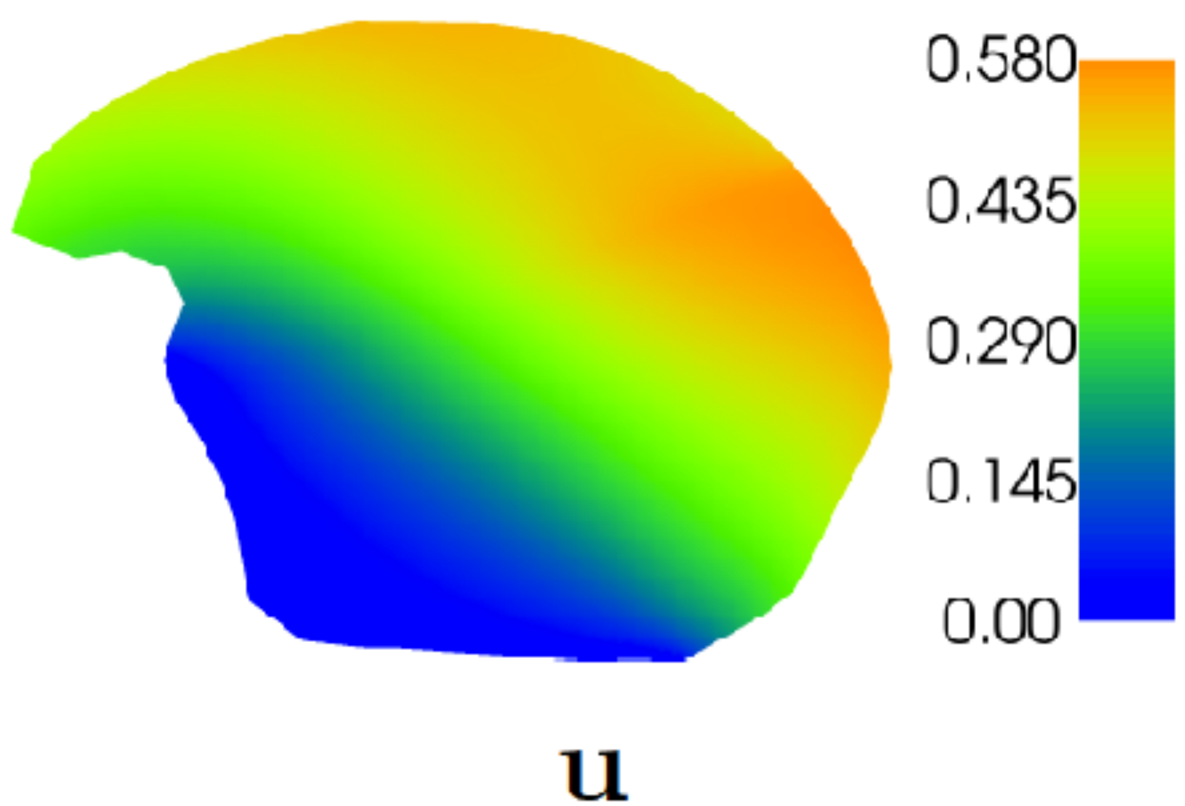
Mathematical Model

↓

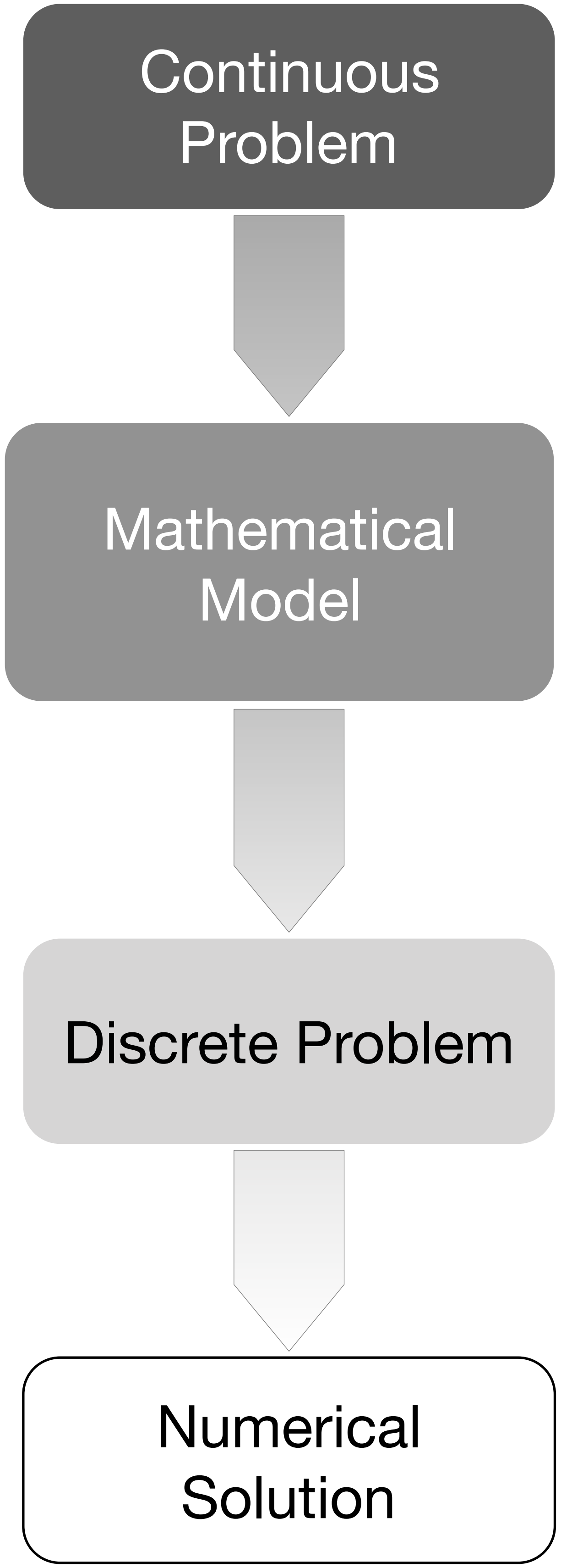
Discrete Problem

↓

Numerical Solution



Mathematical Modelling



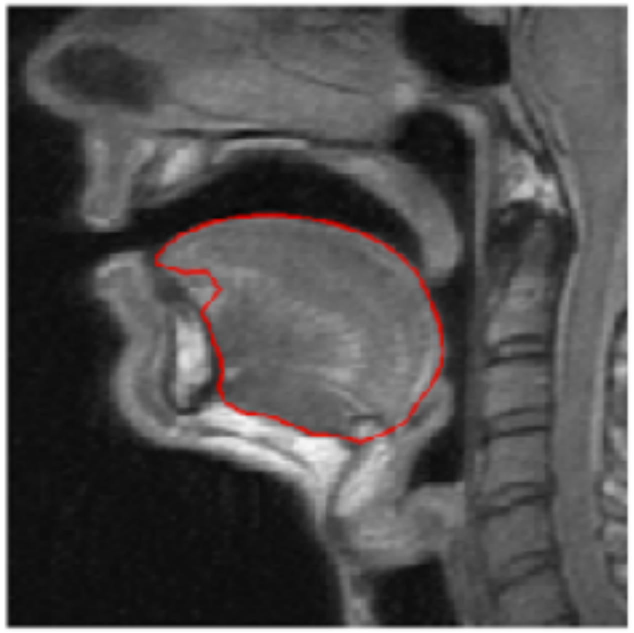
Mathematical Modelling

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

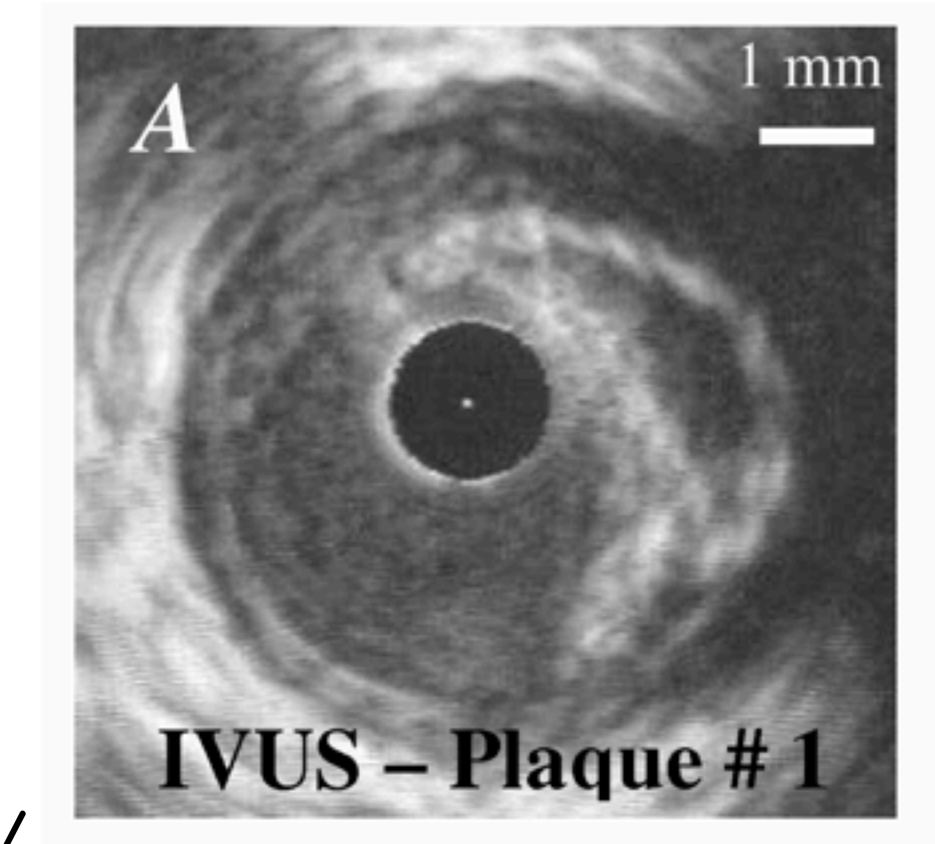
Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error



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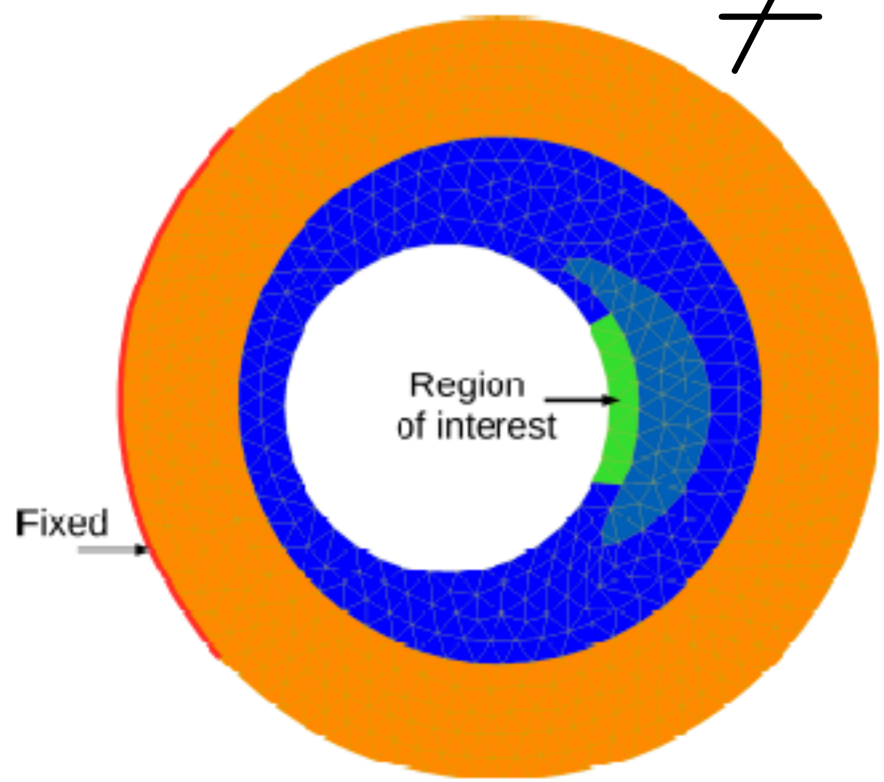

Geometry
Boundary conditions

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Mathematical Modelling

Continuous Problem

↓

Mathematical Model

↓

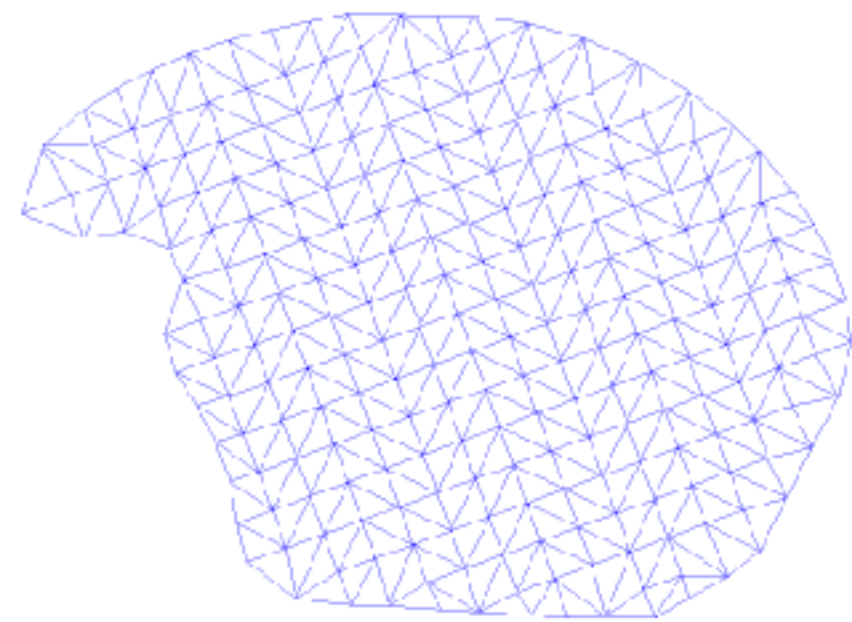
Discrete Problem

↓

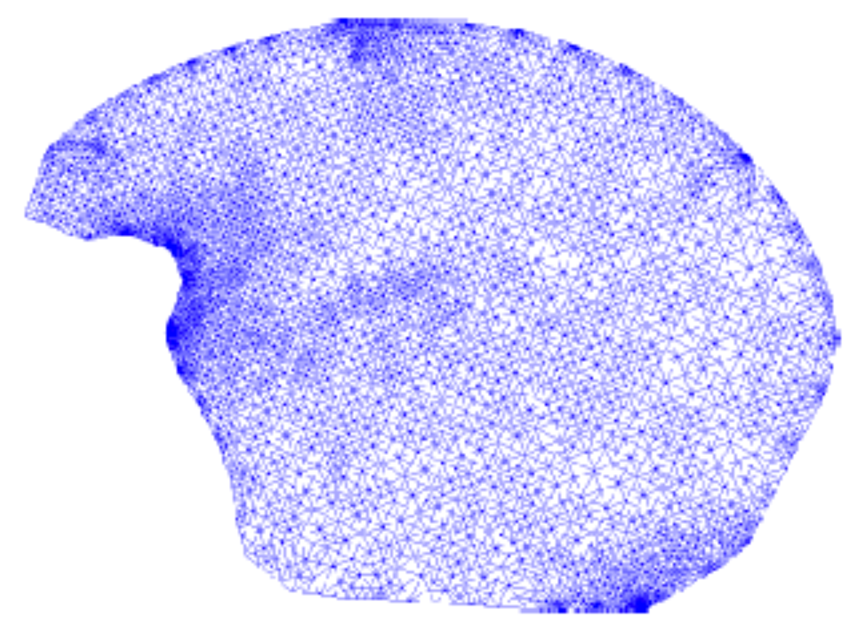
Numerical Solution

Model Error

Discretization Error



vs.



Mathematical Modelling

Continuous Problem

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Mathematical Model

↓

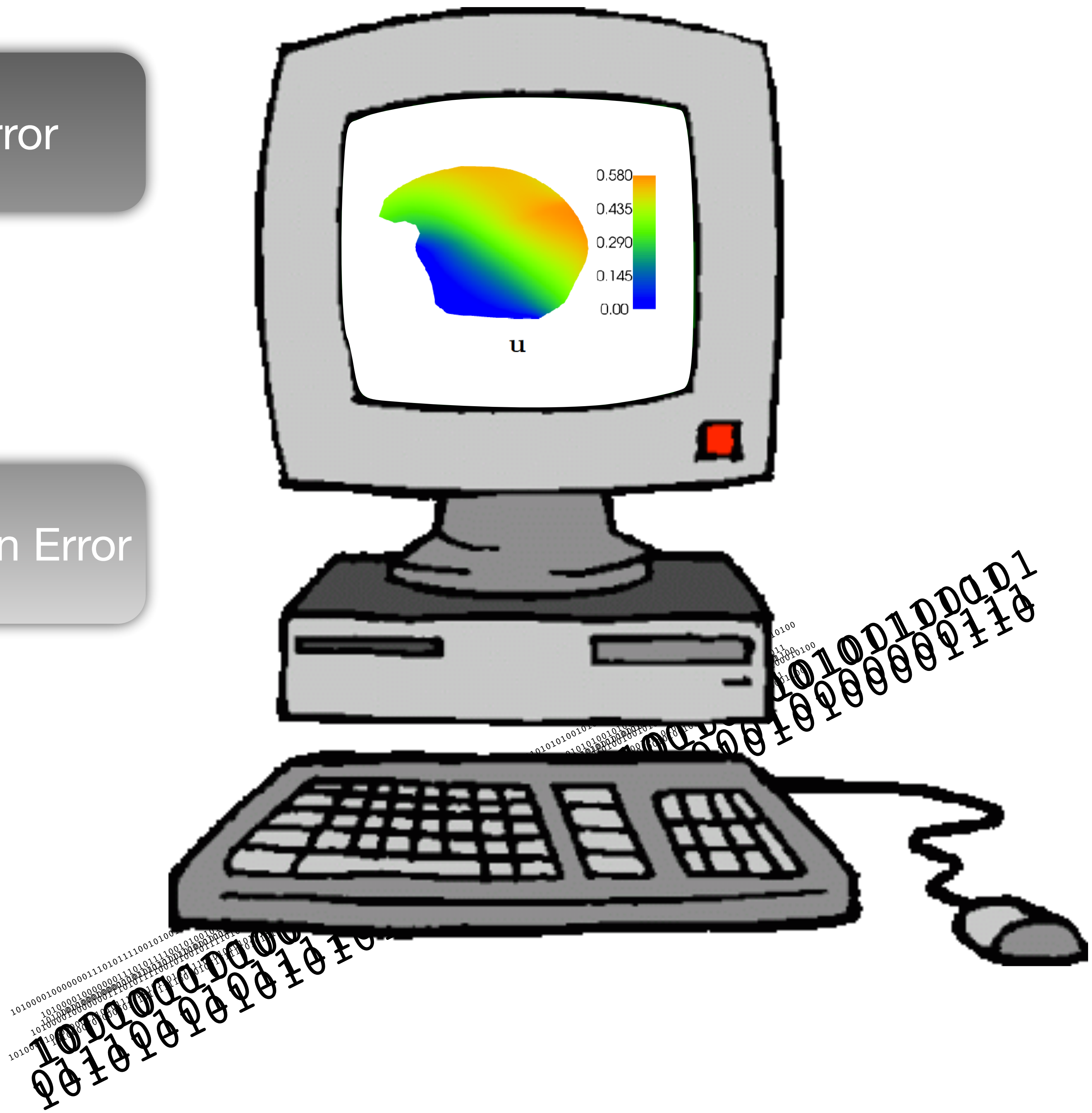
Discrete Problem

↓

Numerical Solution

Model Error

Discretization Error



Mathematical Modelling

32 bit?

64 bit?

Continuous Problem

Model Error

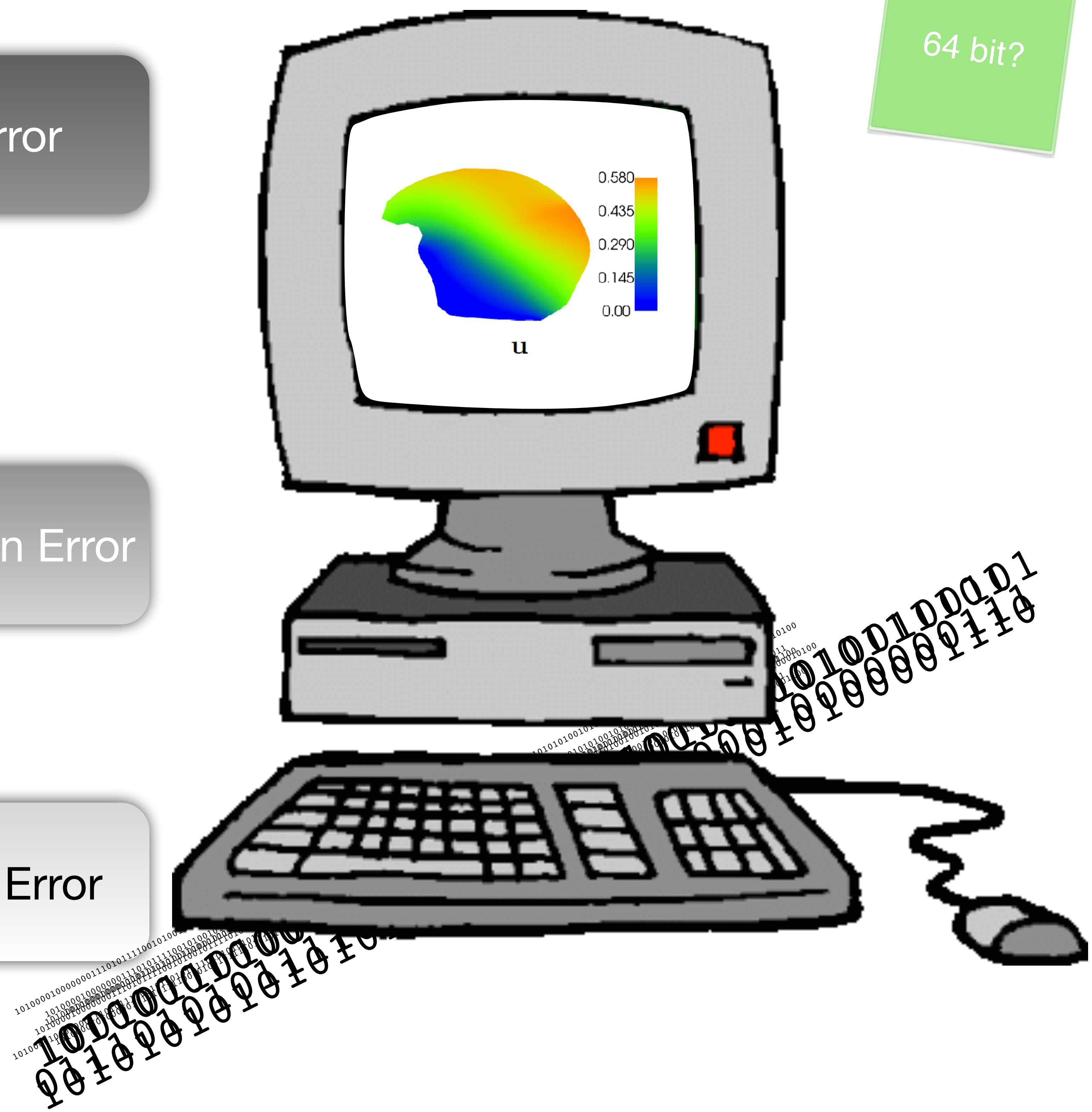
Mathematical Model

Discretization Error

Discrete Problem

Numerical Error

Numerical Solution



Mathematical Modellin

Continuous Problem

Mathematical Model

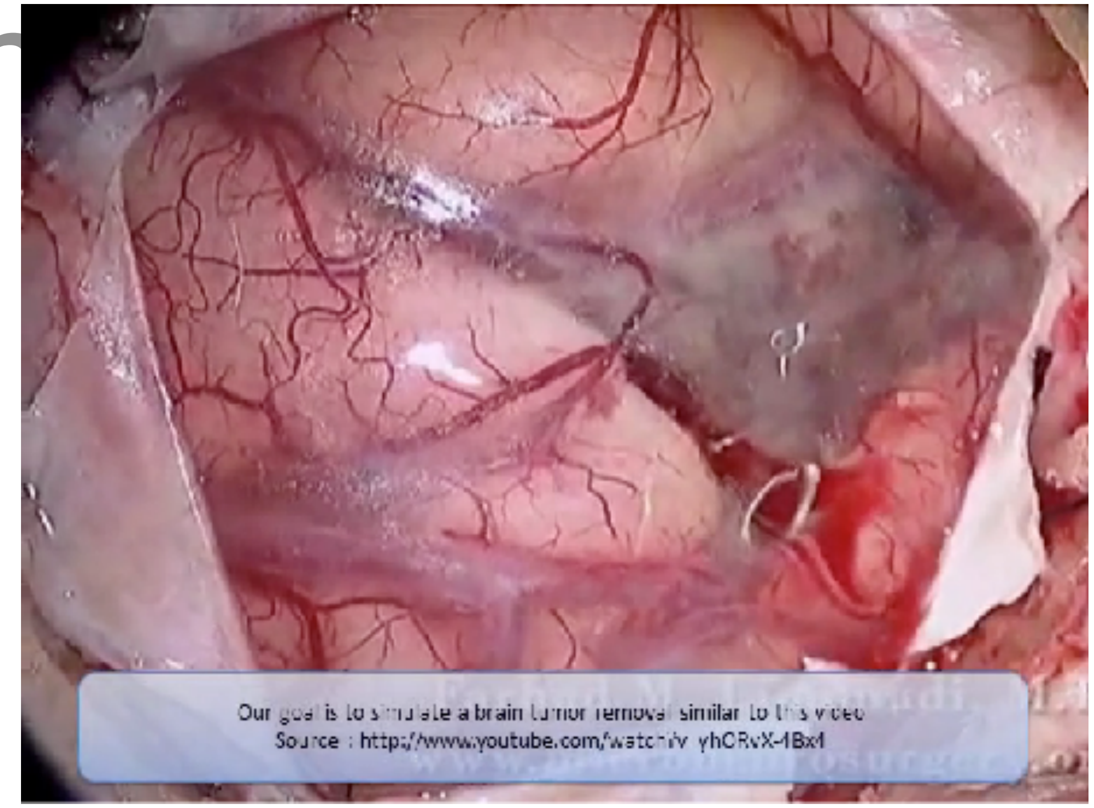
Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error

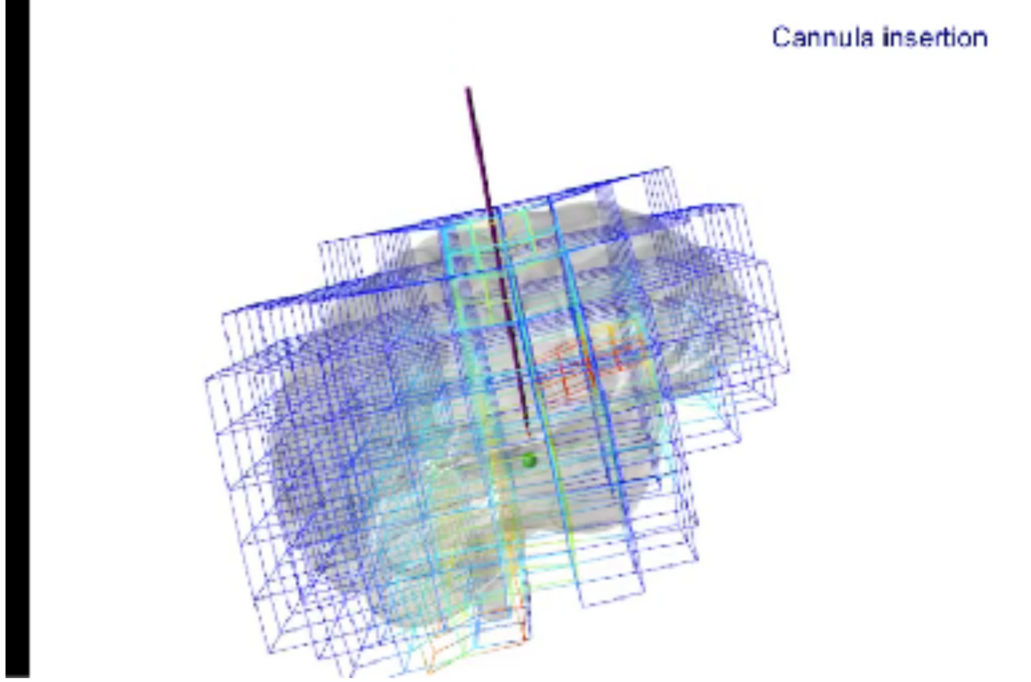


Total Error

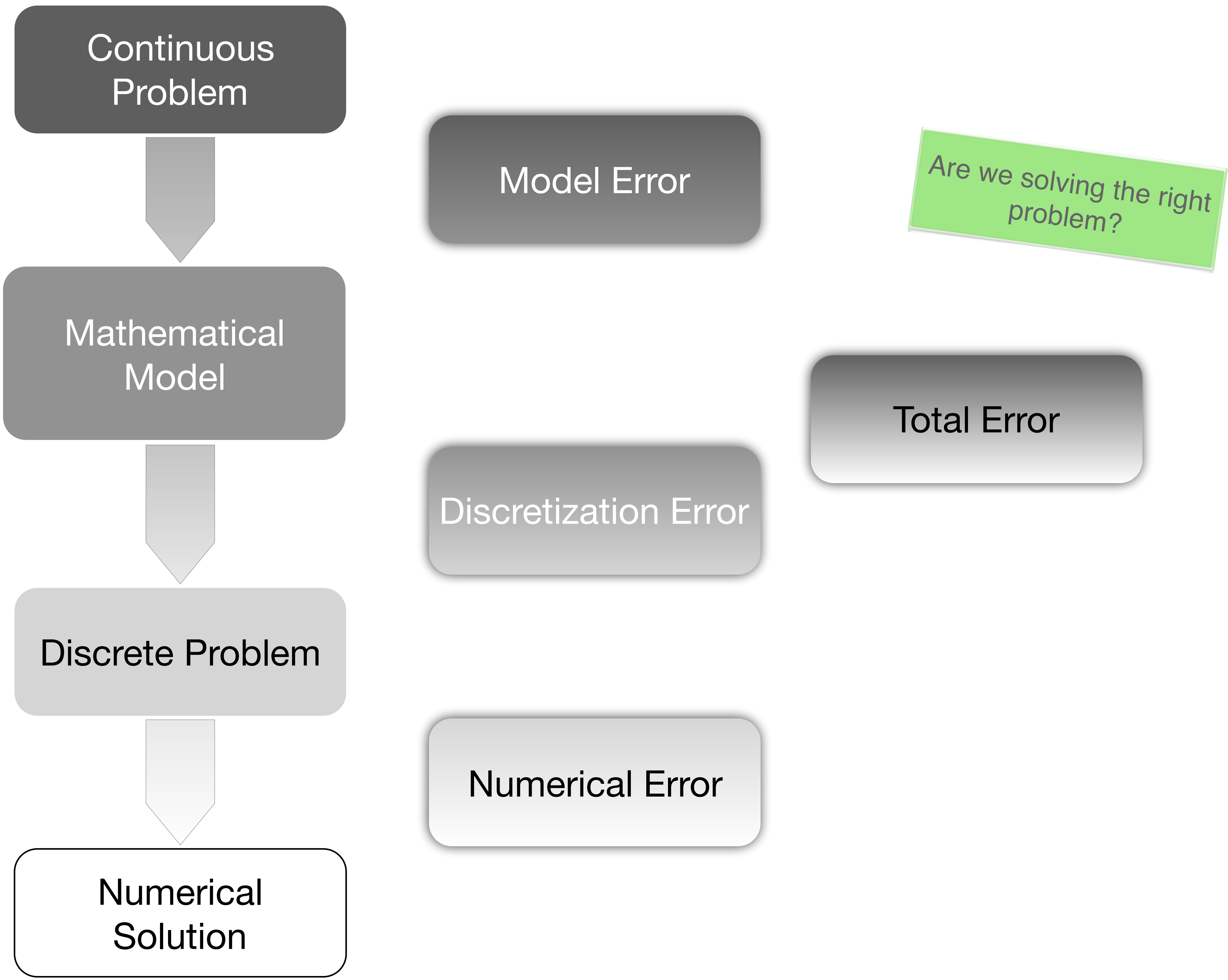
Reality

vs.

Simulation



Mathematical Modelling



Mathematical Modelling

Continuous Problem

Model Error

Are we solving the right problem?

Mathematical Model

Total Error

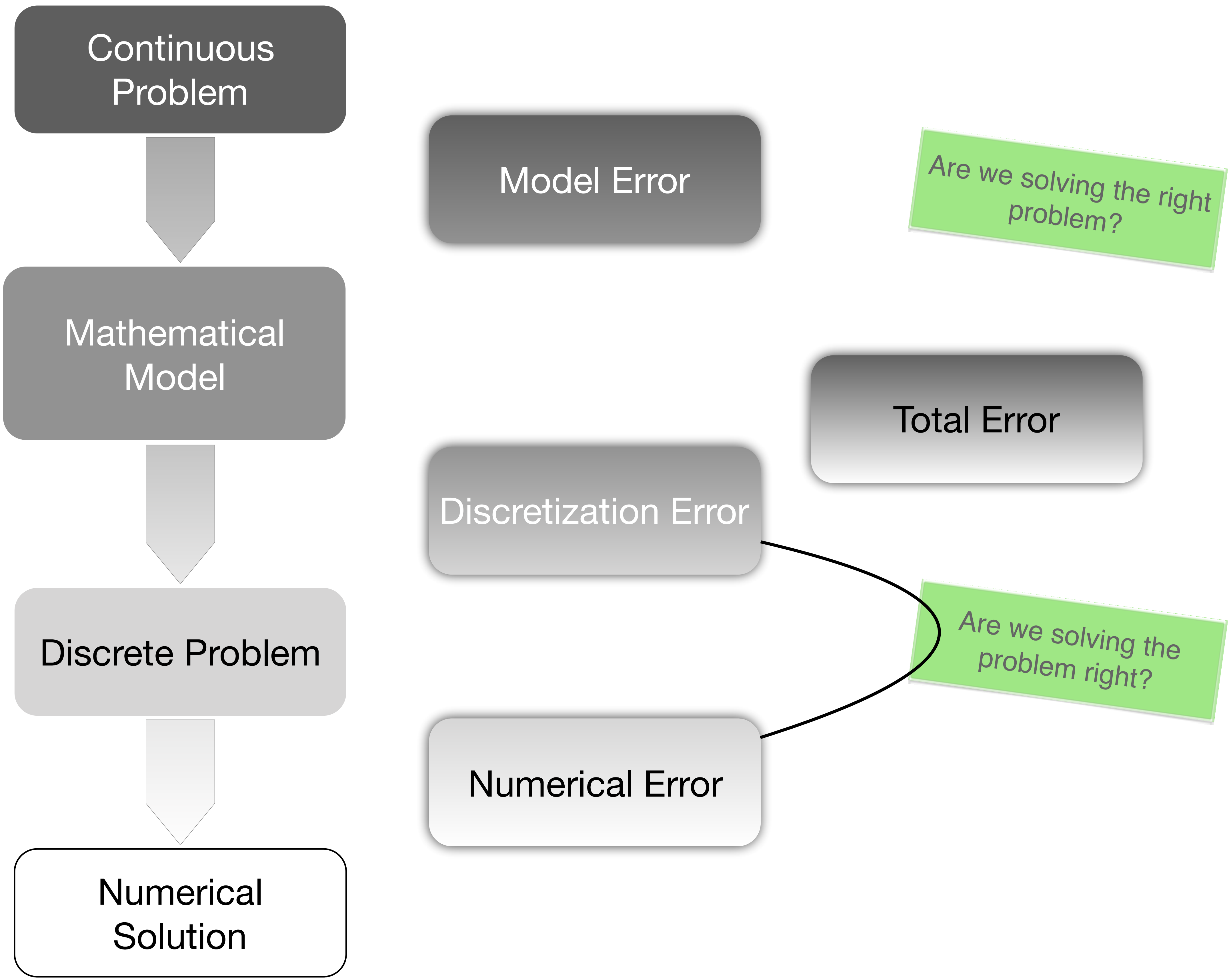
Discretization Error

Discrete Problem

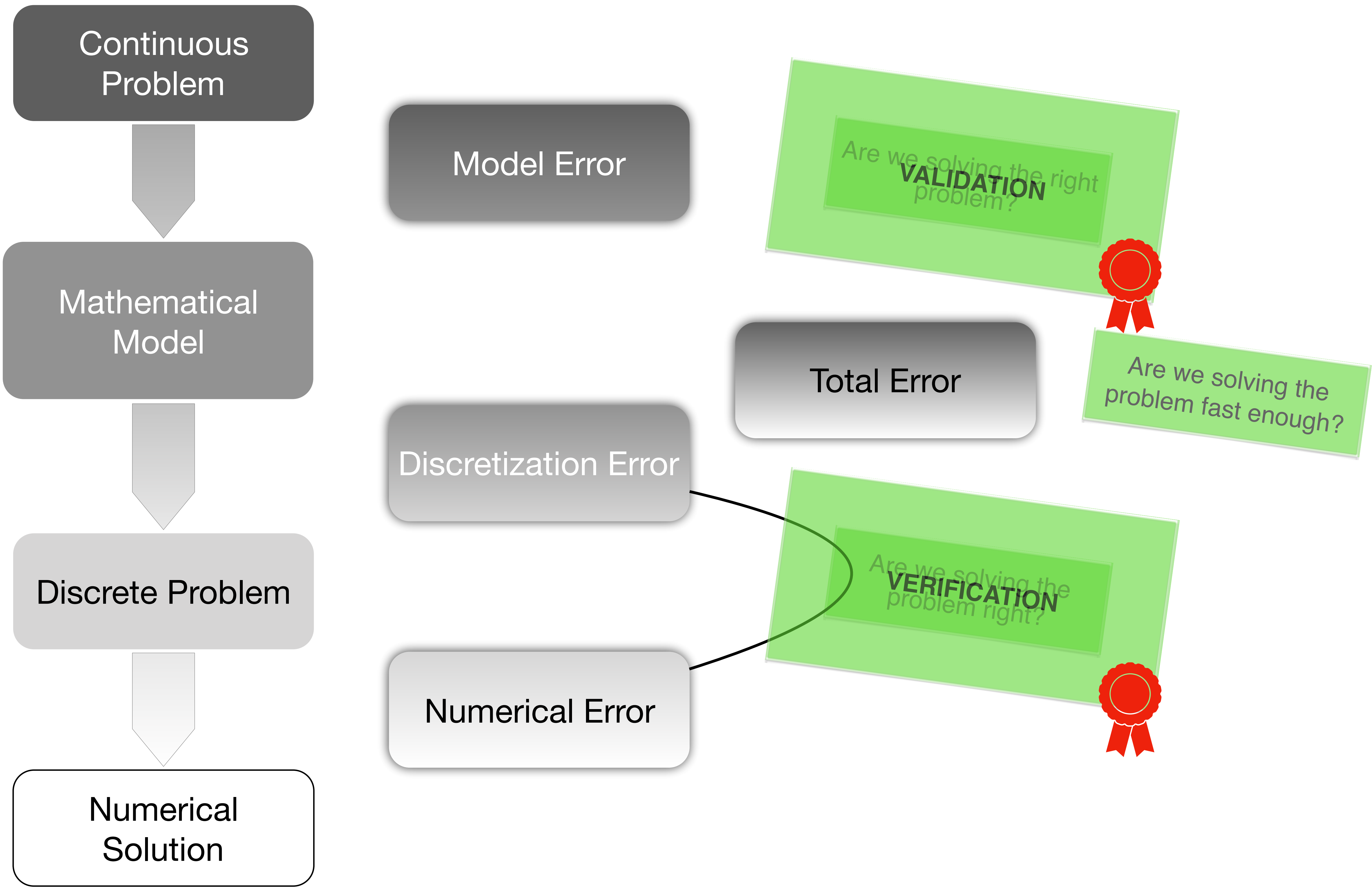
Numerical Error

Numerical Solution

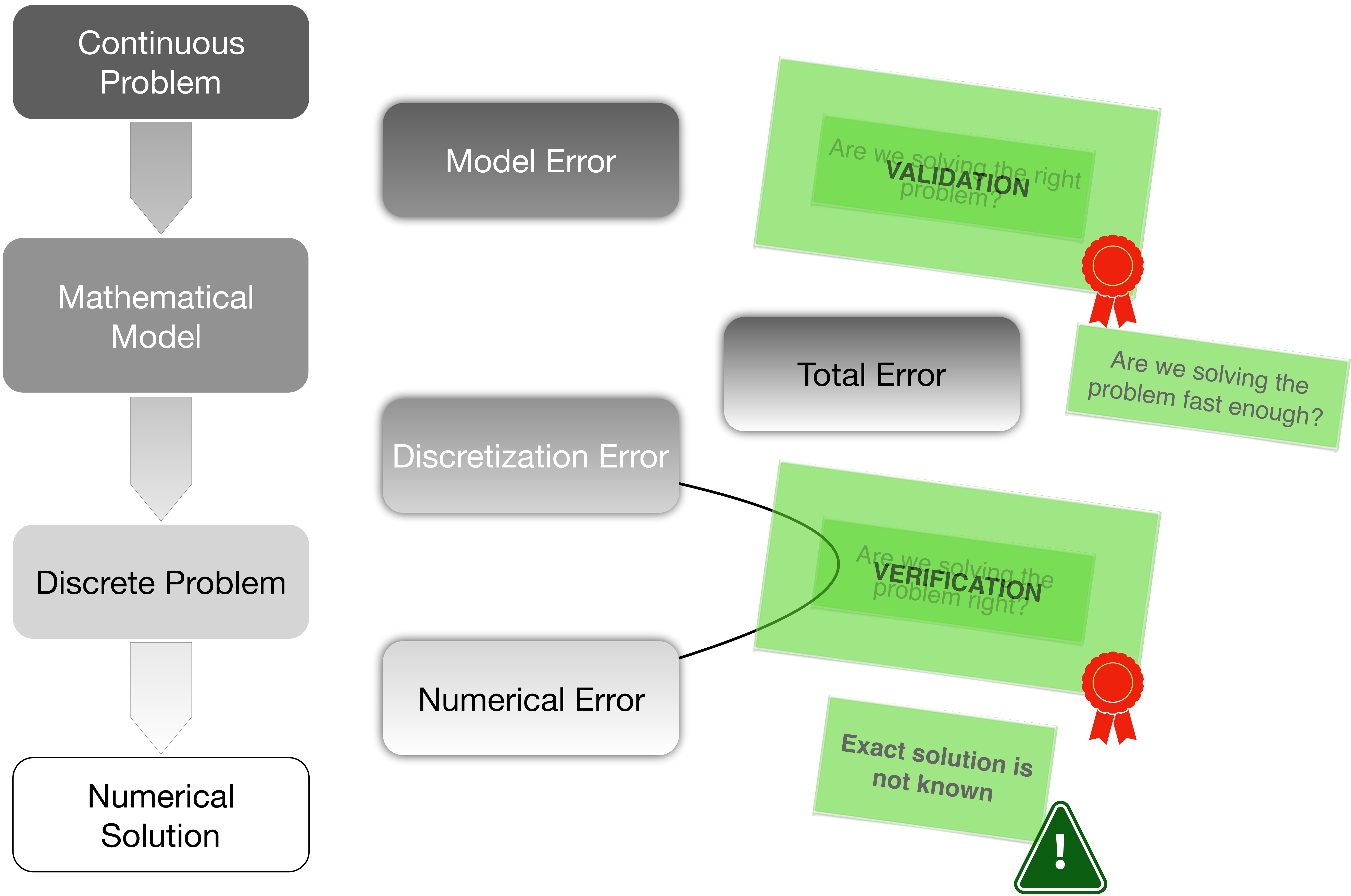
Mathematical Modelling



Mathematical Modelling



Mathematical Modelling



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Interface problems appear naturally

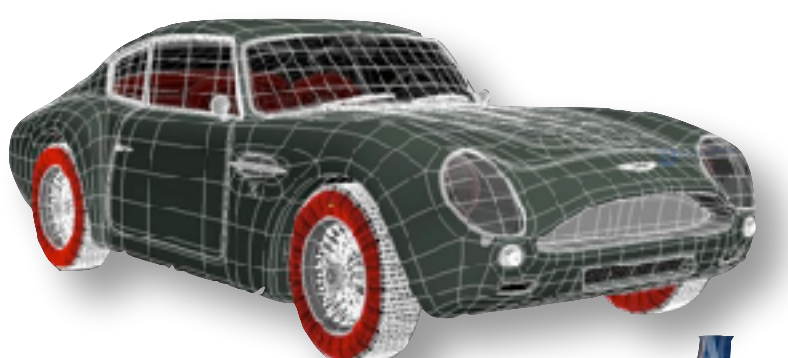
Discontinuities

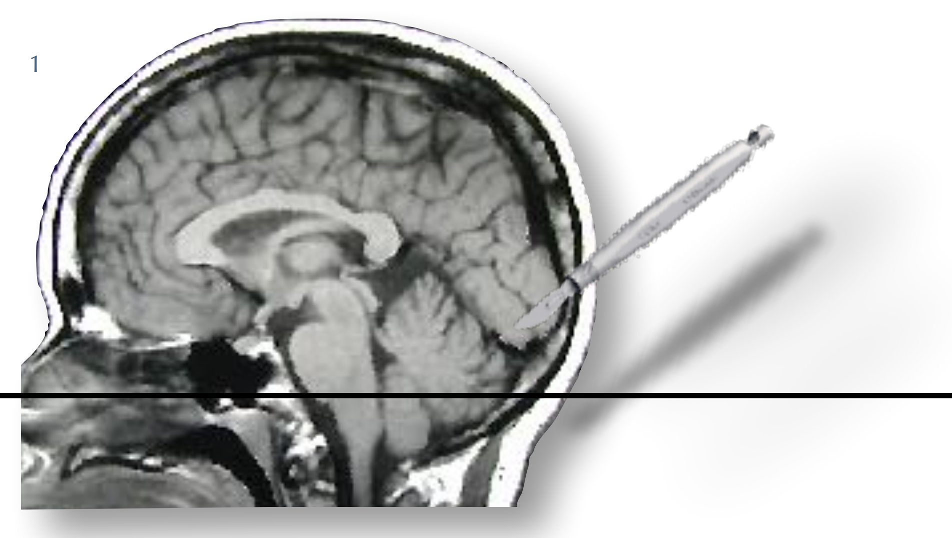
1

Large scale

Small scale

Discontinuities

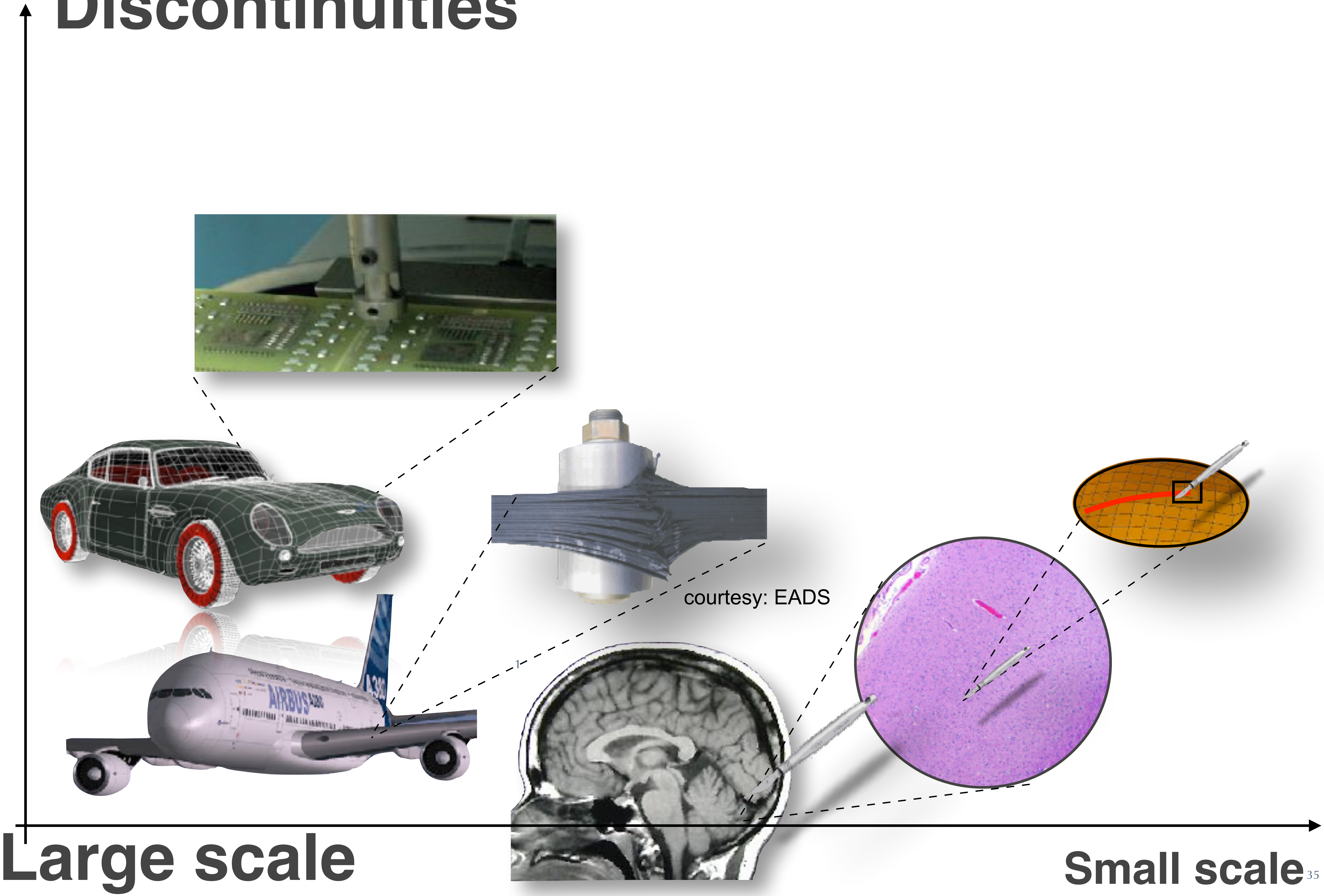


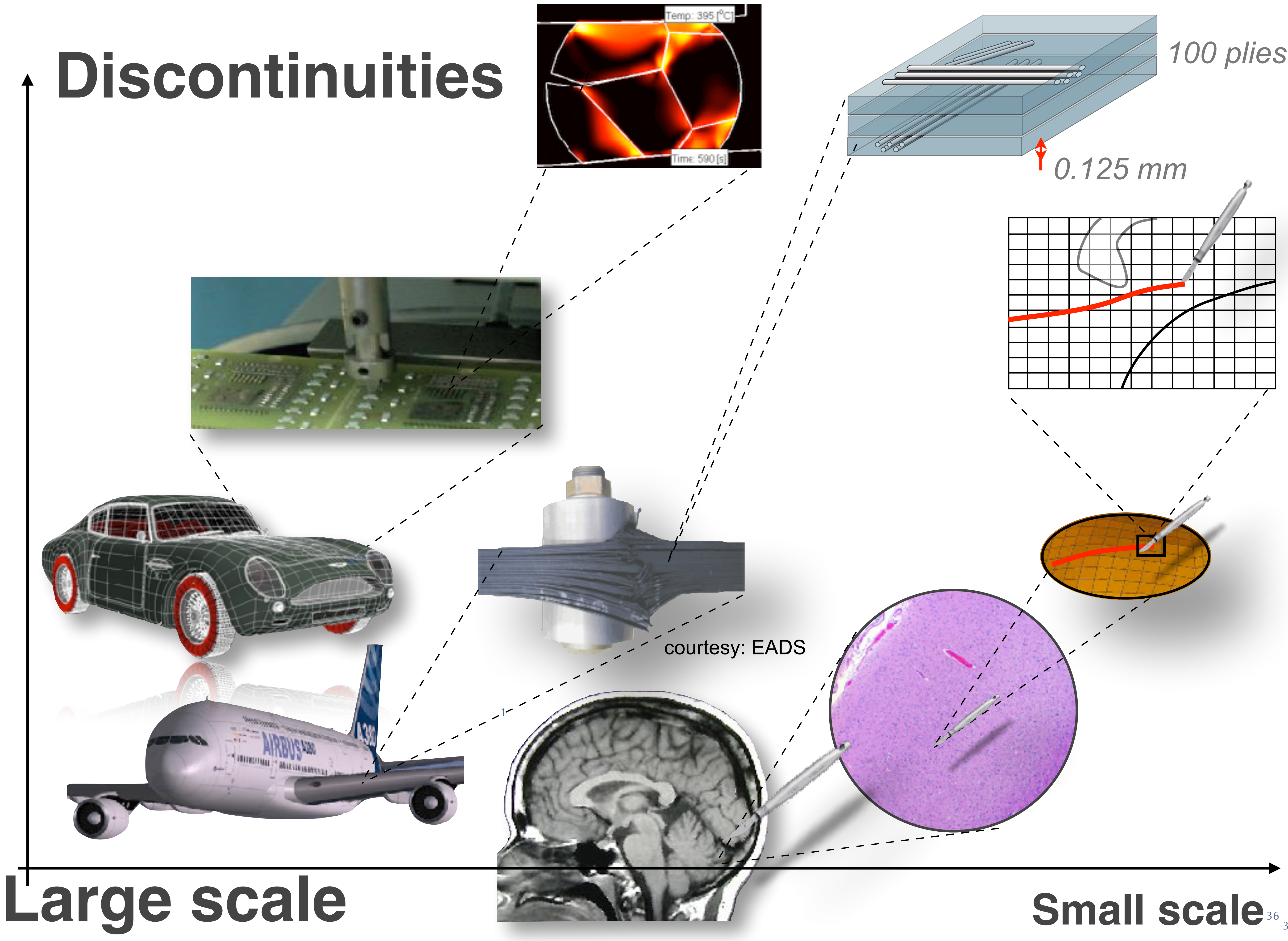


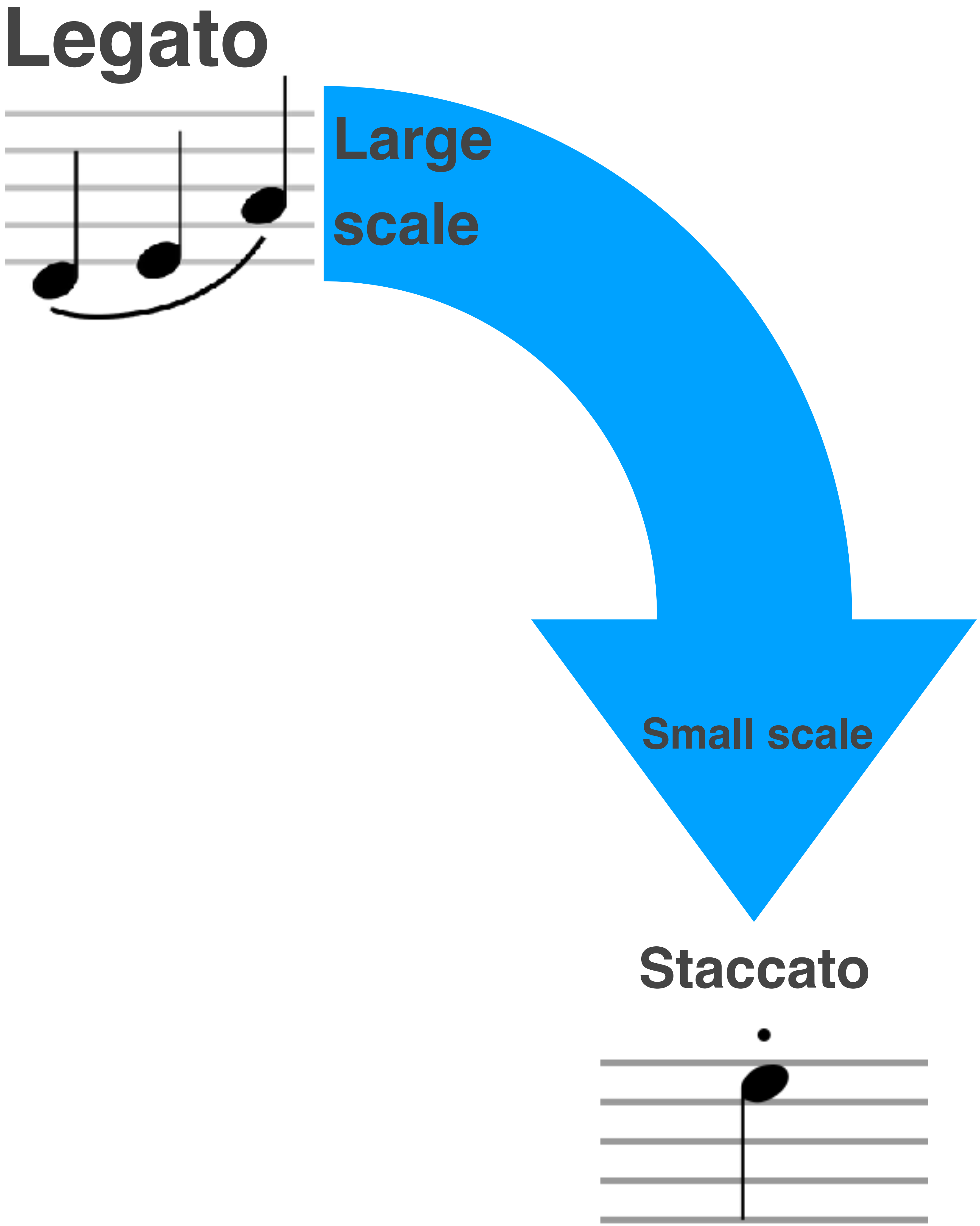
Large scale

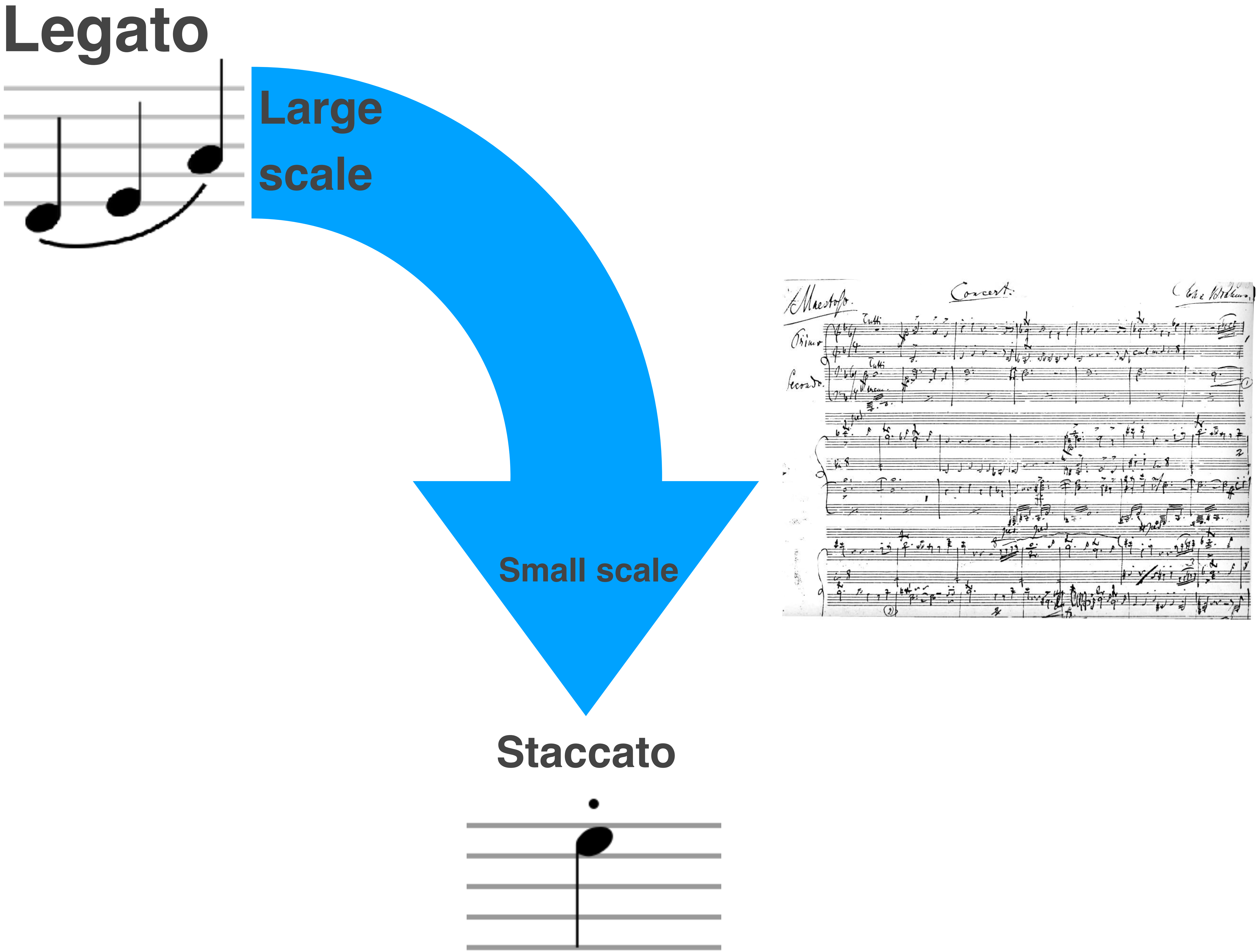
Small scale

Discontinuities




Discontinuities
Temp: 395 [°C]
Time: 590 [s]
100 plies
0.125 mm
courtesy: EADS
Large scale
Small scale

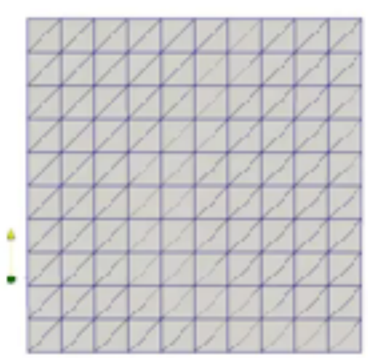

Legato
Large
scale
Small scale
Staccato

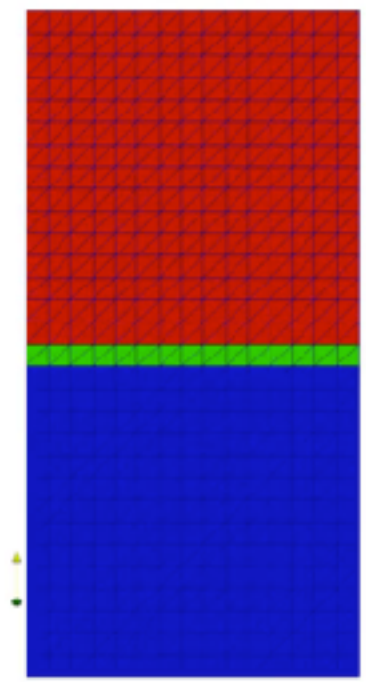

Legato
Large scale
Small scale
Staccato

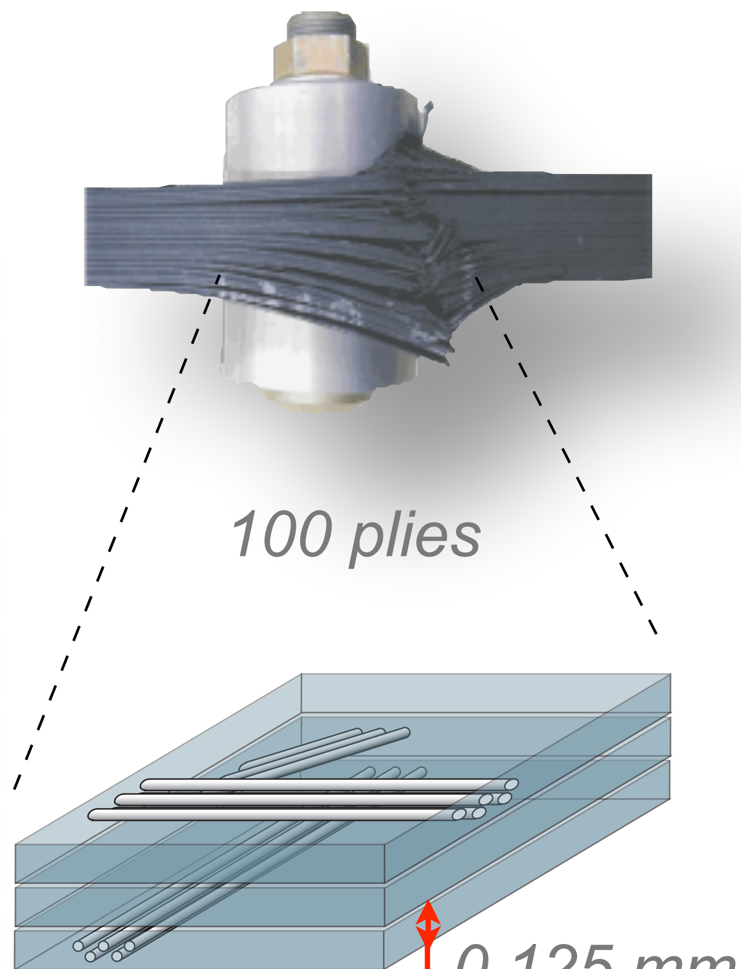
Music of materials

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

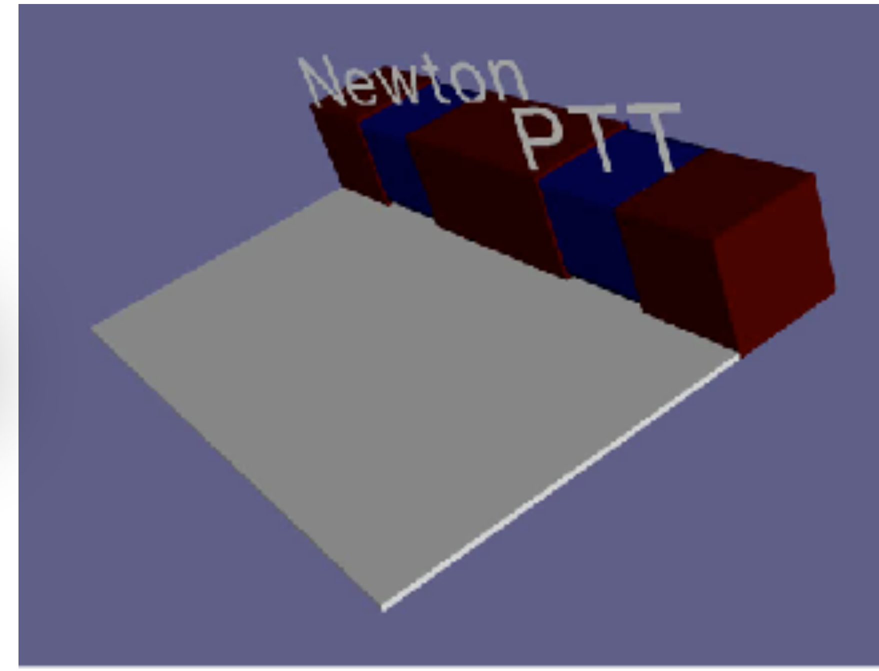
Phases

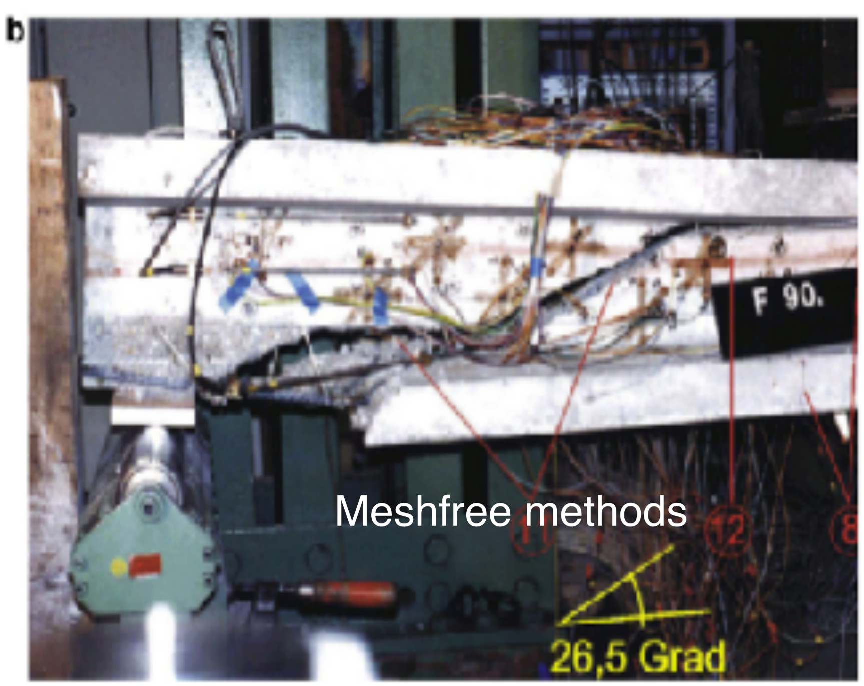


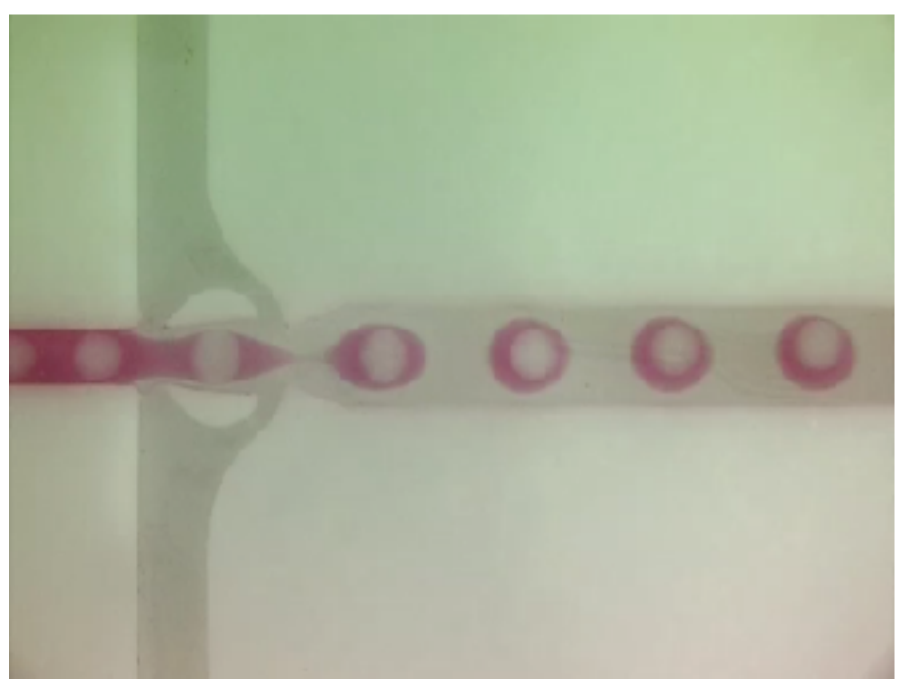




Courtesy, EADS

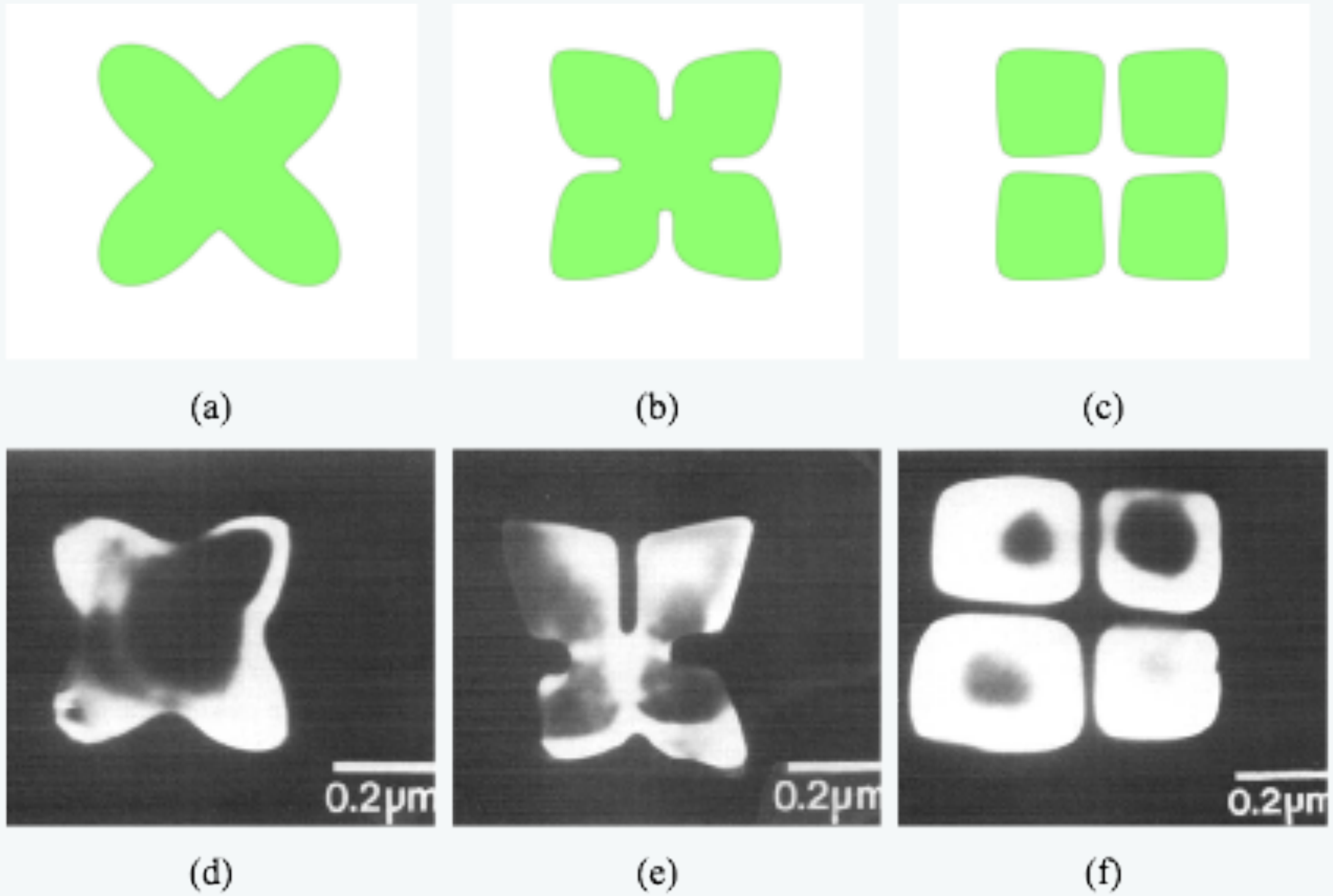






CMECH 2007, EFM2008 CAS 2009, with Timon Rabczuk and Goangseup Zi

Phases at the nano-scale
Surface effects are critical

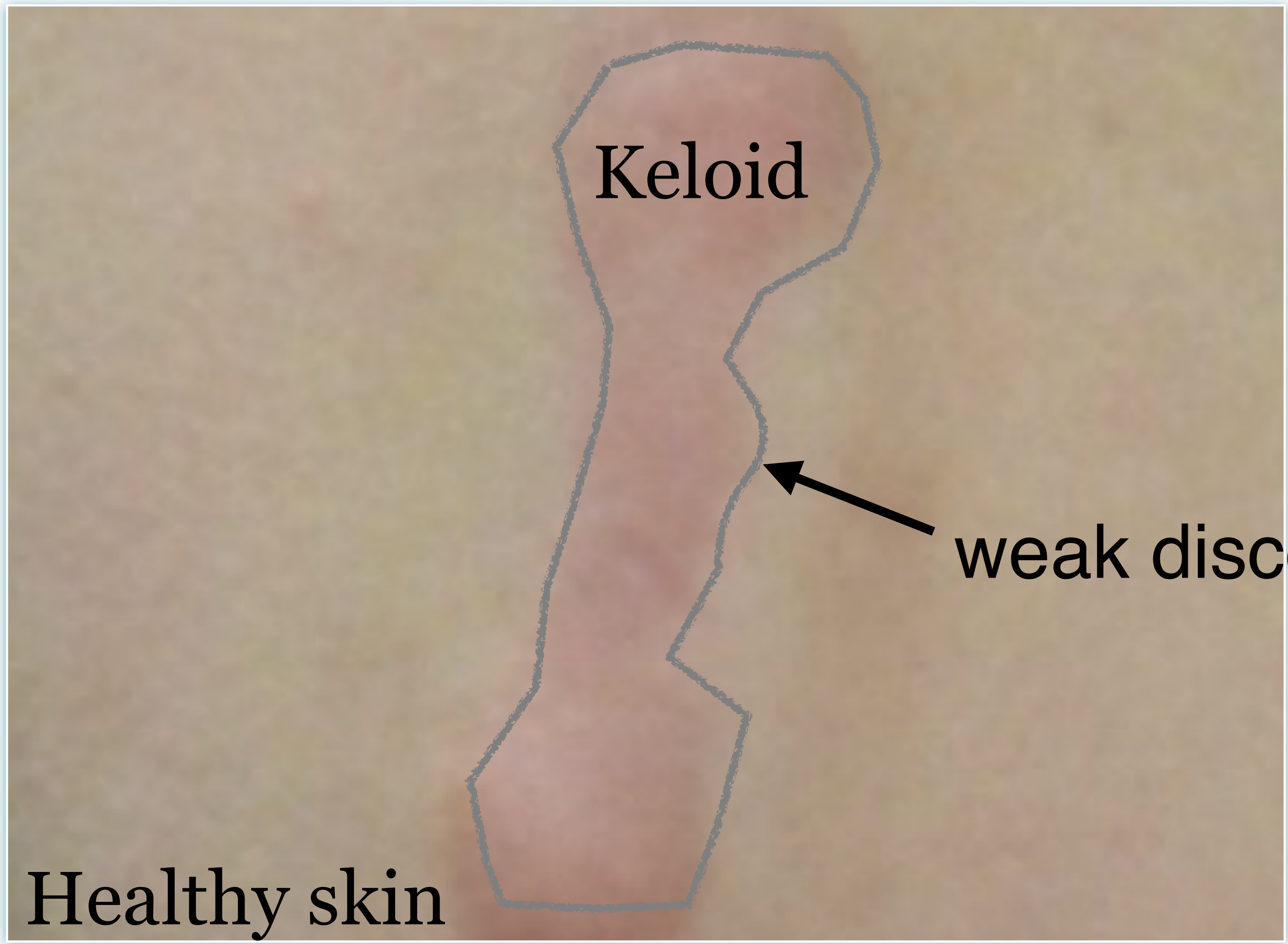


Equilibrium shapes of nano-heterogeneities (with X. Zhao, R. Duddu, J. Qu).

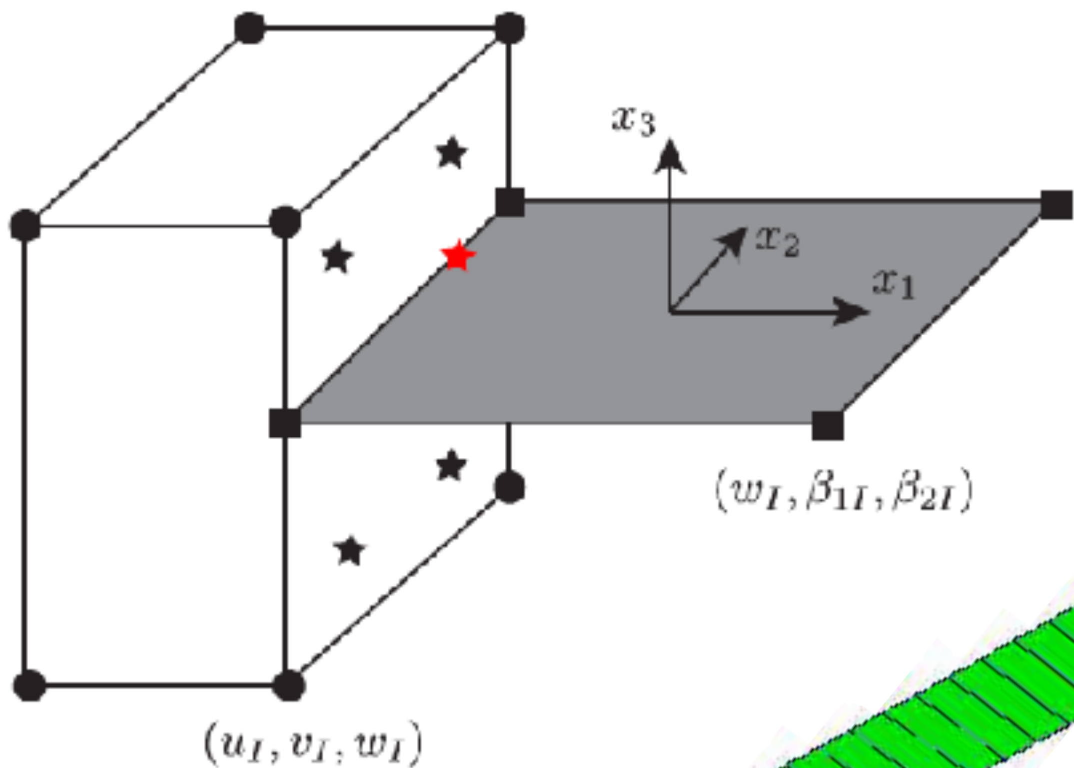
JMPS2015 http://orbilu.uni.lu/bitstream/10993/11024/1/manuscript%20-%20JMPS-D-12-00428.pdf
CMECH2013 http://orbilu.uni.lu/bitstream/10993/11022/1/Manuscript_XZHAO_CMECH_revision.pdf

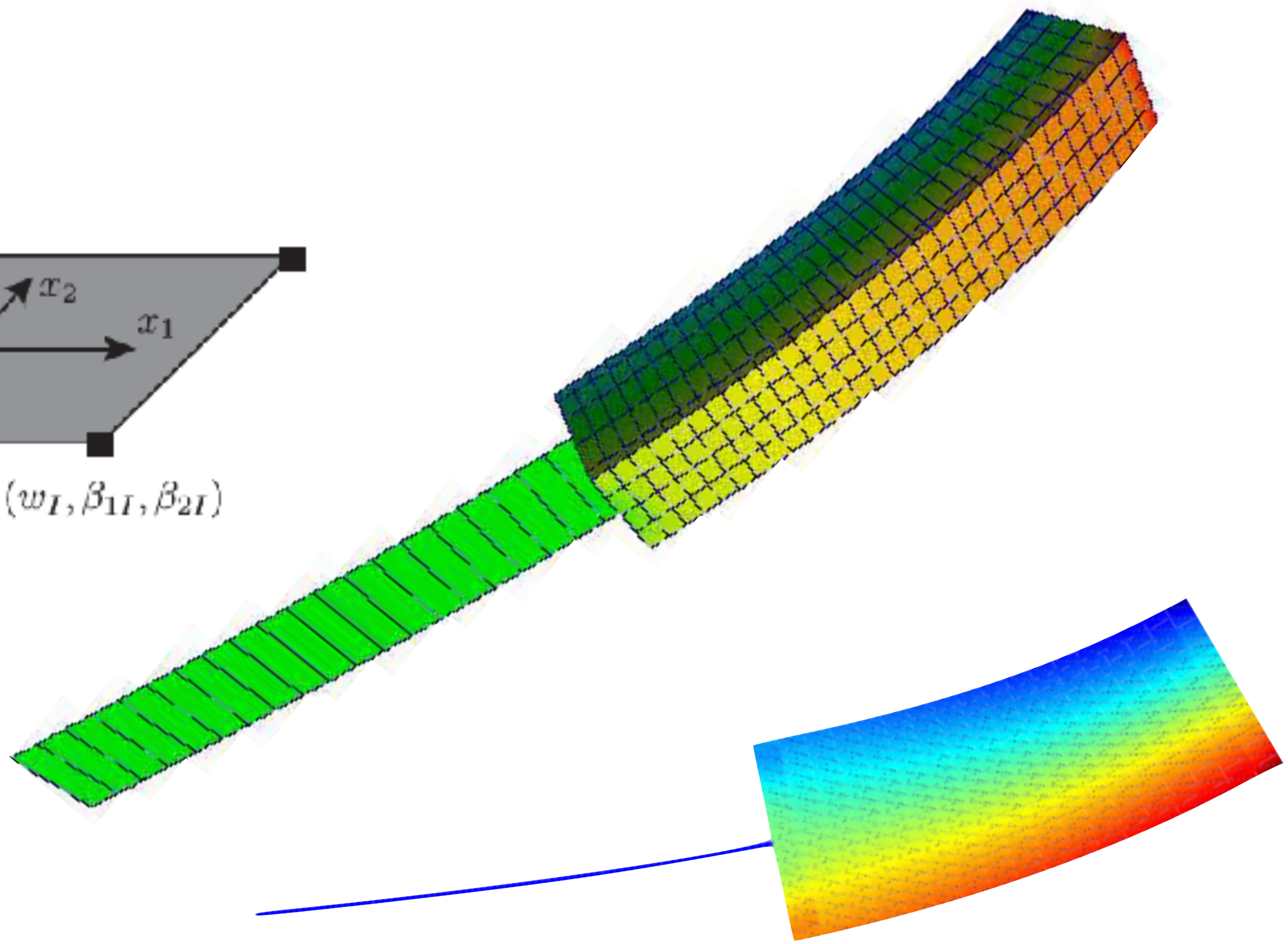
$$\bar{F} = \int_V W dV + \int_\Gamma \gamma dS + \lambda\left(\int_\Omega dV - V_0\right)$$


Keloid
Healthy skin


Keloid
weak discontinuity
Healthy skin

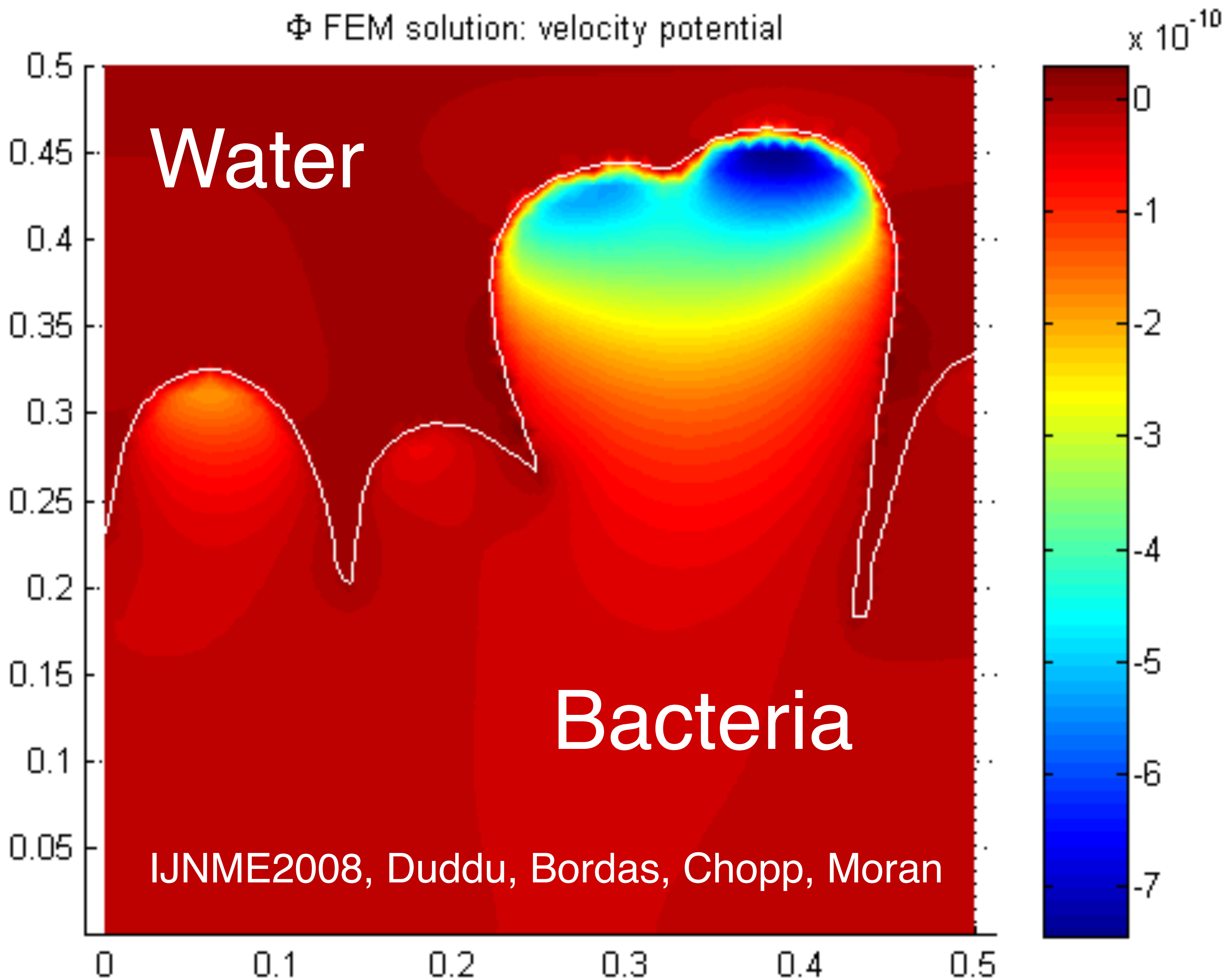
Kinematics interfaces



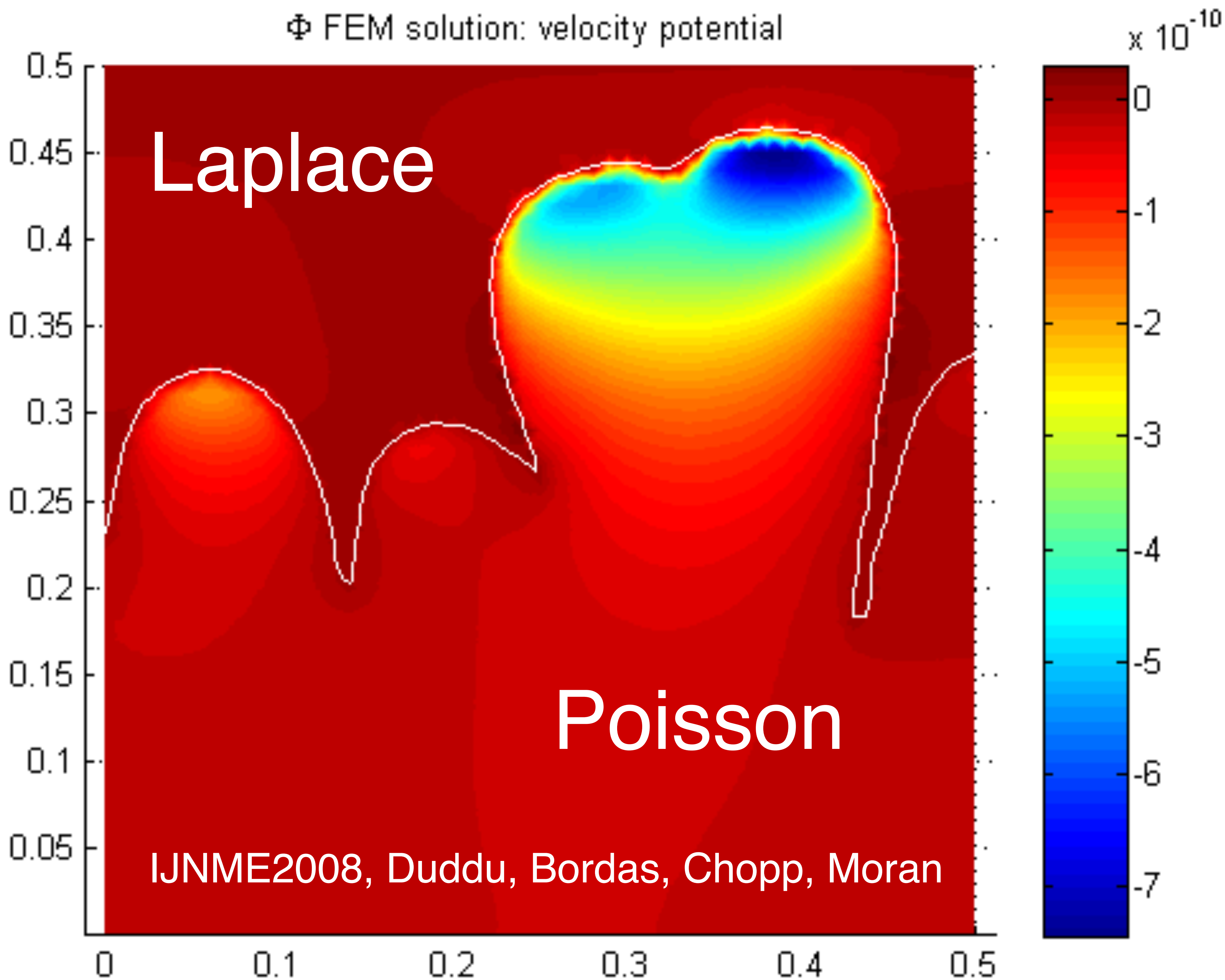


Interfaces between different PDEs

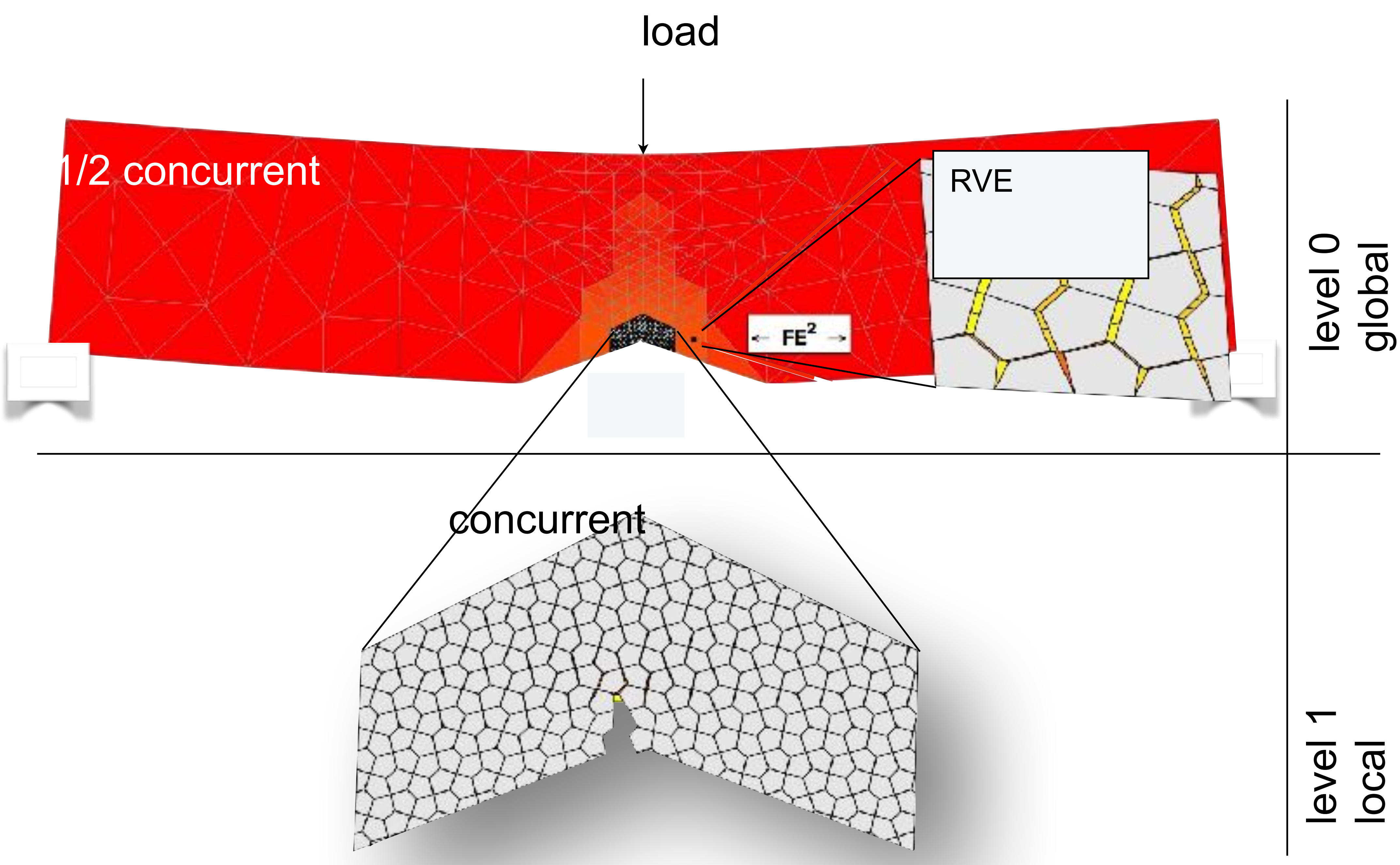
e.g. Biofilms



Interfaces between different PDEs

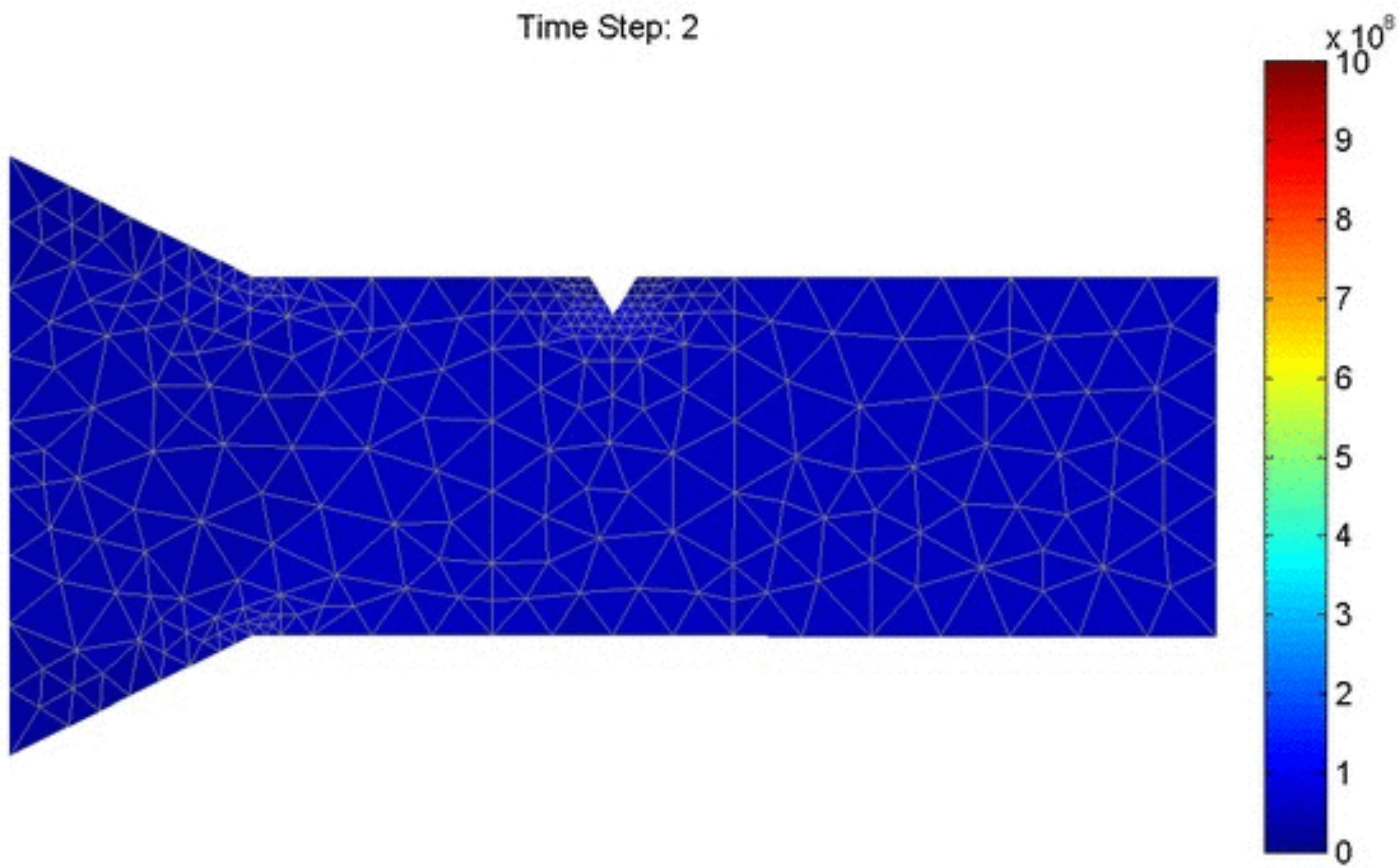


Interfaces between material models

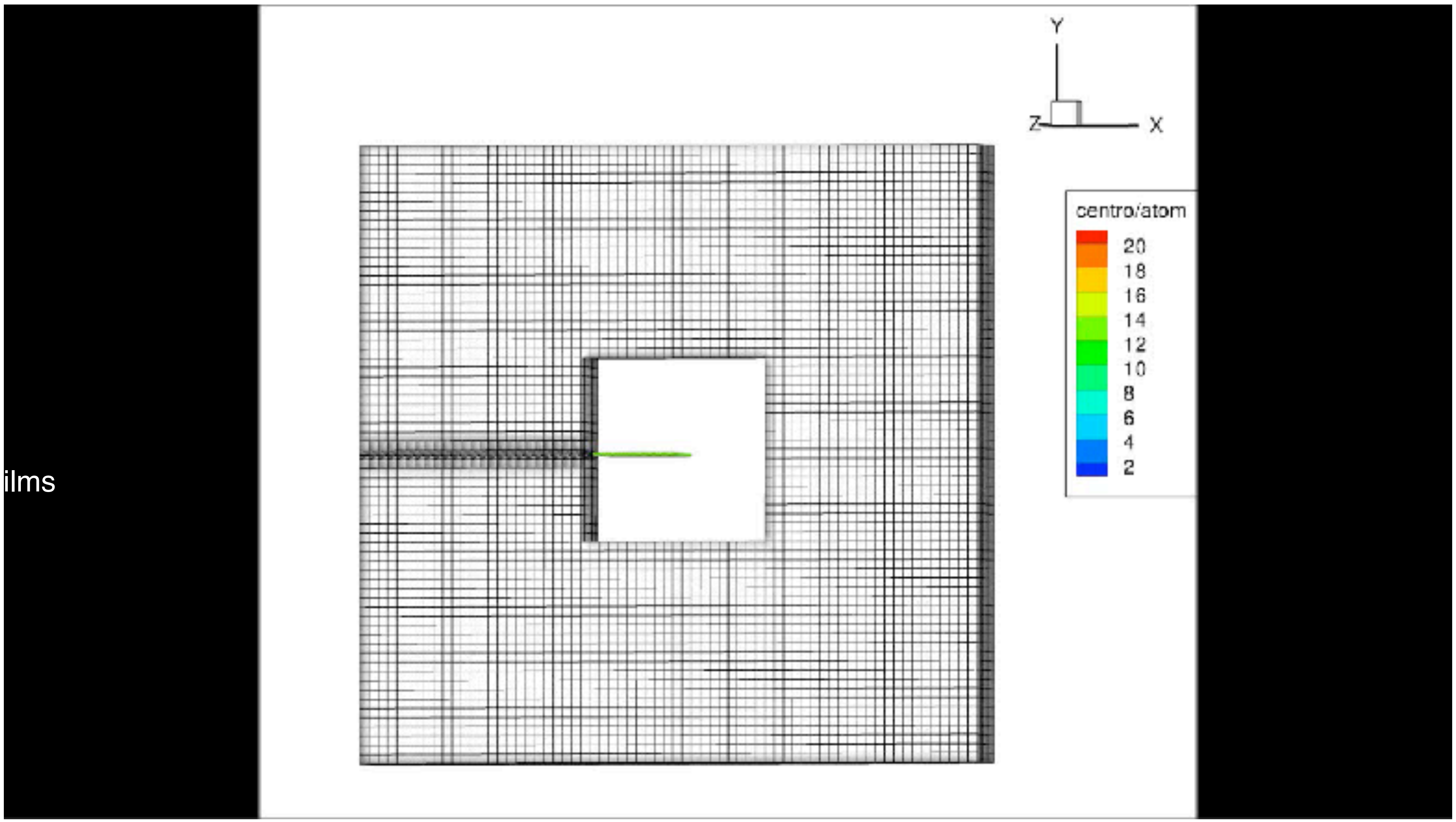


PhilMag15, Akbari
CMAME13,CMECH16, Goury
NMPDES13,CMAME15, Chi

Adaptive model selection



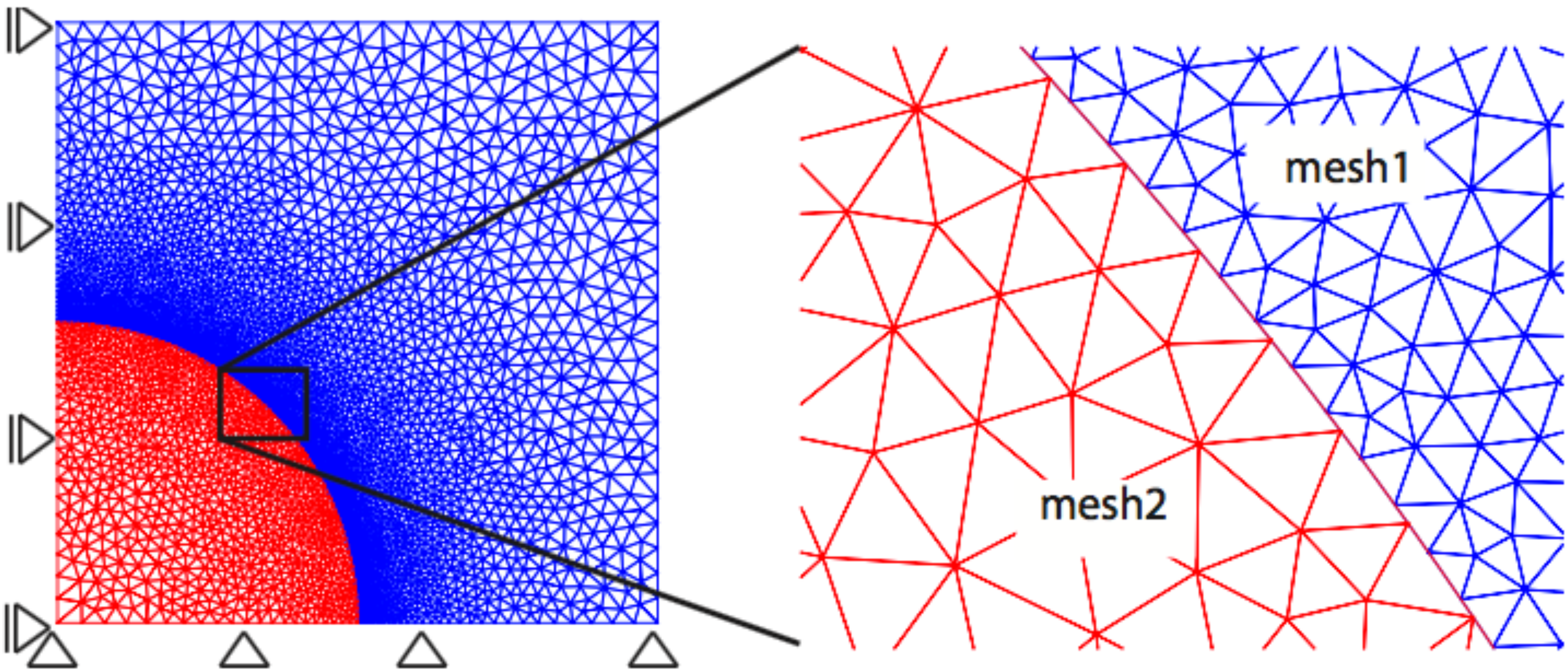
Molecular dynamics - continuum interfaces



CMECH14, IJMSE13 Talebi

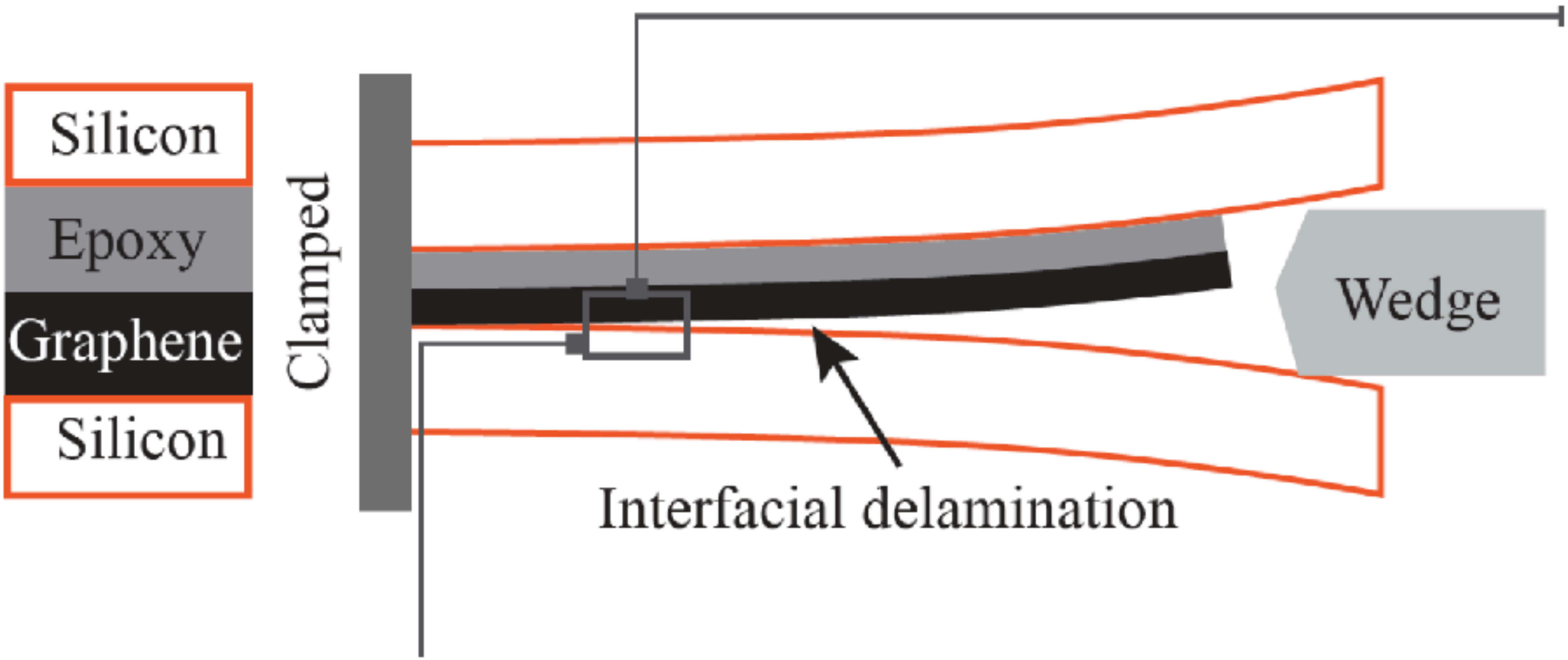
Interfaces between different discretizations

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

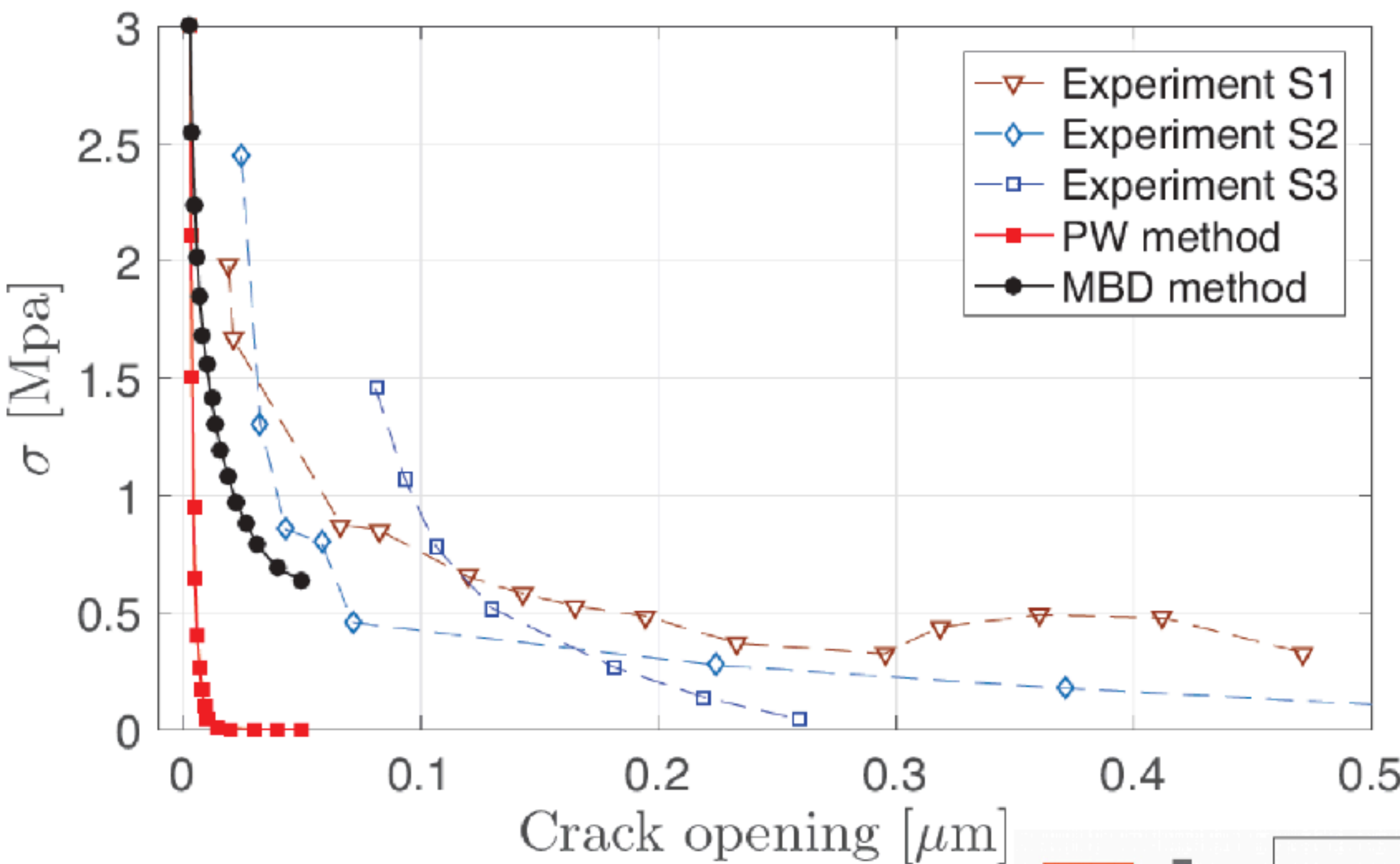
Ultra-long range delimitation mechanics

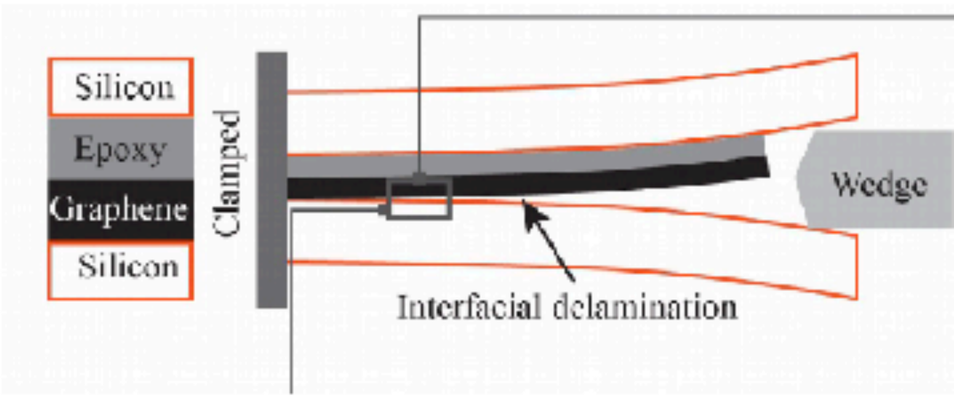


2018 APS - With Tkatchenko, Ambrosetti and Nguyen Thanh-Tung

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).

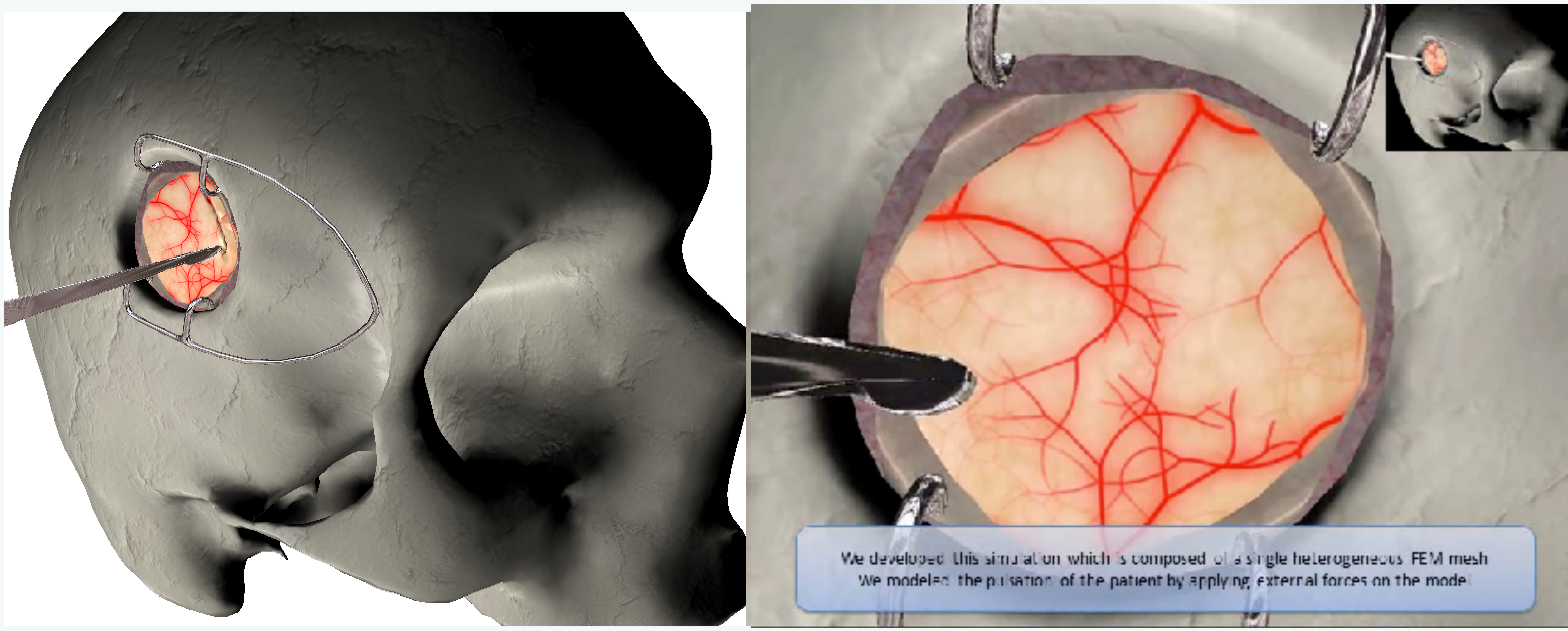
Ultra-long range delimitation mechanics





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

Cutting in soft tissue

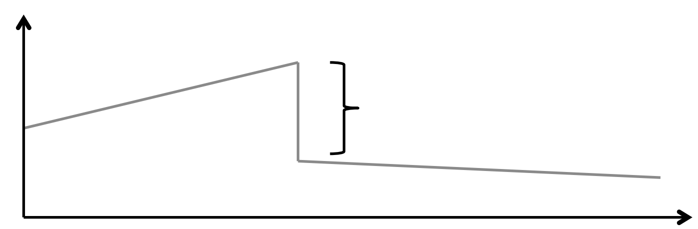


Real-time simulation of cutting during brain surgery
Med. Im. Anal. 2014 Courtecuisse, Cotin, SPAB et al.

Classification of Discontinuities

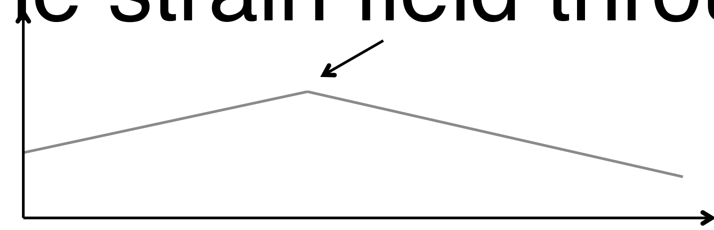
Strong discontinuities

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



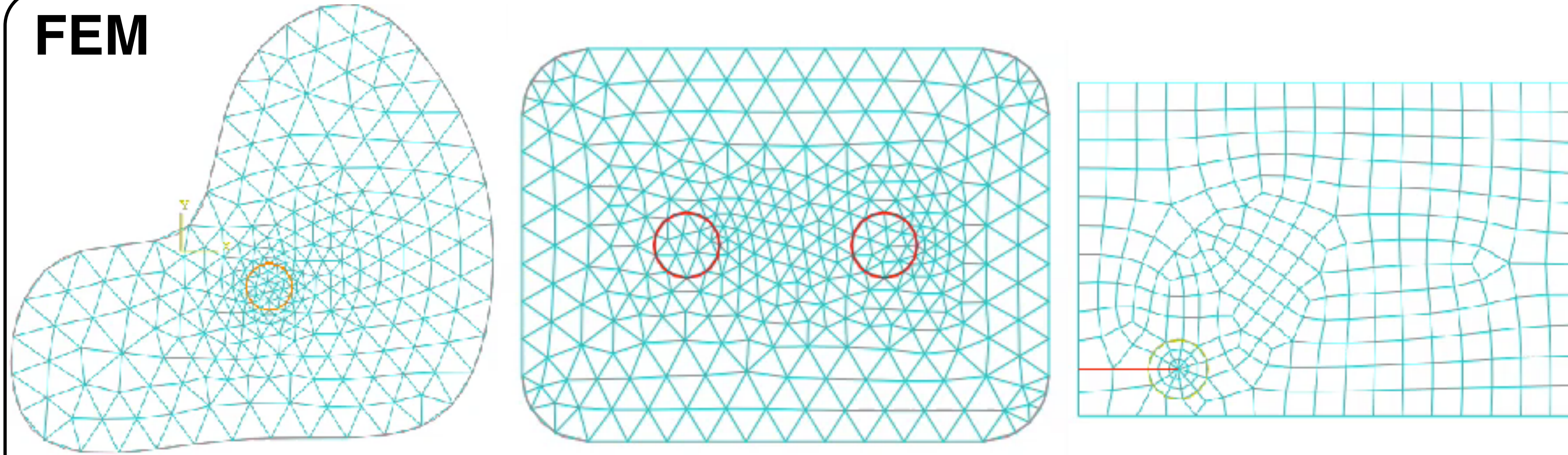
Weak discontinuities

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

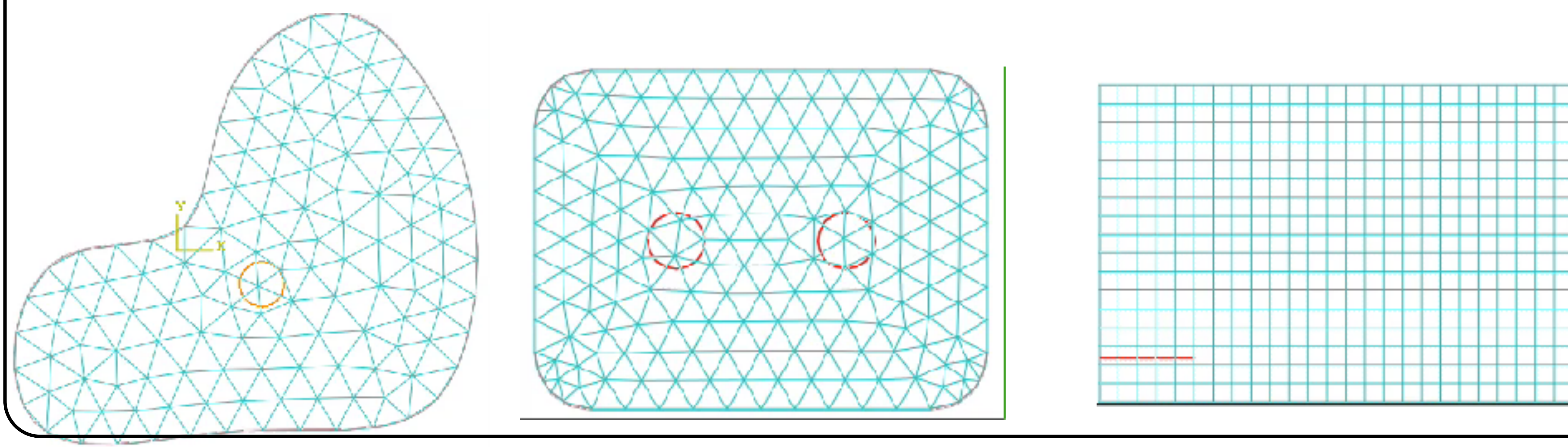


Discretization of interface problems

FEM



XFEM



Discretization of interface problems
Challenges

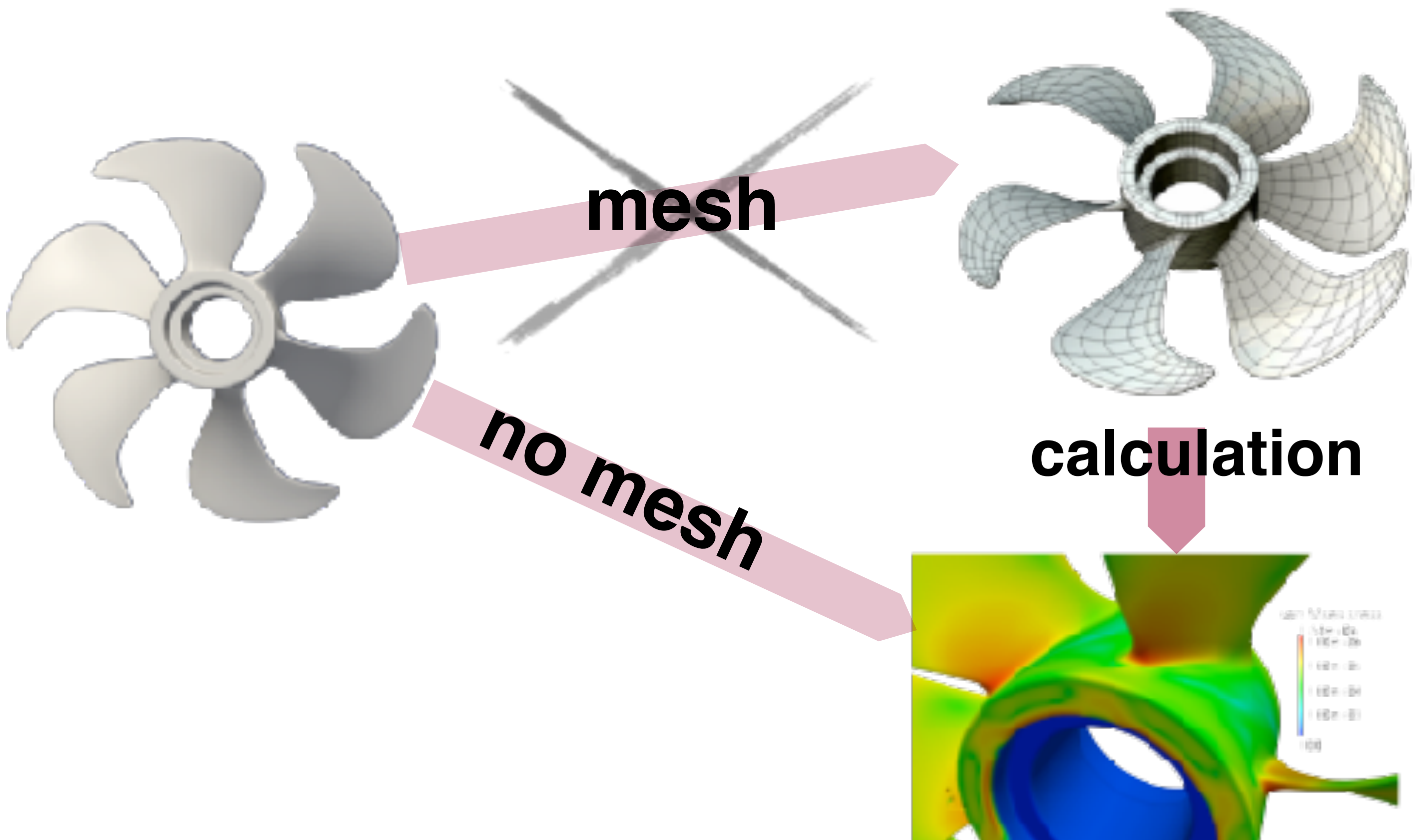
Evolving and complex geometries

Accurate calculations of front velocities

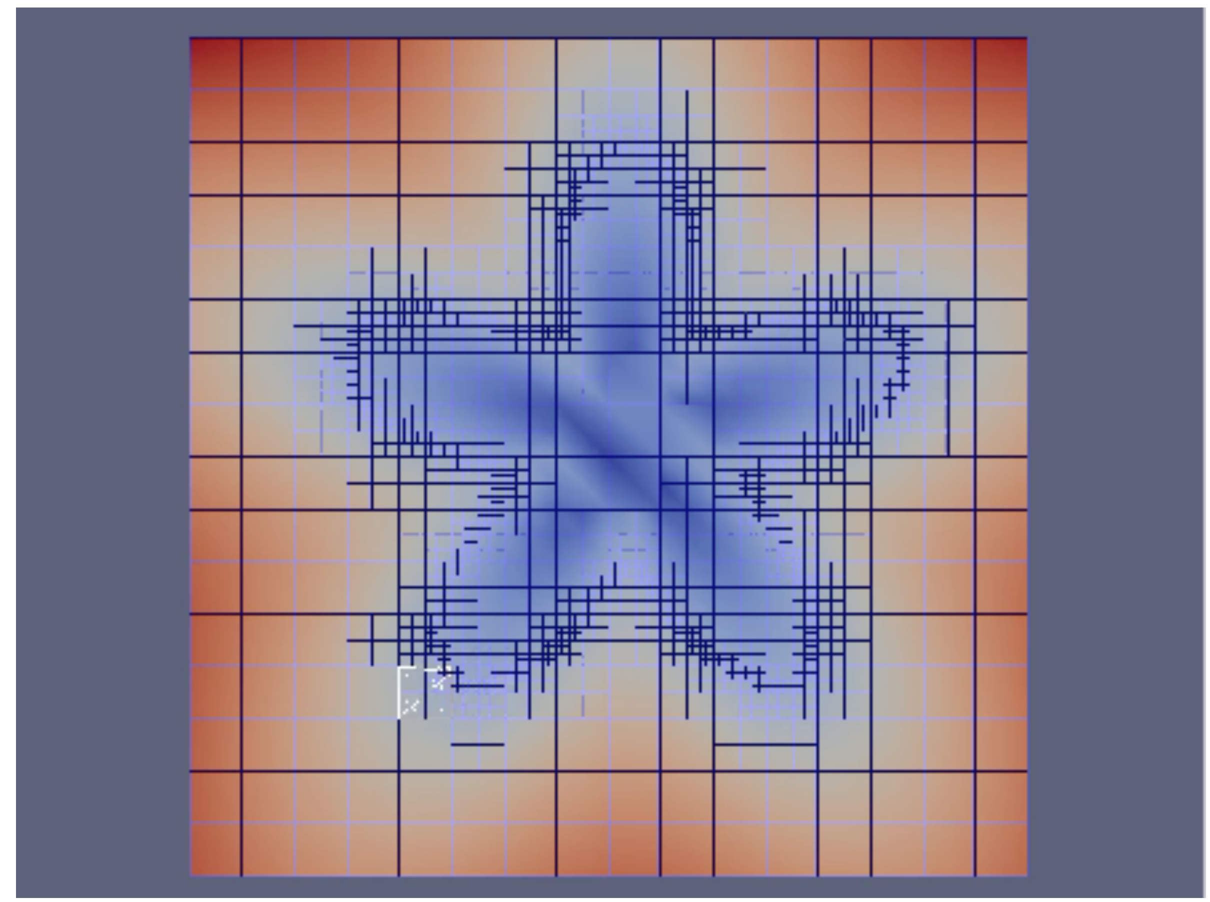
Error estimation and adaptivity

Time stepping schemes

Handling interfaces numerically



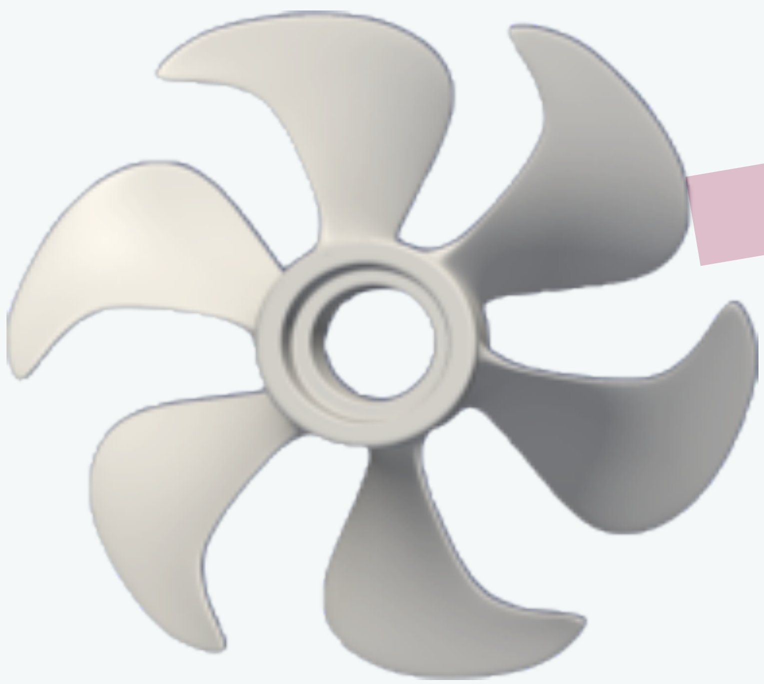
Coupling - isogeometric analysis



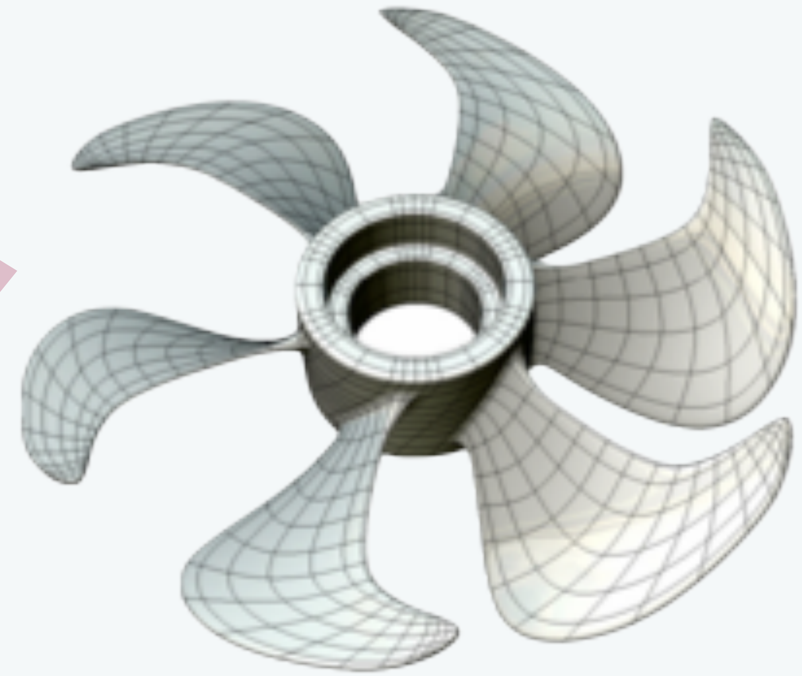
Decoupling - implicit interfaces

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

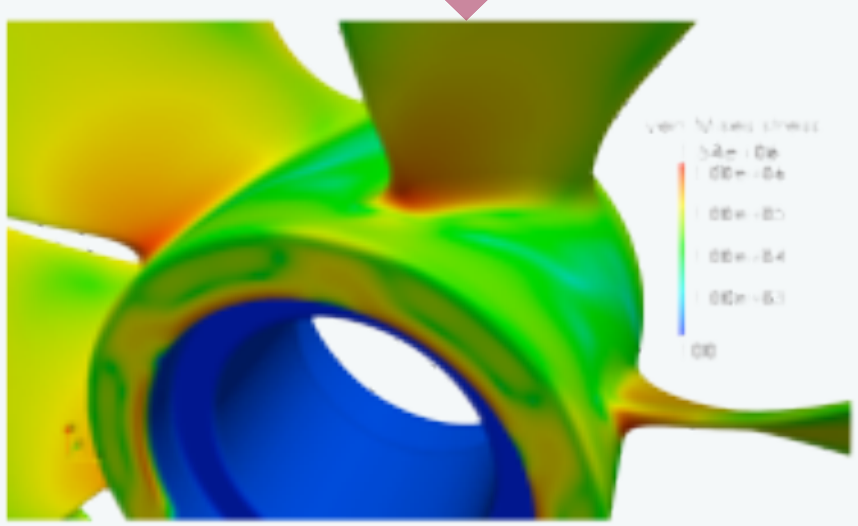
Isogeometric analysis



mesh

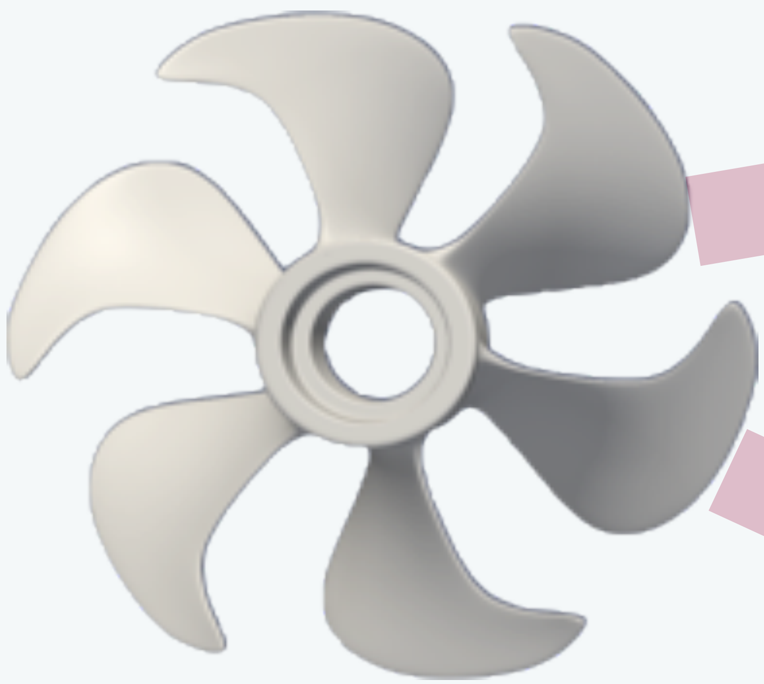


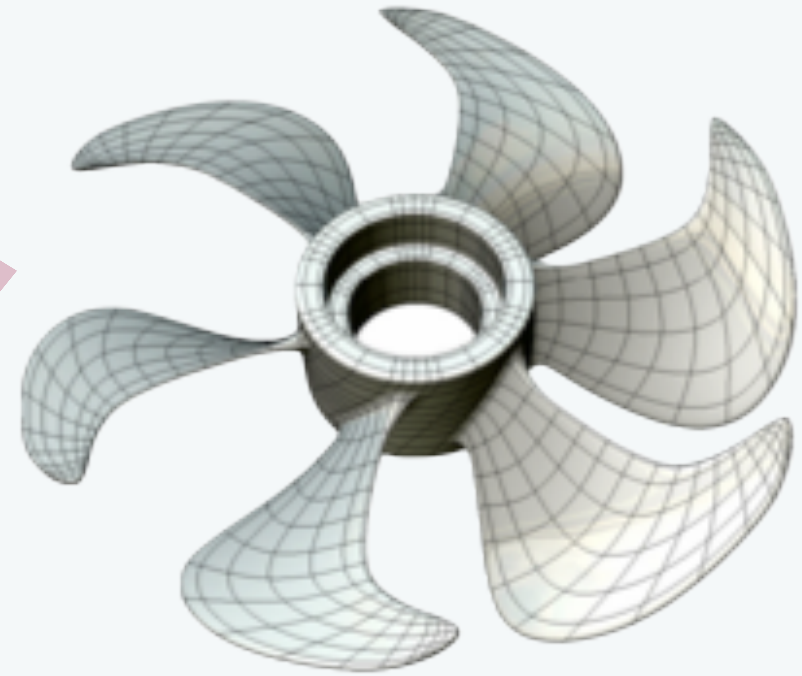
calculation

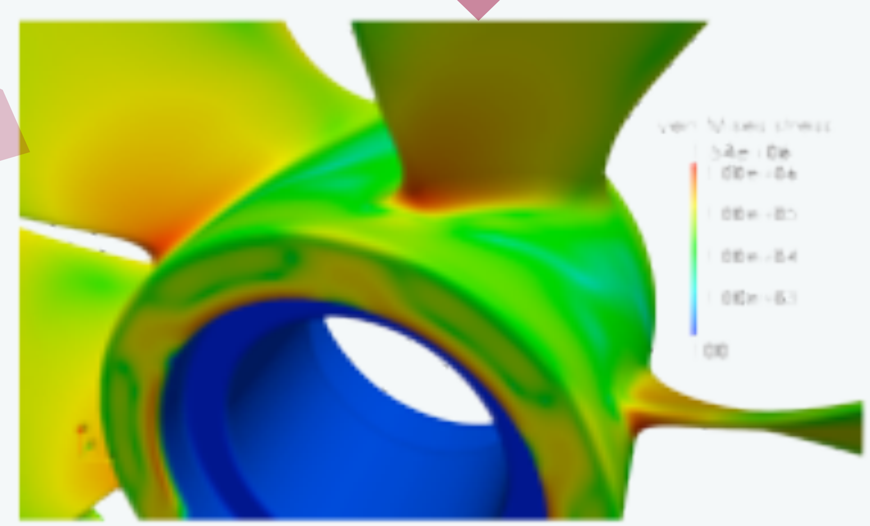


stress analysis

Isogeometric analysis

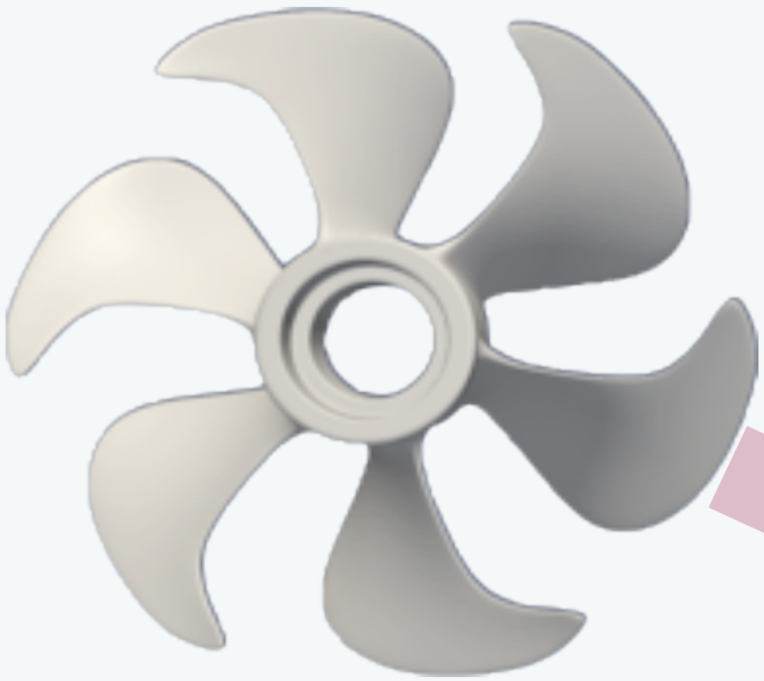




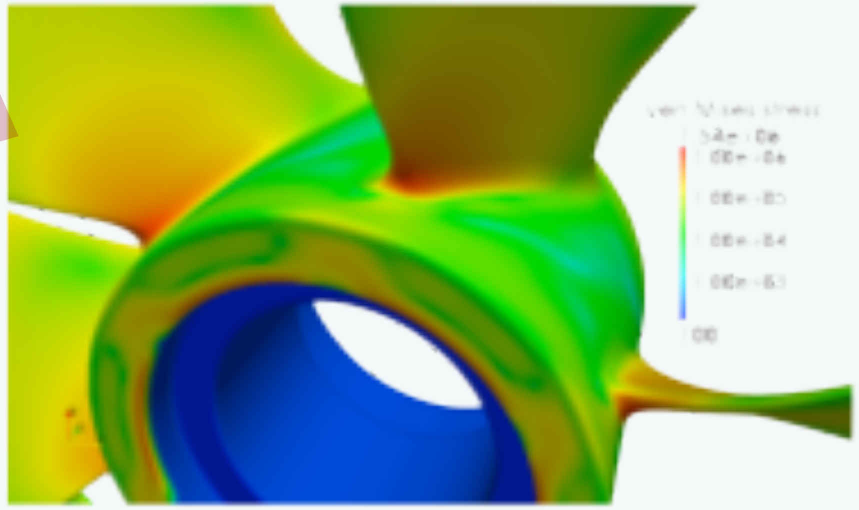


Idea: Hughes et al. 2005. Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.

Isogeometric analysis



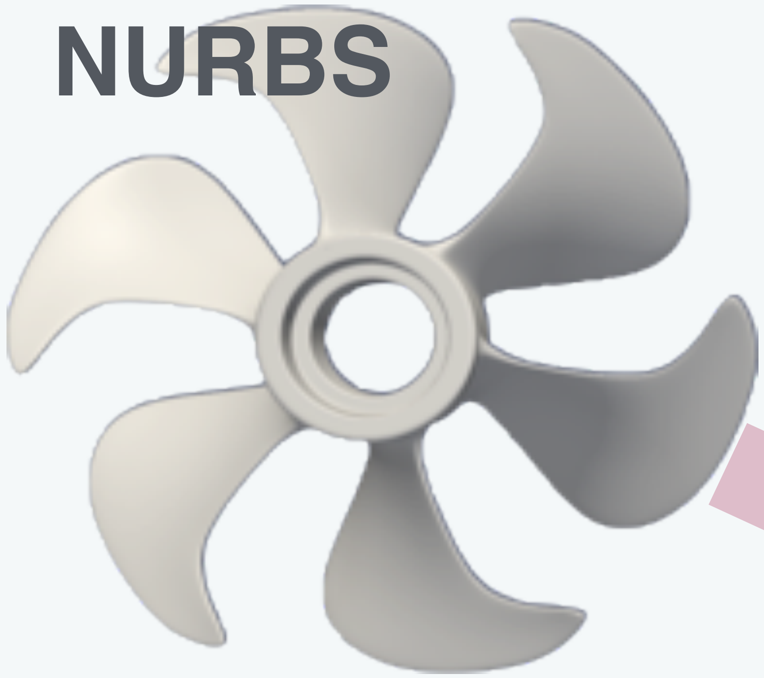
direct calculation



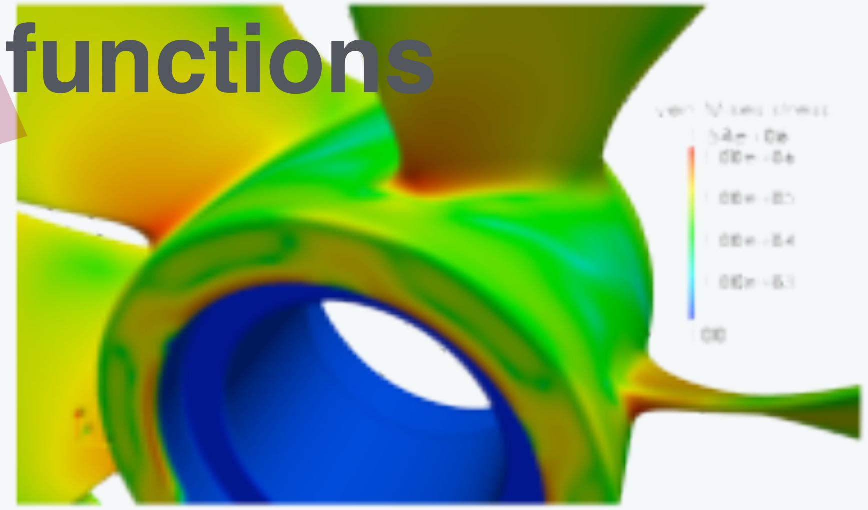
stress analysis

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

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?

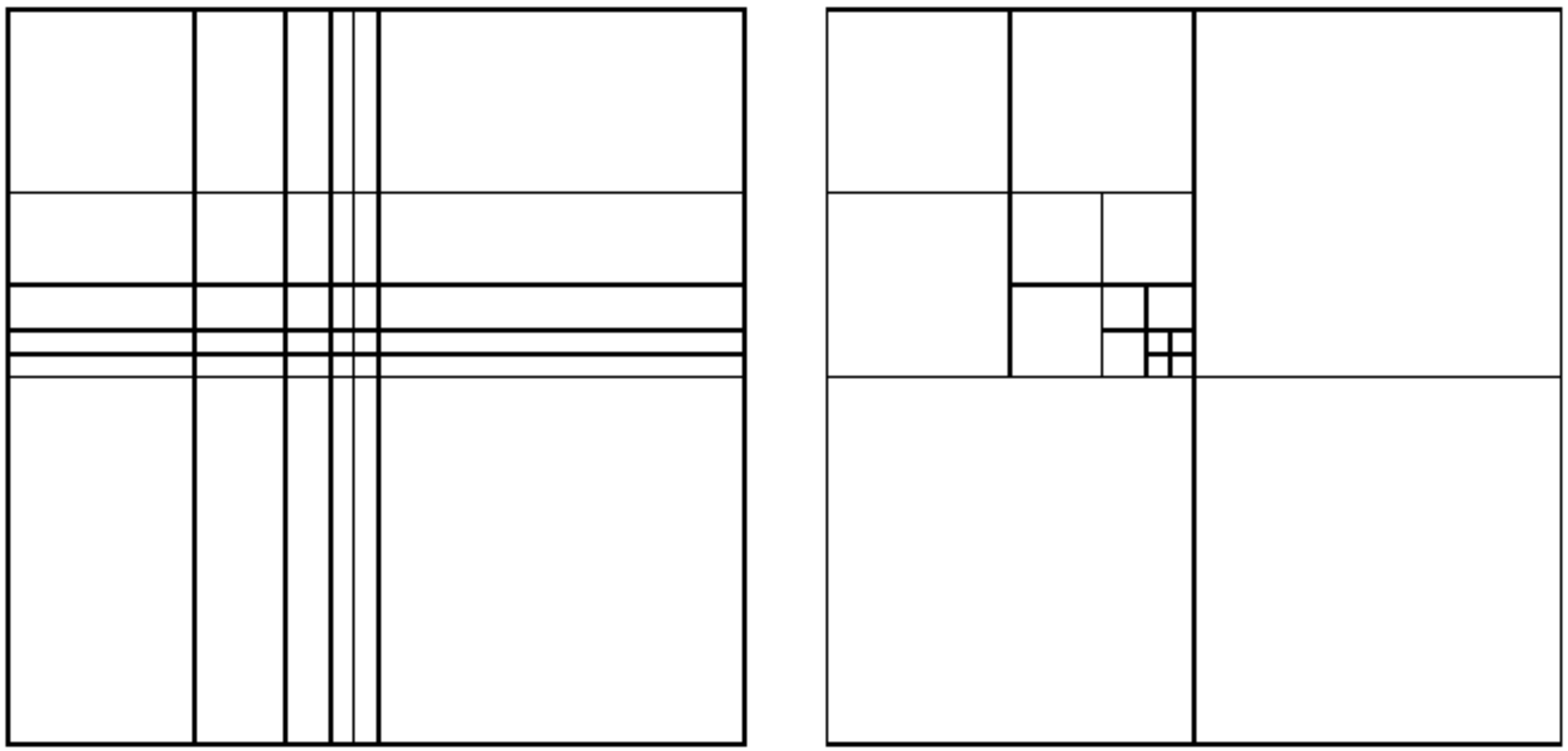
Isogeometric Finite Element Analysis

- [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)

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

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

 erc RealTCut

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)

Isogeometric Boundary Element Analysis

☑ For shell-like domains
☑ For volumes

Stress analysis and shape optimisation directly from CAD

H. Lian et al. (2017). CMAME*:* 317 (2017): 1-41.
H. Lian et al. (2015). IJNME
H. Lian et al. (2013). EACM:166(2):88-99.
M. Scott et al. (2013) CMAME 254: 197-221.
R. N. Simpson et al. (2013) CAS 118: 2-12.
R. N. Simpson et al. (2012) CMAME Feb 1;209:87-100.

Fracture mechanics directly from CAD

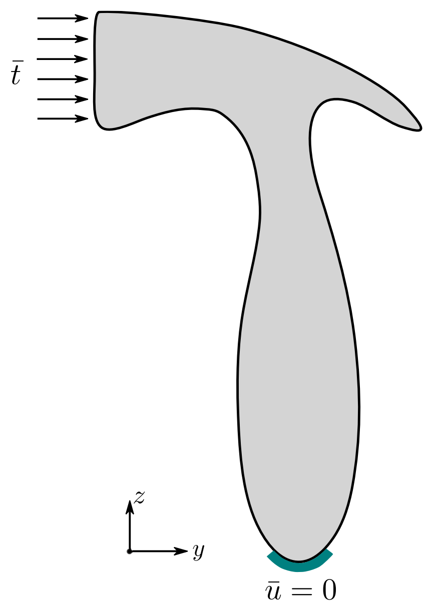
X. Peng, et al. (2017). *IJF*, 204(1), 55–78.
X. Peng, et al. (2017). *CMAME*, 316, 151–185.

Handling (complex) interfaces numerically

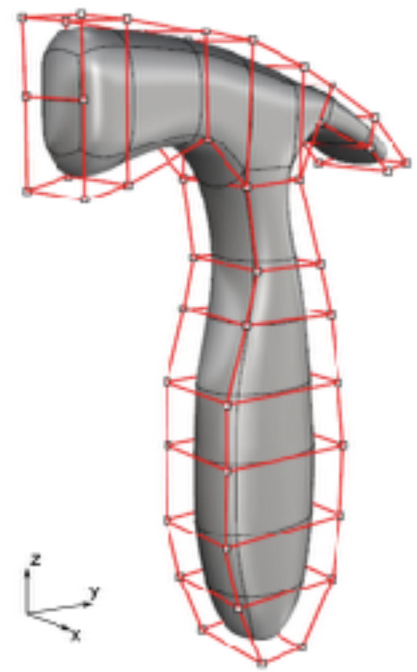
Example applications
Isogeometric Boundary Element Analysis (IGABEM)

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

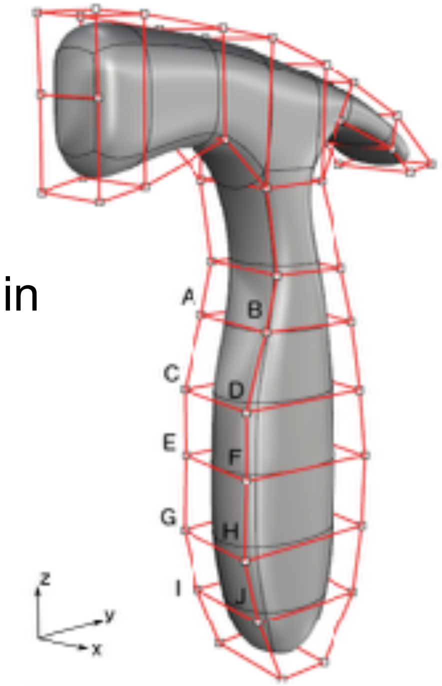
Shape optimisation



Model construction with CAD



Design points selection in control points



Problem definition

Control points

Design points

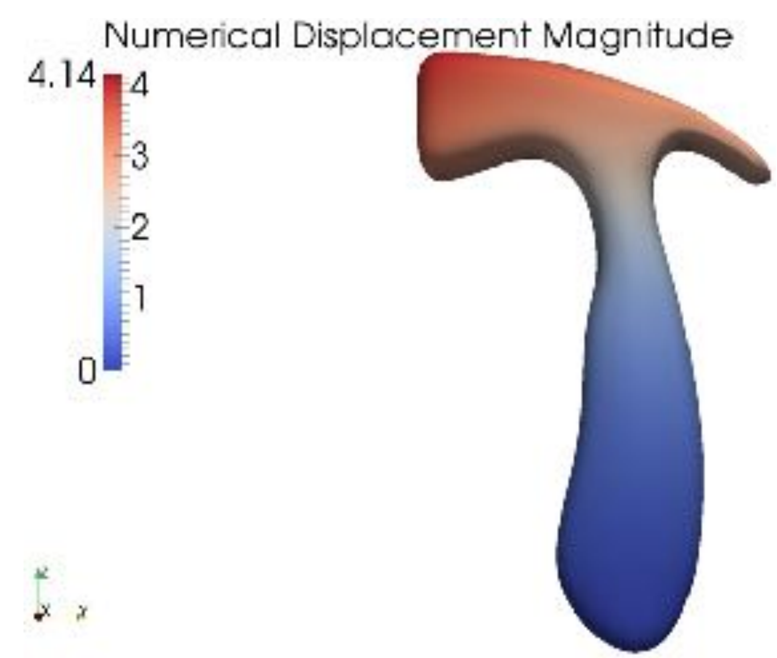
Objective function: $$\int_S t_i u_i \mathrm{d}S$$

Volume constraint: $$V - V_0 \leq 1$$

Side constraints:

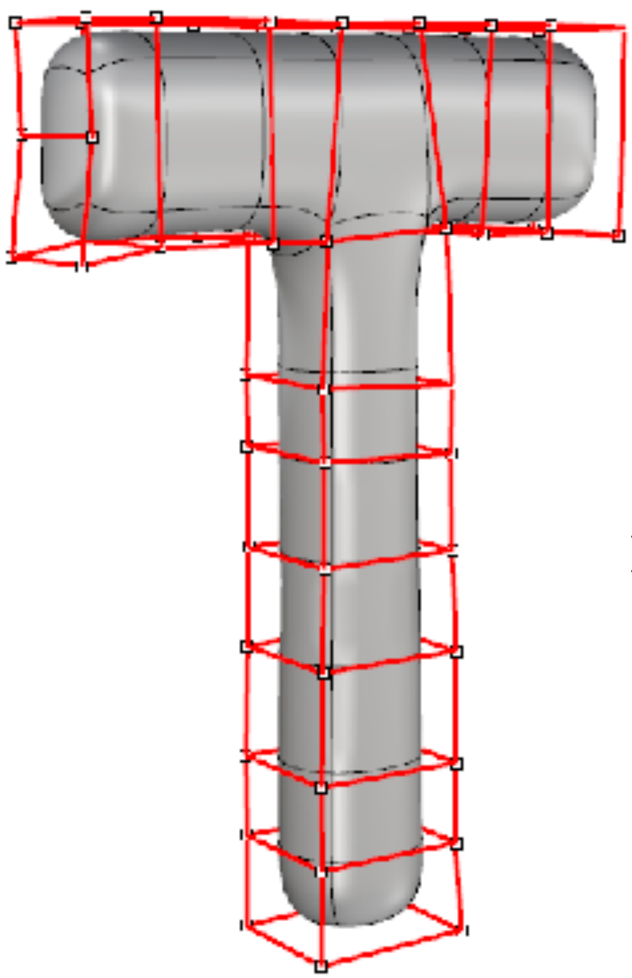
Design variable	Lower bound	Upper bound	Initial value
t_1	0	4	2.45
t_2	0	4	1.25
t_3	0	4	1.33
t_4	0	4	1.28
t_5	0	4	2.30

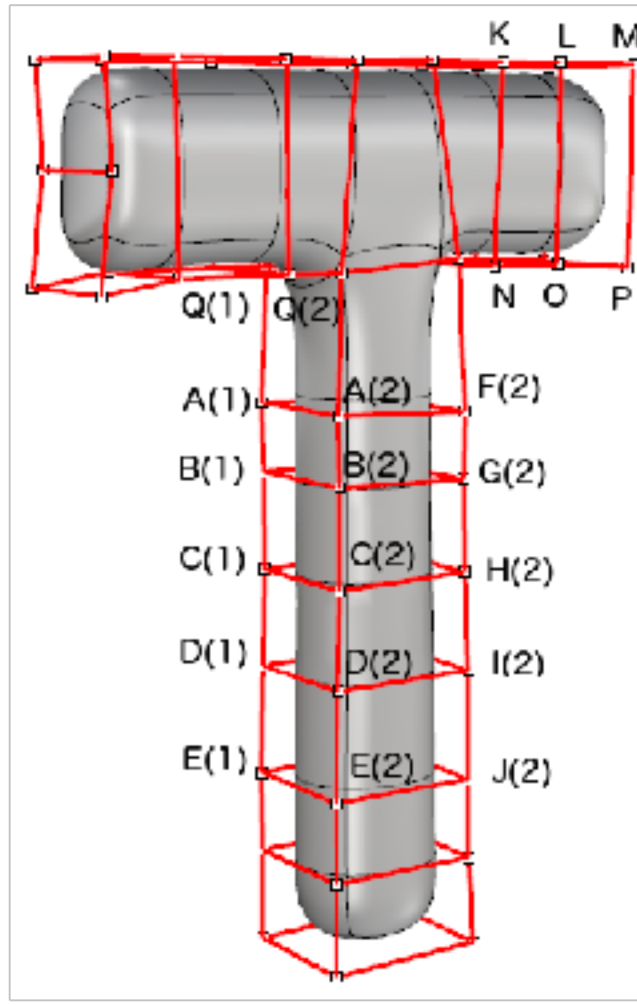
Structural analysis;
Sensitivity analysis;
gradient-based optimizer



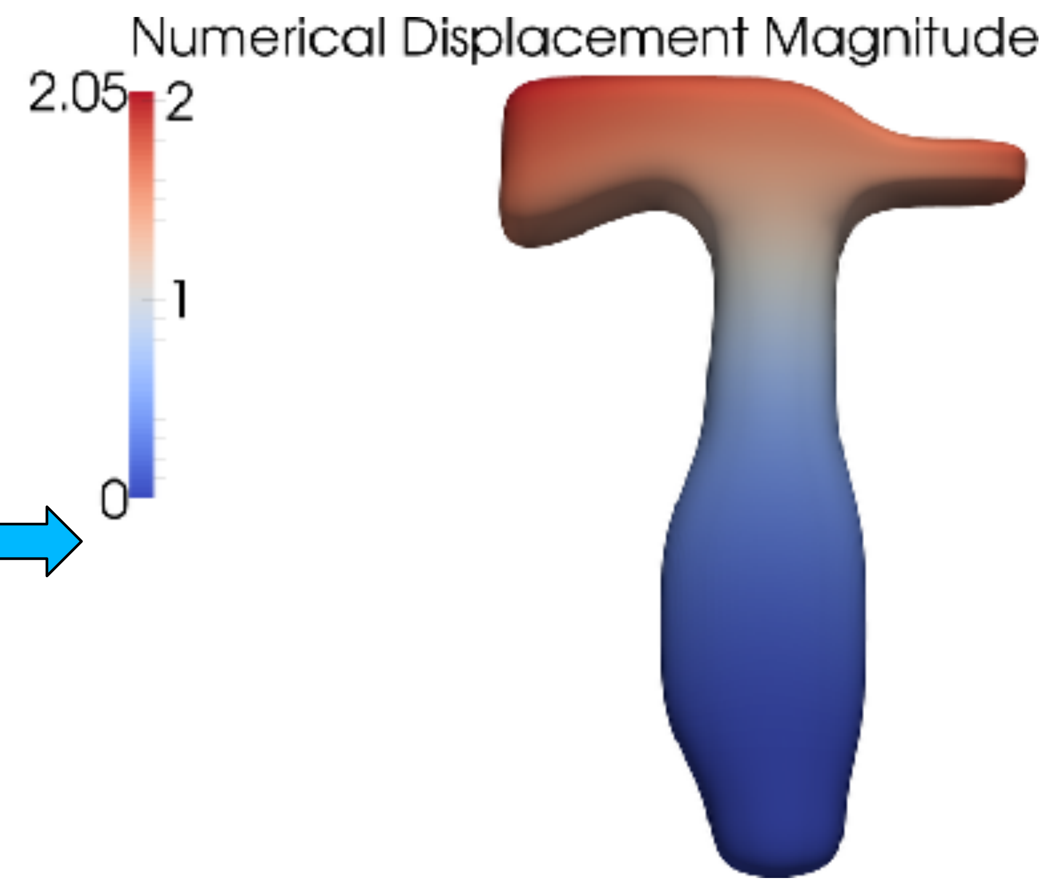
Optimized solution

Shape optimization





Choose design points from the control points



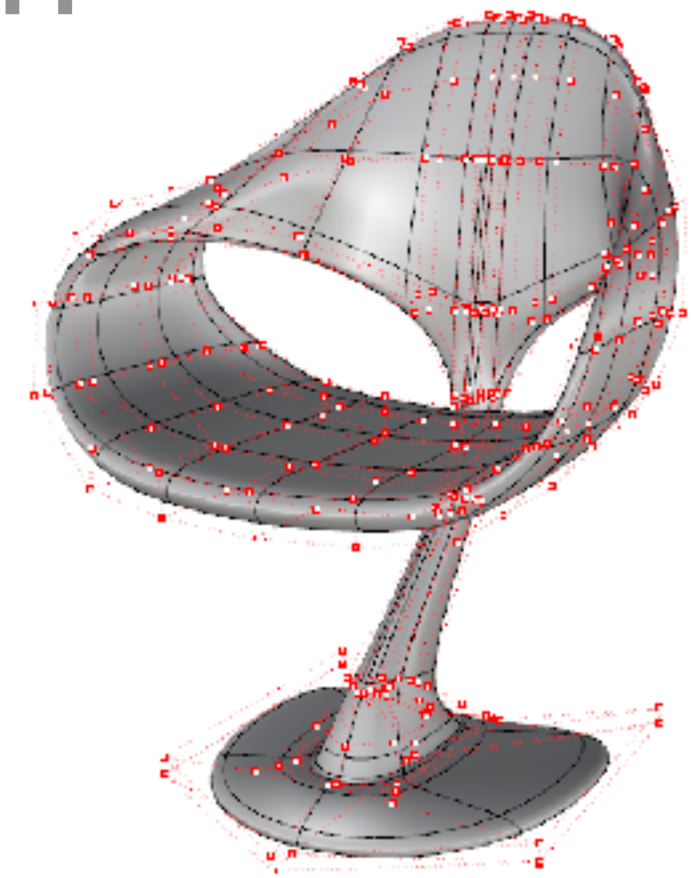
Conduct sensitivity analysis to converge to the optimized solution

Stress analysis and shape optimisation directly from CAD

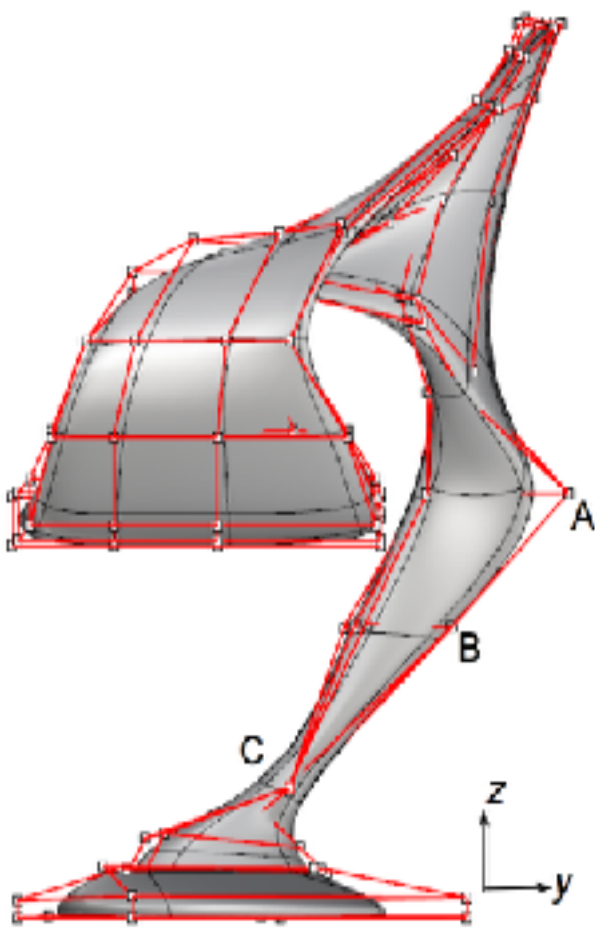
H. Lian et al. (2017). CMAME*:* 317 (2017): 1-41.
H. Lian et al. (2015). IJNME
H. Lian et al. (2013). EACM:166(2):88-99.

M. Scott et al. (2013) CMAME 254: 197-221.
R. N. Simpson et al. (2013) CAS 118: 2-12.
R. N. Simpson et al. (2012) CMAME Feb 1;209:87-100.

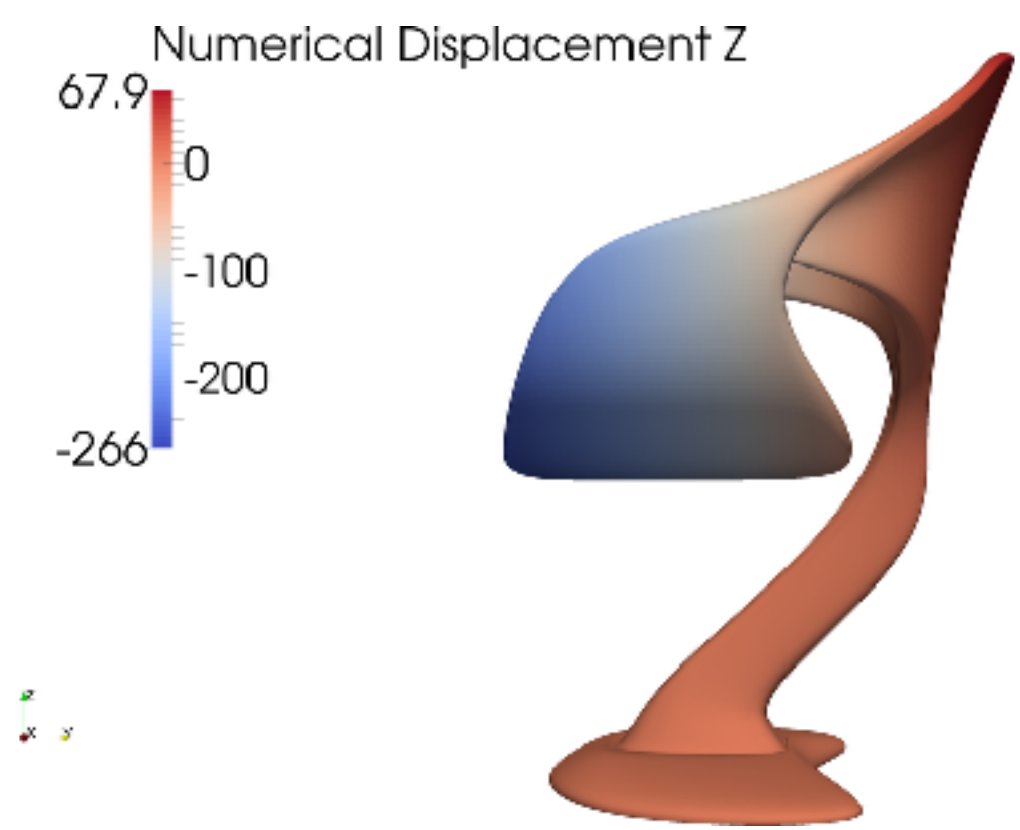
Shape optimization



Construct the geometric model (imported from Rhino)



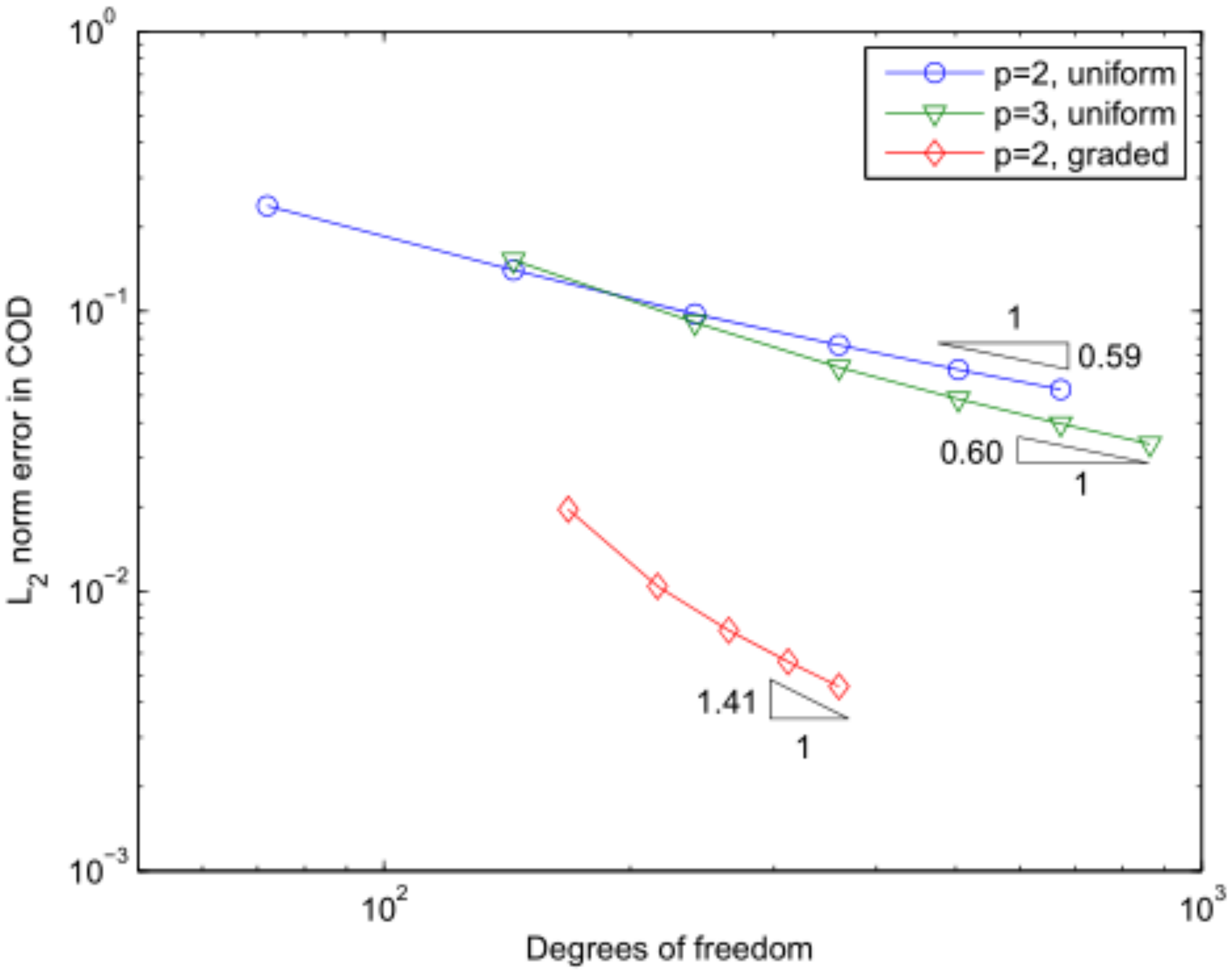
Select design points from control points



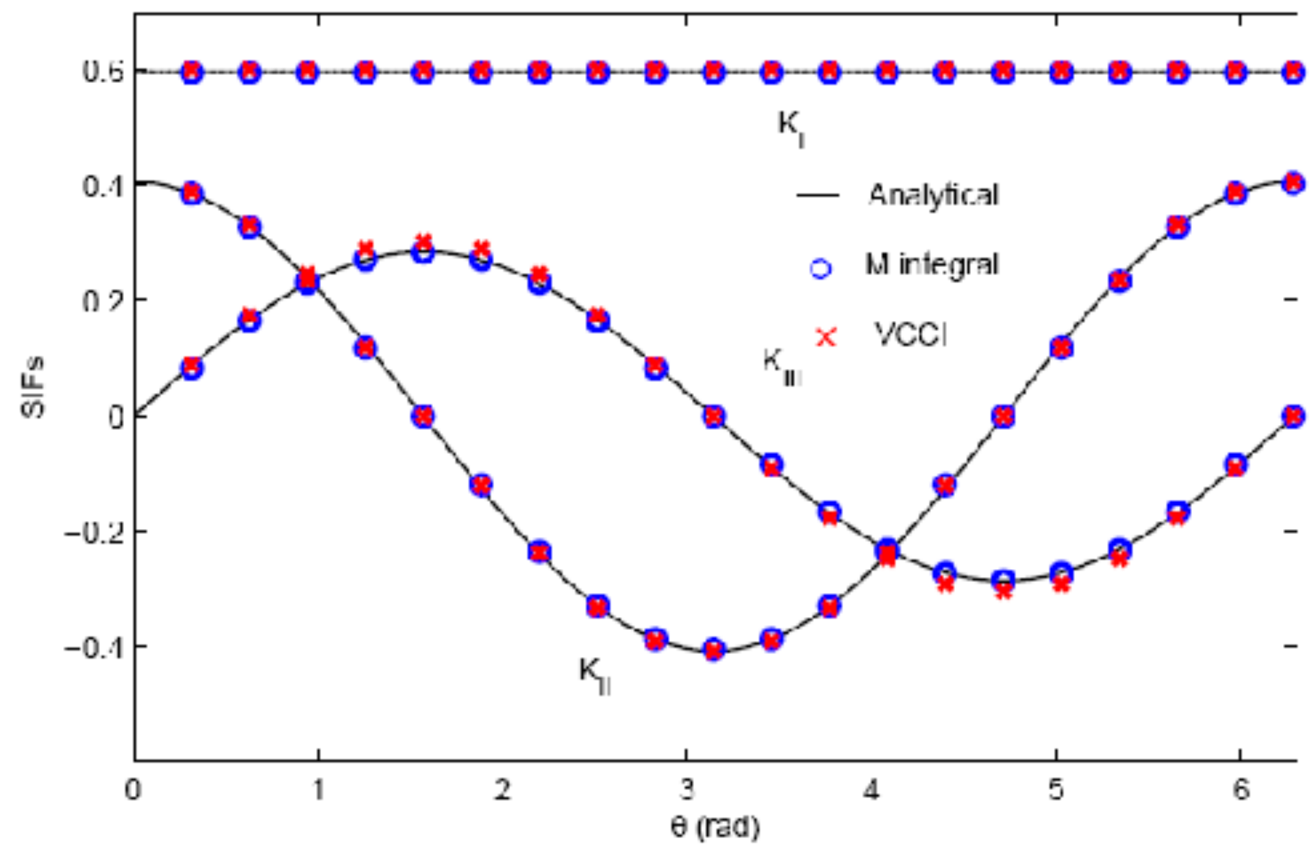
Find optimized solution

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



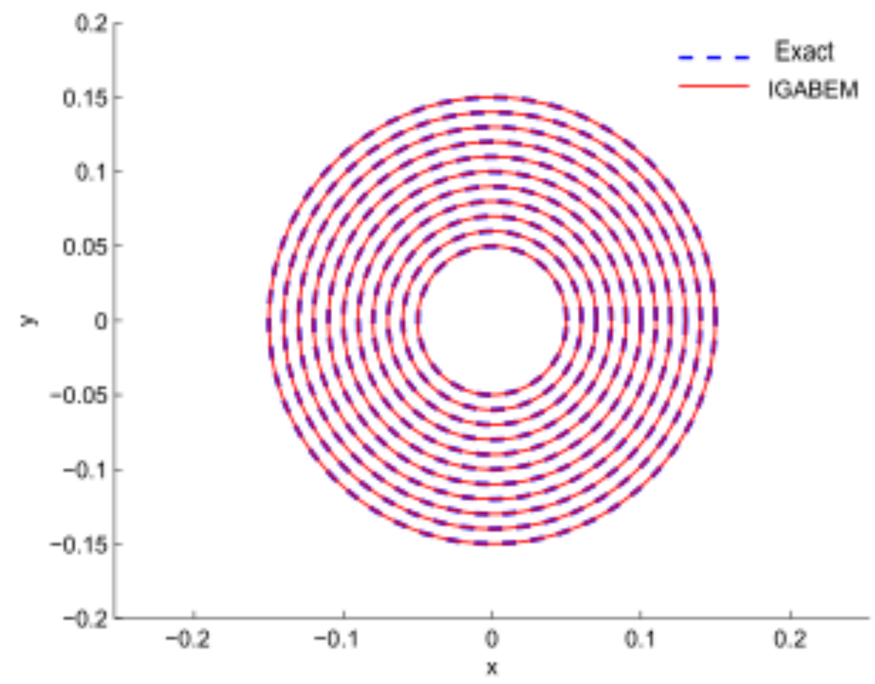
stress intensity factors for penny crack with $\varphi = \pi/6$

Fracture mechanics directly from CAD

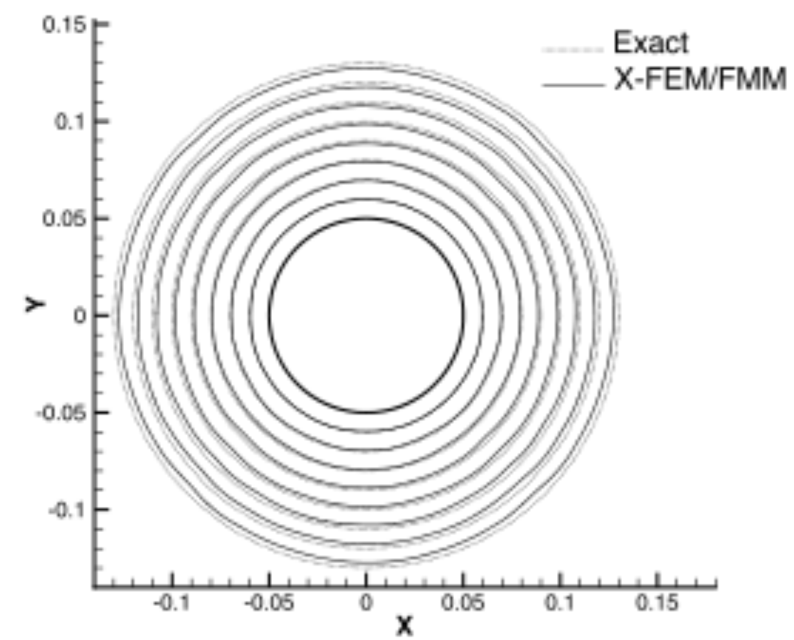
X. Peng, et al. (2017). *IJF*, 204(1), 55–78.

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

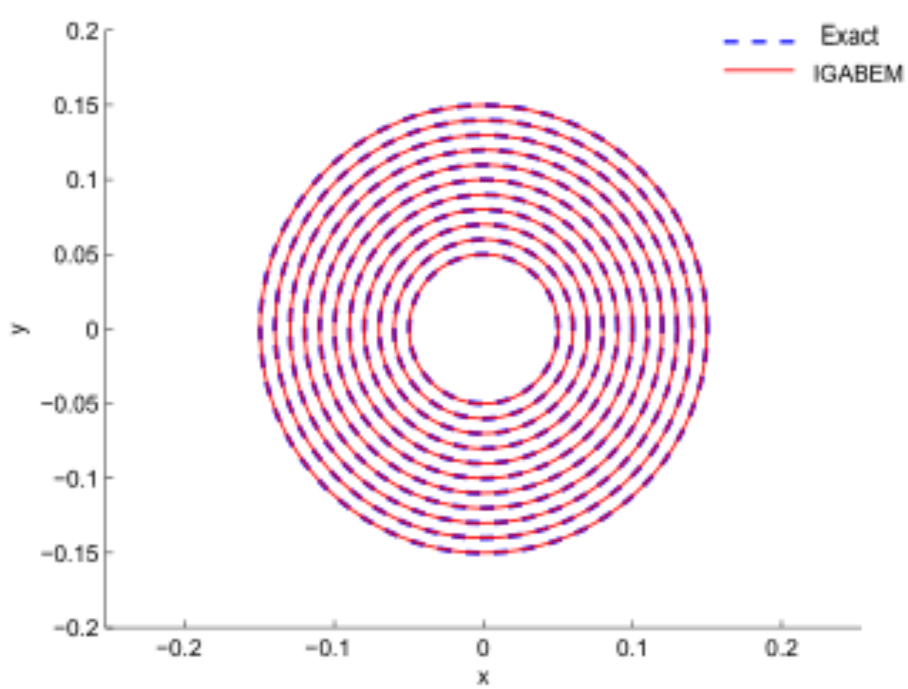
Penny crack growth



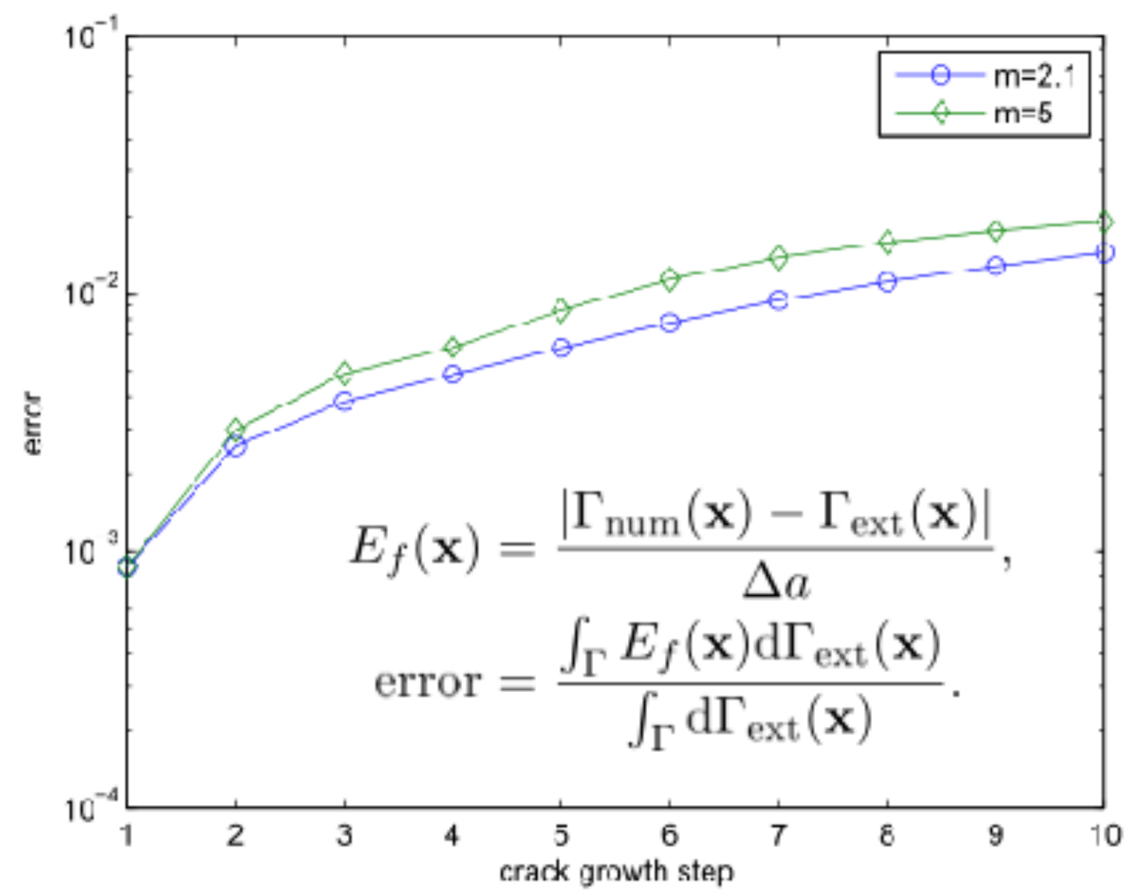
(a) IGABEM, $m = 2.1$



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



(c) IGABEM, $m = 5$

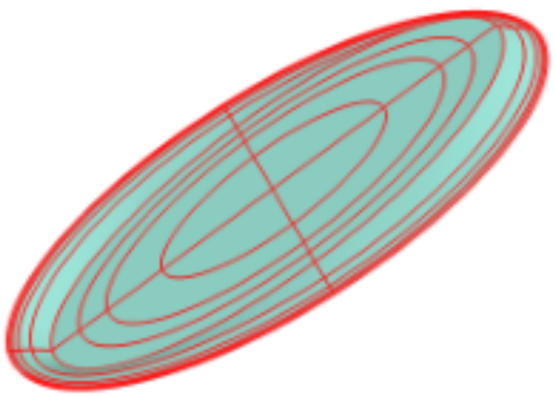


$$E_f(\mathbf{x}) = \frac{|\Gamma_{\text{num}}(\mathbf{x}) - \Gamma_{\text{ext}}(\mathbf{x})|}{\Delta a},$$

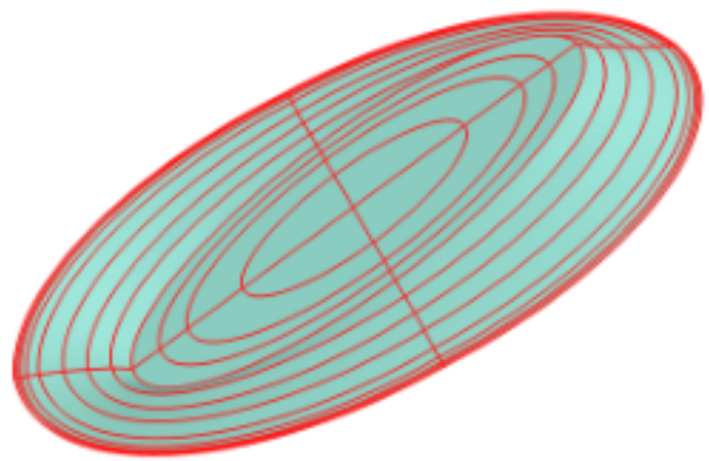
$$\text{error} = \frac{\int_\Gamma E_f(\mathbf{x}) d\Gamma_{\text{ext}}(\mathbf{x})}{\int_\Gamma d\Gamma_{\text{ext}}(\mathbf{x})}.$$

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

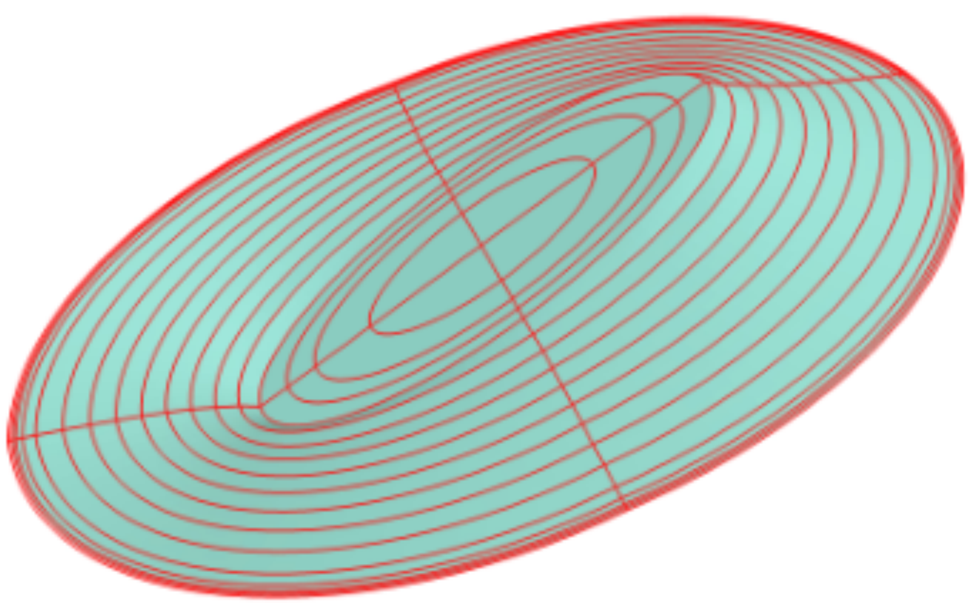
Inclined penny crack growth



(a) Step 2



(b) Step 5



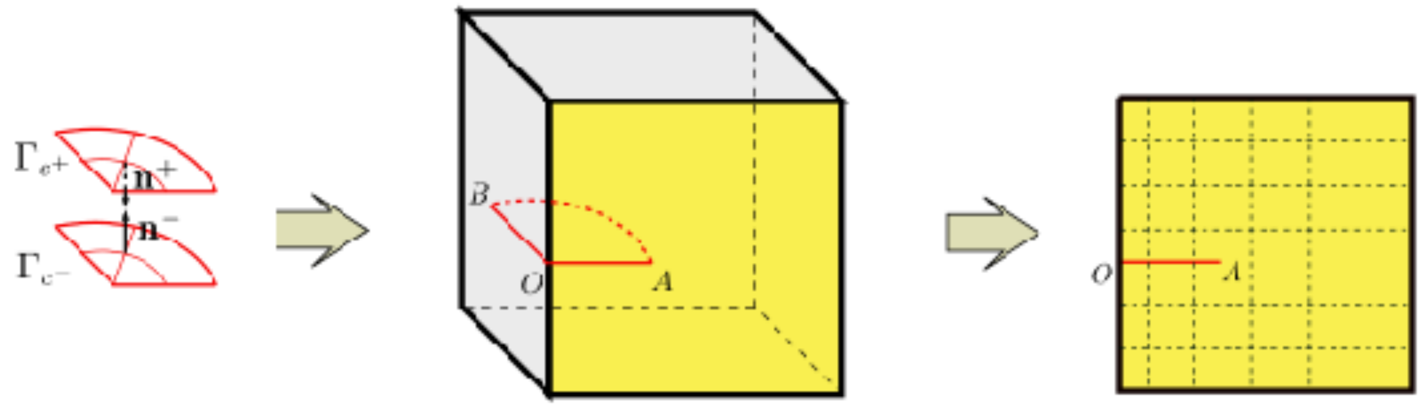
(c) Step 10

Fracture mechanics directly from CAD

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

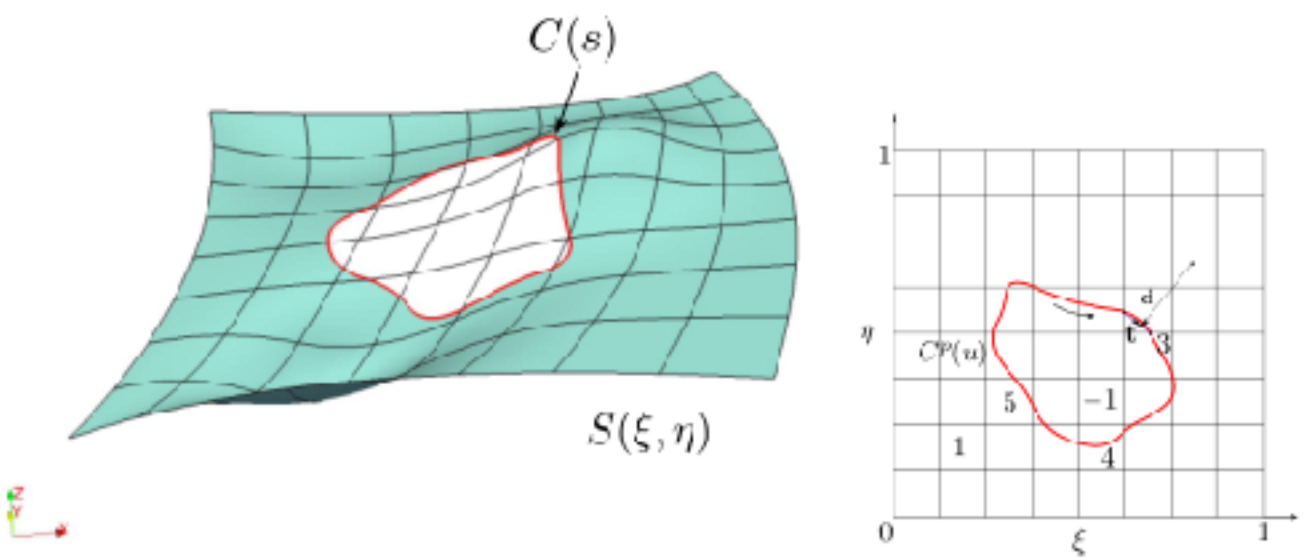
X. Peng, et al. (2017). *CMAME*, 316, 151–185.

Surface cracks



(a) (b) (c)

Surface discontinuity is introduced



(a) (b)

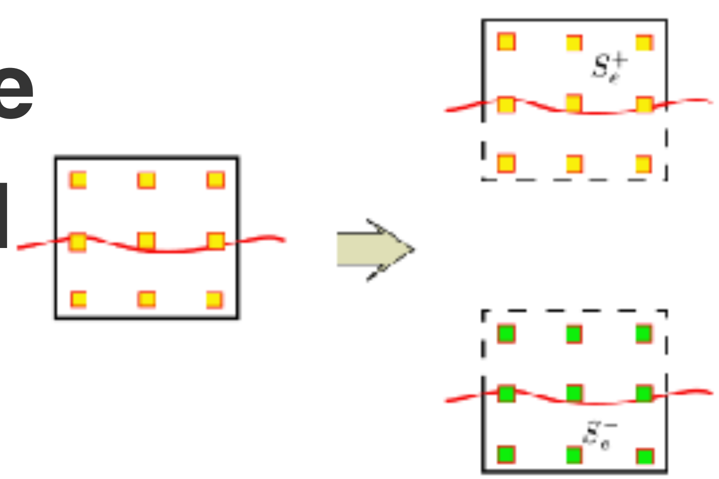
Trimmed NURBS technique

Crack = trimming curve

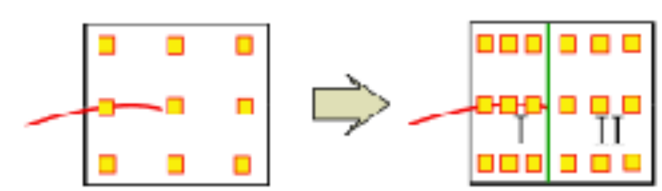
Phantom node method

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

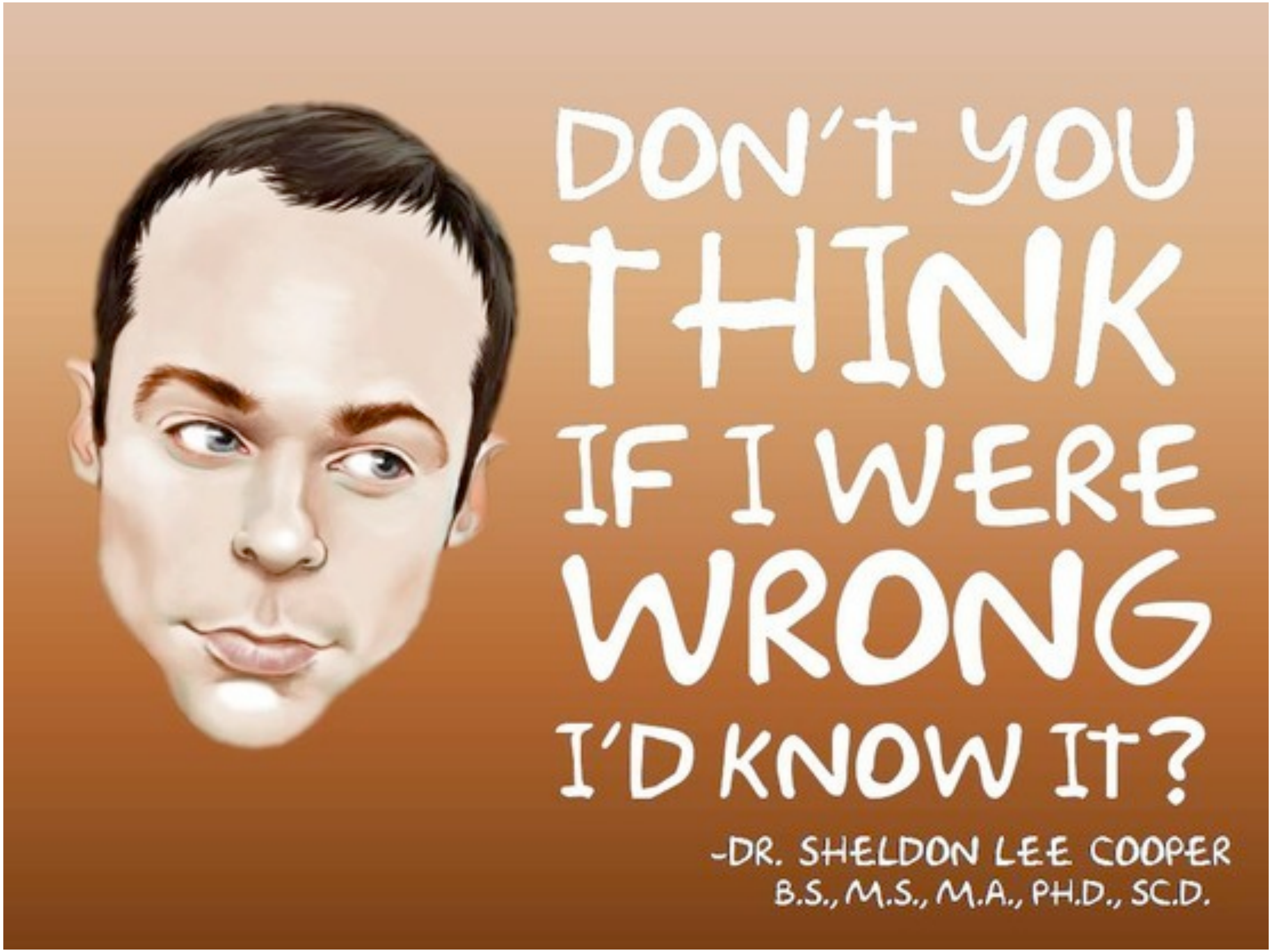
$$\mathbf{u}^-(\mathbf{x}) = \sum_{k}^{N^e} \mathbf{R}_k(\mathbf{x})\mathbf{d}_k, \quad \mathbf{x} \in S_e^-$$



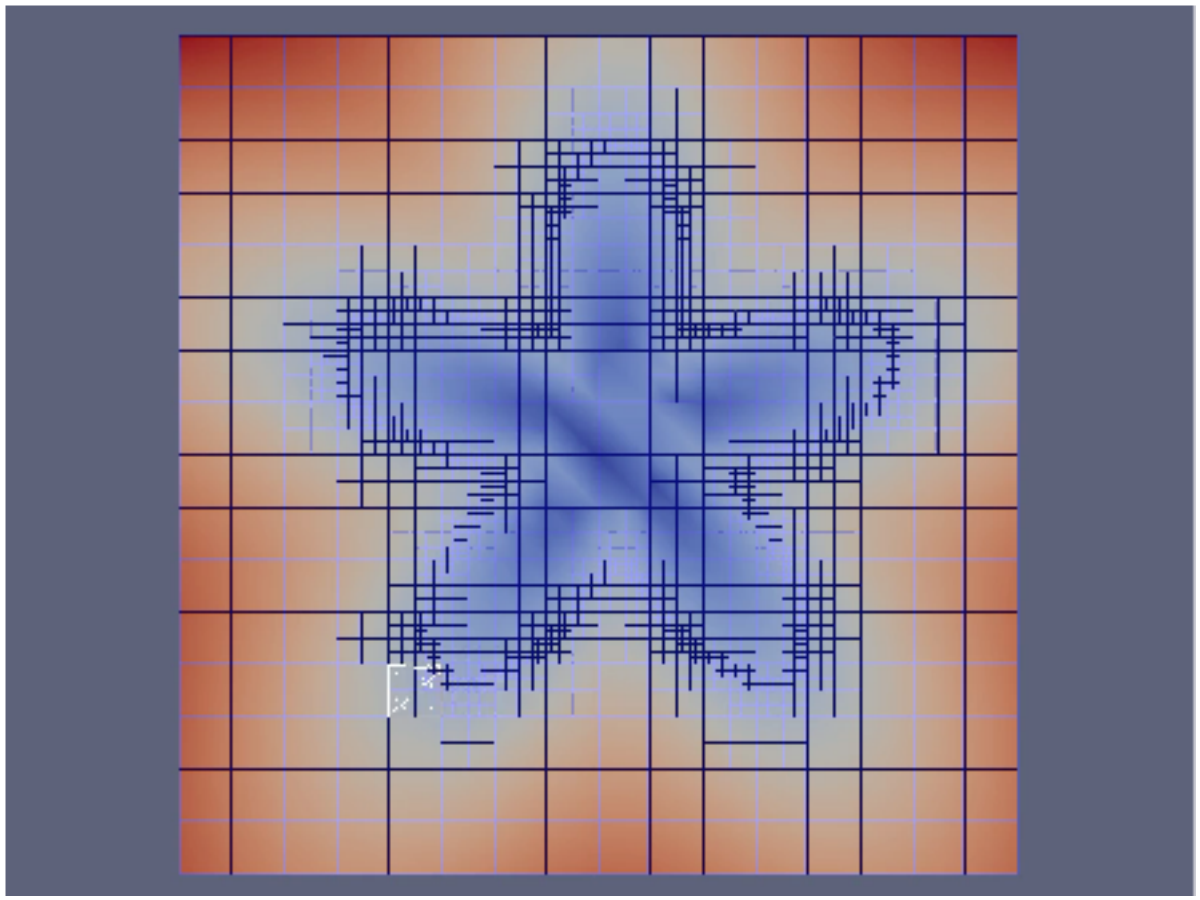
(a)

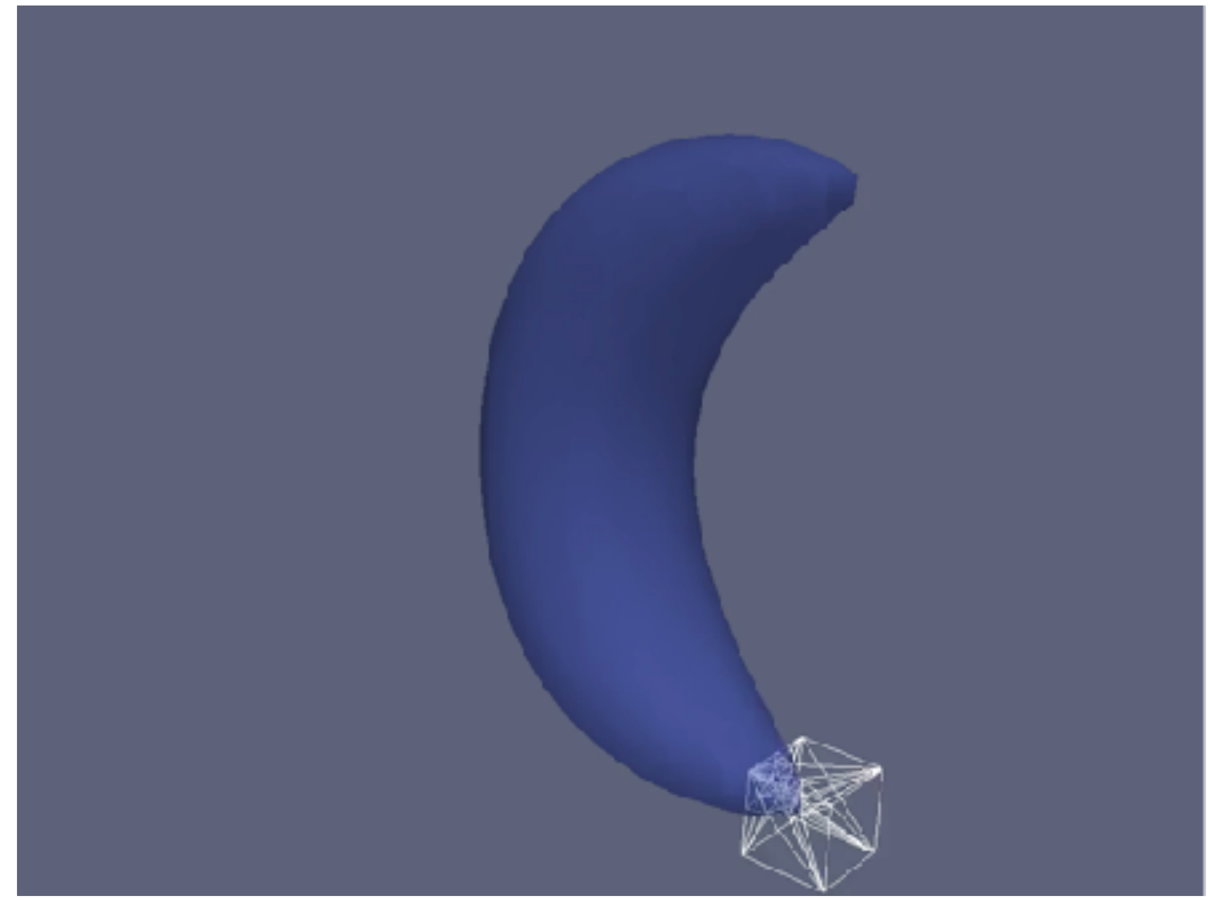


(b)


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.

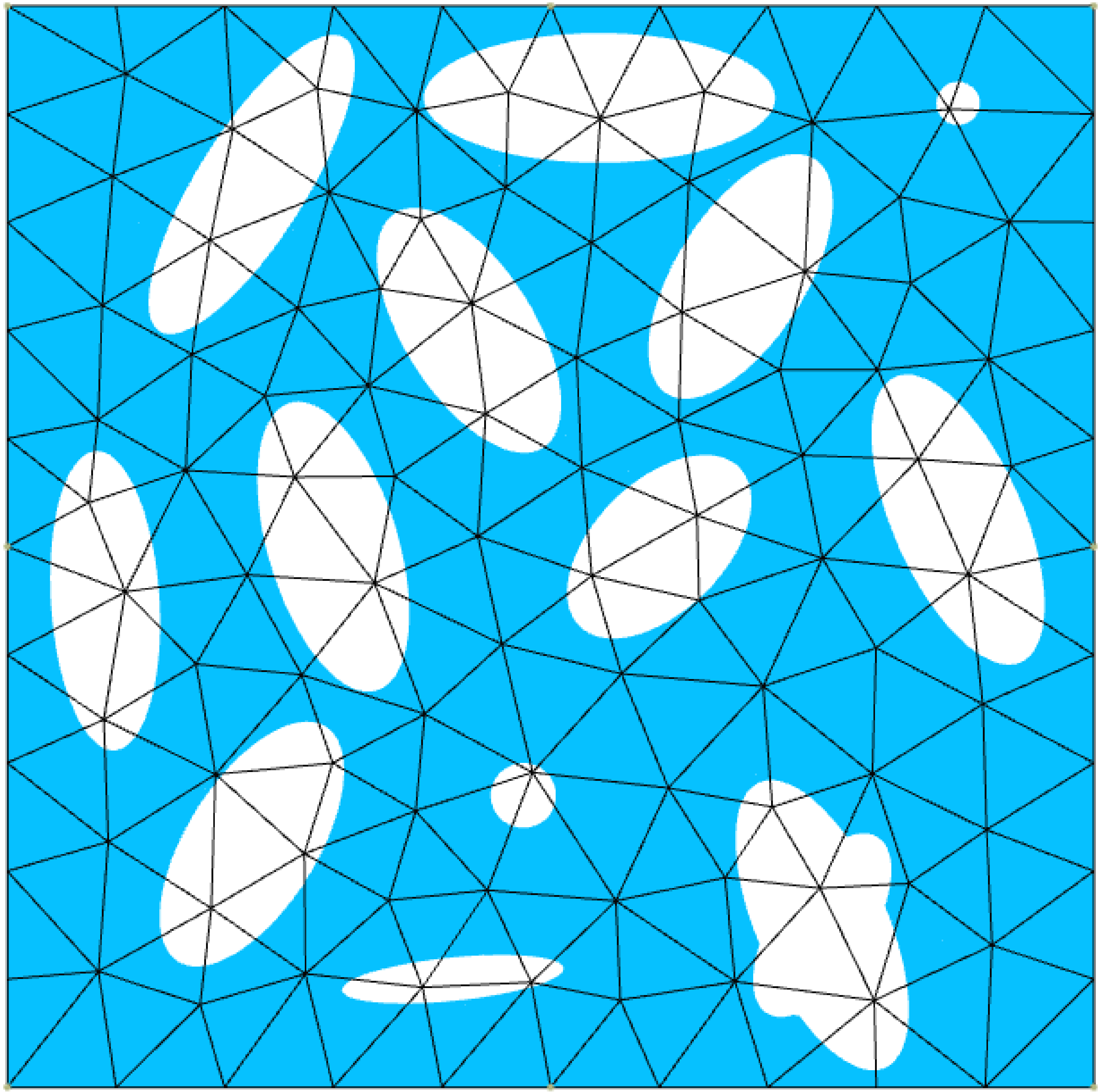


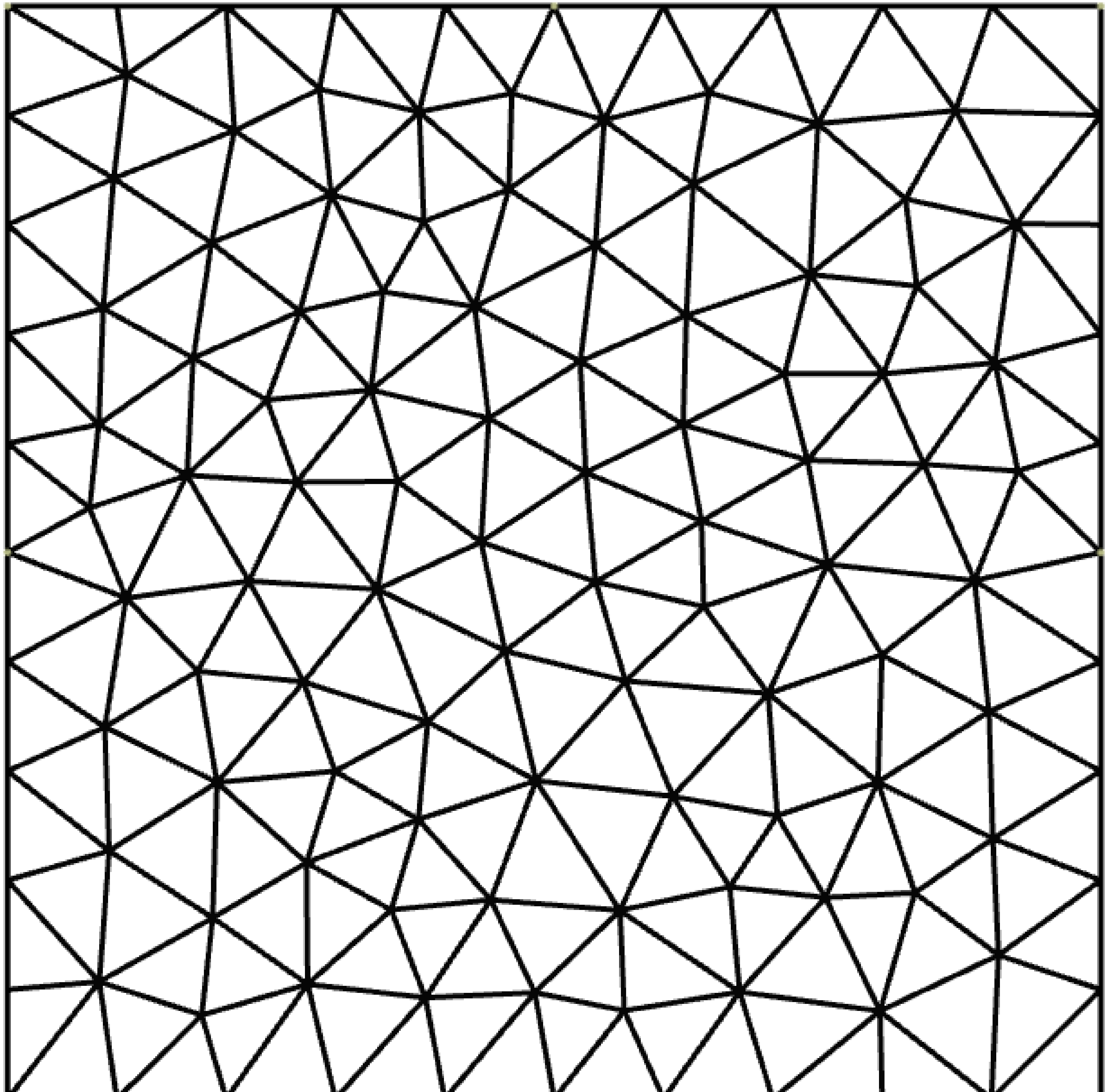


Question: for which problems are we better off coupling/decoupling the geometry from the field approximation?

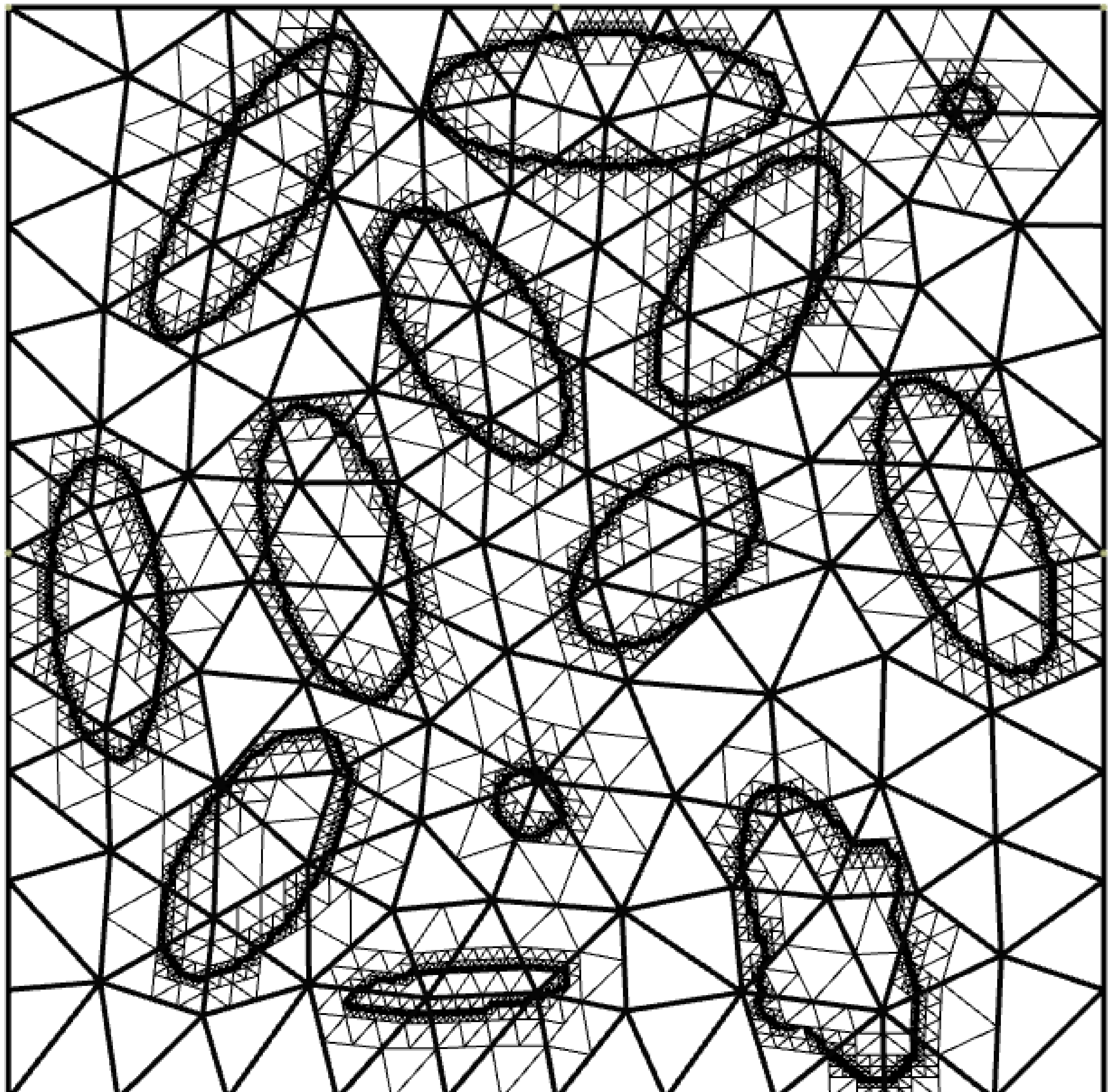
Implicit surfaces

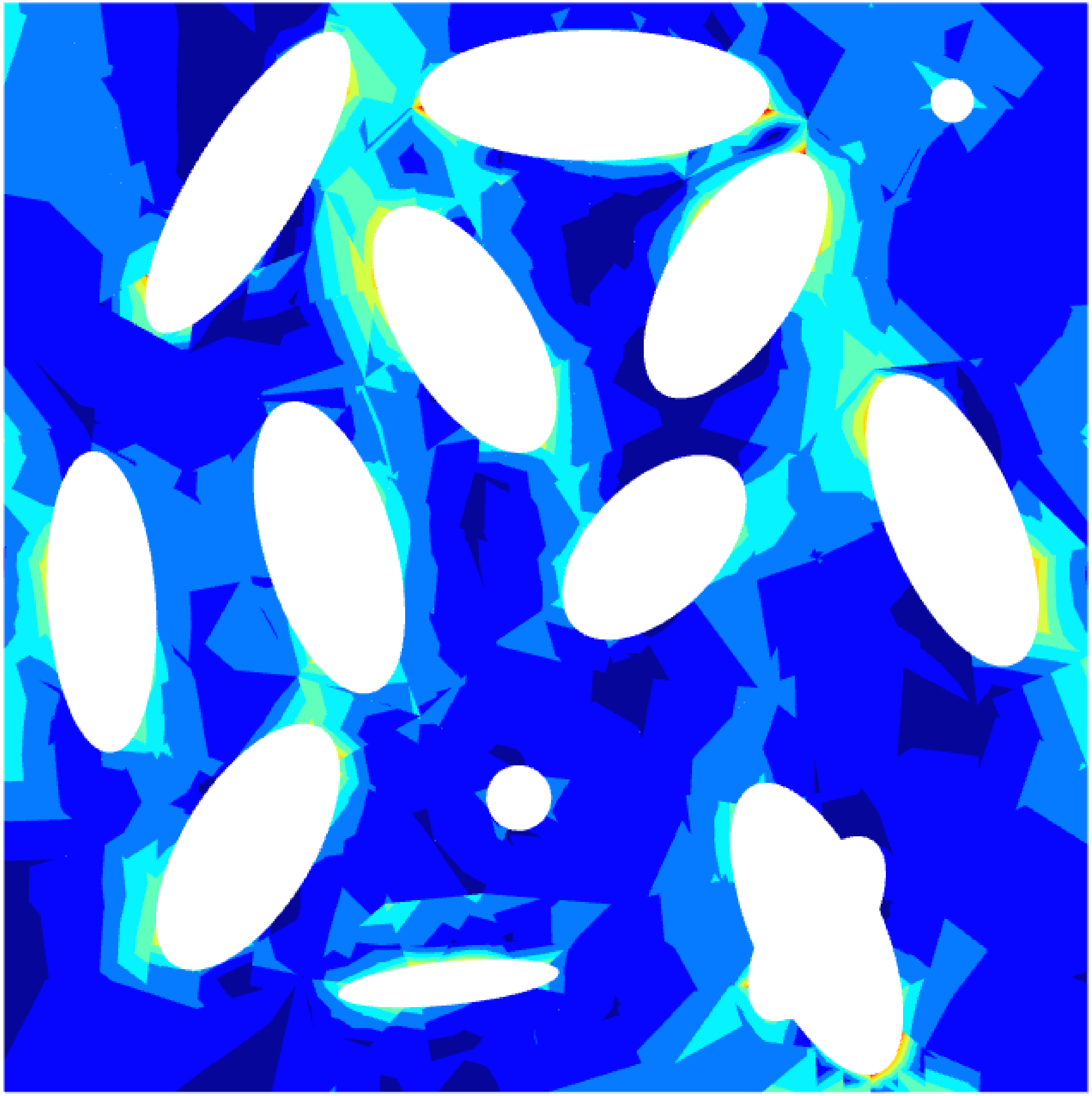
T. Rüberg (2016) Advanced Modeling and Simulation in Engineering Sciences 3 (1), 22
M. Moumnassi (2011) CMAME *200*(5): 774-796. (CSG and multiple level sets)
N. Moës (2003) CMAME192.28 (2003): 3163-3177. (Single level set)
T. Belytschko IJNME 56.4 (2003): 609-635. (Structured XFEM)
…



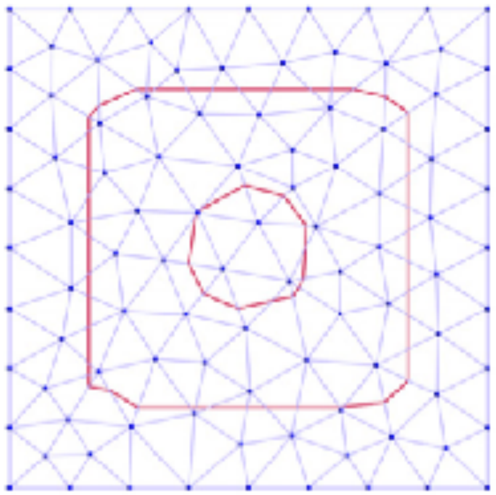


erc RealTCut

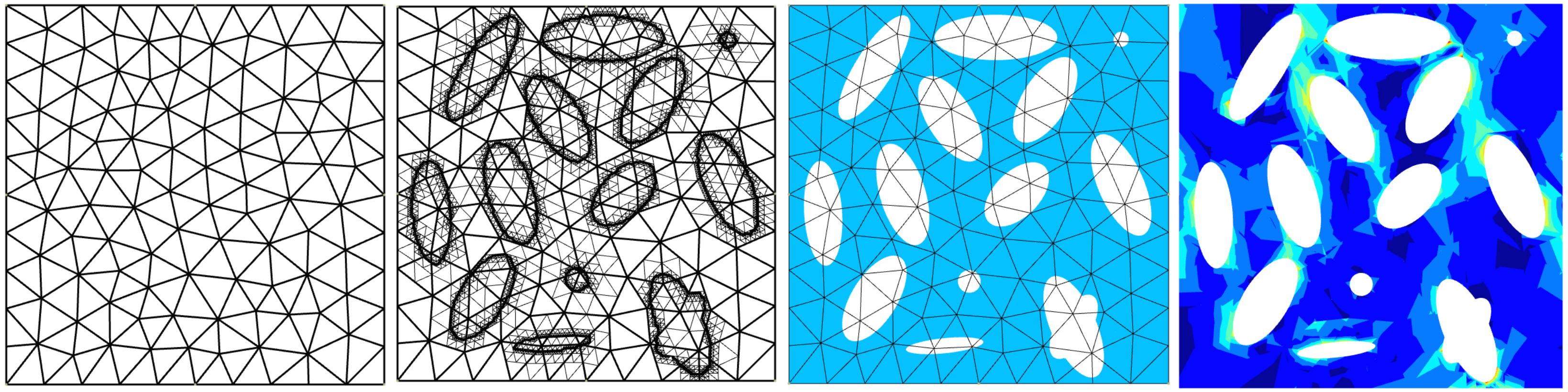


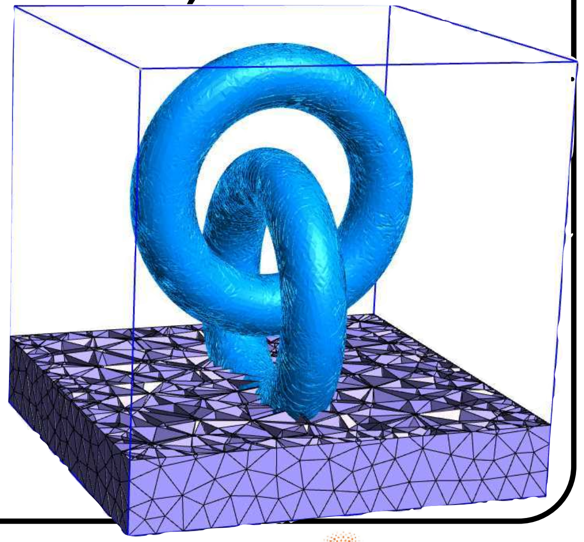


Immersed boundary method (Mittal, *et al.* 2005)
Fictitious domain (Glowinski, *et al.* 1994)
Embedded boundary method (Johansen, *et al.* 1998
Virtual boundary method (Saiki, *et al.* 1996)
Cartesian grid method (Ye, *et al.* 1999, Nadal, 2013)

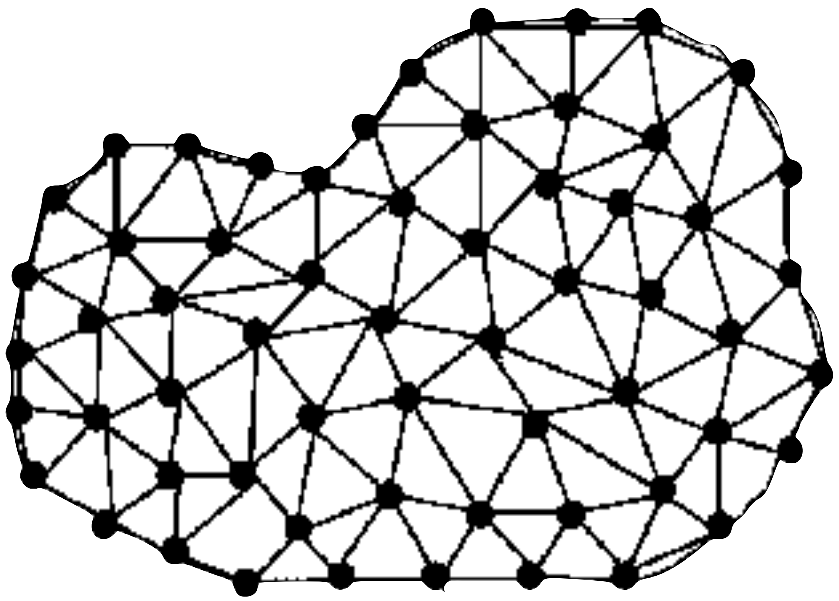


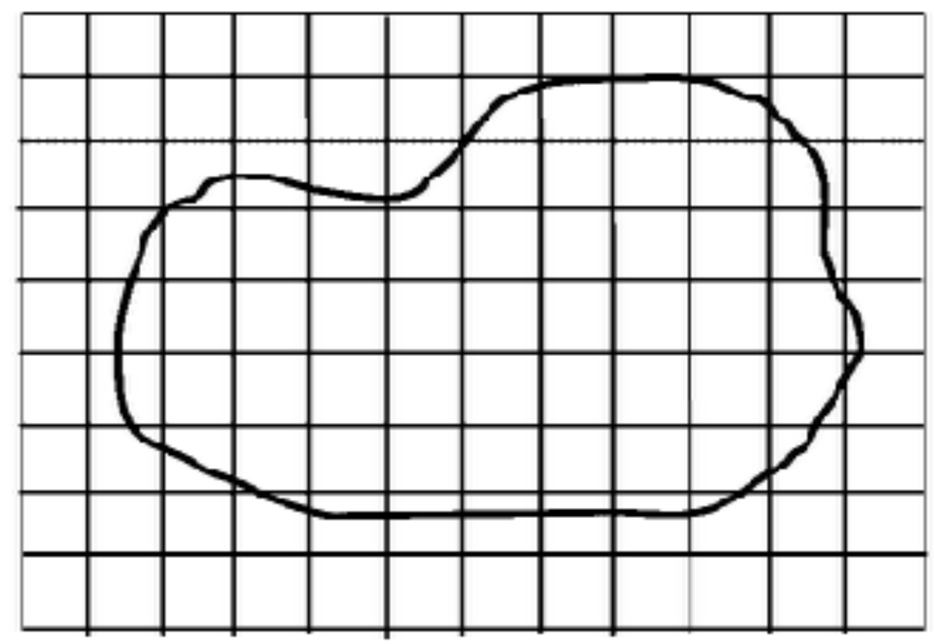
- ✓ Easy adaptive refinement + error estimation (Nadal, 2013)
- ✓ Flexibility of choosing basis functions
- • Accuracy for complicated geometries? BCs on implicit surfaces?
- ➡ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi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



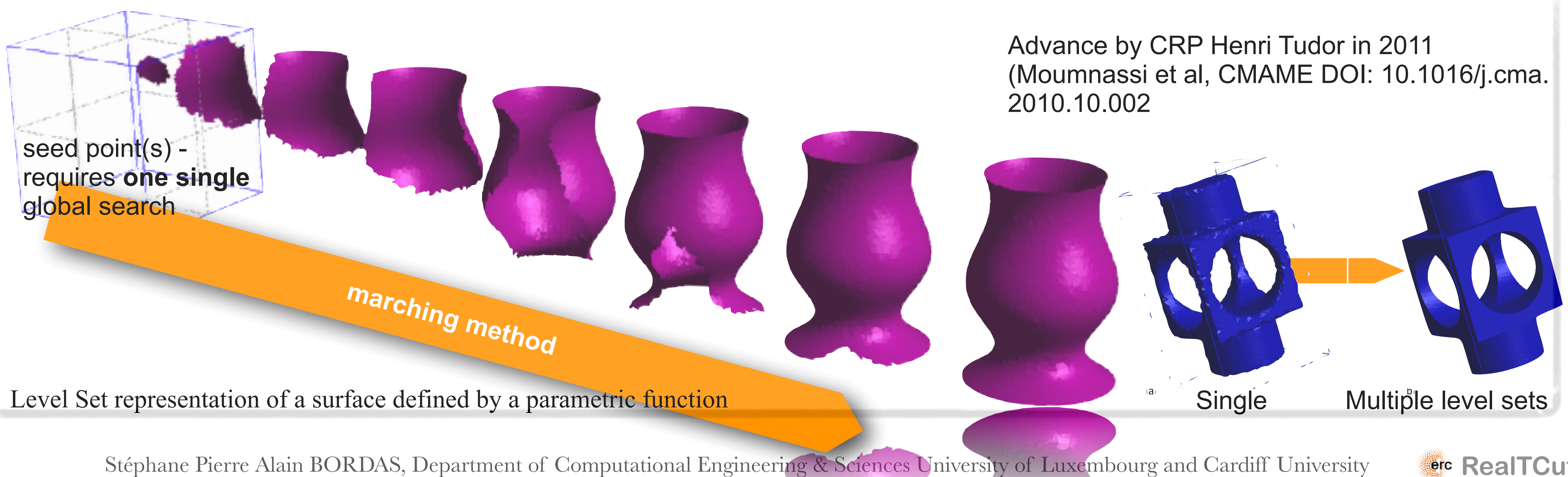


Moumnassi et al, CMAME DOI:10.1016/j.cma.2010.10.002



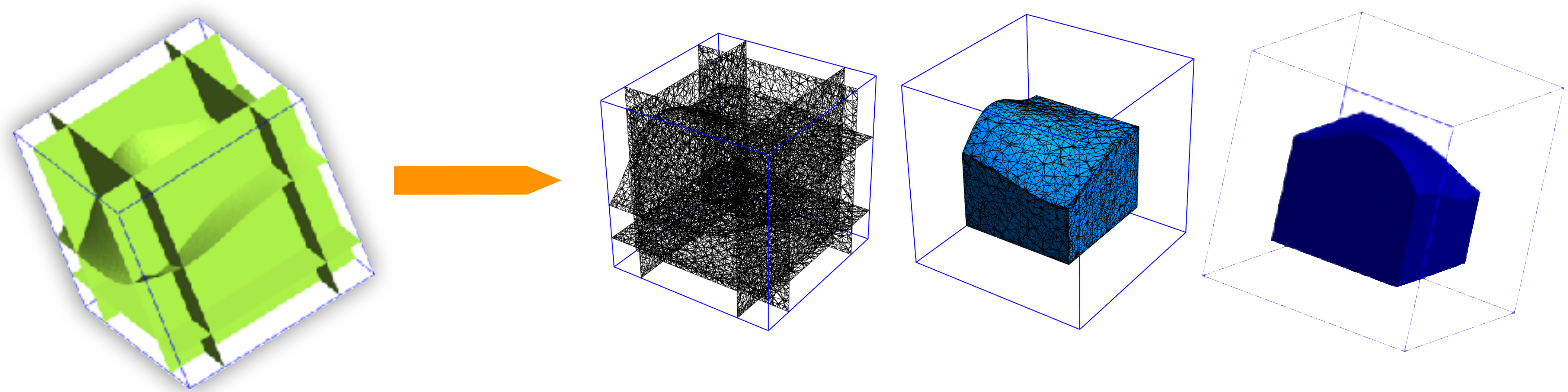


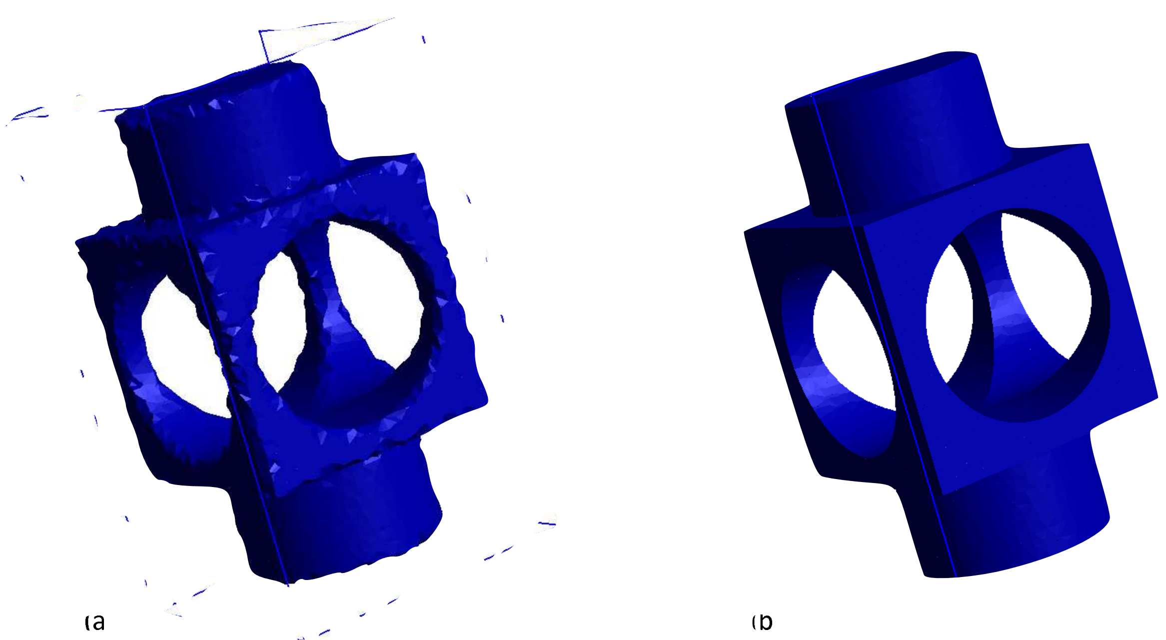
Question: How can we generate level set functions from CAD descriptions (including corners/vertices)?

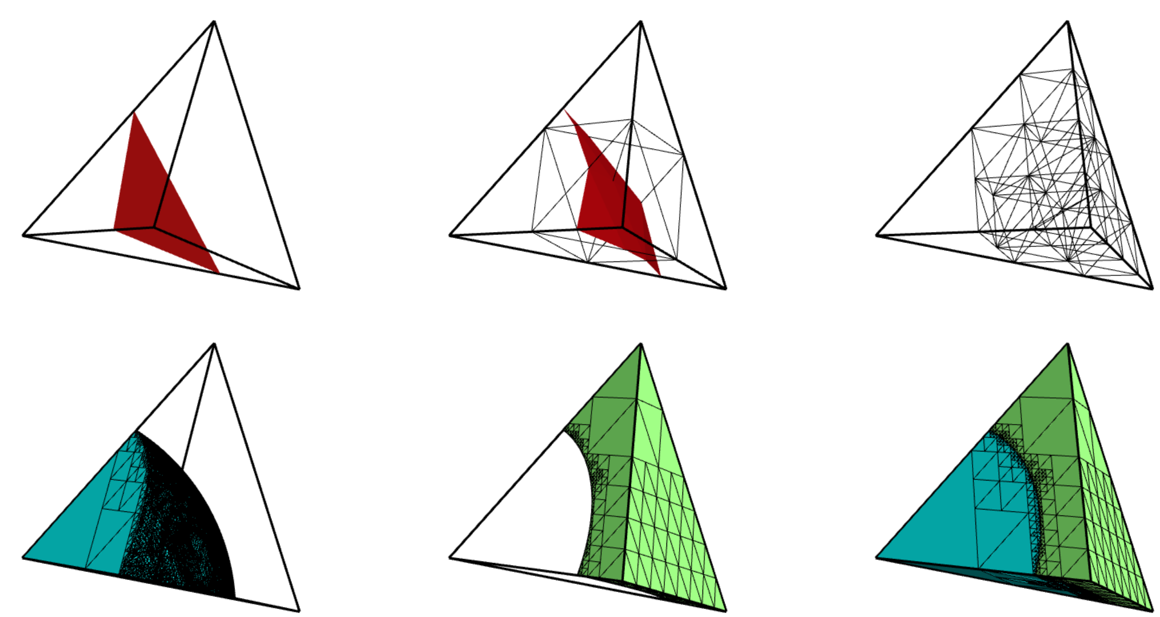


Level Set representation of a surface defined by a parametric function

Examples

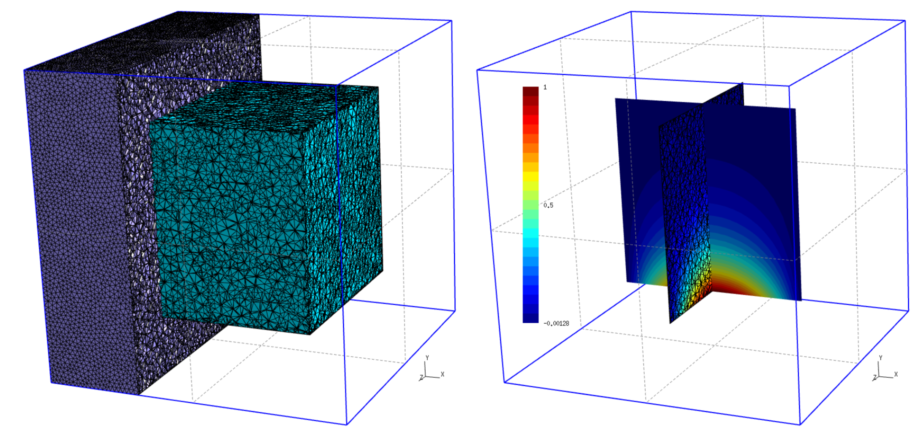




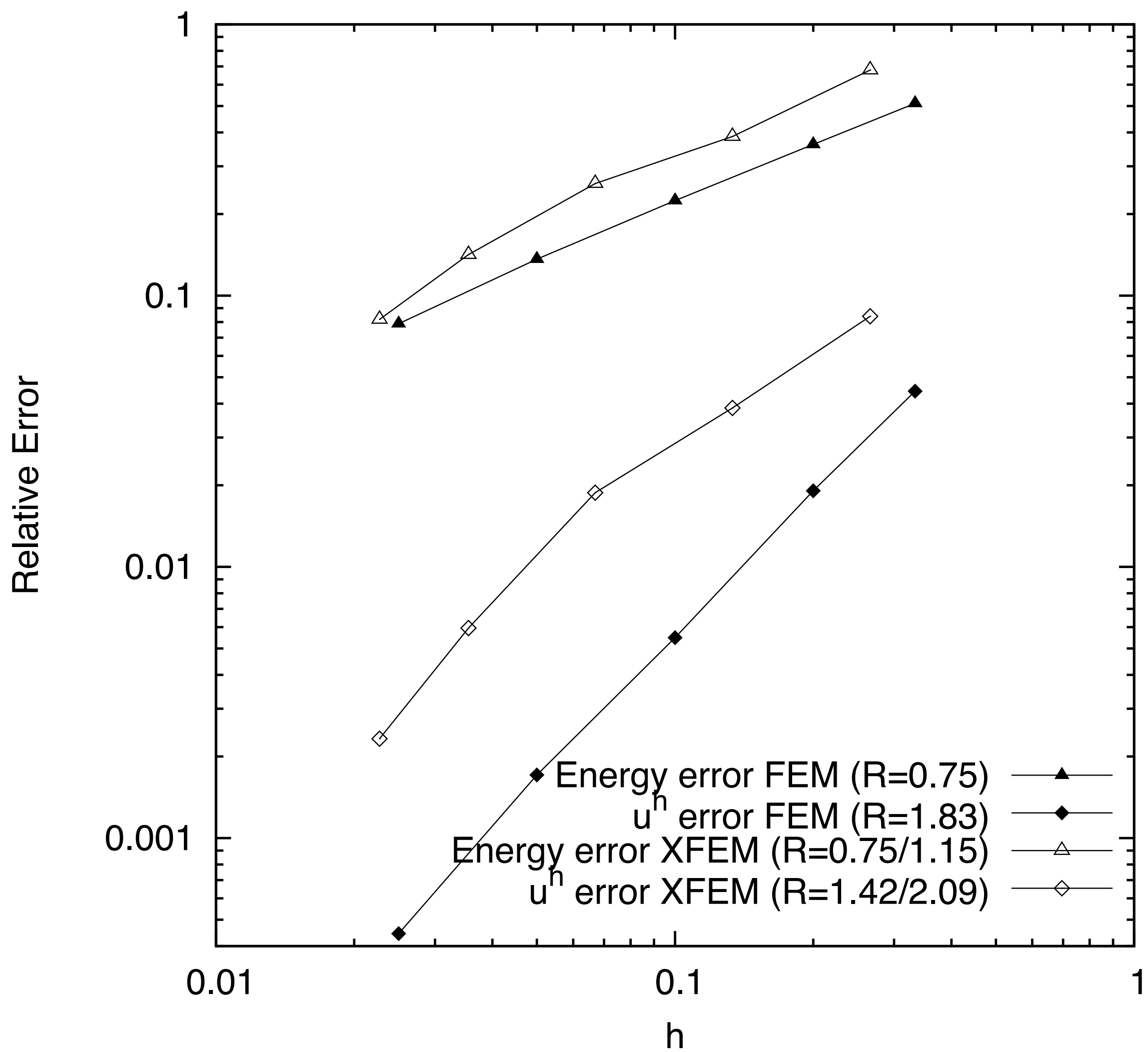


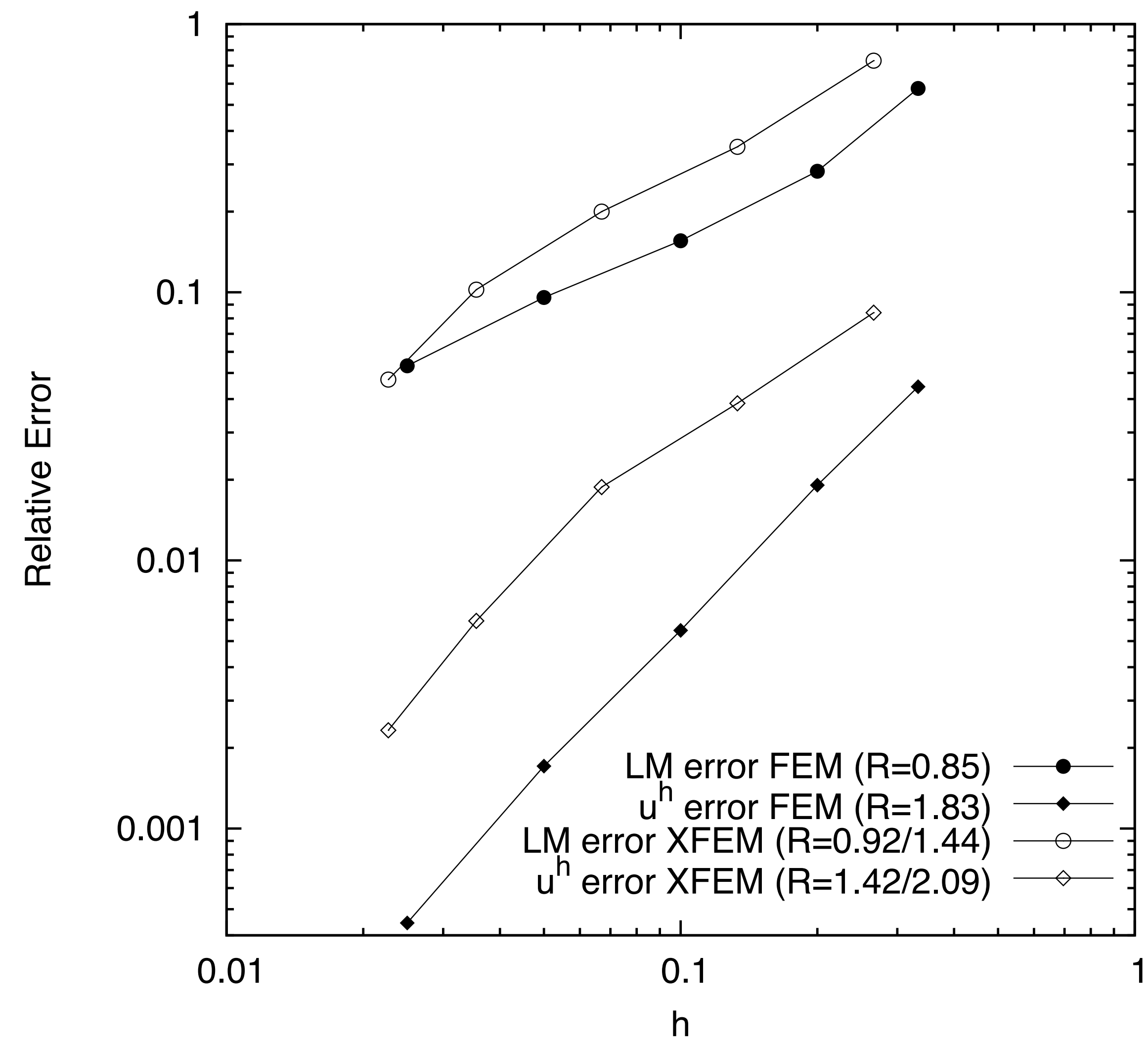
Single level set **Multi level sets**

Three-dimensional model problem



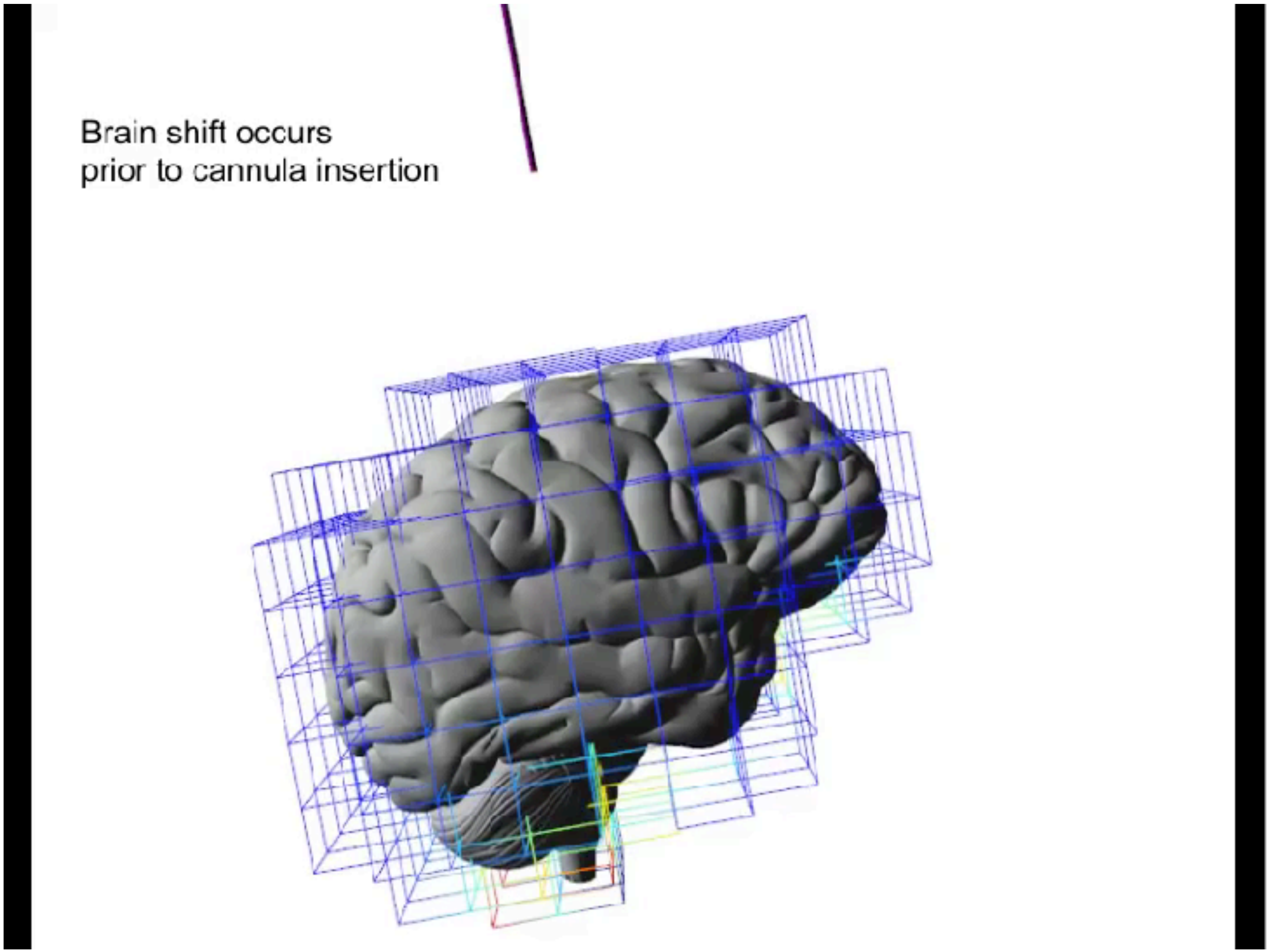
(a) (b)





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

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

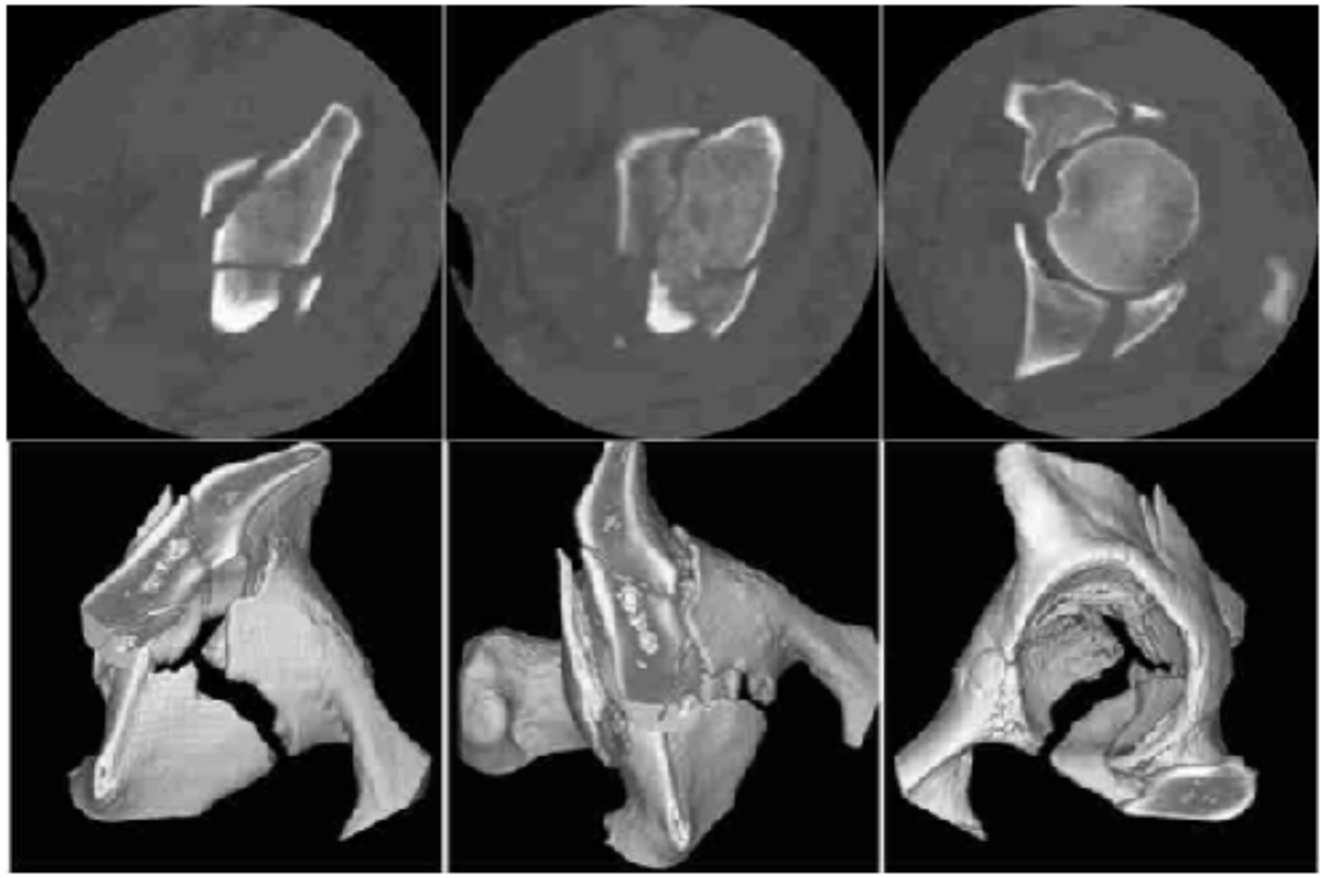
Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg and Cardiff University

Shuttle crash, 2003

Landslide, Colorado

Taiwan earthquake, 2003

Fragmentation of concrete



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?)

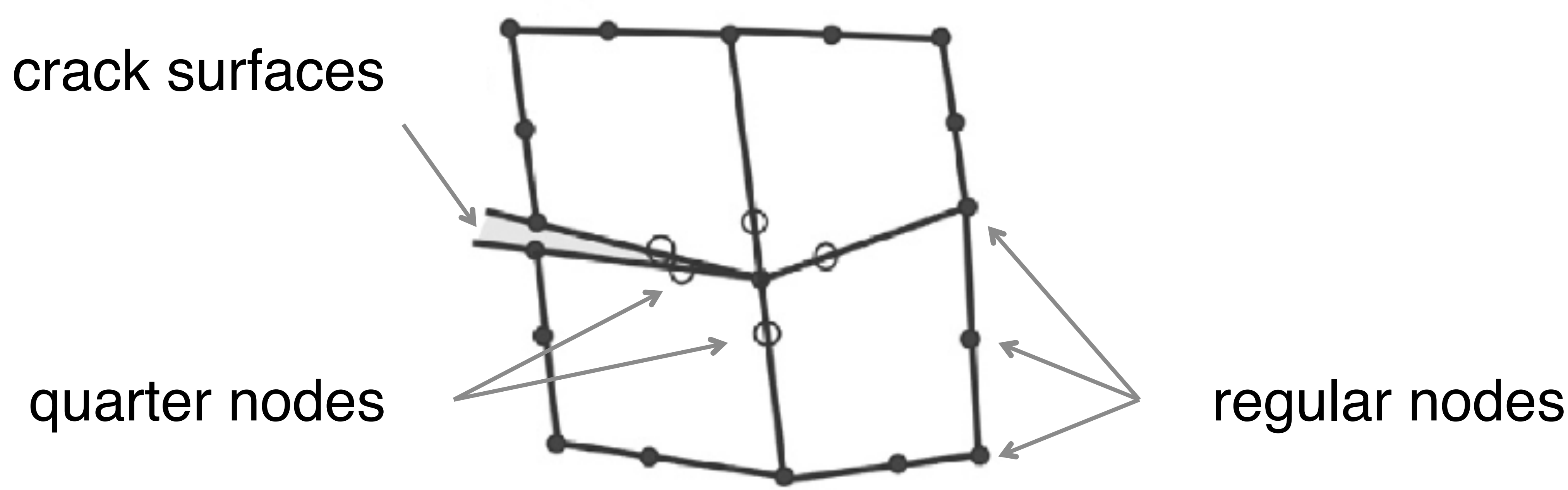
Extended finite element methods (multi-crack?)

Meshfree methods (cost? stability? robustess?)

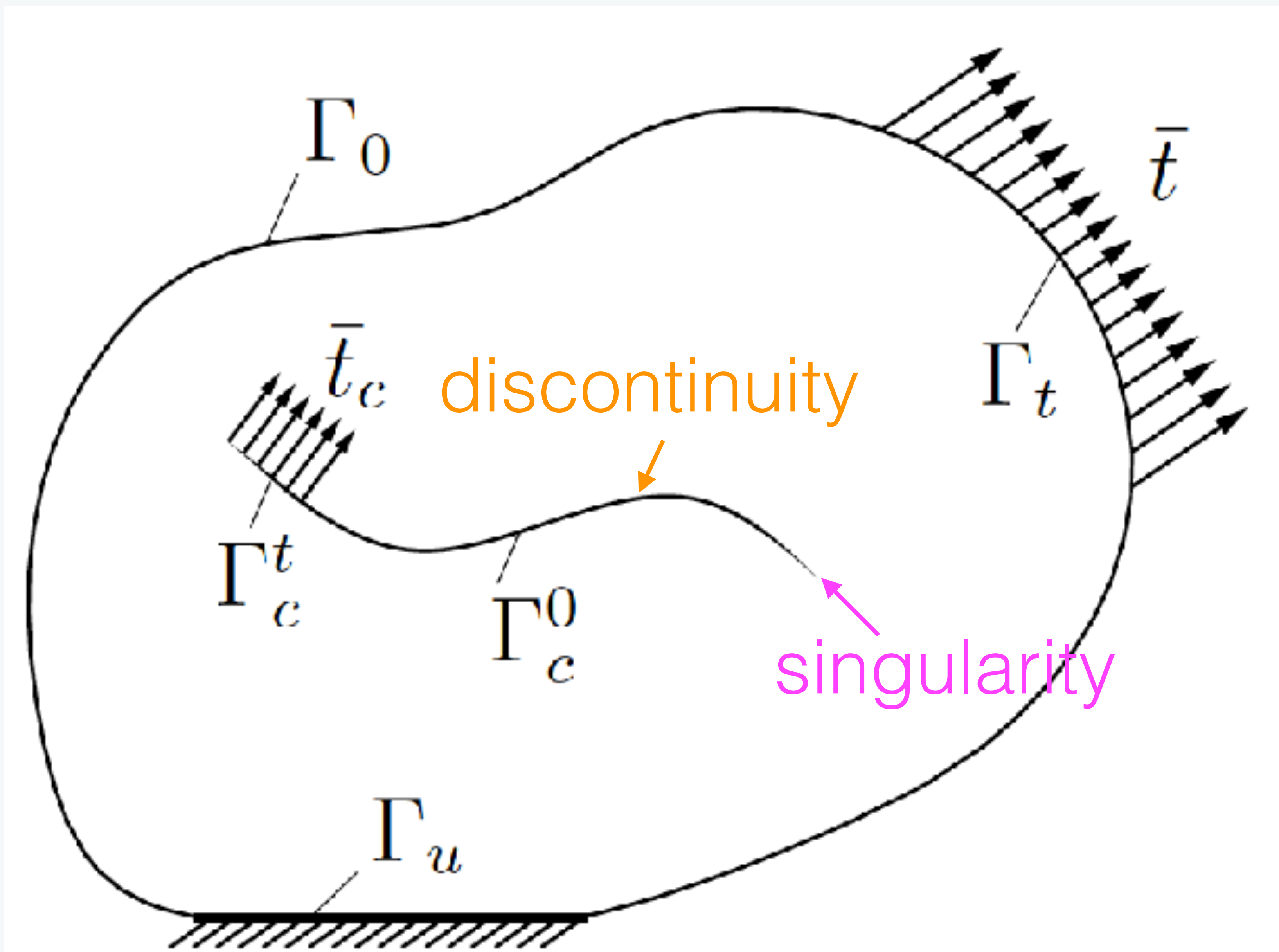
Singular elements - Barsoum 1974

For simulating the crack tip singular field in LEFM

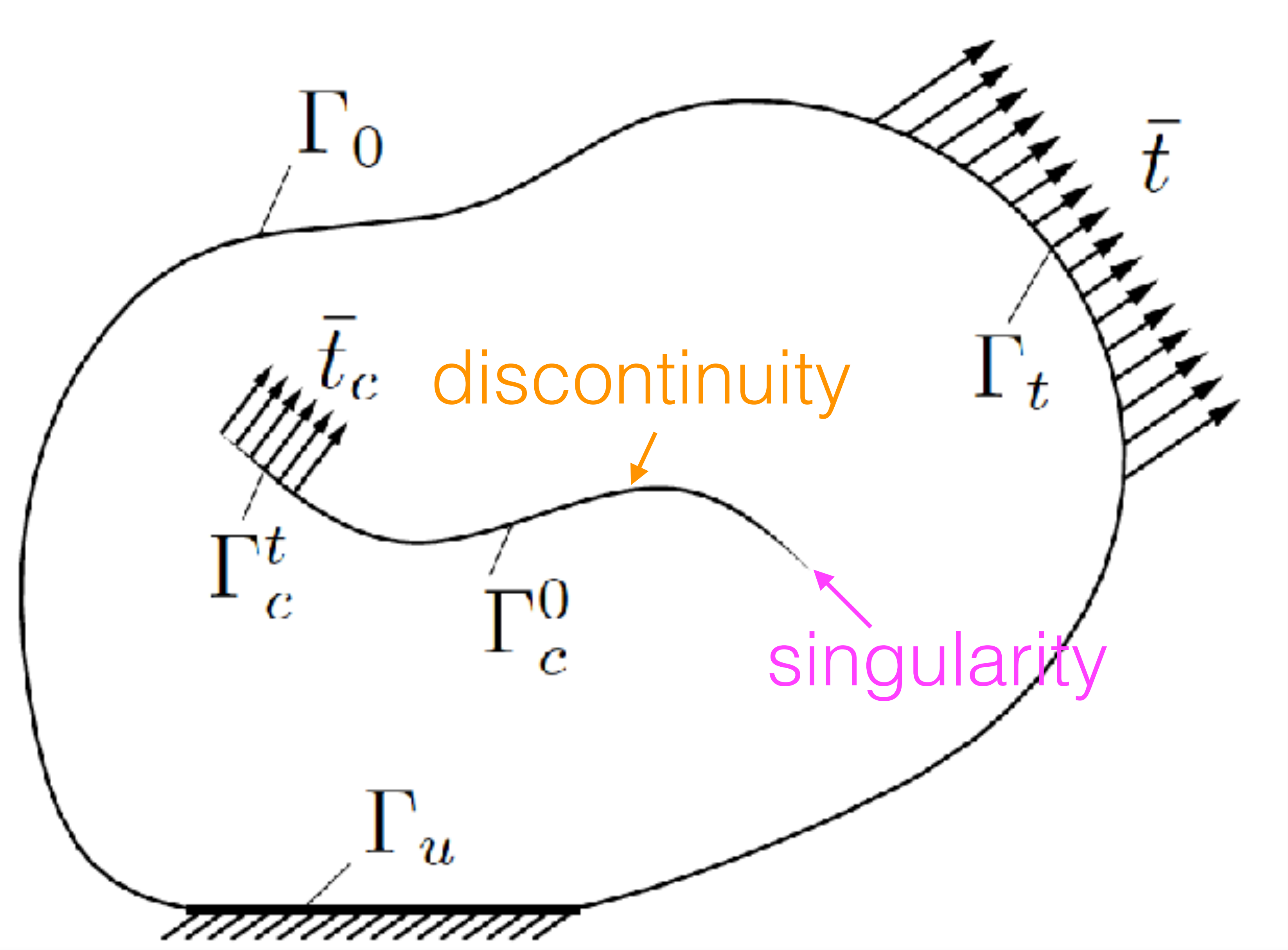
- A simple way how to introduce a singularity of $1/\sqrt{r}$ in isoperimetric finite elements is by displacing the mid-side nodes of two adjacent edges to one quarter of the element edge length from the node where the singularity is desired.



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



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



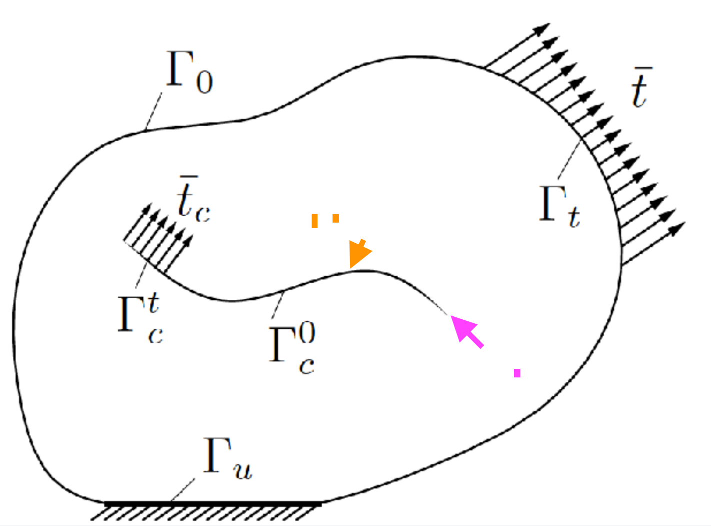
The idea of Partition of Unity Enrichment (PUFEM, GFEM, XFEM, hp clouds, enriched IGA, enriched mesfhree methods, enriched BEM…)

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

Singularities?

Discontinuities?

Boundary layers?



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*

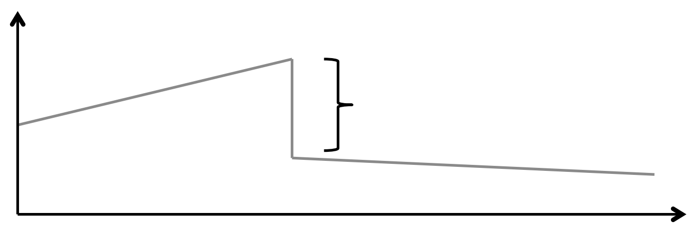
- The approximation space can be extended by introducing of an *a priori* knowledge about the sought solution, and thereby:

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

Classification of discontinuities

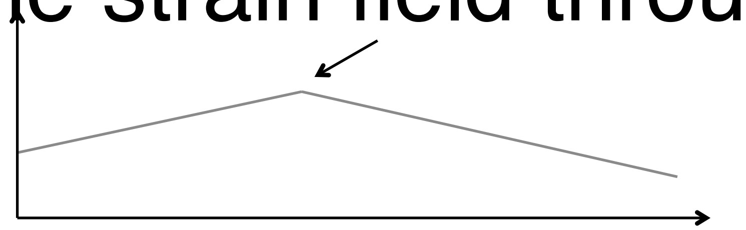
Strong discontinuities

- 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.



Partition of Unity FEM

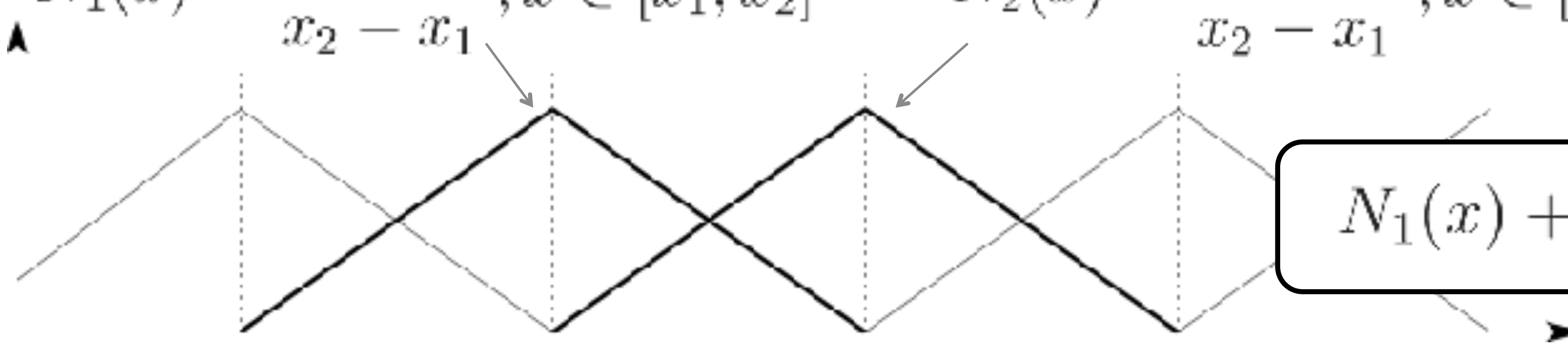
Partition of unity (PU)

- 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:

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



$$\boxed{N_1(x) + N_2(x) = 1}$$

Partition of Unity FEM

Reproducibility of PU

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

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:

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

- 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:

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

$$\Downarrow$$

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

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

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

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

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

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

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

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:

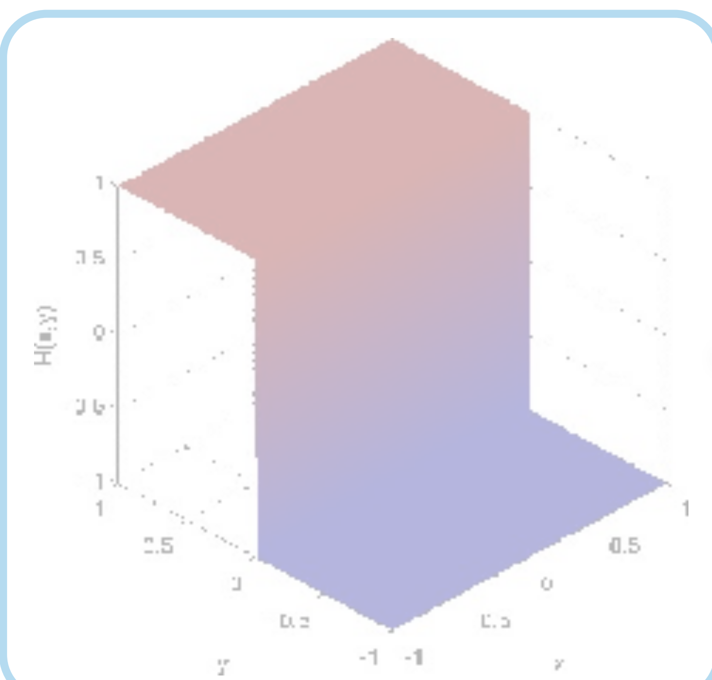
- Belytschko and Black (1999)
- Moës et. al. (1999)
- Dolbow (1999)

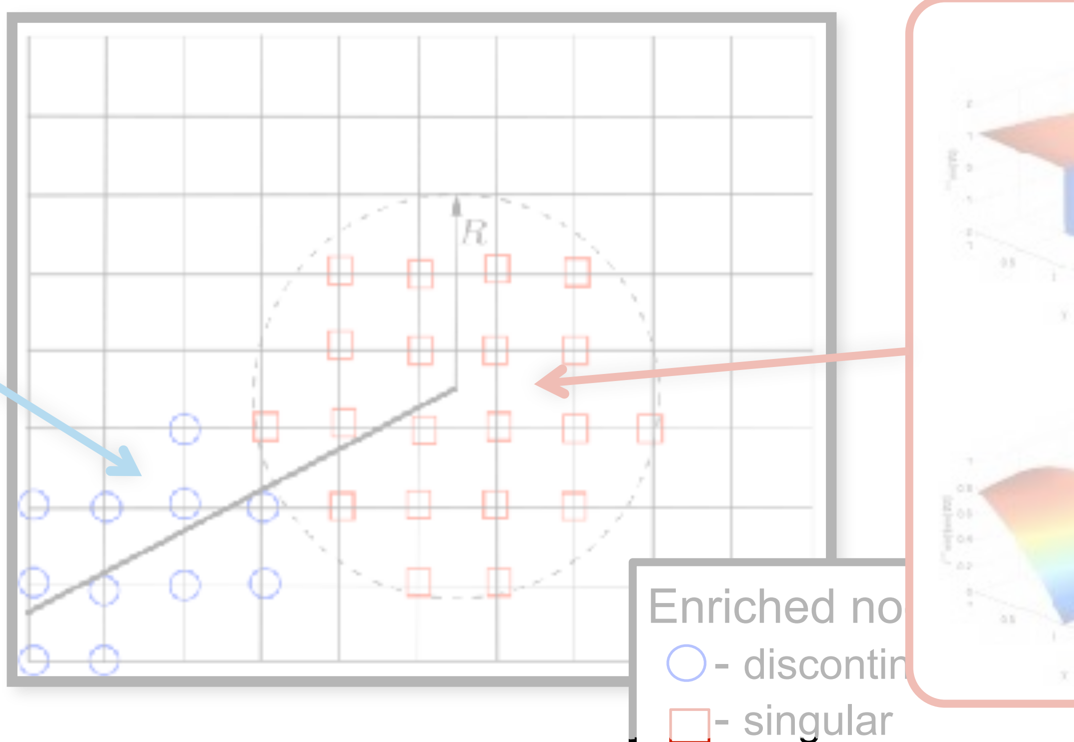
Formulation for crack growth:

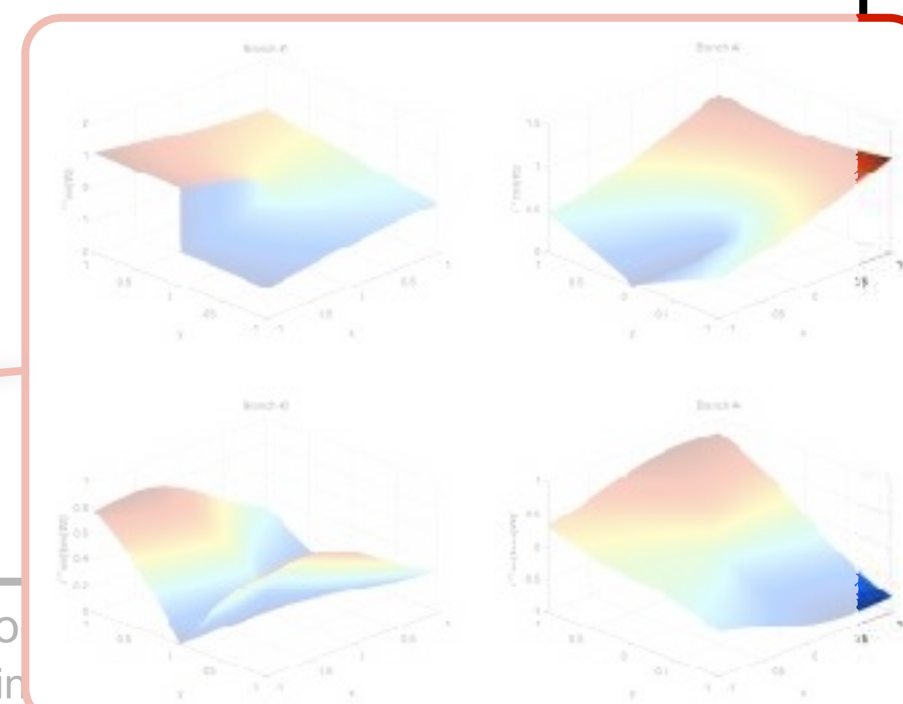
$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I\in\mathcal{N}_I} N_I(\mathbf{x})\mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J\in\mathcal{N}_J} N_J(\mathbf{x})H(\mathbf{x})\mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K\in\mathcal{N}_K} N_K(\mathbf{x})\sum_{\alpha=1}^{4}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

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

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







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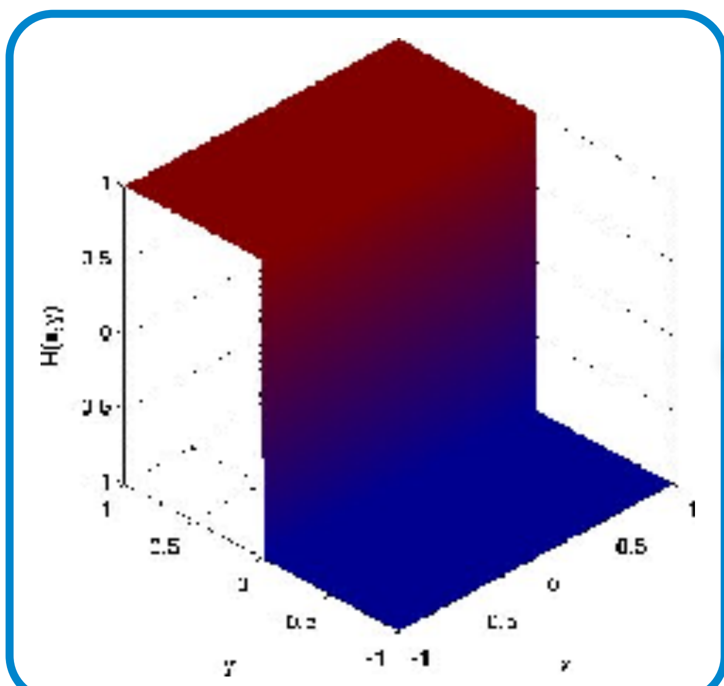

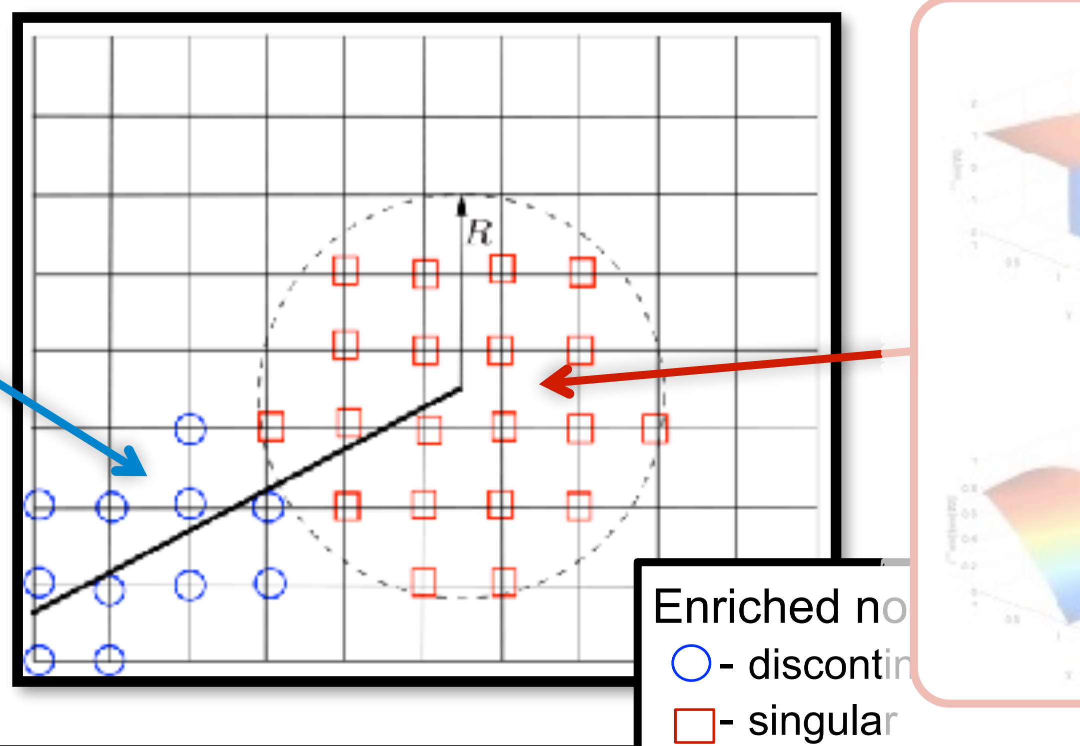

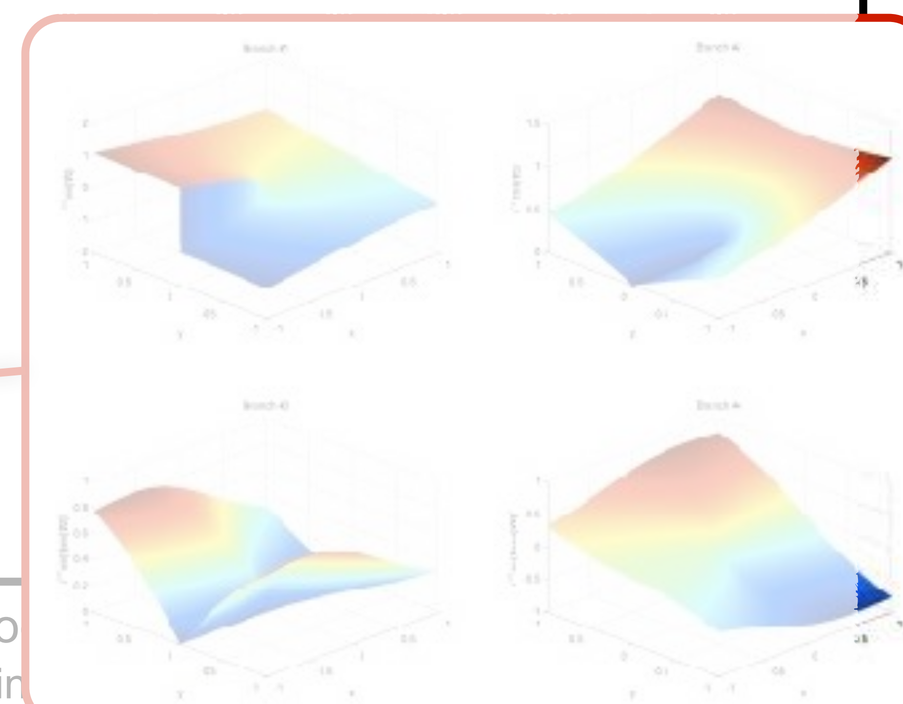

XFEM/GFEM

Formulation for crack growth:

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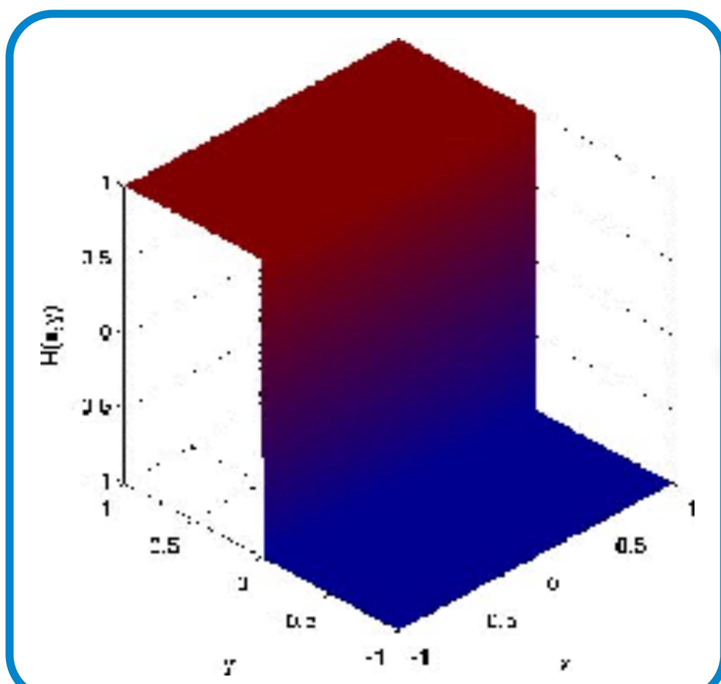
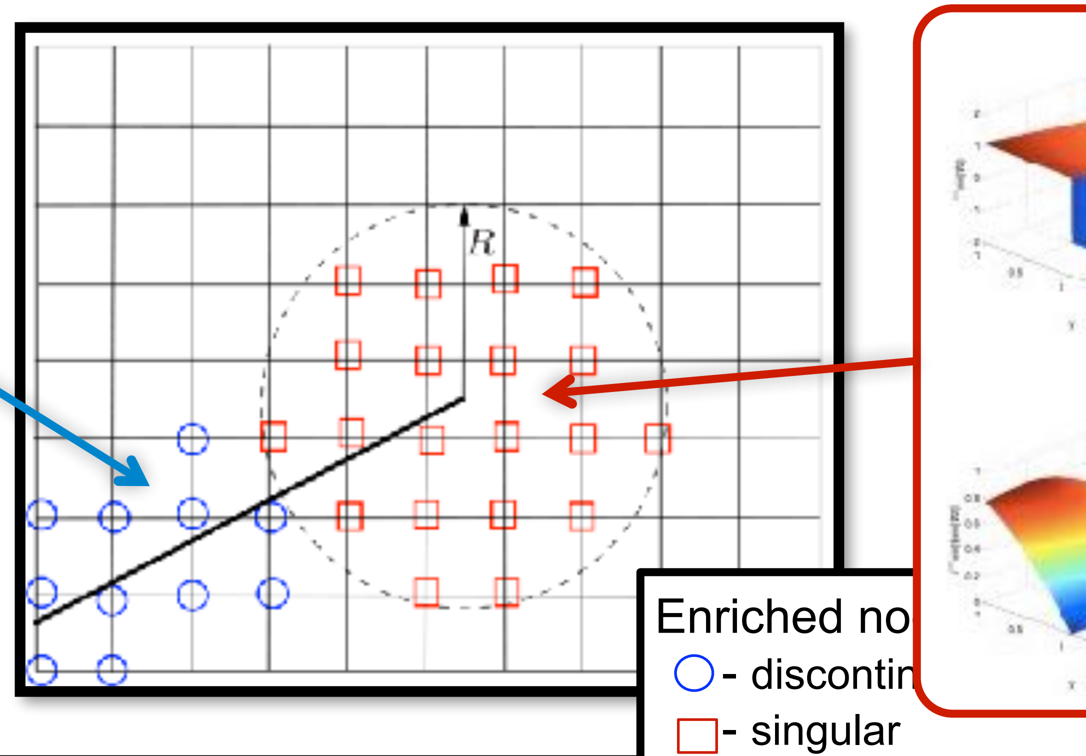
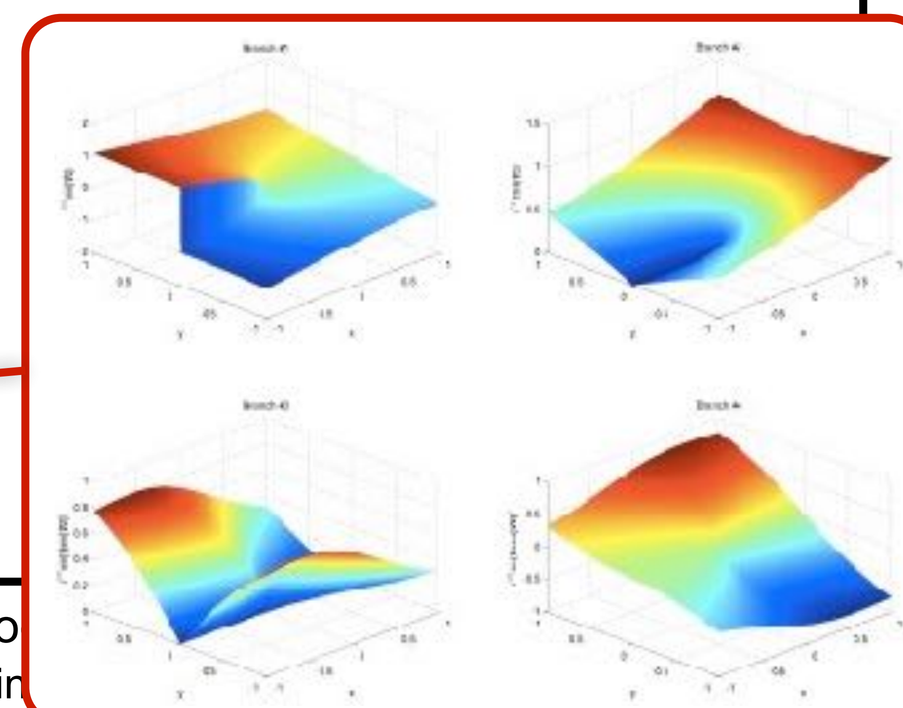
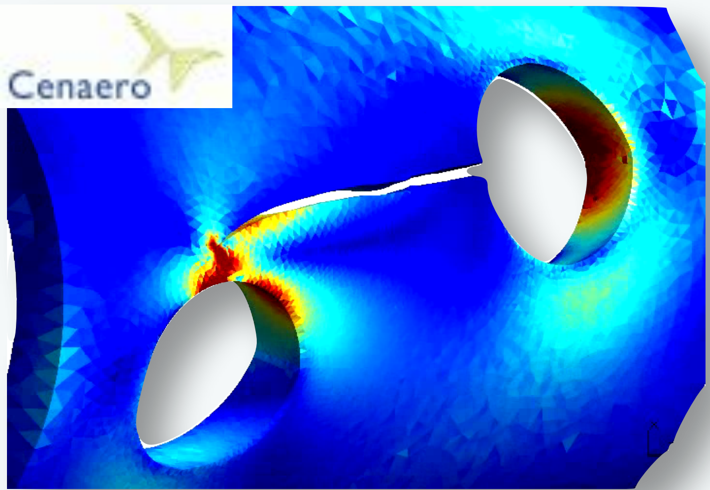


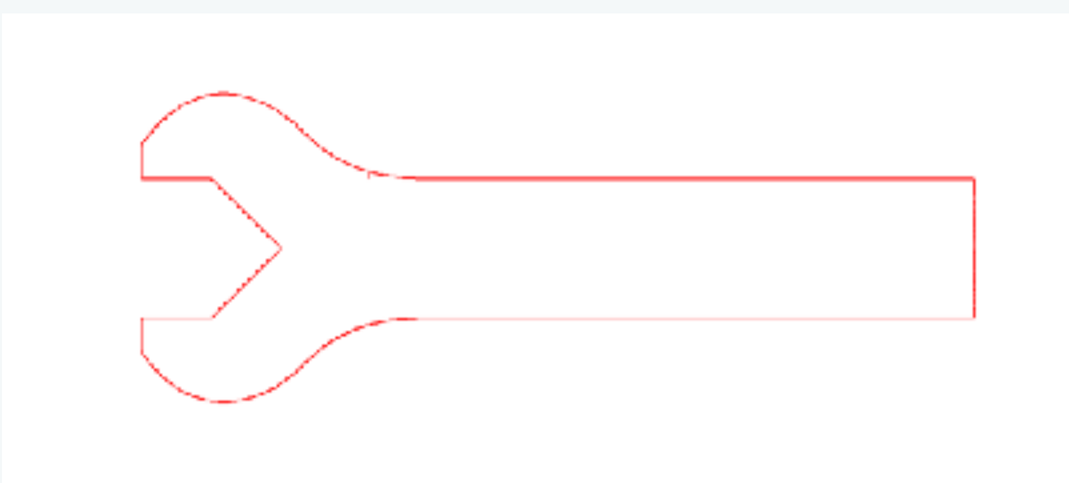




Fracture of homogeneous materials

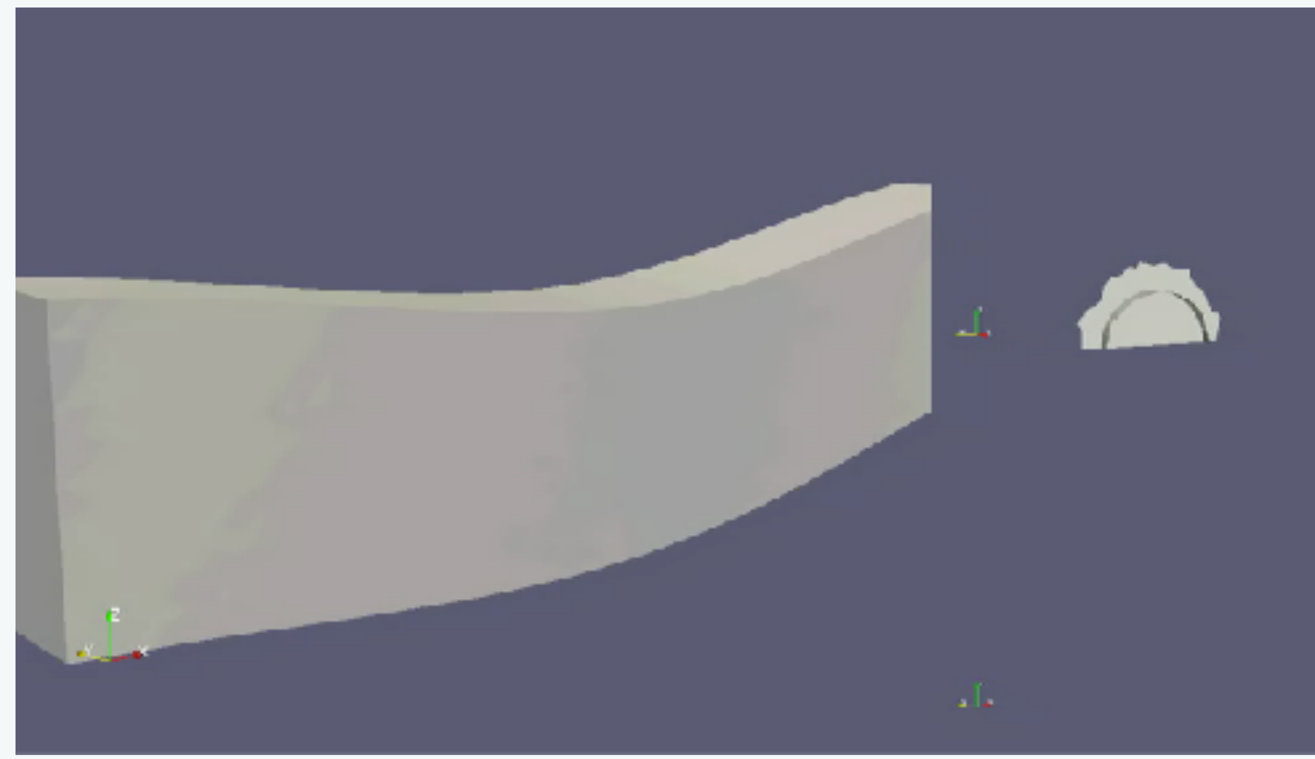
Question: How to control accuracy and simplify/avoid meshing?





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

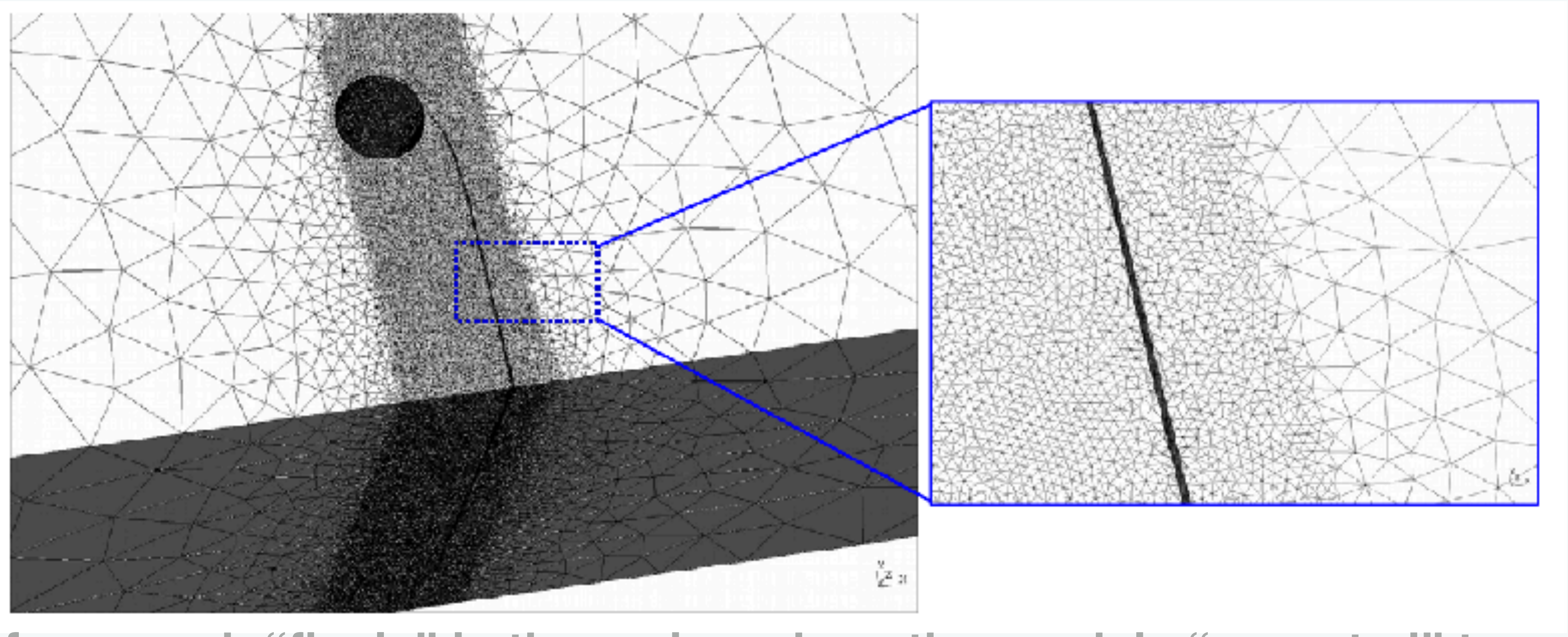
How to avoid meshing completely for crack propagation simulations?



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?

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

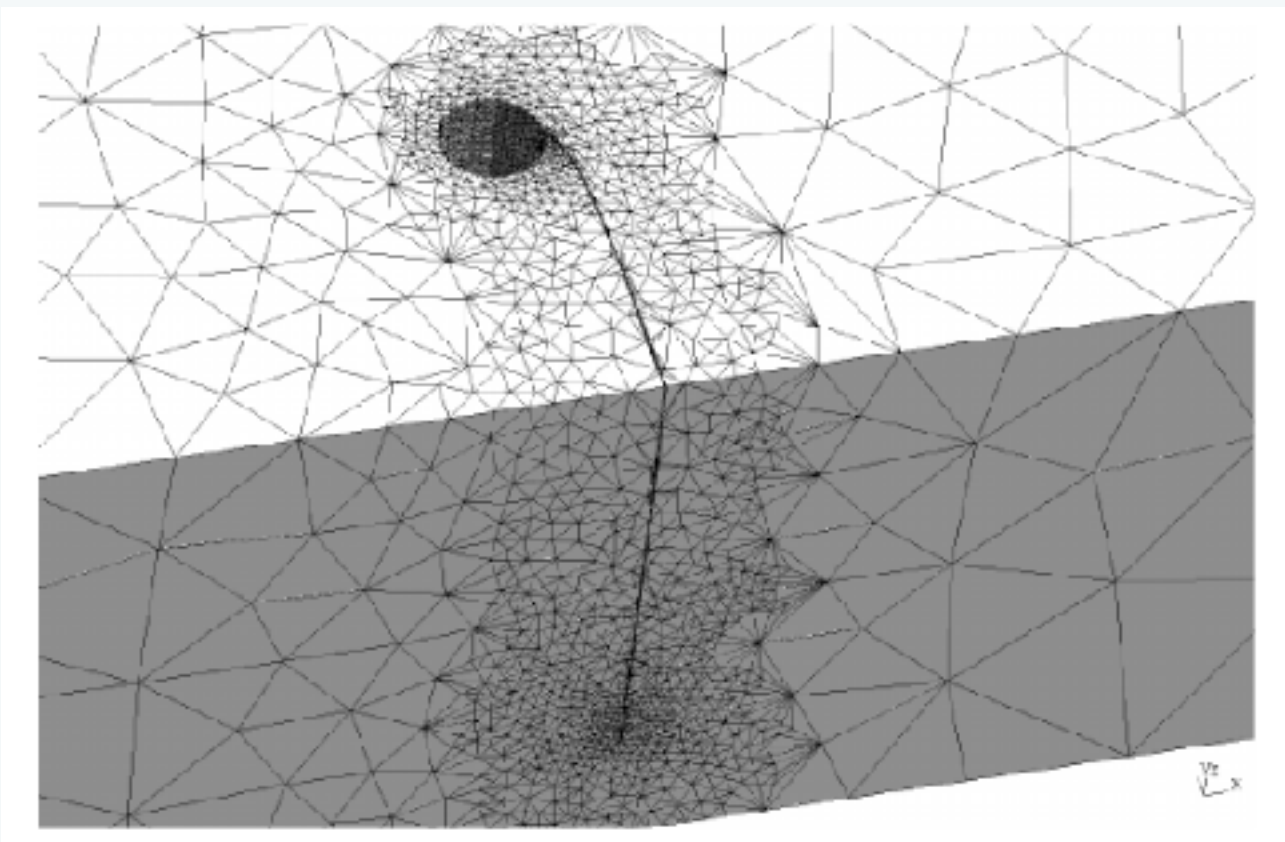


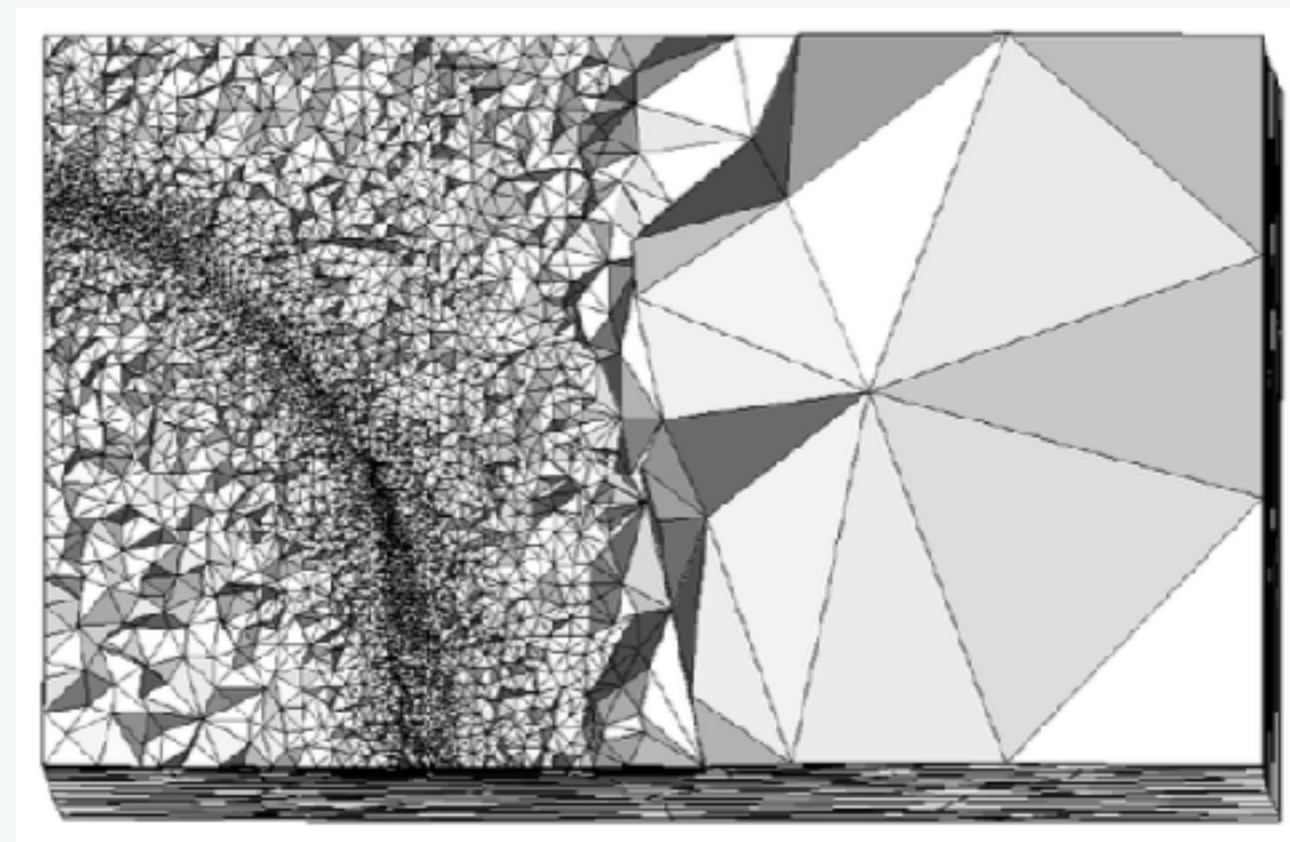
Before: mesh "finely" in the region where the crack is "expected" to propagate

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

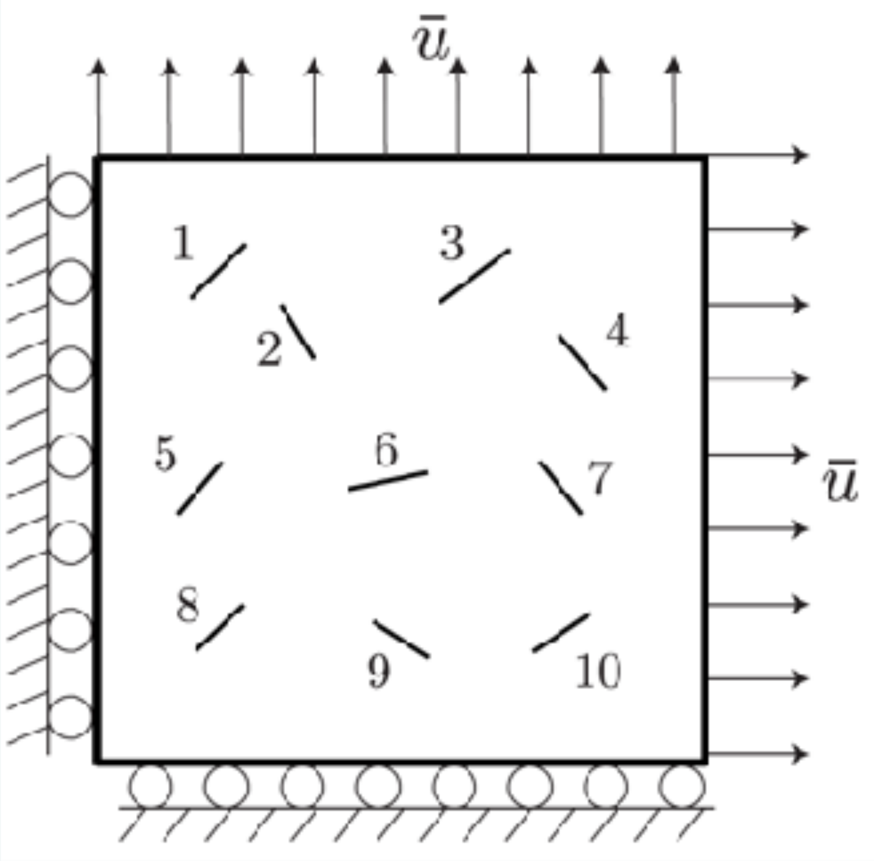
Fracture of homogeneous materials: error estimation and adaptivity





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.


$\bar{u}$
1
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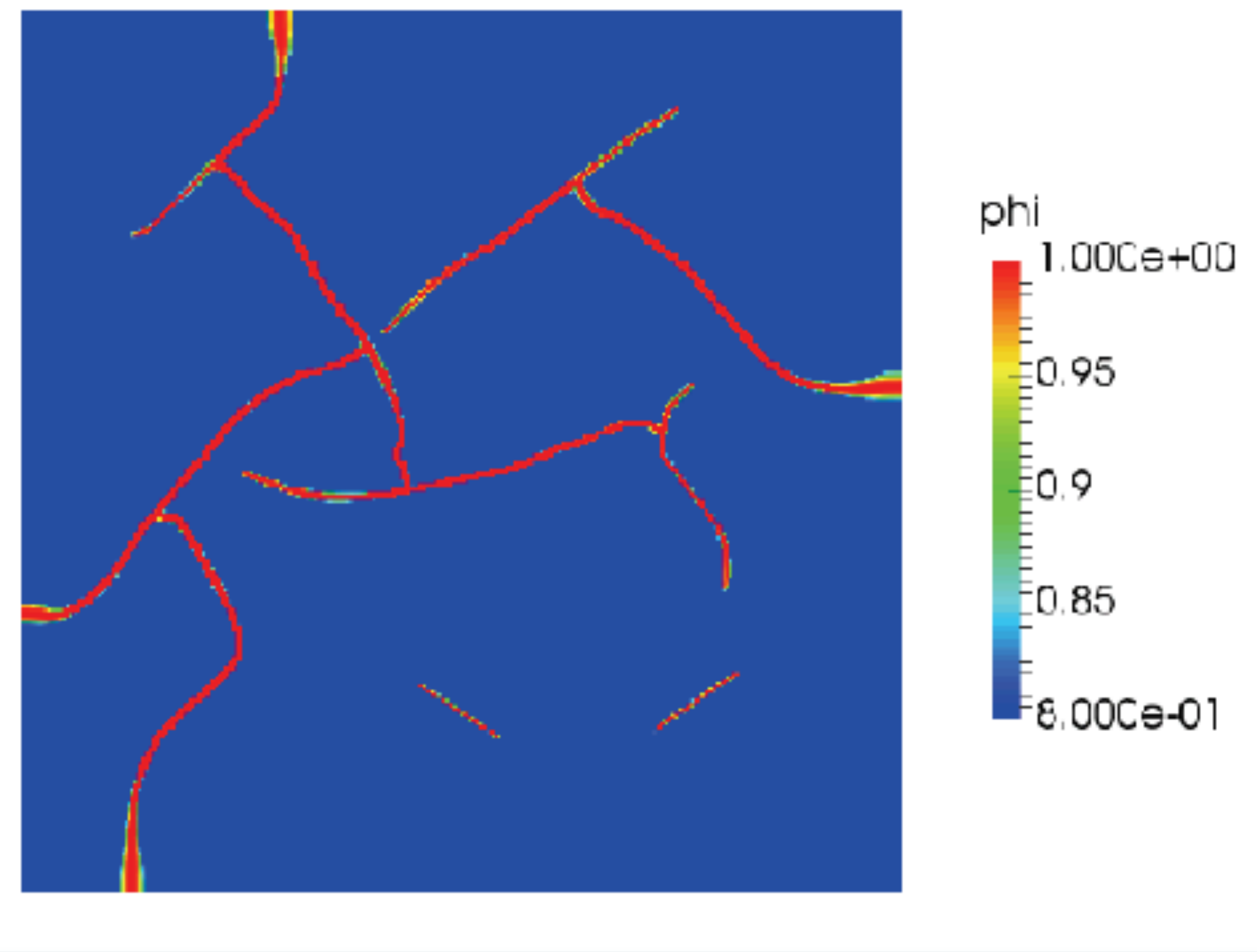
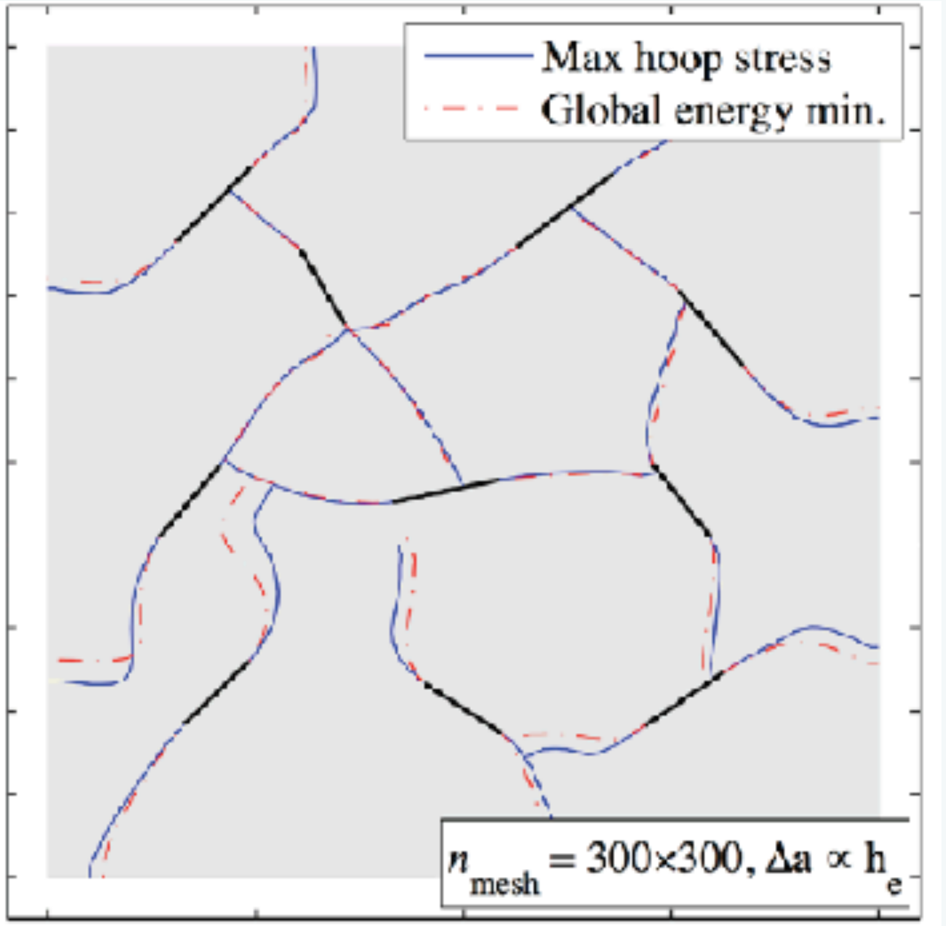
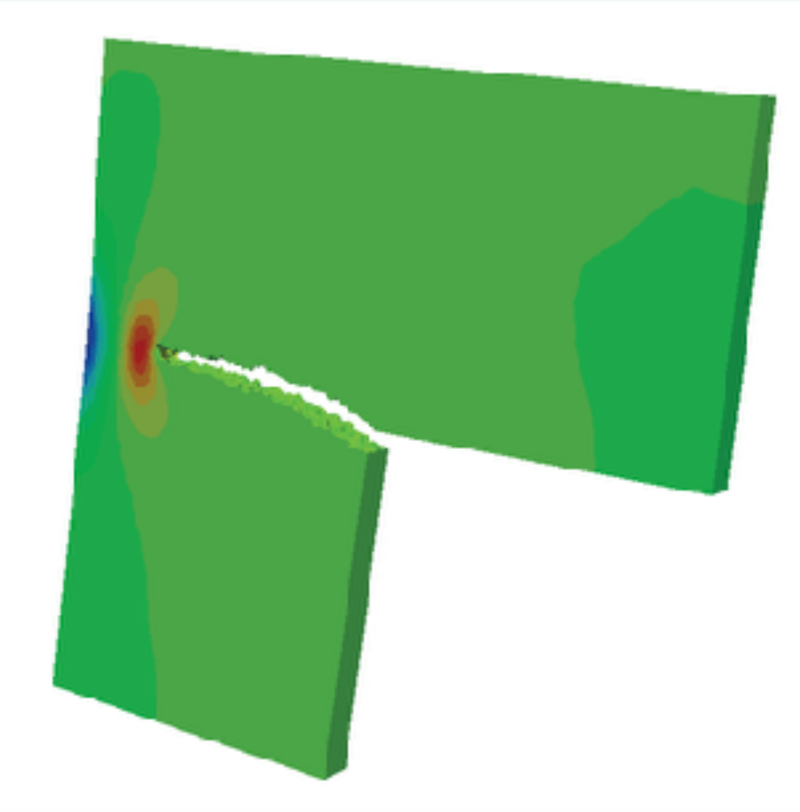
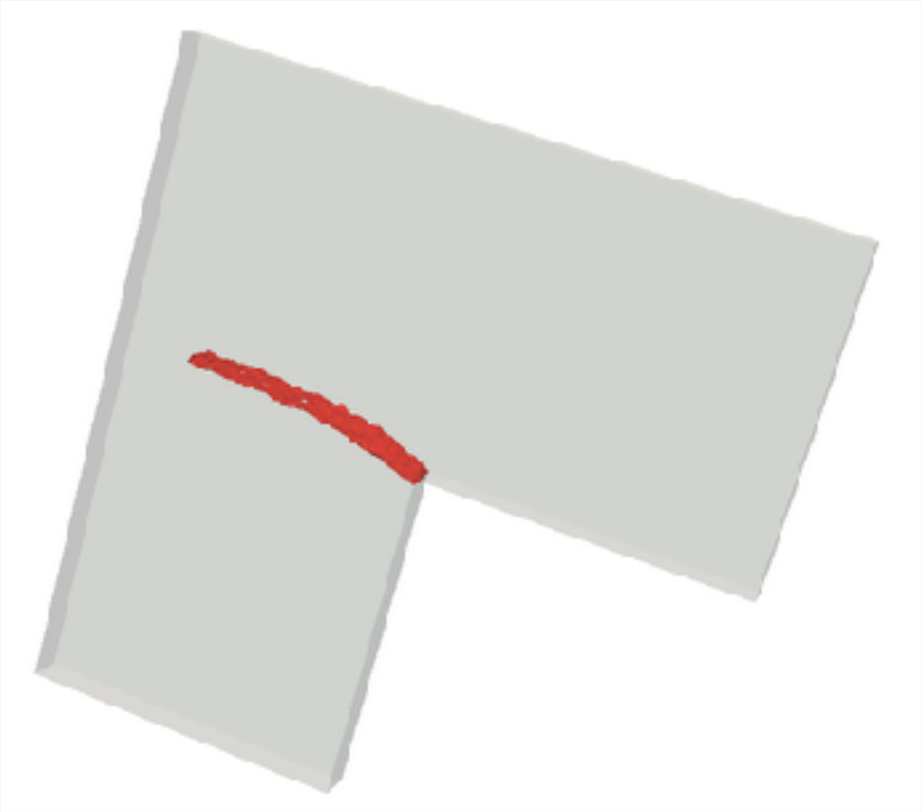
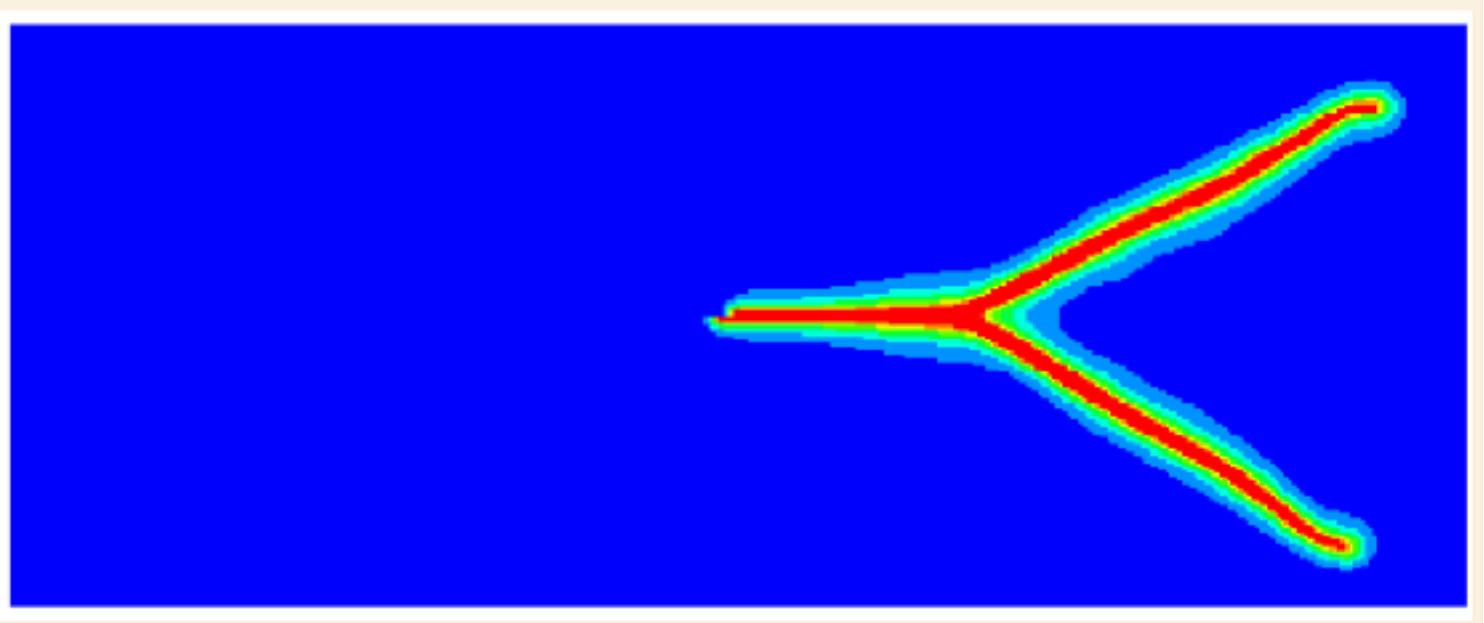

phi
1.000e+00
0.95
0.9
0.85
8.000e-01


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

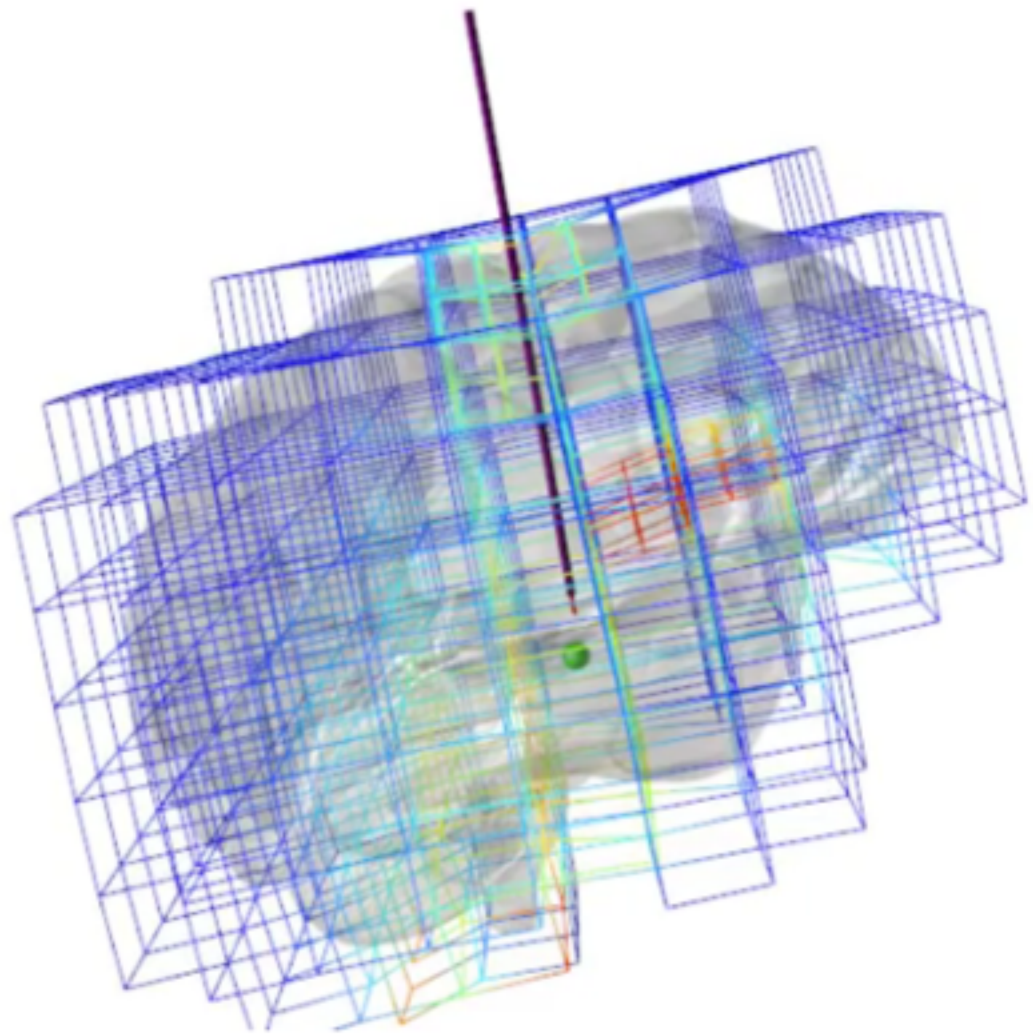




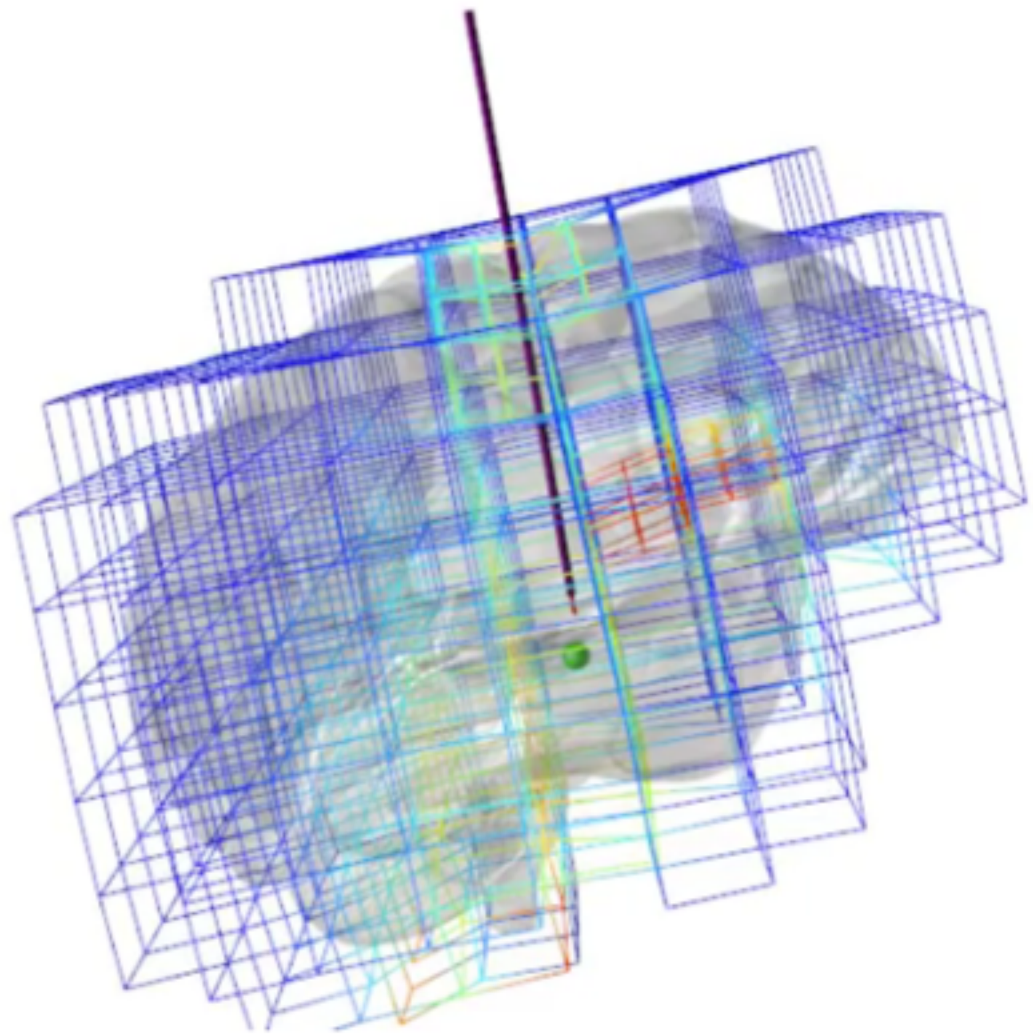


With Danas Sutula and Nguyen Vinh Phu (Monash)
9TH Australasian Congress on Applied Mechanics (ACAM9)
27 - 29 November 2017
phu.nguyen@monash.edu

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?

RealTCut

QUESTIONS

Local mesh refinement is necessary, but where? how?

What else is missing?

Model of contractile tissue

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

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

where

Cowin & Humphrey 2001

Payan & Ohayon 2017

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

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. $a(\mathbf{v},\mathbf{z}) = J(\mathbf{v}) \quad \forall\, \mathbf{v} \in \mathbf{V}$ (dual problem)

➡ **global estimator** : η_h

Local representation

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

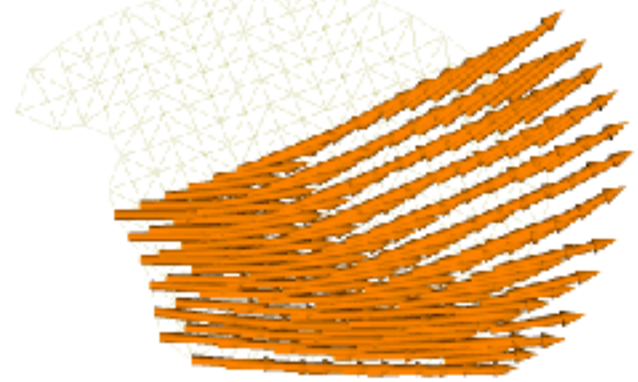
$\pi_h \mathbf{z}$: interpolant of dual solution
R_K / $R_{\partial K}$: residual contributions on K / ∂K

➡ **local estimators** : η_K

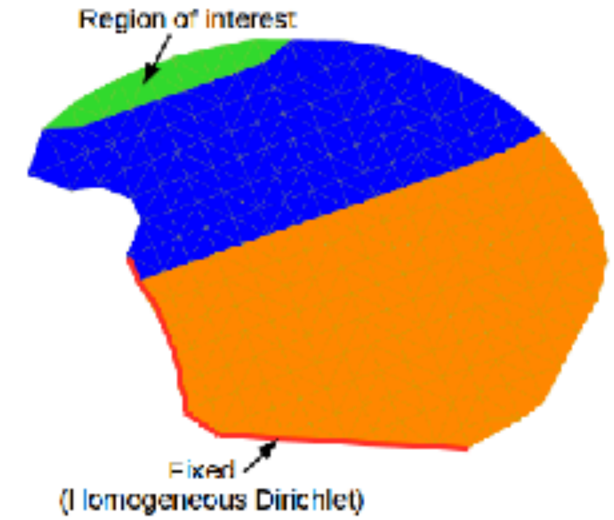
Becker & Rannacher 1997, 2001
Rognes & Logg 2013 (FEniCS)

Genioglossus activation

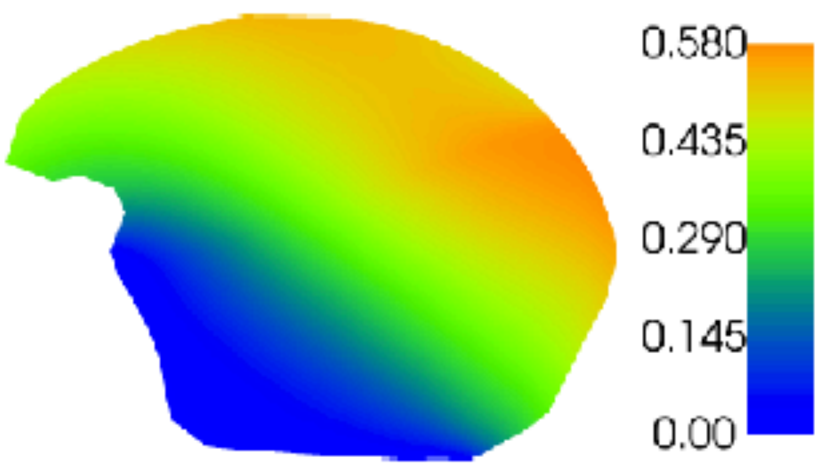
Bijar, Rohan, Perrier & Payan 2015



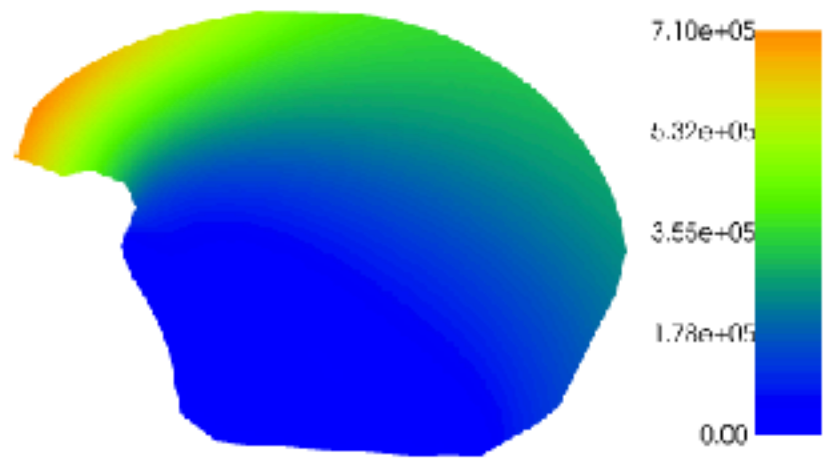
fibers (genioglossus)



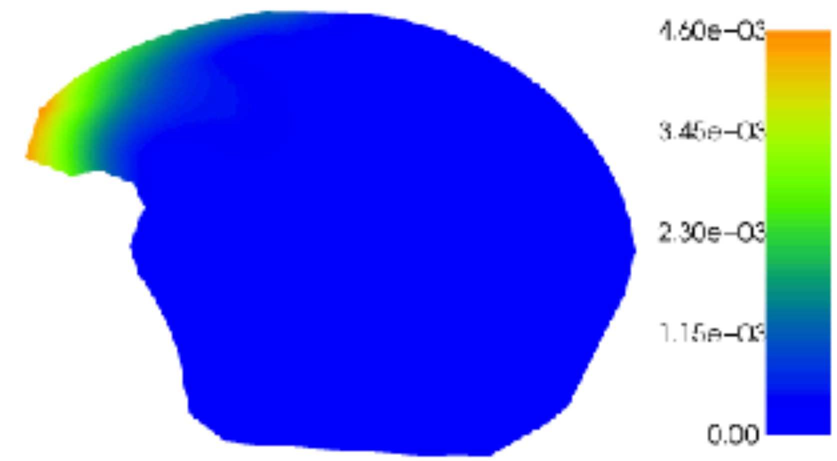
region of interest ω (green)



$\mathbf{u}$



$\mathbf{z}$ / J_1

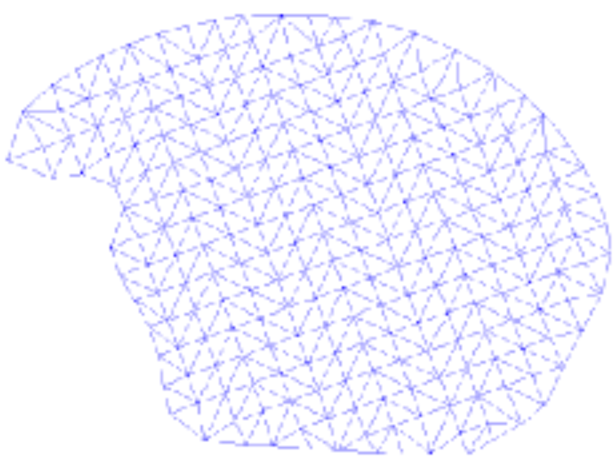


$\mathbf{z}$ / J_2

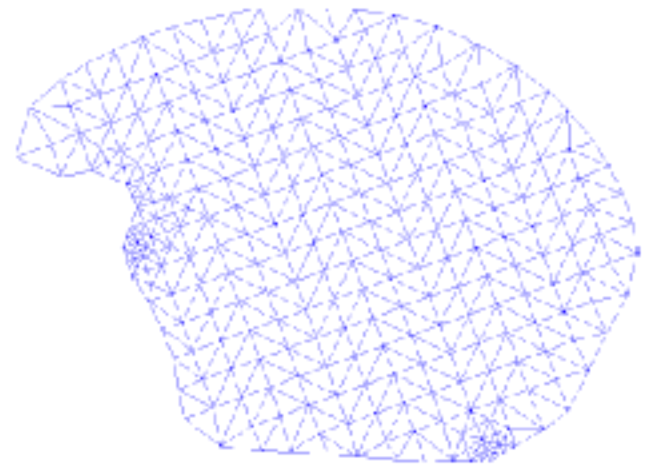
$$J_1(\mathbf{u}) := \int_\omega (u_x + u_y)\, d\mathbf{x} \qquad J_2(\mathbf{u}) := \int_\omega \operatorname{div} \mathbf{u}\, d\mathbf{x}$$

Genioglossus activation

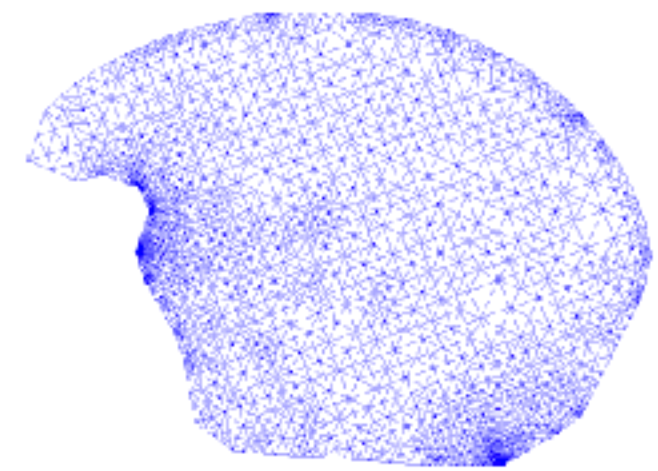
J_1 :



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

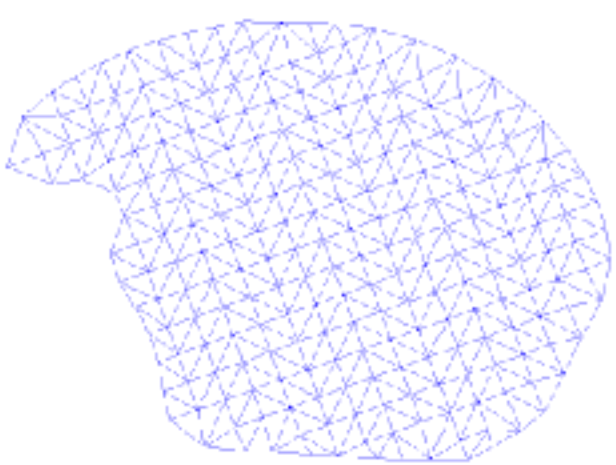


2nd iteration
(N=523, $\varepsilon = 3.10^{-3}$)

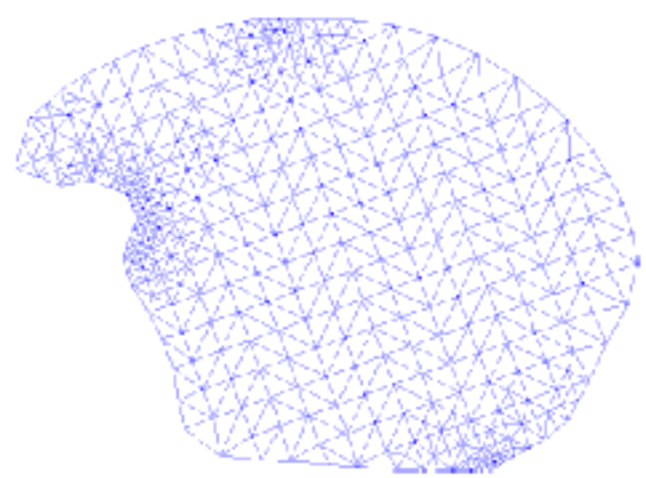


8th iteration
(N=5143, $\varepsilon = 4.10^{-5}$)

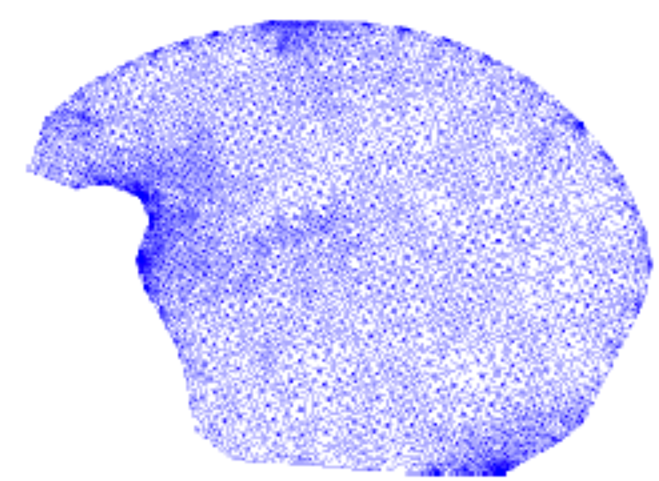
J_2 :



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

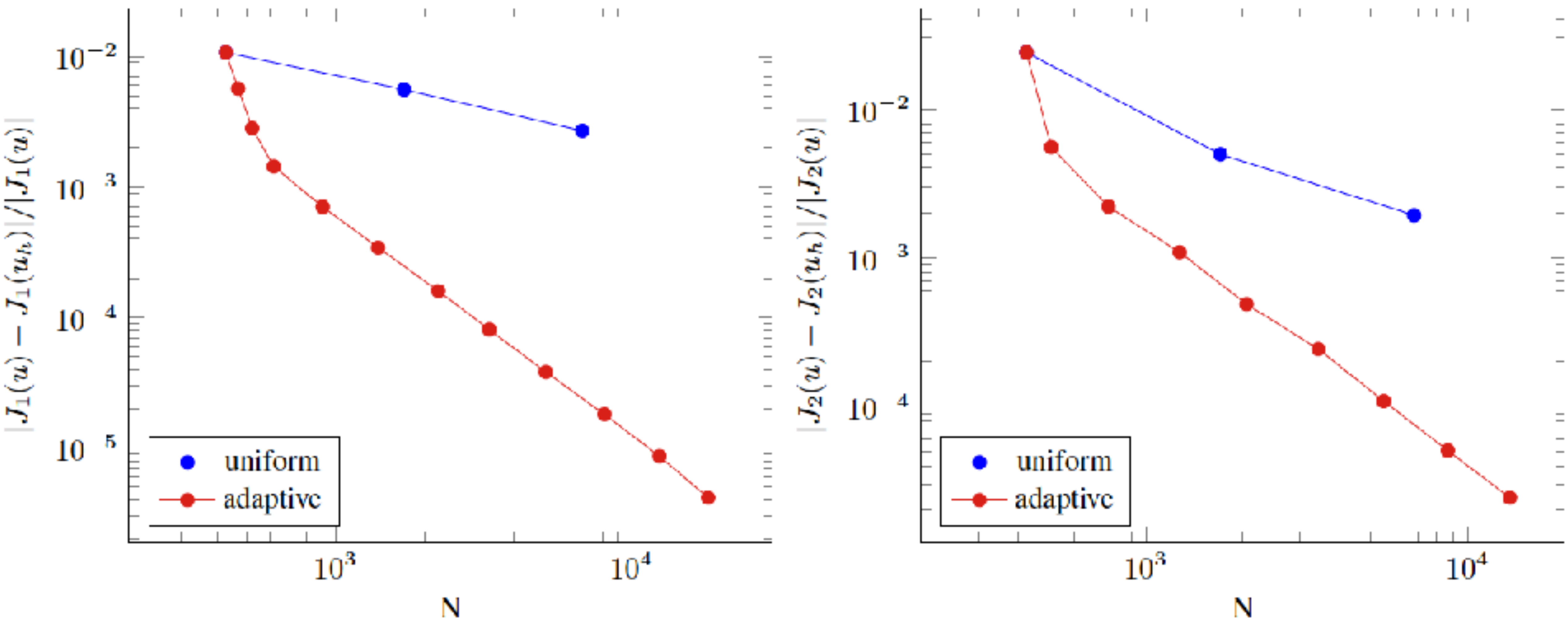


2nd iteration
(N=766, $\varepsilon = 2.10^{-3}$)



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

Effect of adaptive refinement



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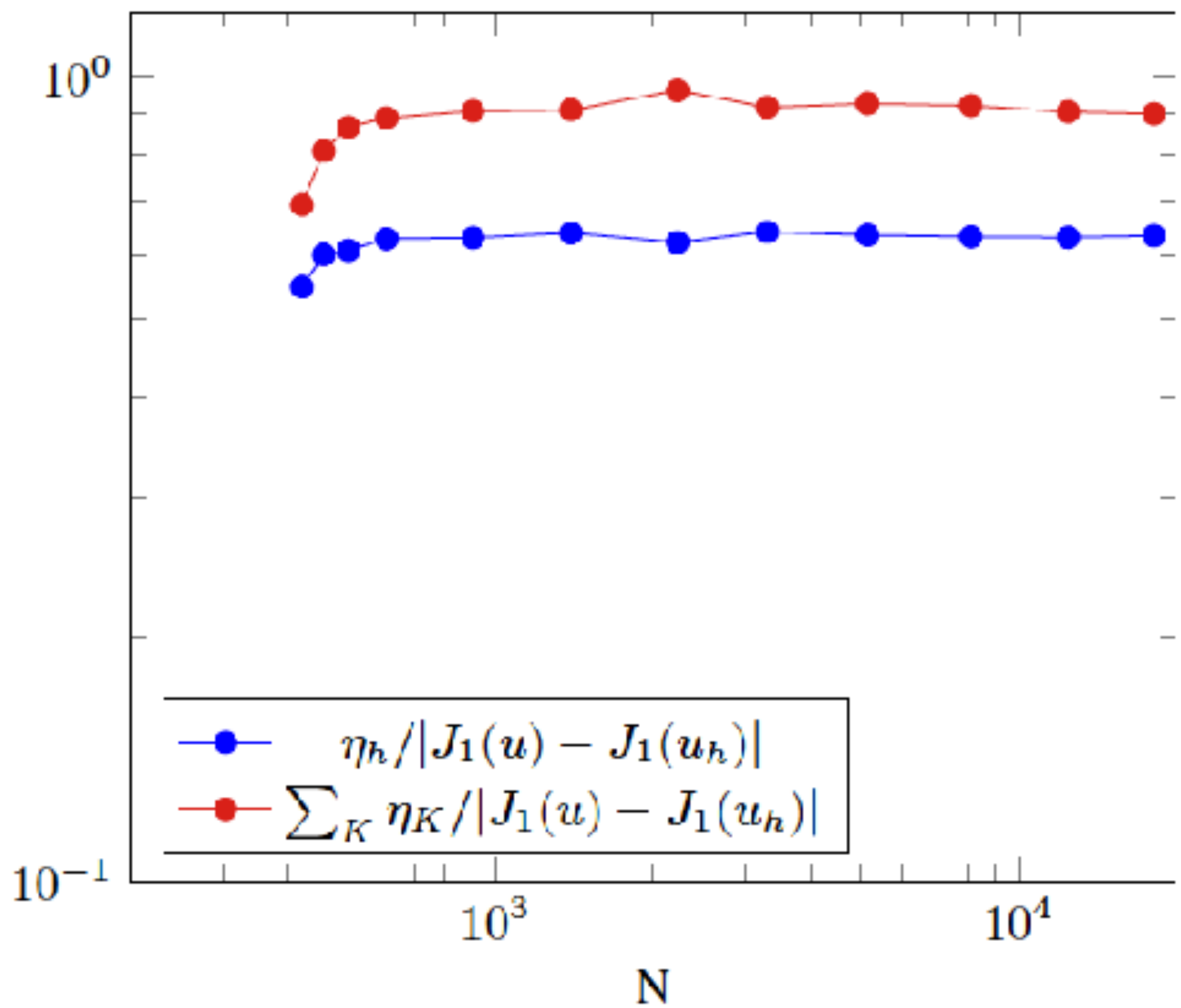
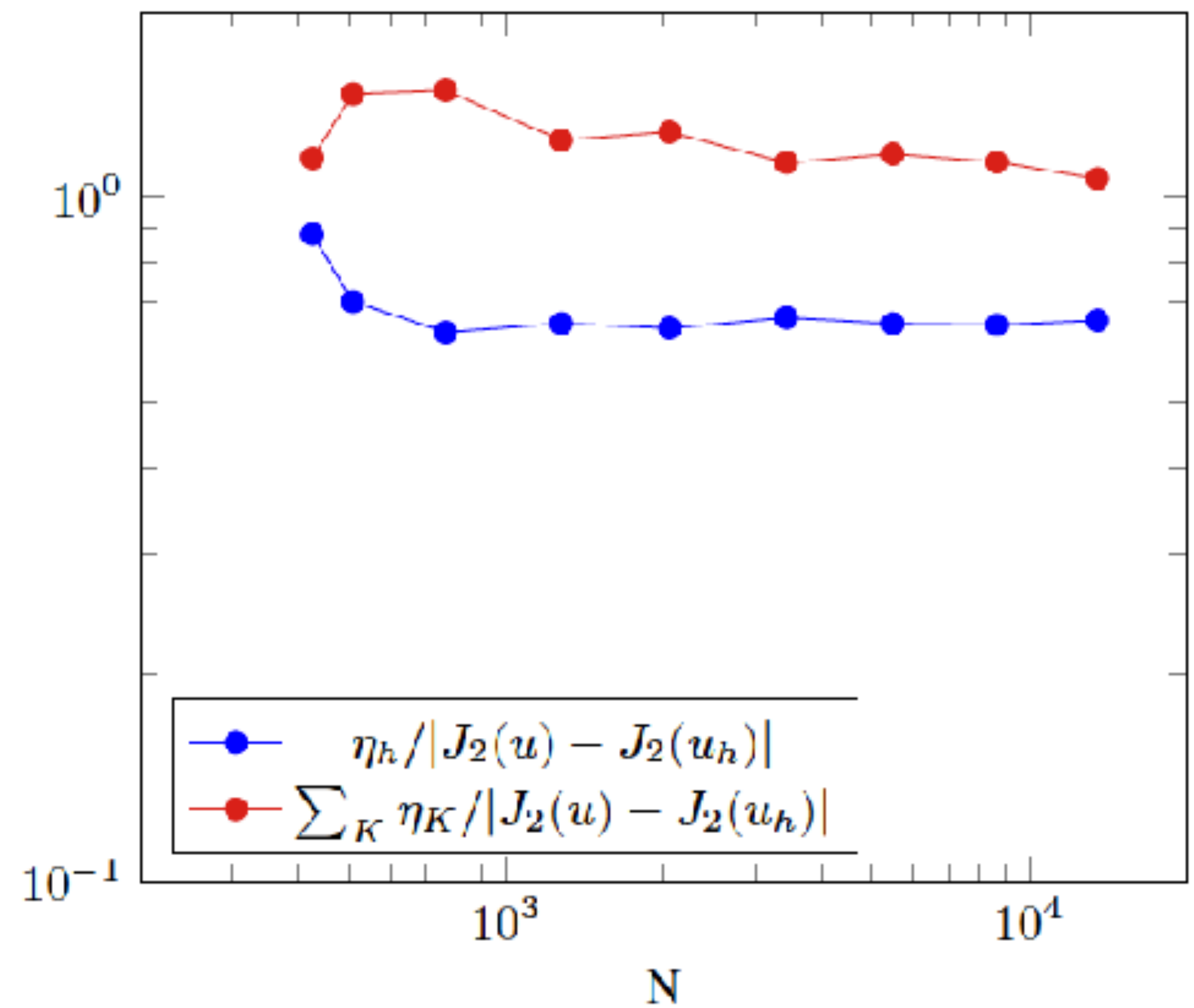
Effectivity of the error indicator





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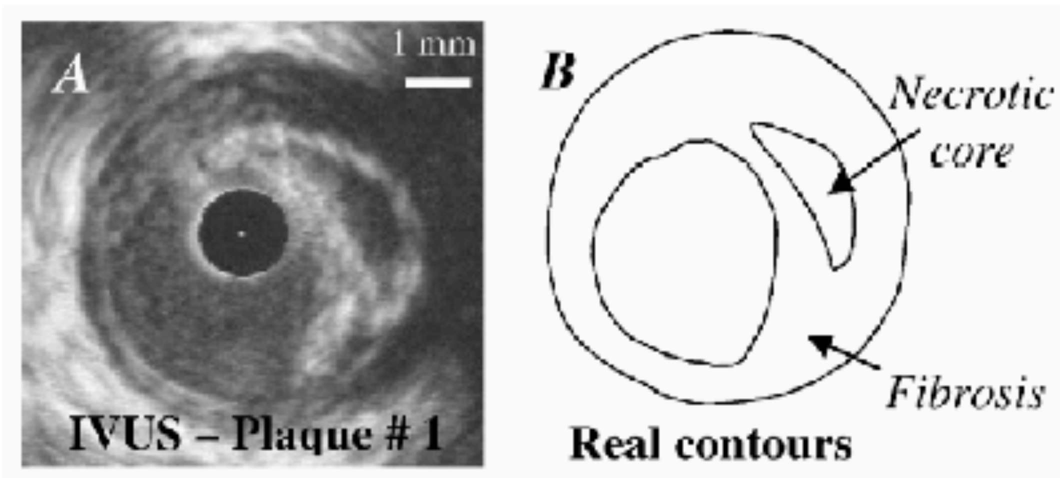
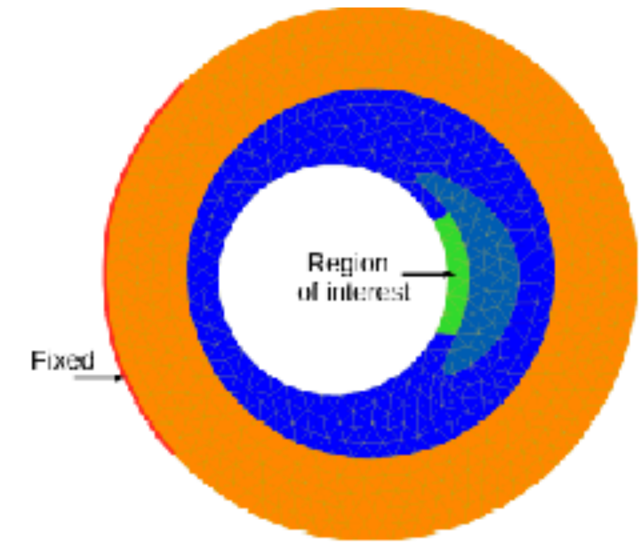
Arterial wall activation

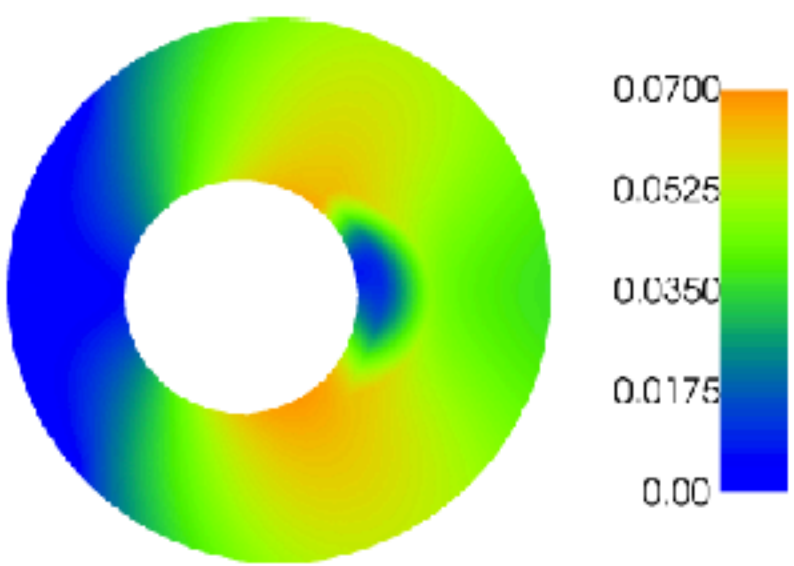


Le Floc'h et.al 2008

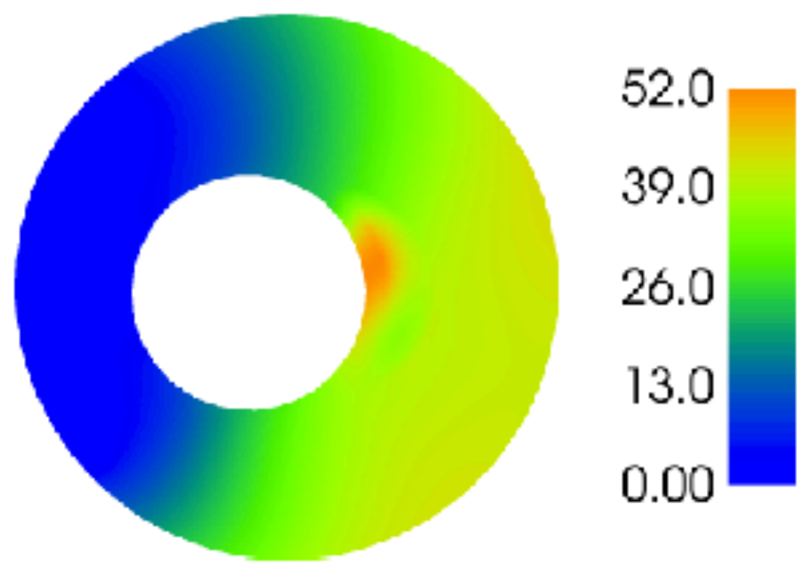
media



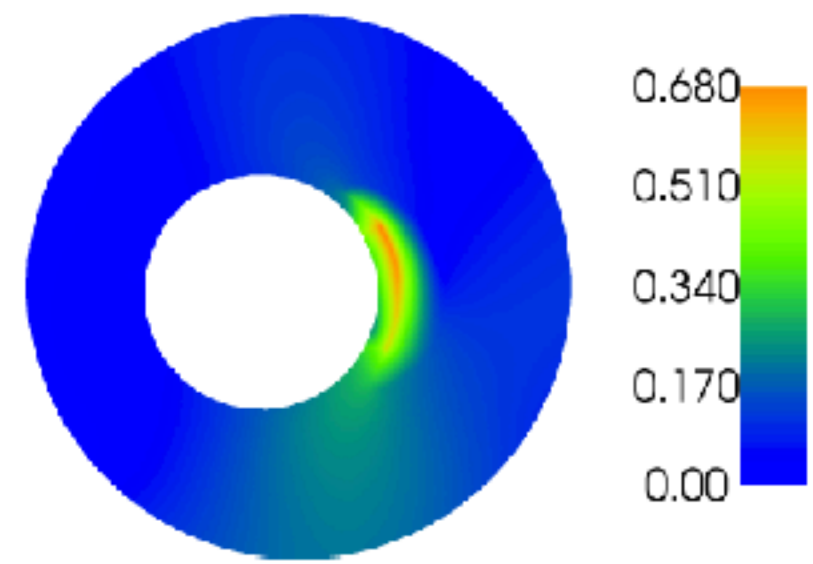
region of interest ω (green)



$\mathbf{u}$



$\mathbf{z}$ / J_1



$\mathbf{z}$ / J_2

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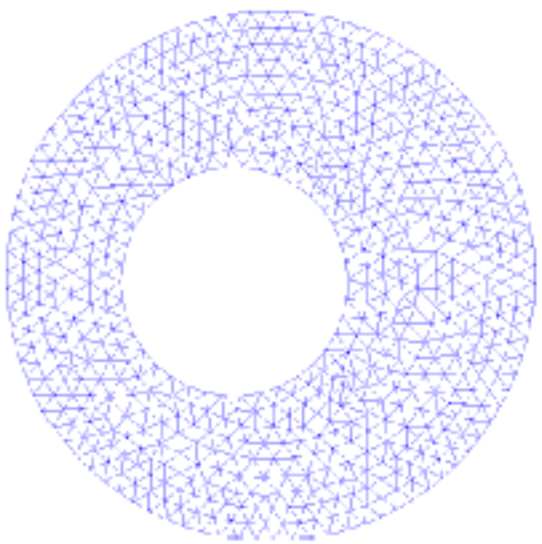
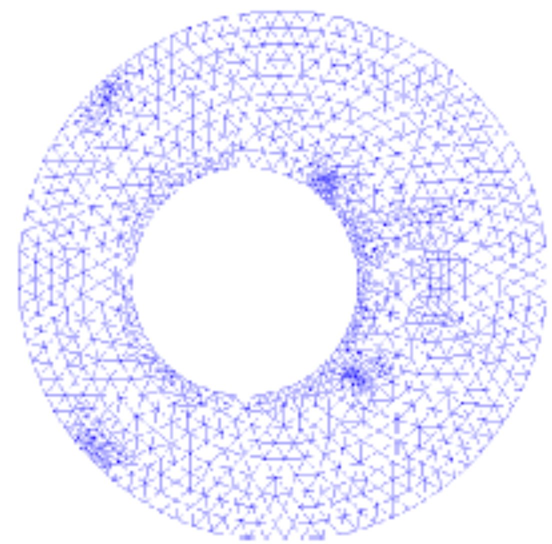
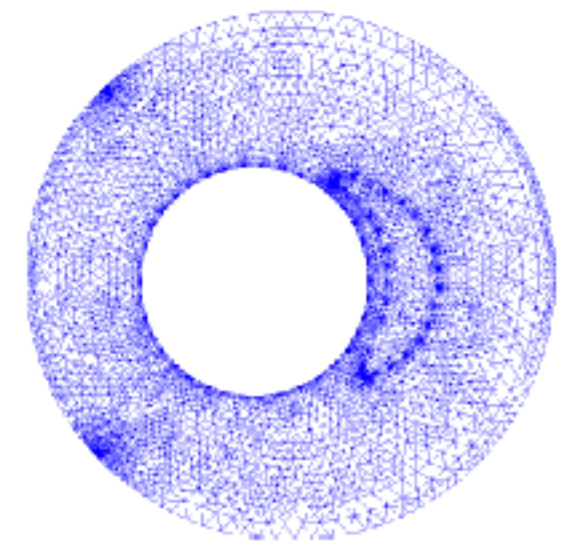
J_1 :



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



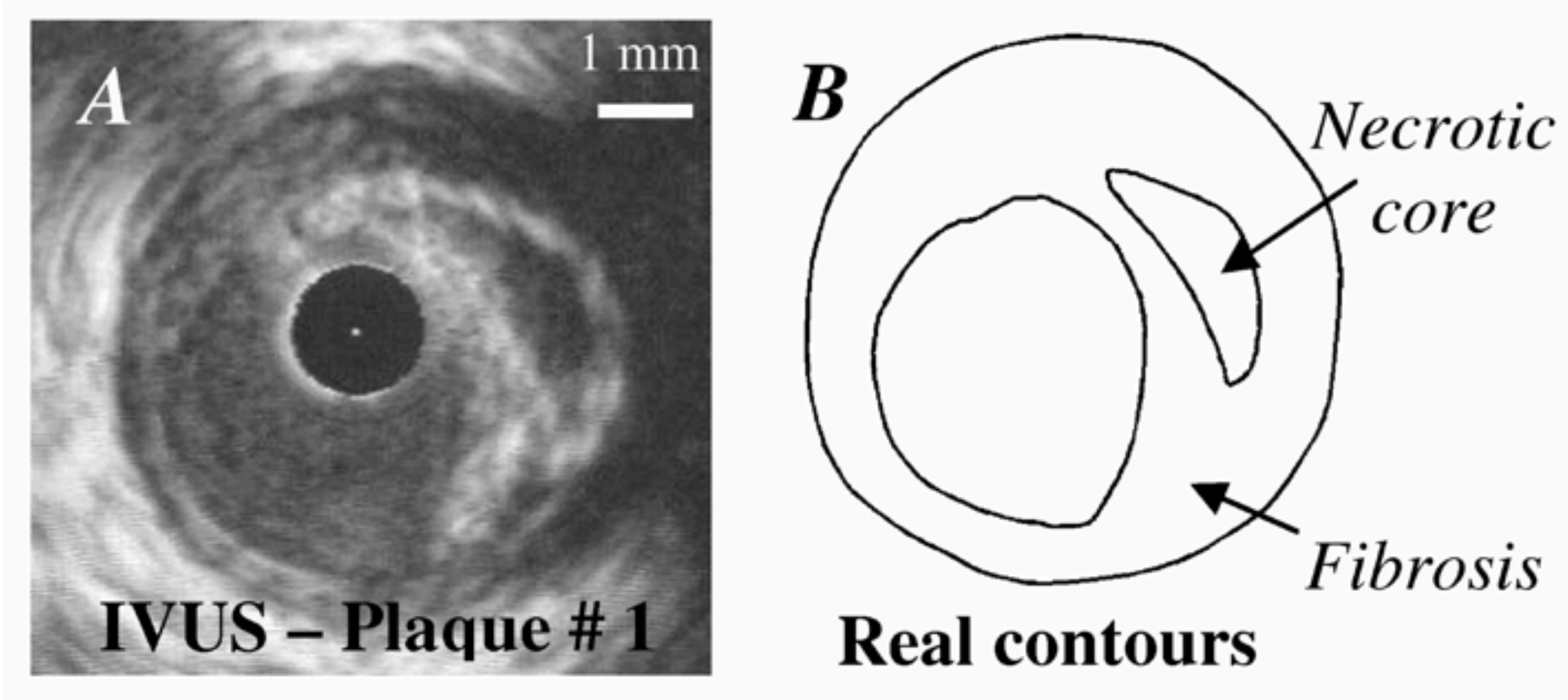
2nd iteration
(N=2079, $\varepsilon = 0.05$)

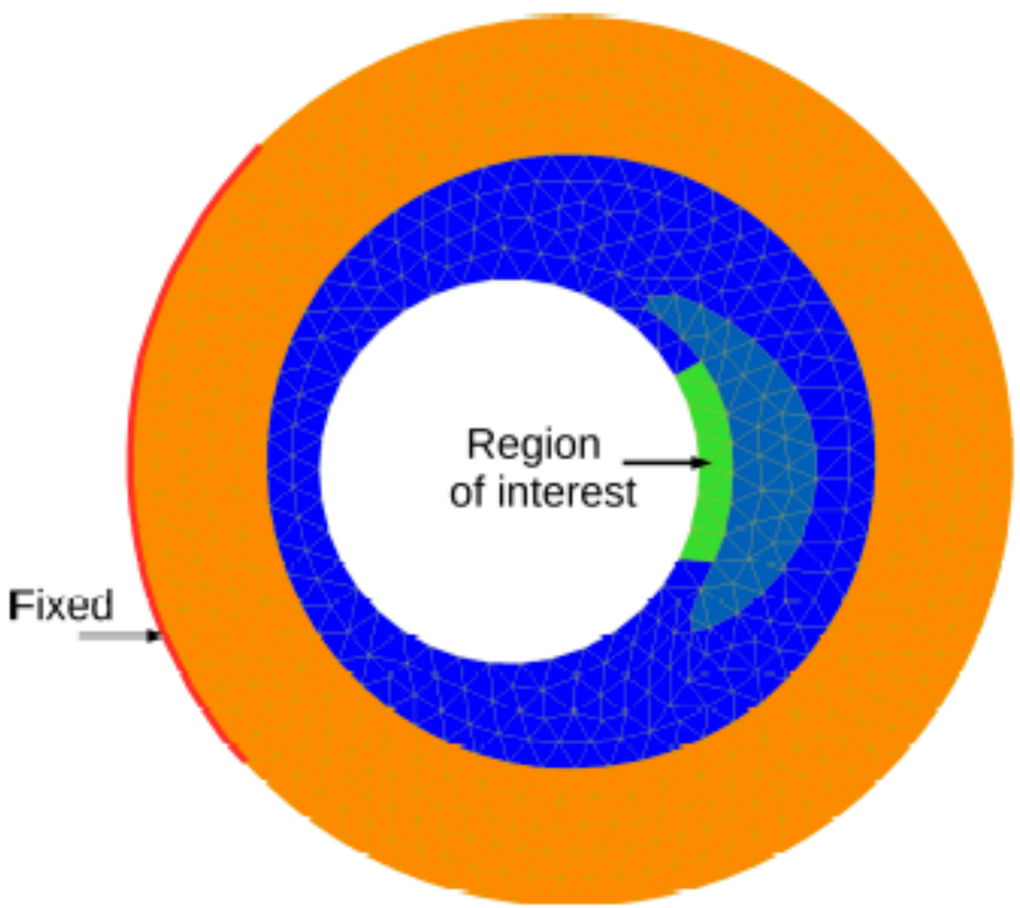


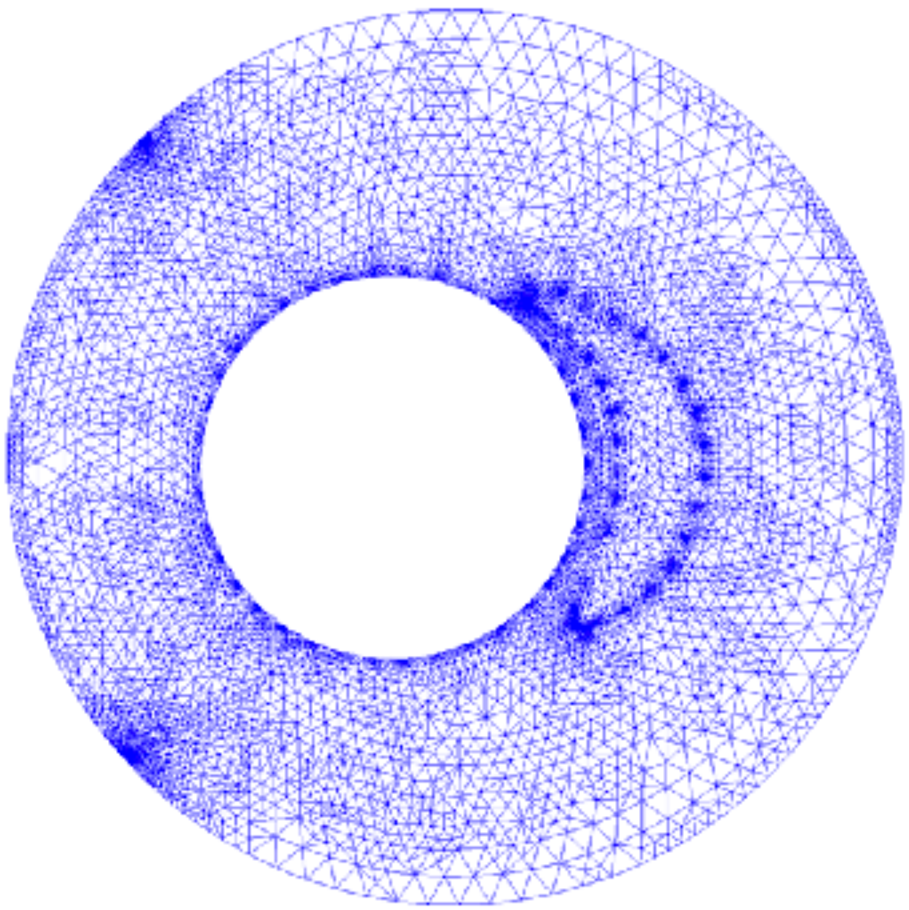
6th iteration
(N=15028, $\varepsilon = 3.10^{-3}$)

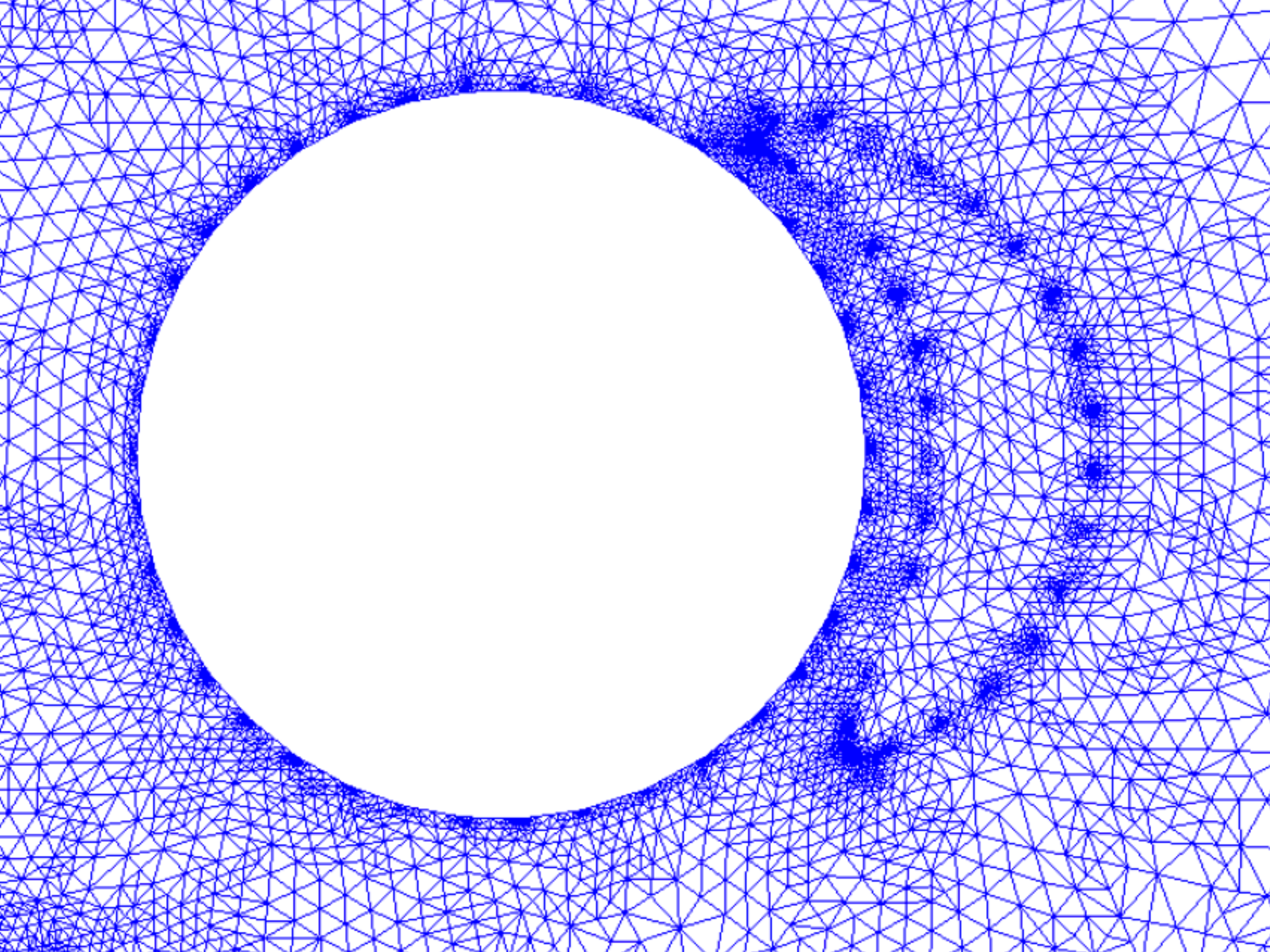
J_2 : similar results.

RealTCut

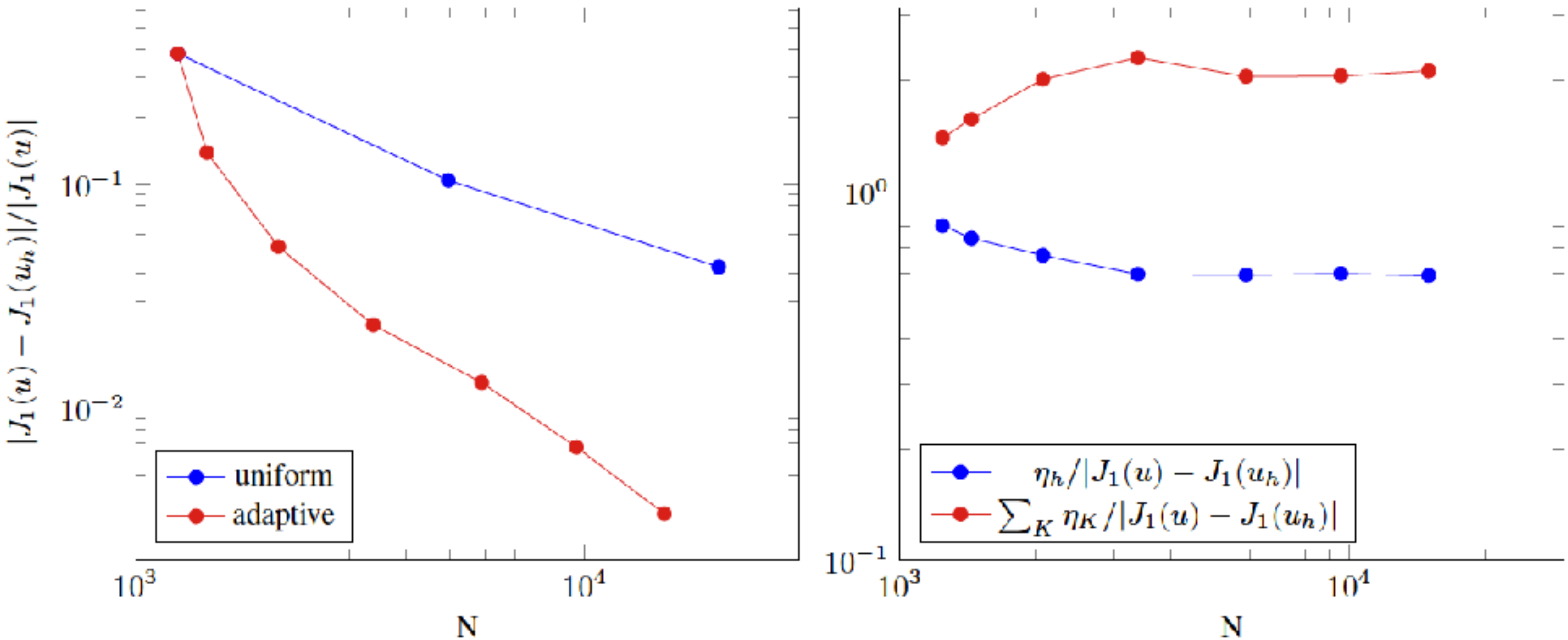

A
1 mm
IVUS – Plaque # 1
B
Necrotic core
Fibrosis
Real contours


Region of interest
Fixed





Effectivity



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

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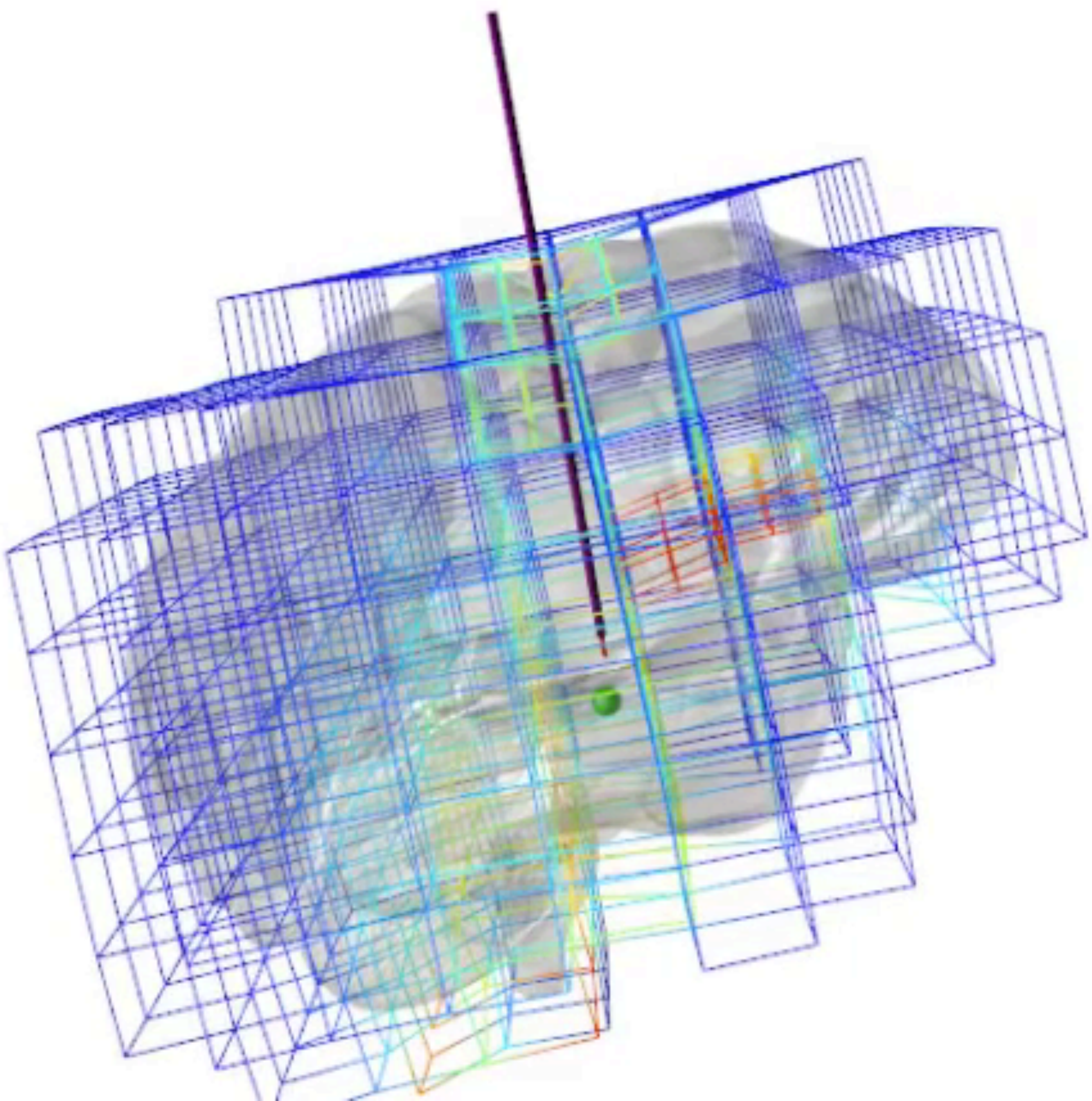
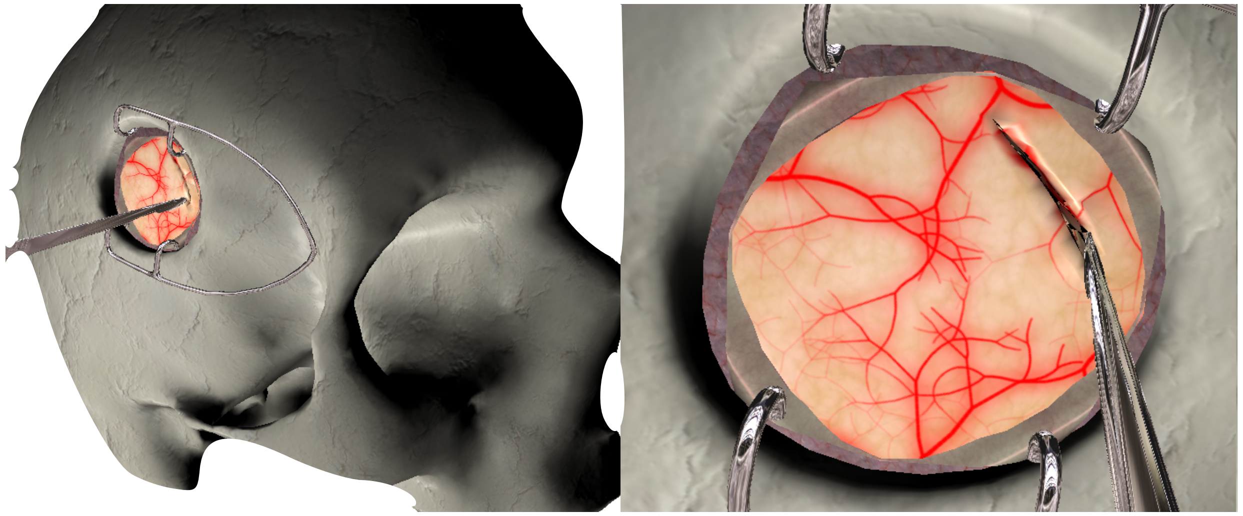
Cannula insertion



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).

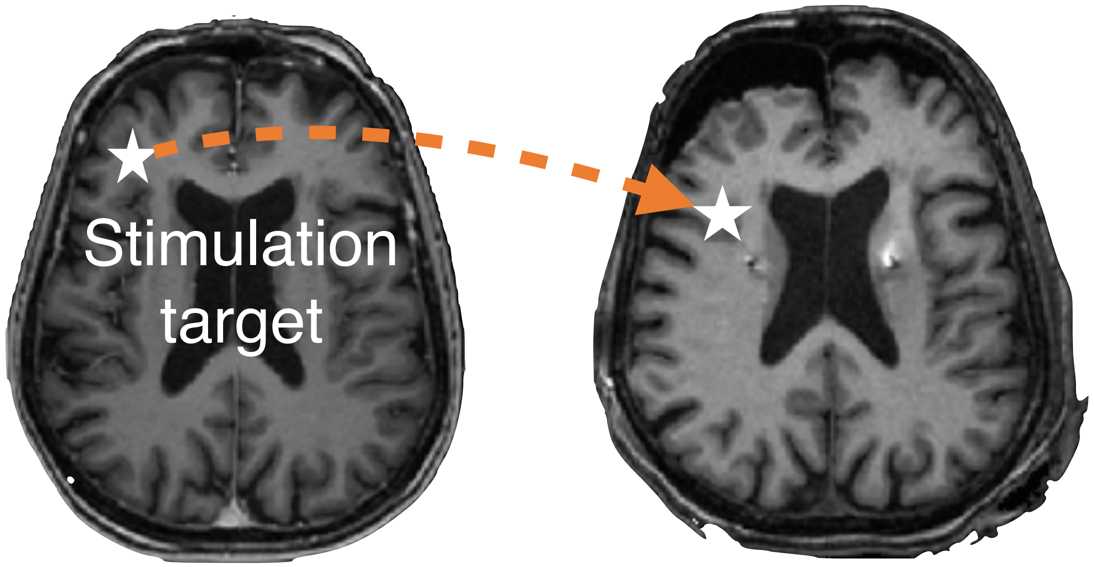


Courtecuisse, 2014, Implicit method for cutting in real-time. MEDIA

A generic organ is sufficient.

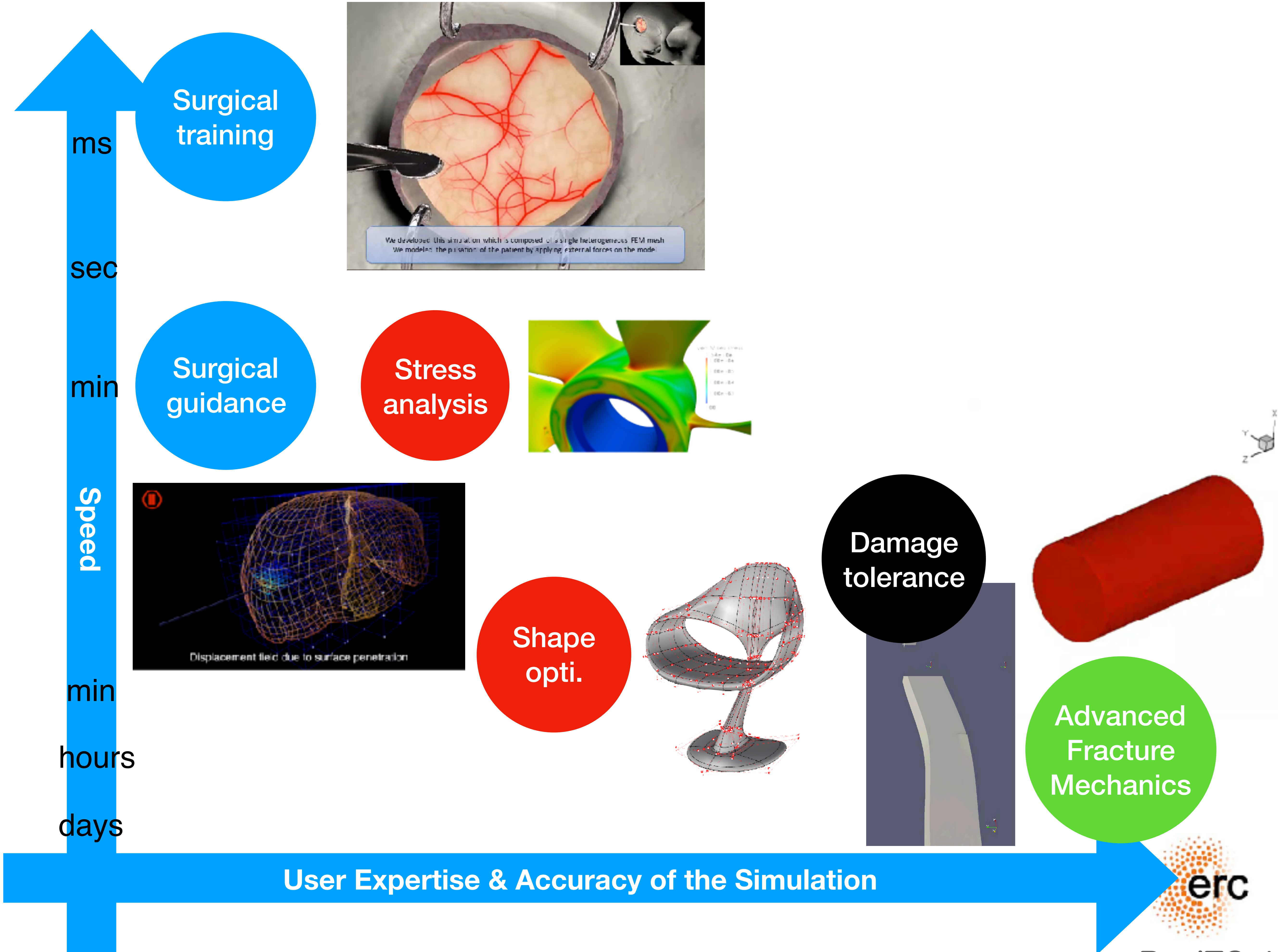
Future
Surgical assistance and planning

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



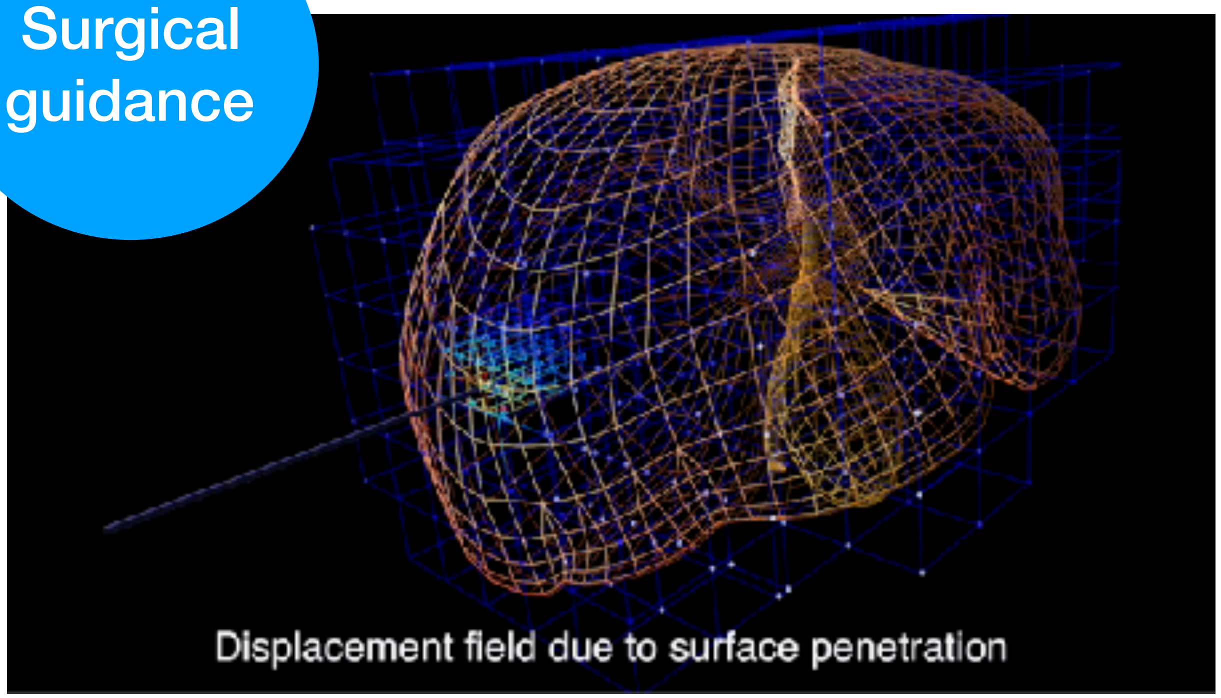
Predict shift of brain target.

Patient specificity is


Surgical training
We developed this simulation which is composed of a single heterogeneous FEM mesh
We modeled the pulsation of the patient by applying external forces on the model
ms
sec
min
Surgical guidance
Stress analysis
Speed
Displacement field due to surface penetration
Damage tolerance
Shape opti.
min
hours
days
Advanced Fracture Mechanics
User Expertise & Accuracy of the Simulation
erc
RealTCut

From surgical training to surgical planning and assistance

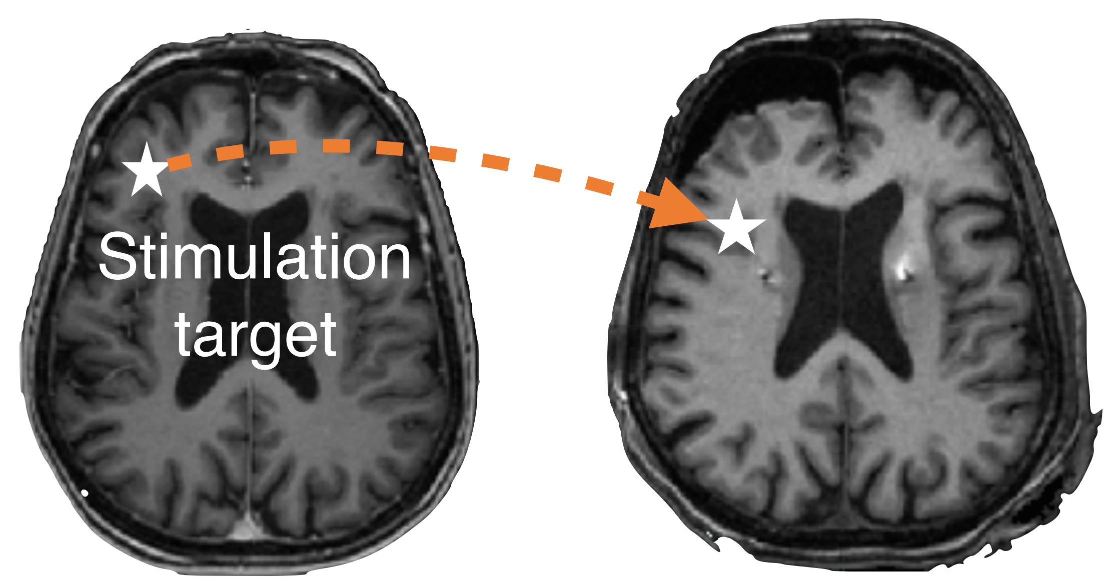
Surgical guidance



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

Future
Surgical assistance and planning

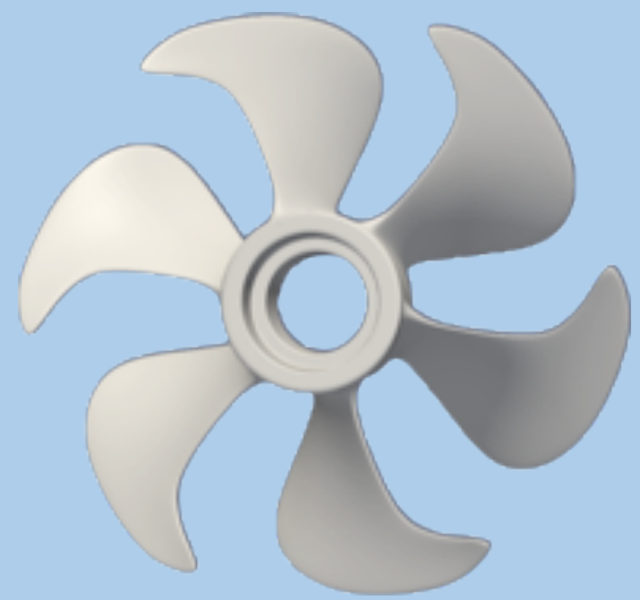
- Data-driven material models (real-time).
- Error control in quantities of interest for strong non-linearities, multi-field…
- Clinical time scales (solution in minutes).



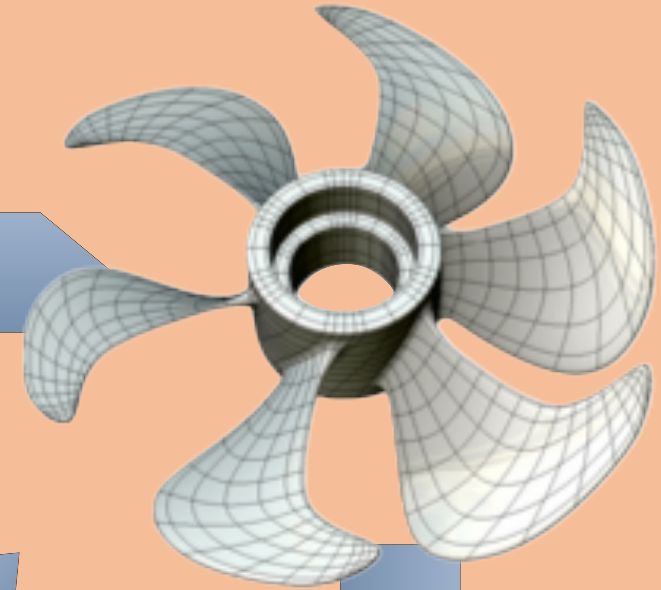
Predict shift of brain target.

Patient specificity is

GEOMETRY



DISCRETISATION



Verification

A POSTERIORI ERROR

MATERIAL MODELS

Phenomenological

Elasticity/Plasticity

Crack growth law (Paris…)

Fracture energy

Maximum tensile strength

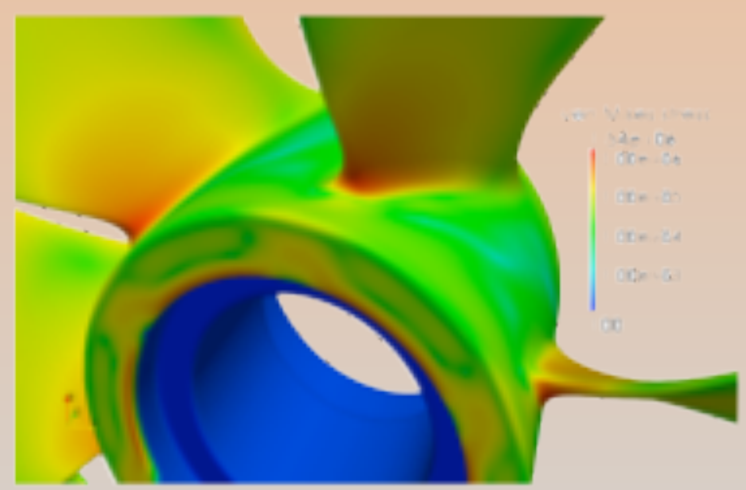
Multi-scale

Debonding, Fibre pull-out

Fibre breakage, interface

fracture, grains, dislocations,

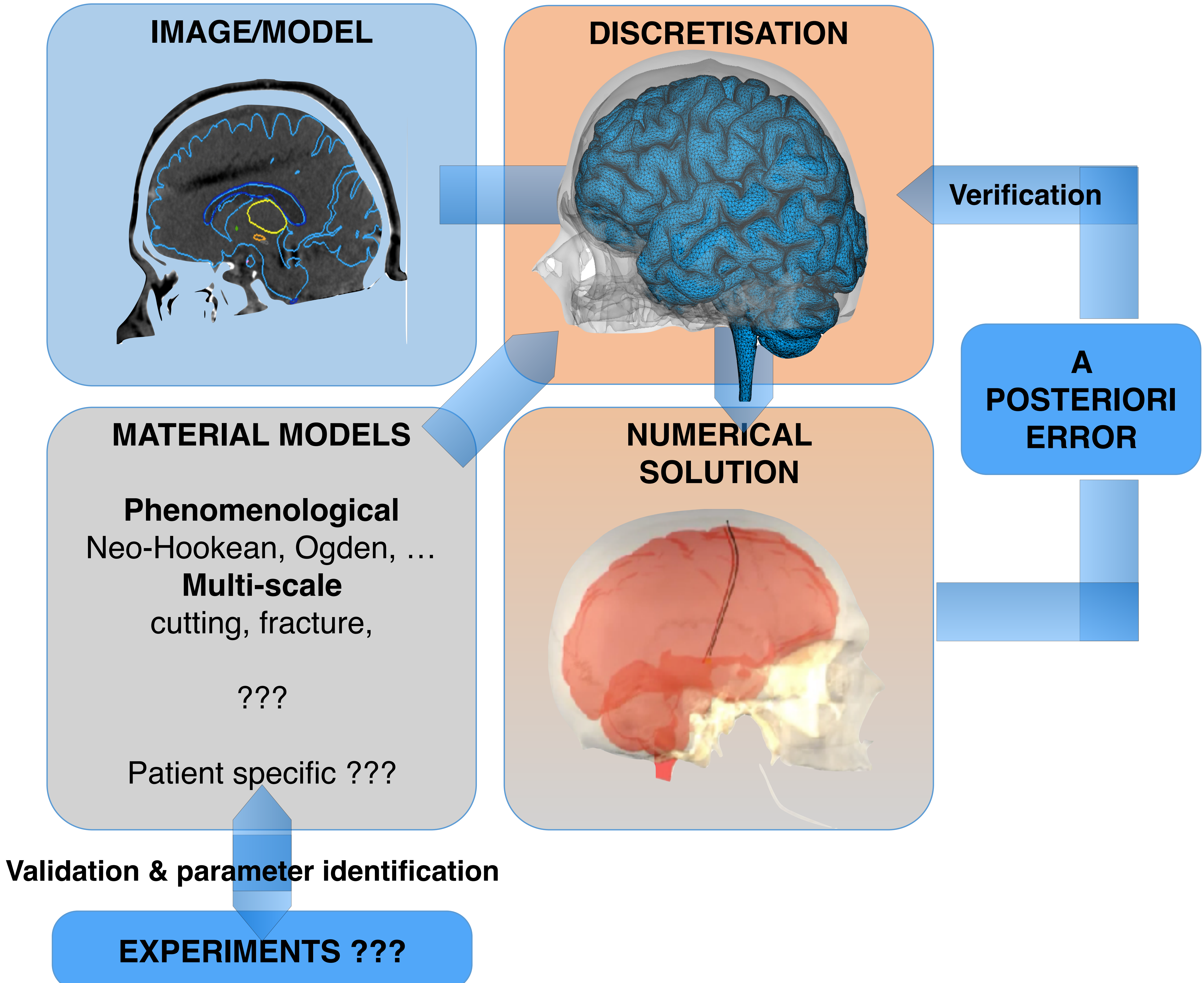
NUMERICAL SOLUTION



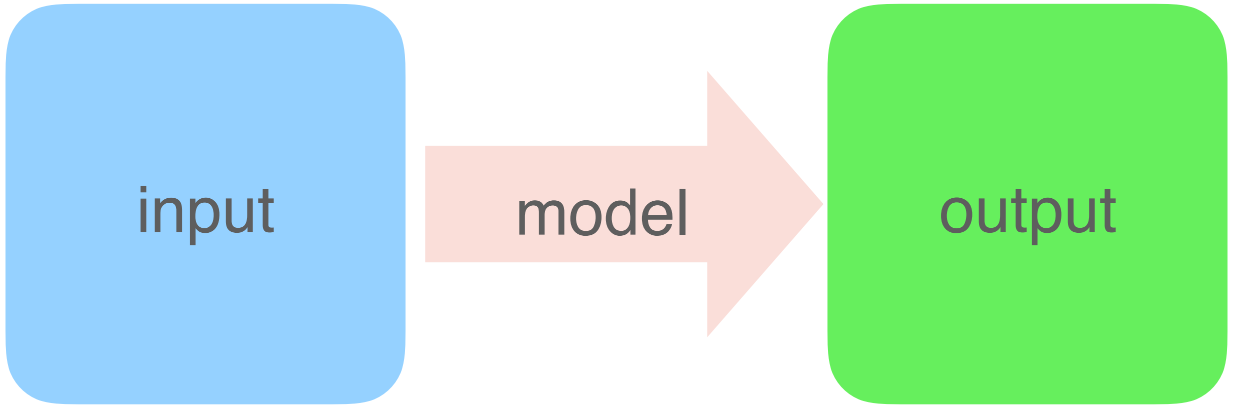
Validation & parameter identification

EXPERIMENTS

CONVENTIONAL APPROACH

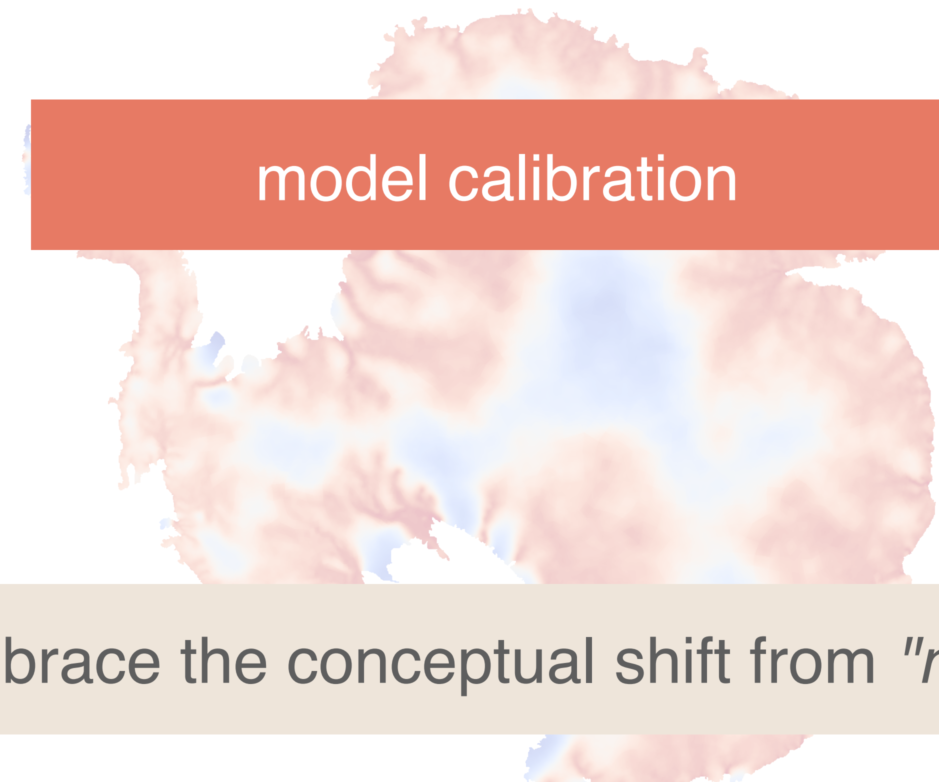

IMAGE/MODEL
DISCRETISATION
Verification
A POSTERIORI ERROR
MATERIAL MODELS
Phenomenological
Neo-Hookean, Ogden, …
Multi-scale
cutting, fracture,
???
Patient specific ???
NUMERICAL SOLUTION
Validation & parameter identification
EXPERIMENTS ???

Data-driven Modelling



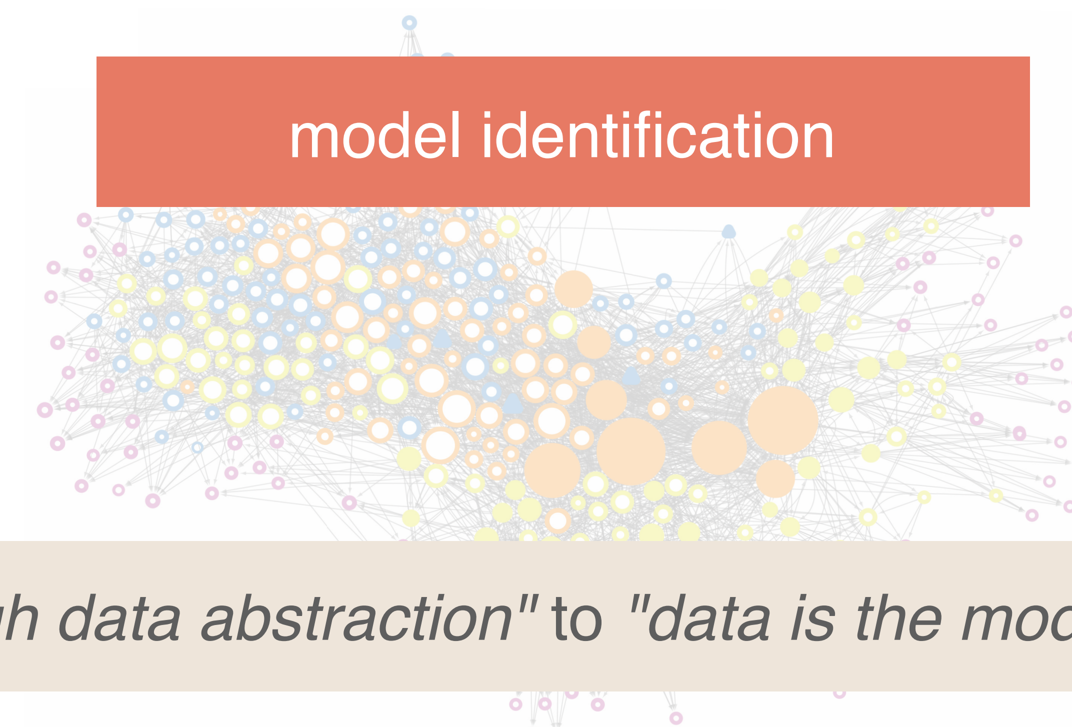
$$f : \mathbf{x} \rightarrow \mathbf{y}$$

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



model calibration

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

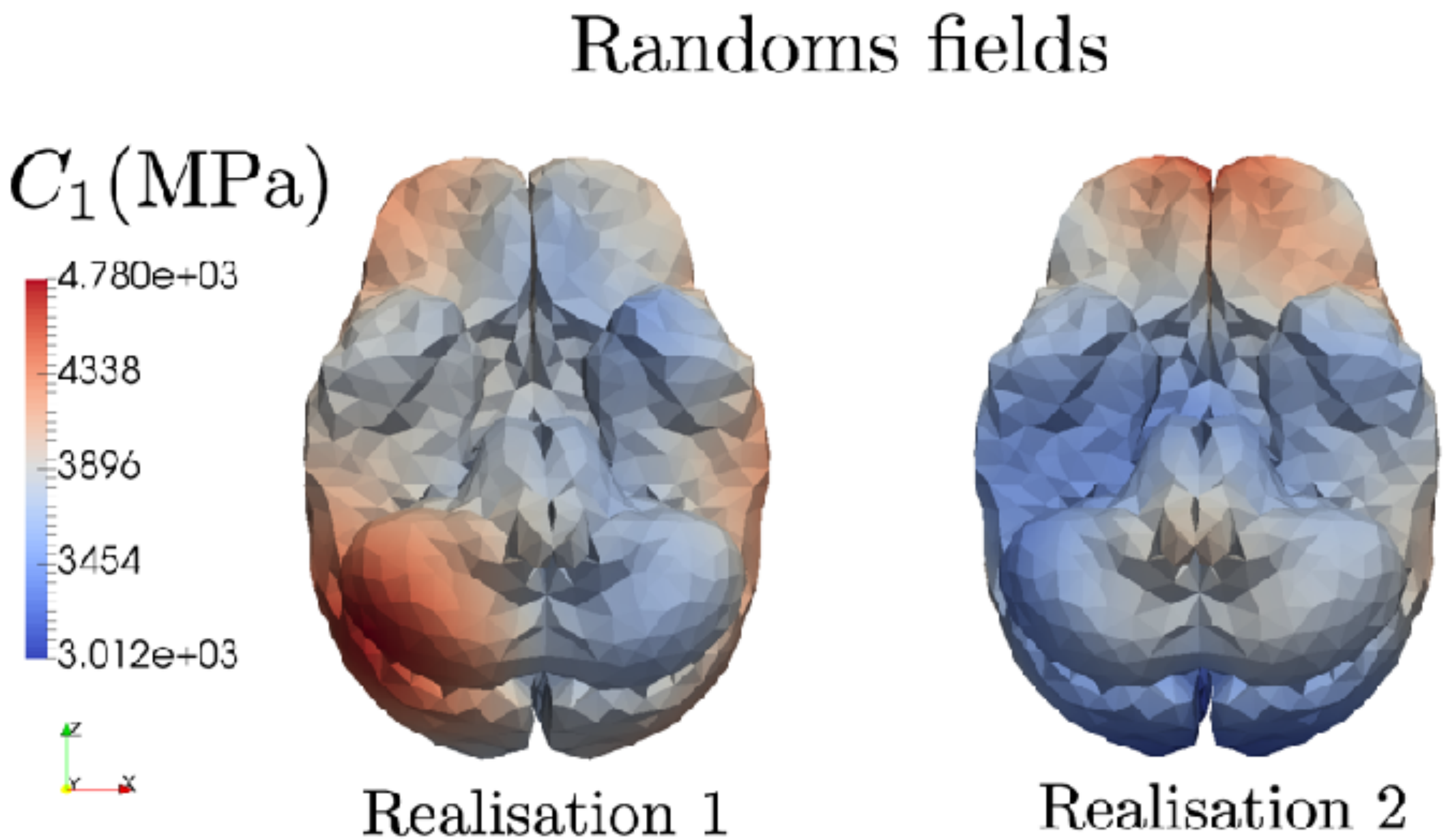


model identification

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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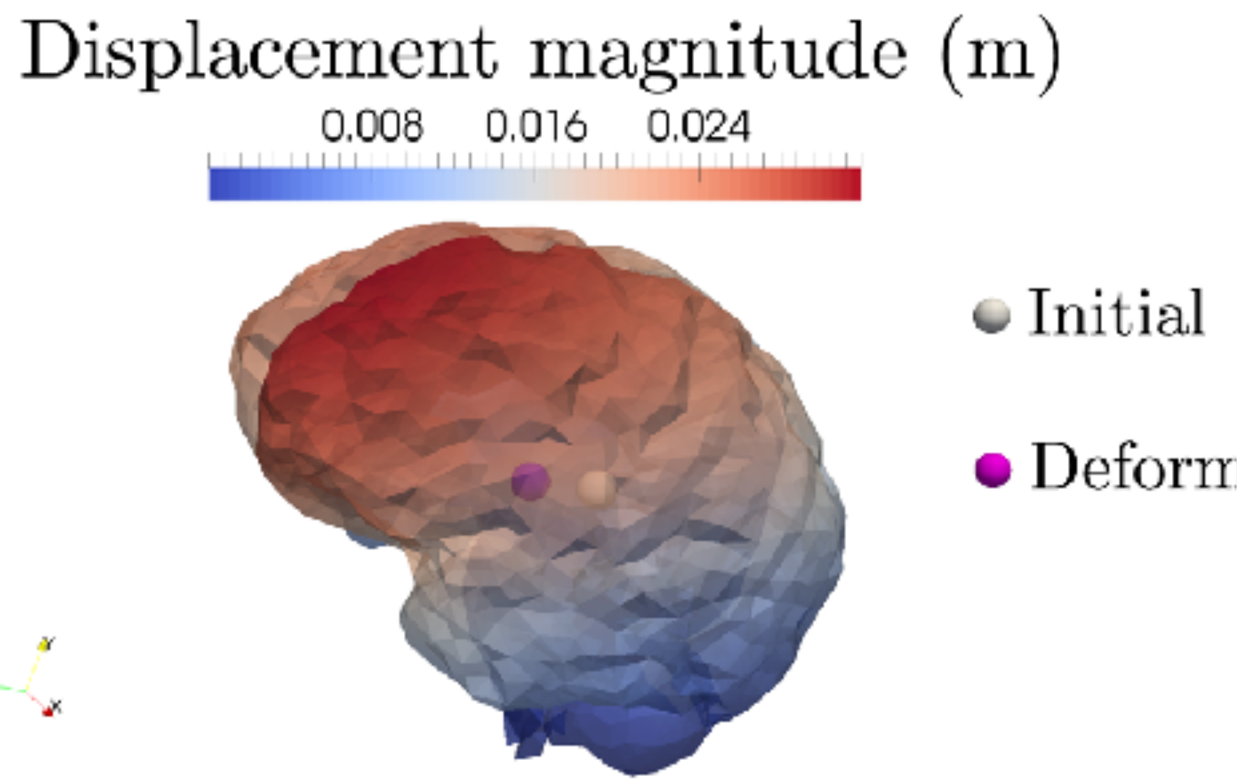
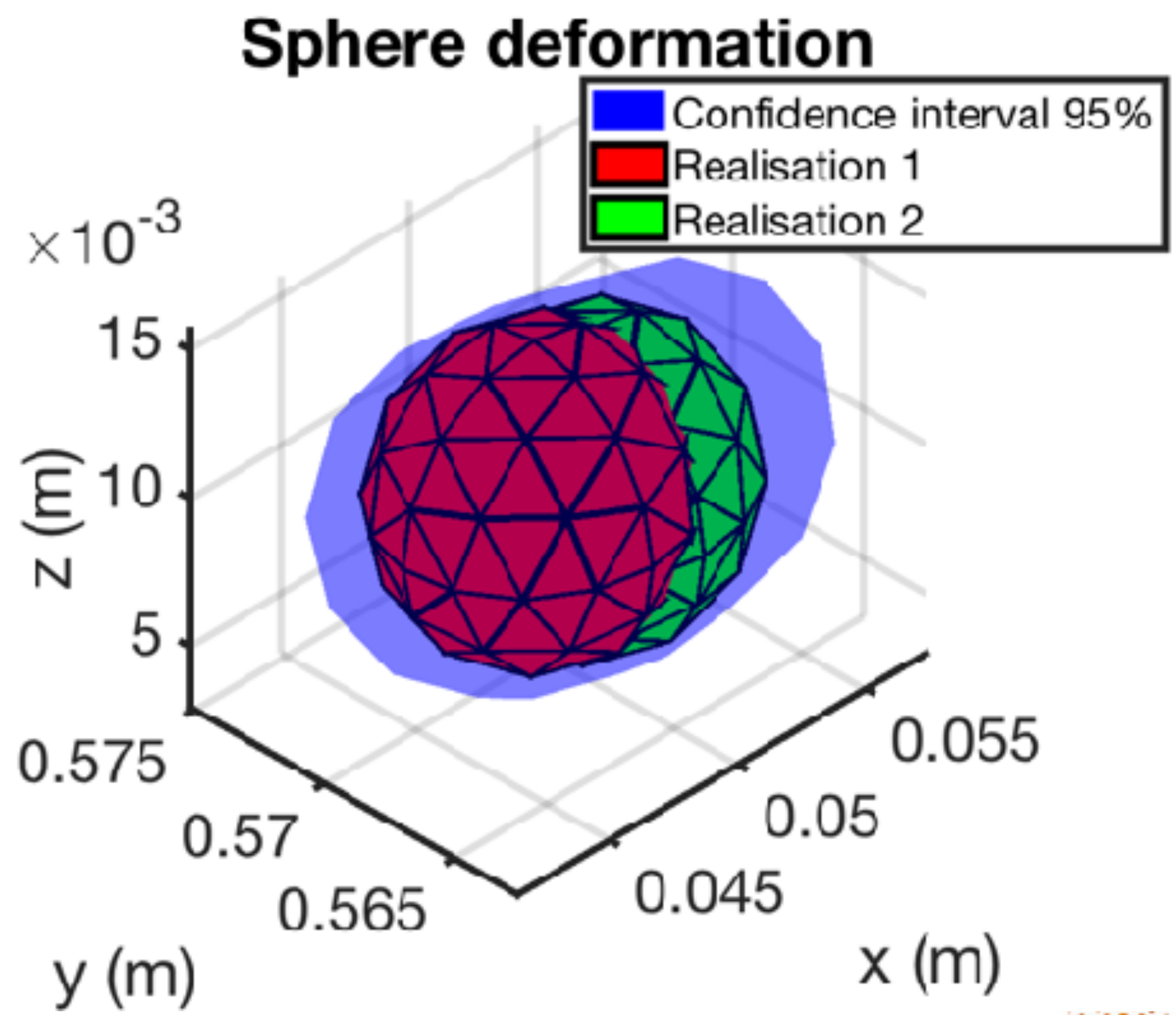
Confidence level in predicting the target location

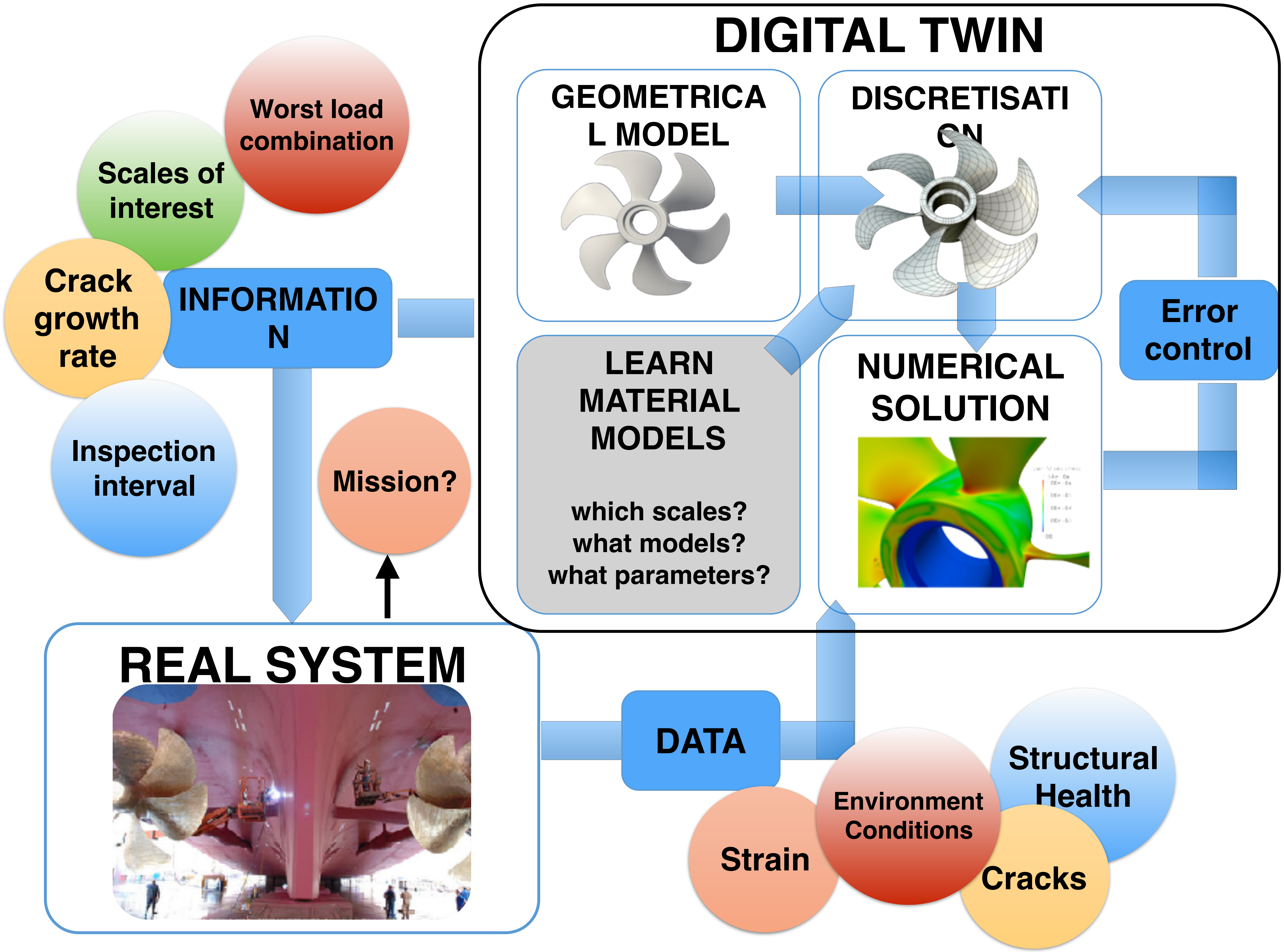


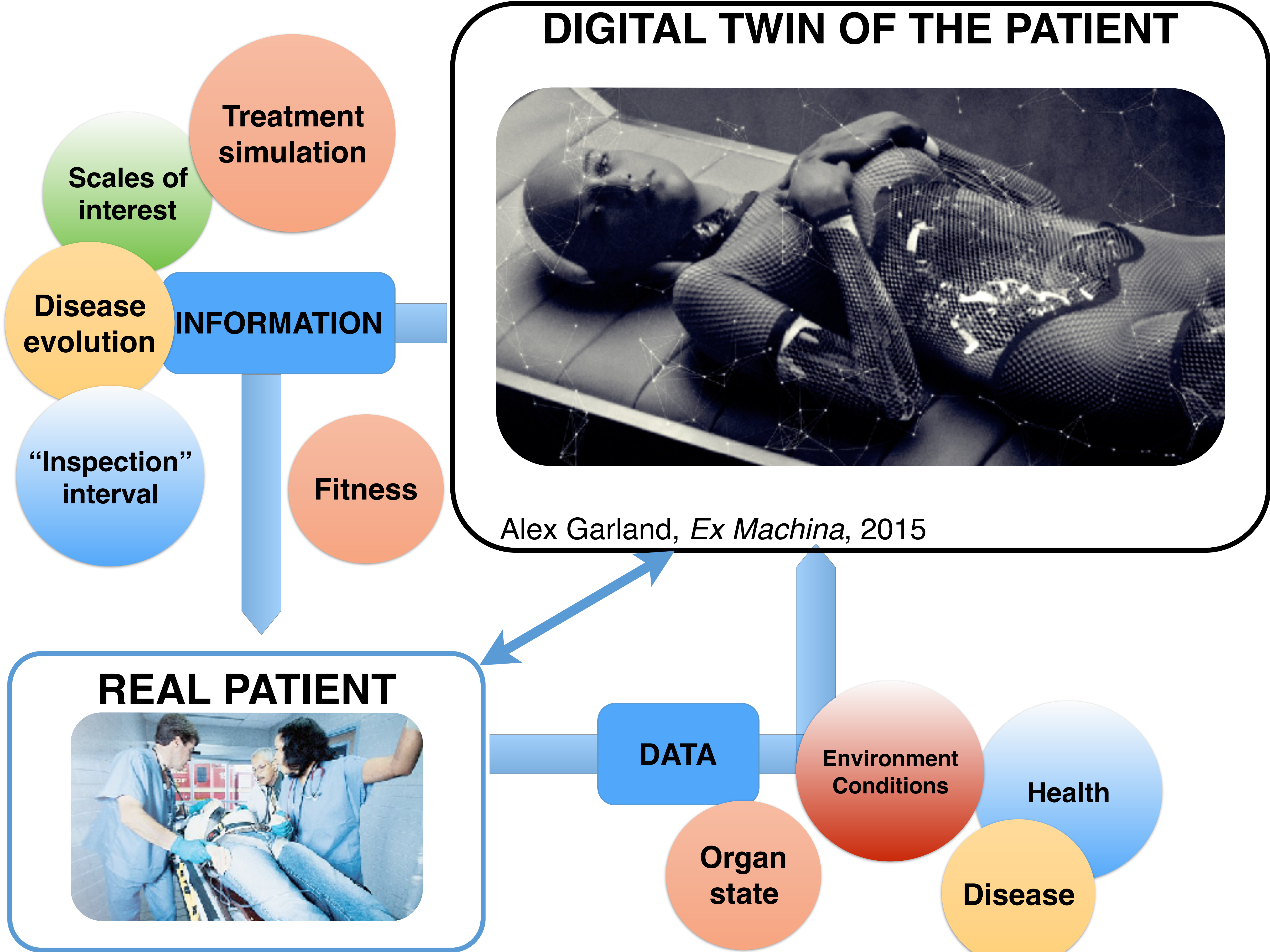


What is the influence of material parameters on computed quantities of interest?

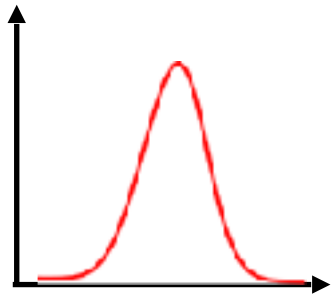
RealTCut

Possible approach

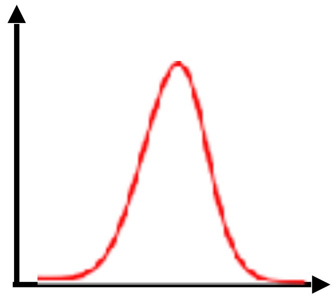



DIGITAL TWIN OF THE PATIENT
Alex Garland, *Ex Machina*, 2015
Treatment simulation
Scales of interest
Disease evolution
INFORMATION
"Inspection" interval
Fitness
REAL PATIENT
DATA
Environment Conditions
Health
Organ state
Disease

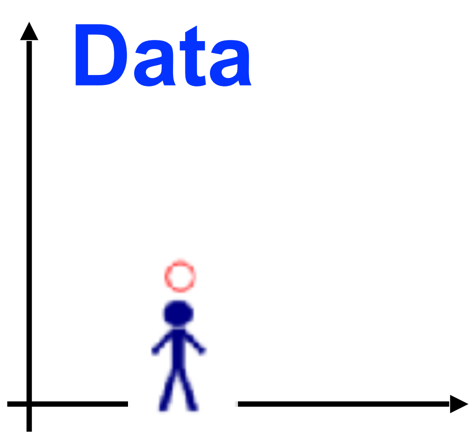
Prior Knowledge



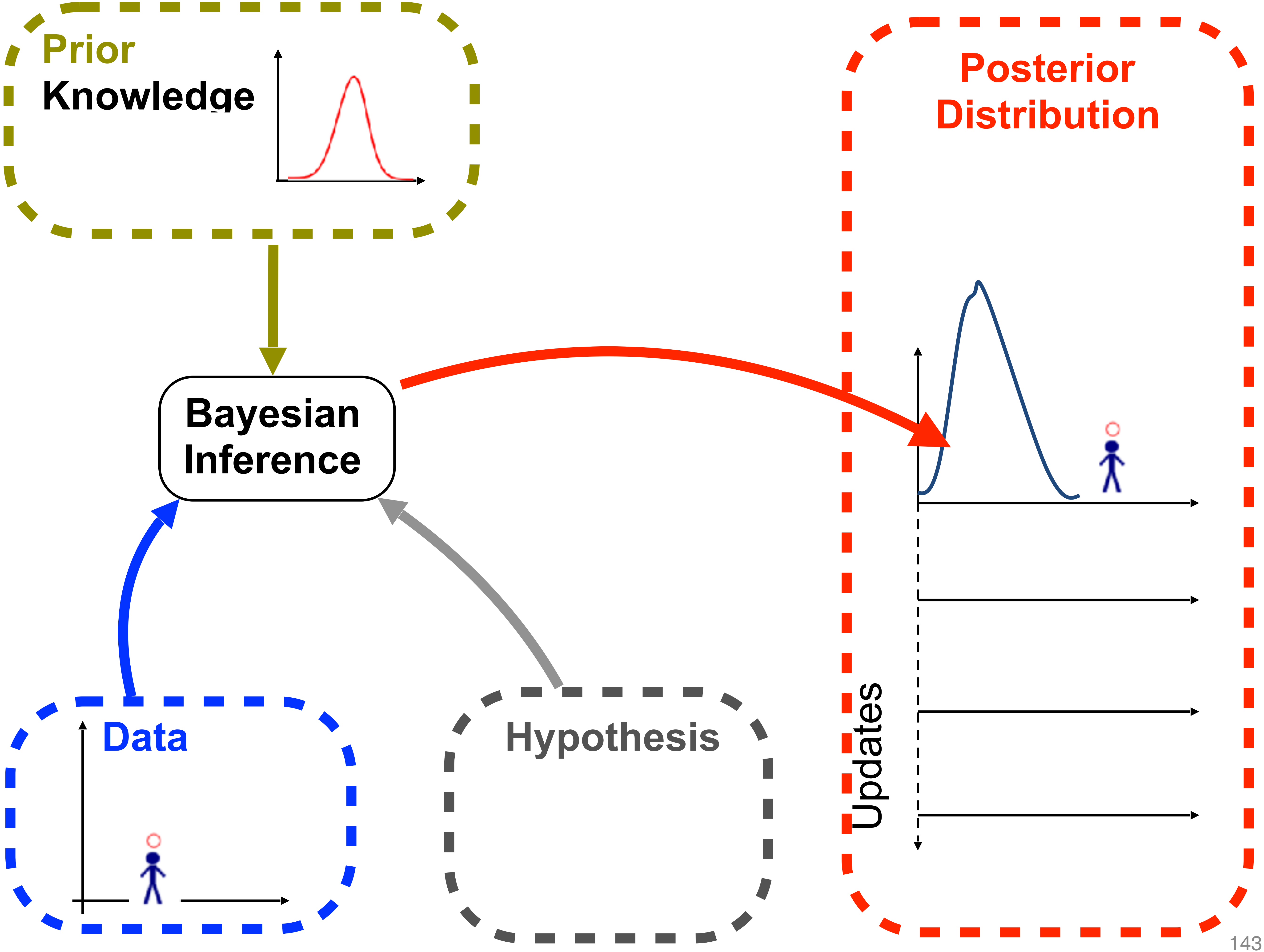
Prior Knowledge



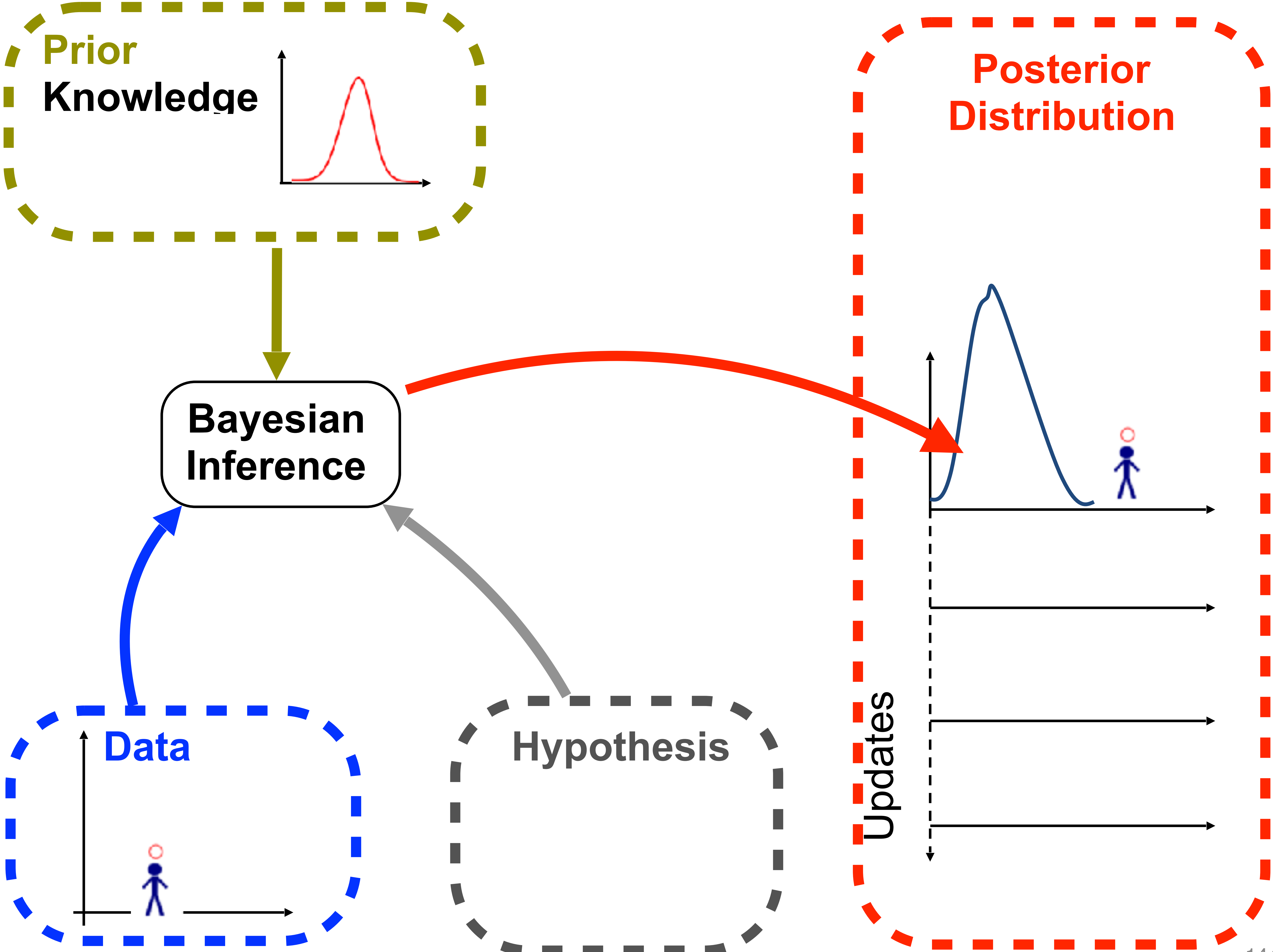
Data



Hypothesis



Prior
Knowledge
Bayesian
Inference
Posterior
Distribution
Data
Hypothesis
Updates


Prior
Knowledge
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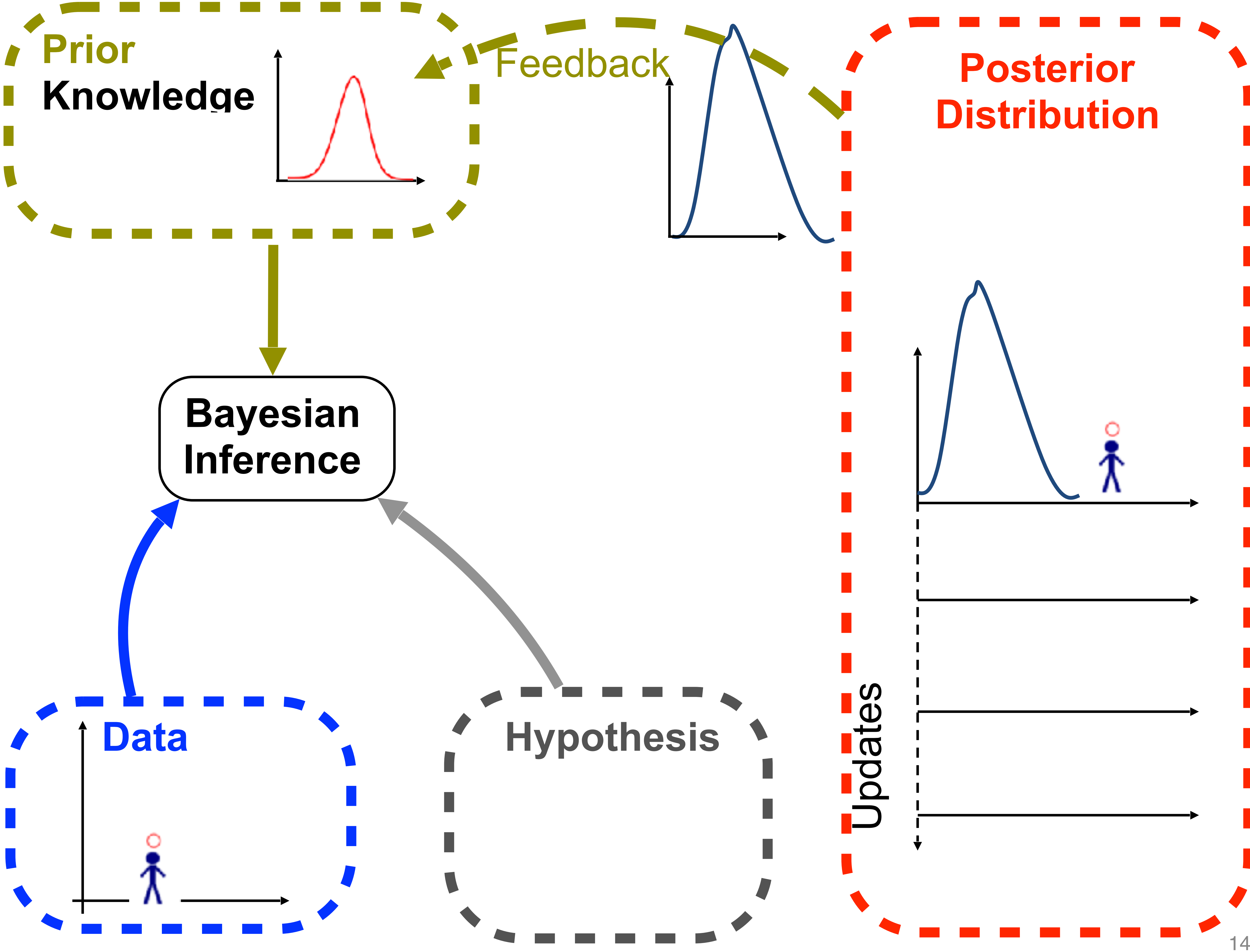
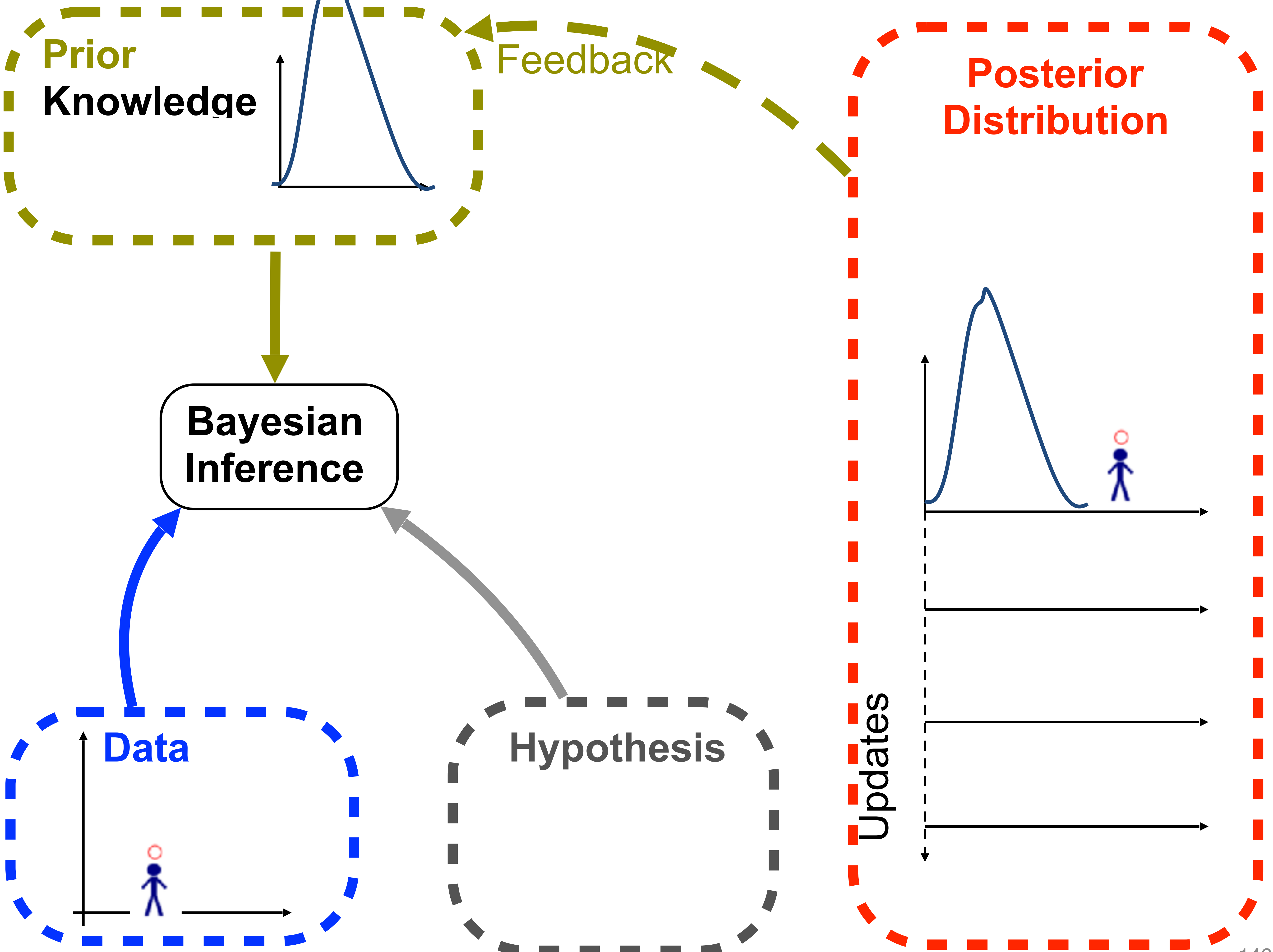
Posterior
Distribution
Data
Hypothesis
Updates


Prior
Knowledge
Feedback
Posterior
Distribution
Bayesian
Inference
Updates
Data
Hypothesis


Prior
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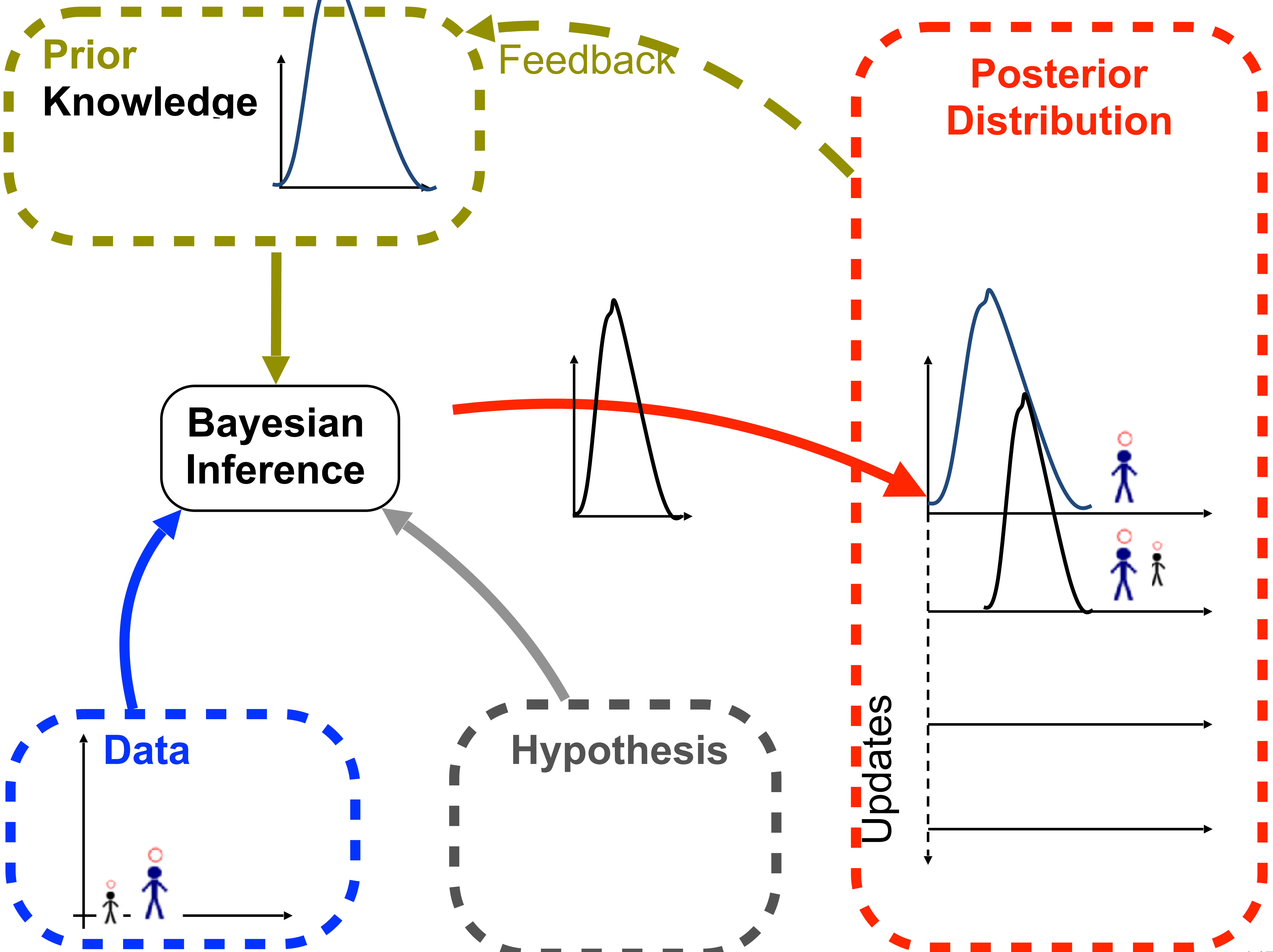
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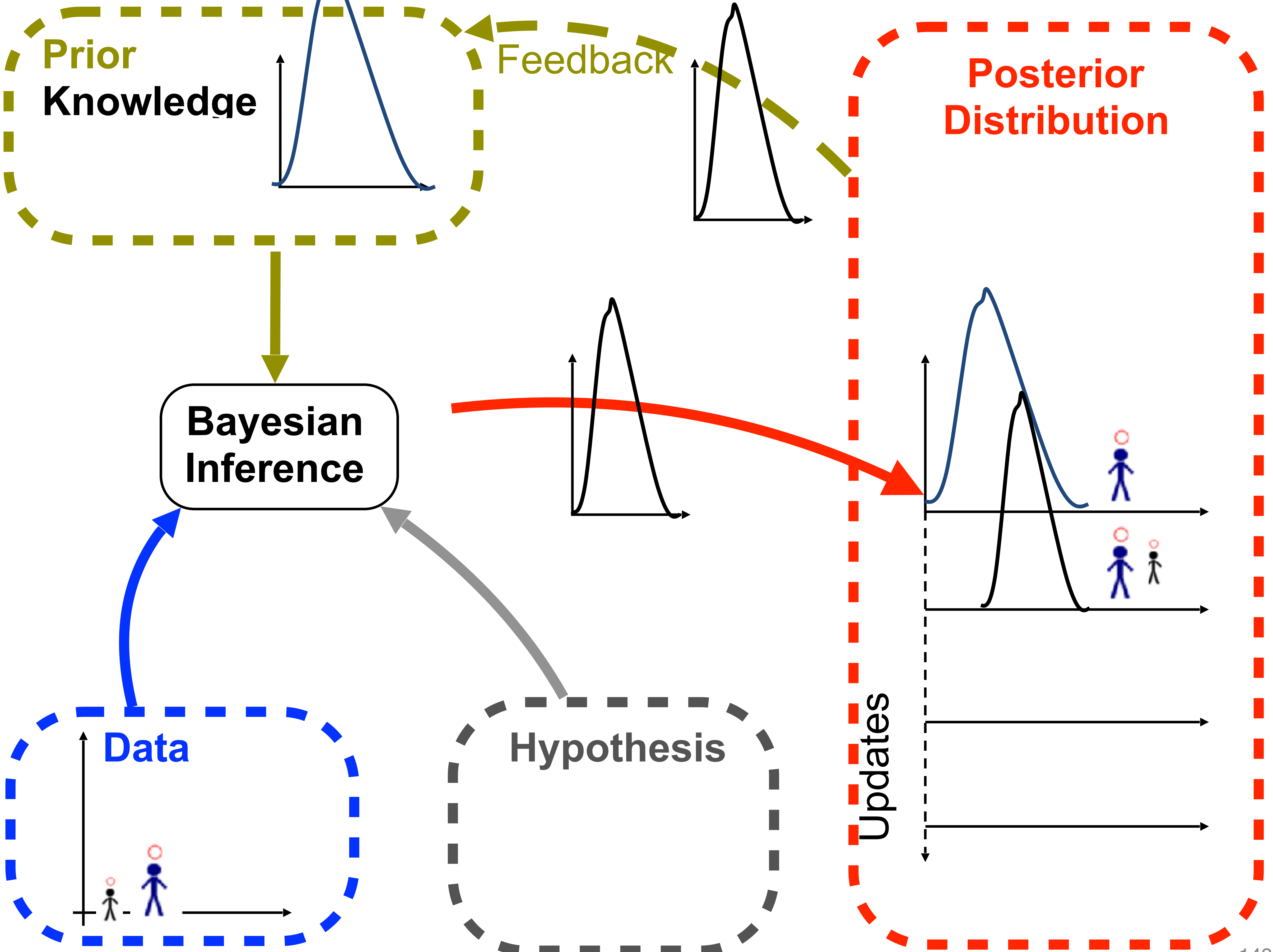
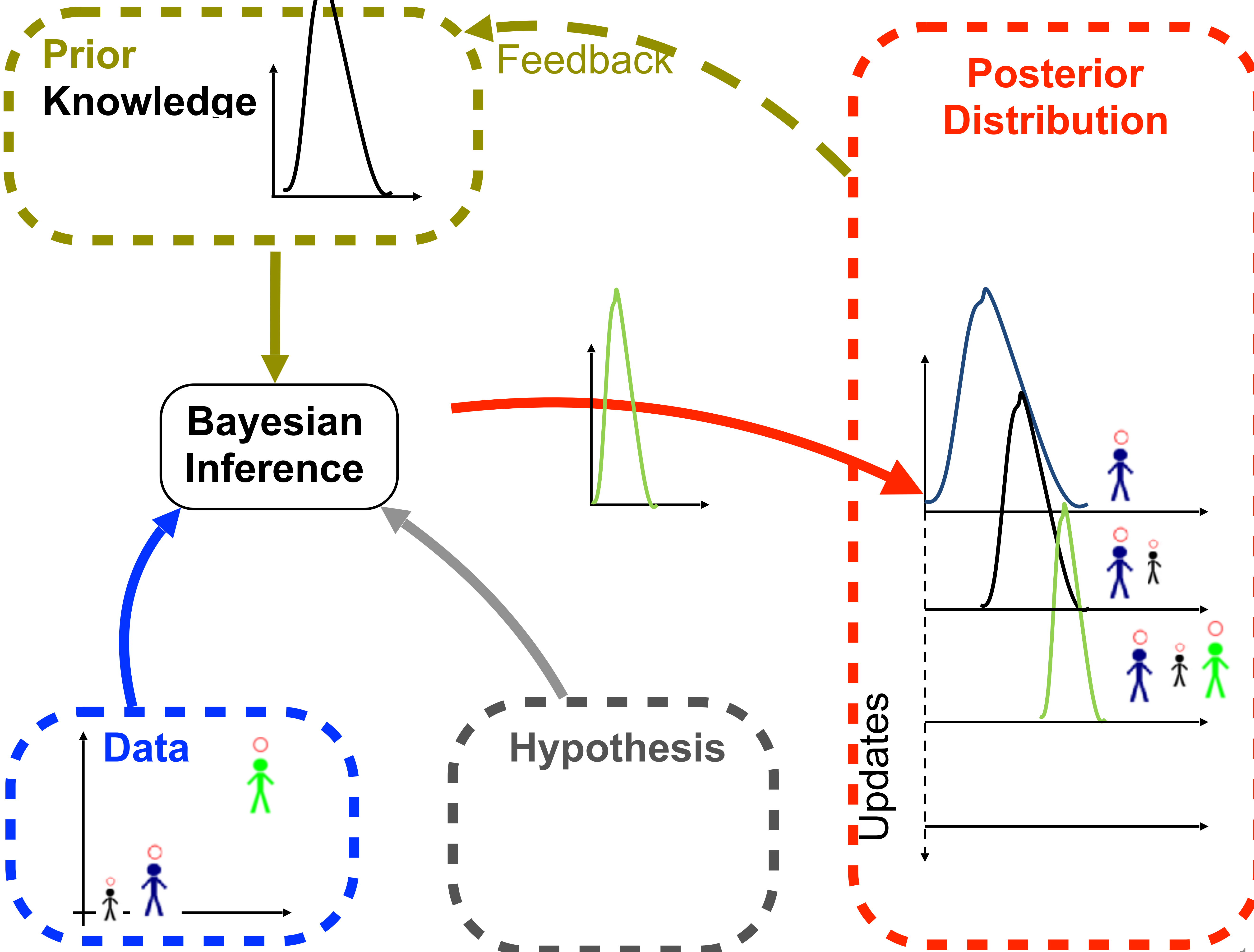
Hypothesis


Prior
Knowledge
Feedback
Posterior
Distribution
Bayesian
Inference
Updates
Data
Hypothesis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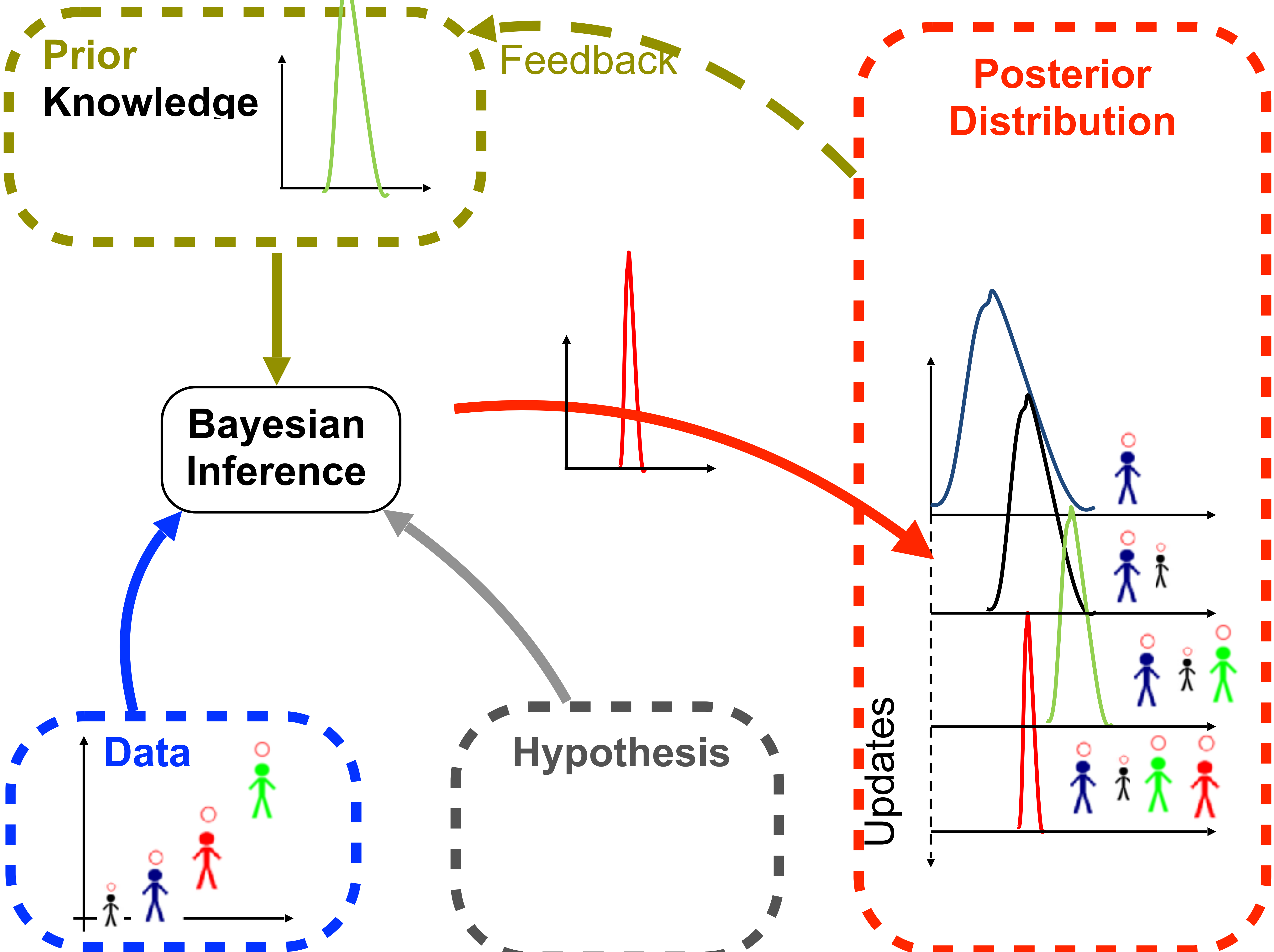
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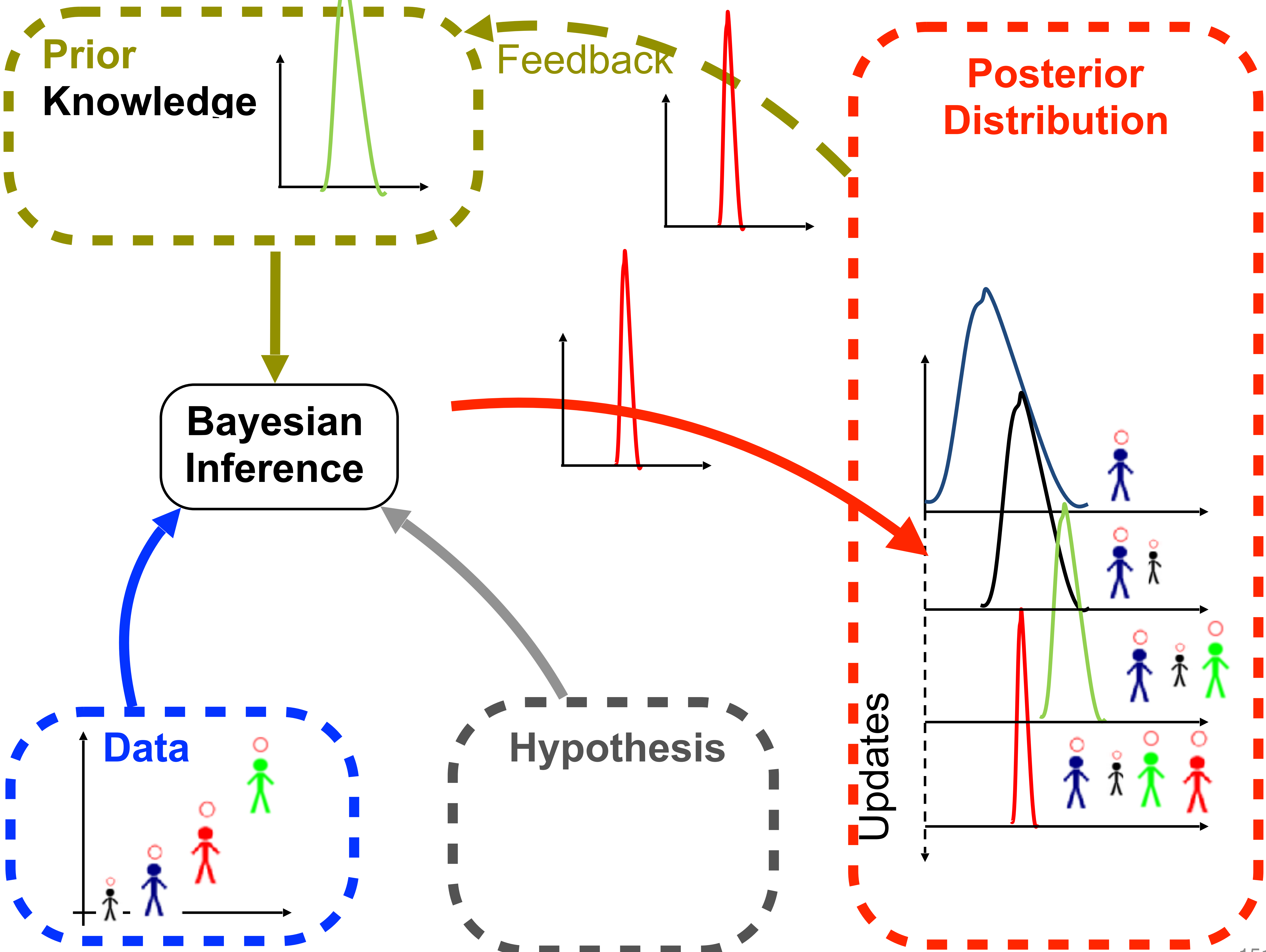
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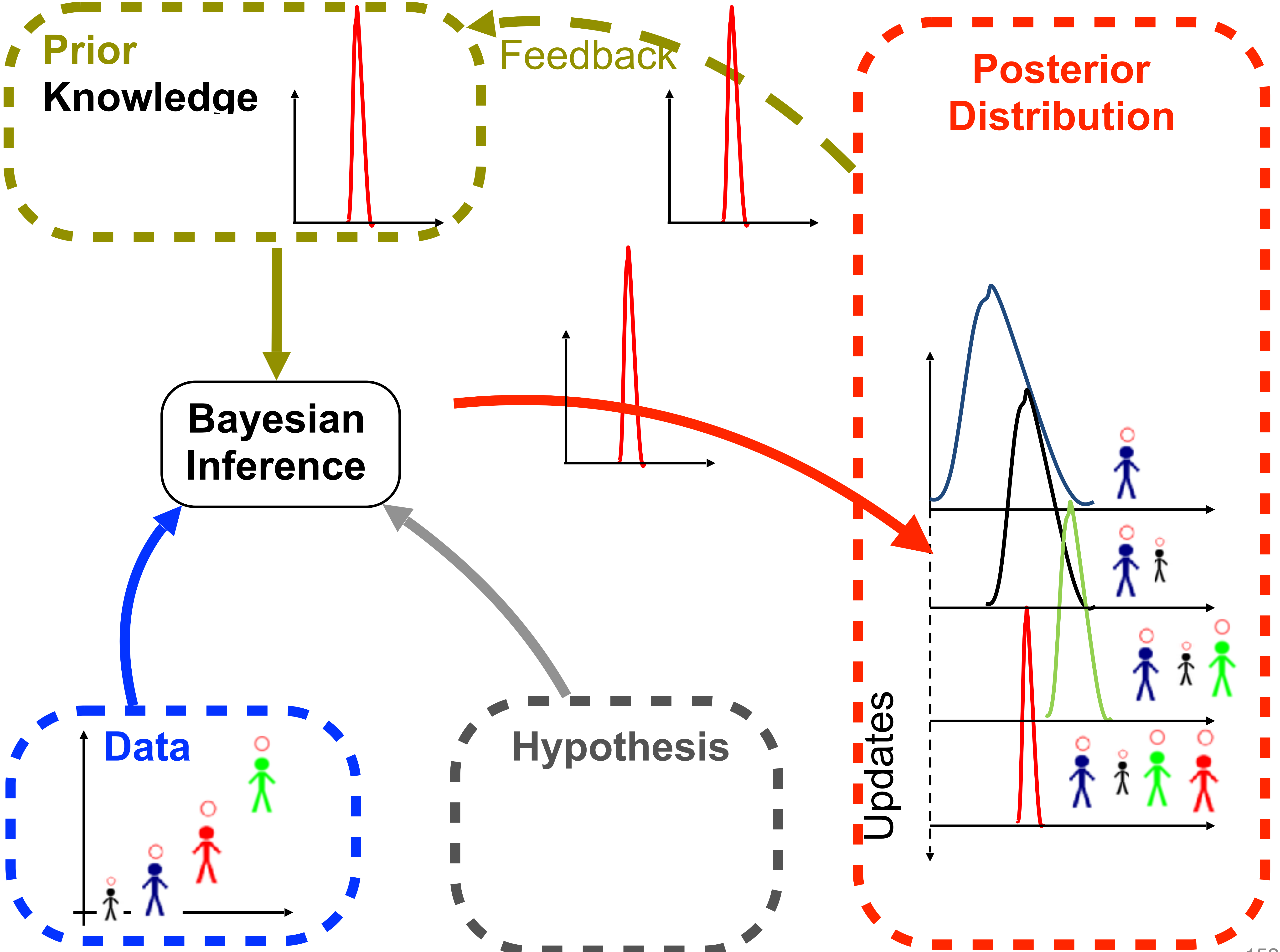
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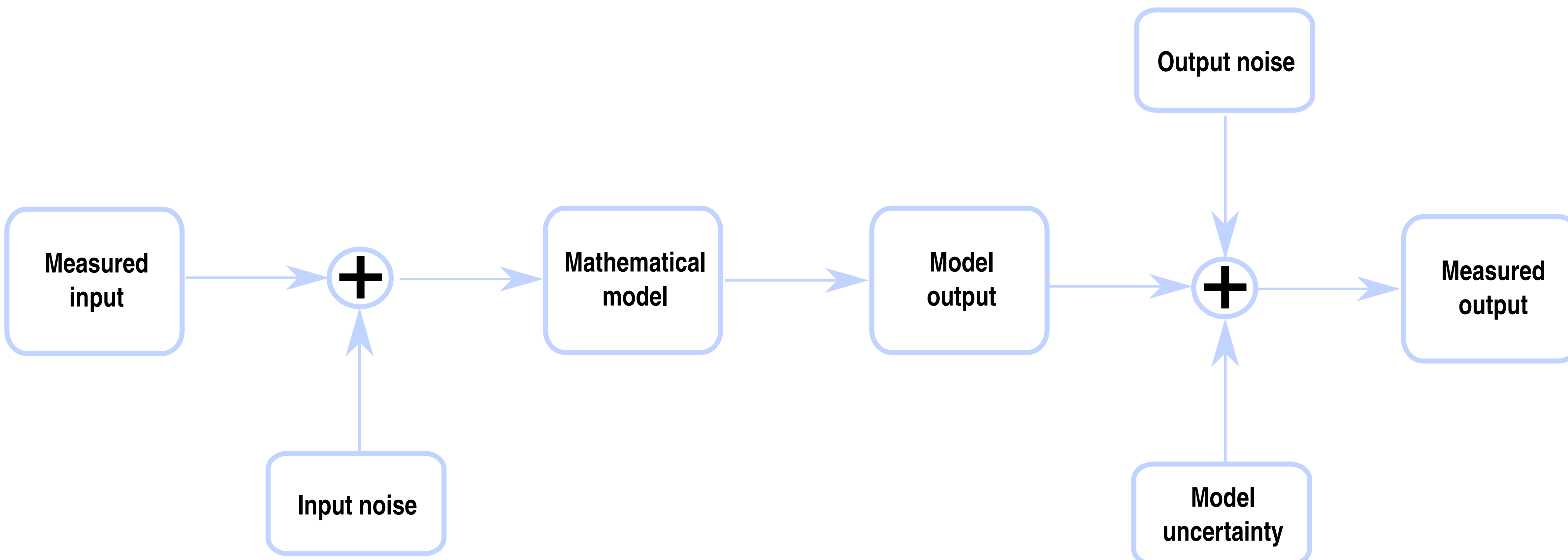
Uncertainties and errors in parameter identification



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