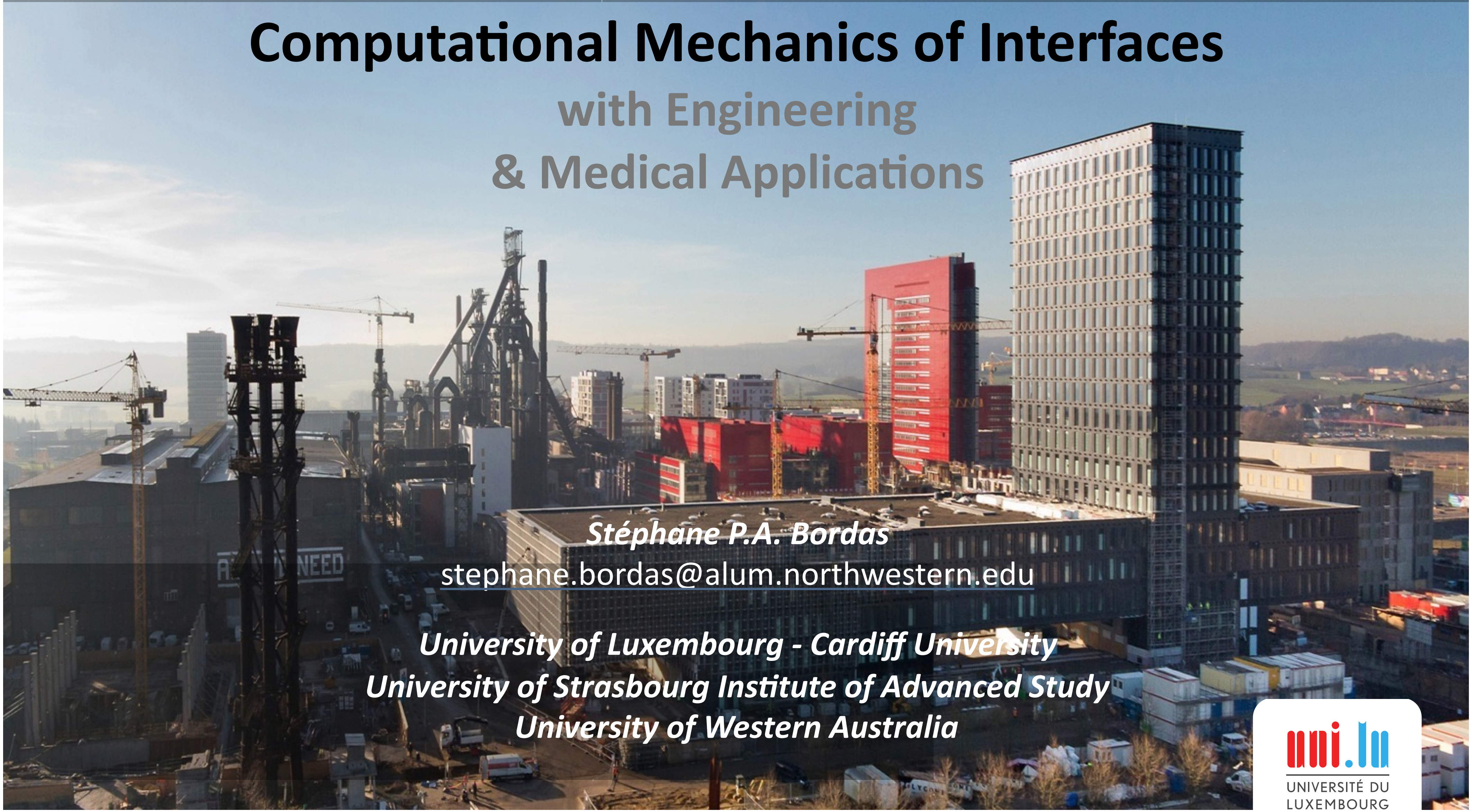
Computational Sciences Luxembourg
Department of Computational Engineering Sciences

Computed in Luxembourg



Computational Mechanics of Interfaces

with Engineering & Medical Applications

Stéphane P.A. Bordas
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University of Luxembourg - Cardiff University
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University of Western Australia

UNIVERSITÉ DU LUXEMBOURG

Outline

Part I. Computational approaches for industrial-scale fracture mechanics simulations and surgical simulation

- Adaptive partition of unity enrichment
- (Multi-scale fracture)
- Adaptivity in IGA through Geometry-Independent Field approximaTion

Part II. Model Selection and Uncertainties in surgical simulation (quick introduction)

Department of Computational Engineering Sciences

Legato Team

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

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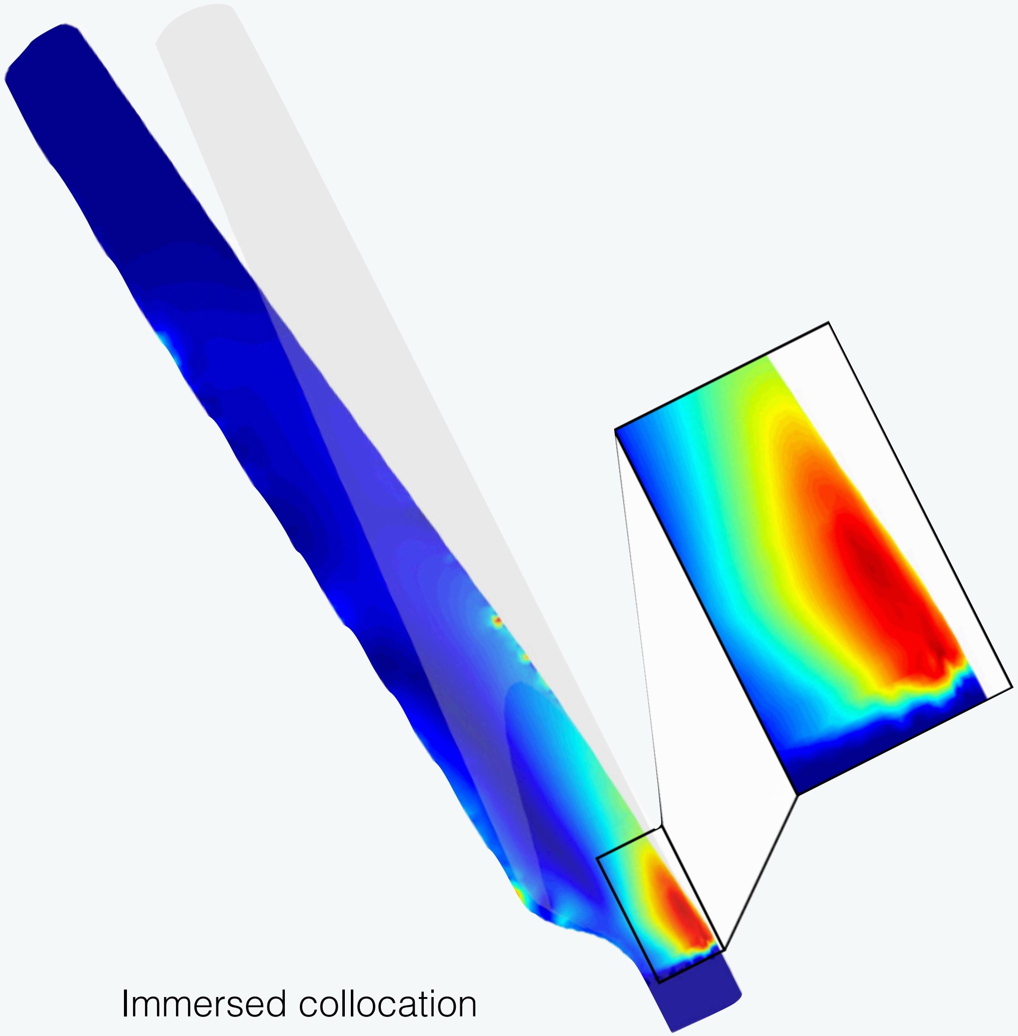
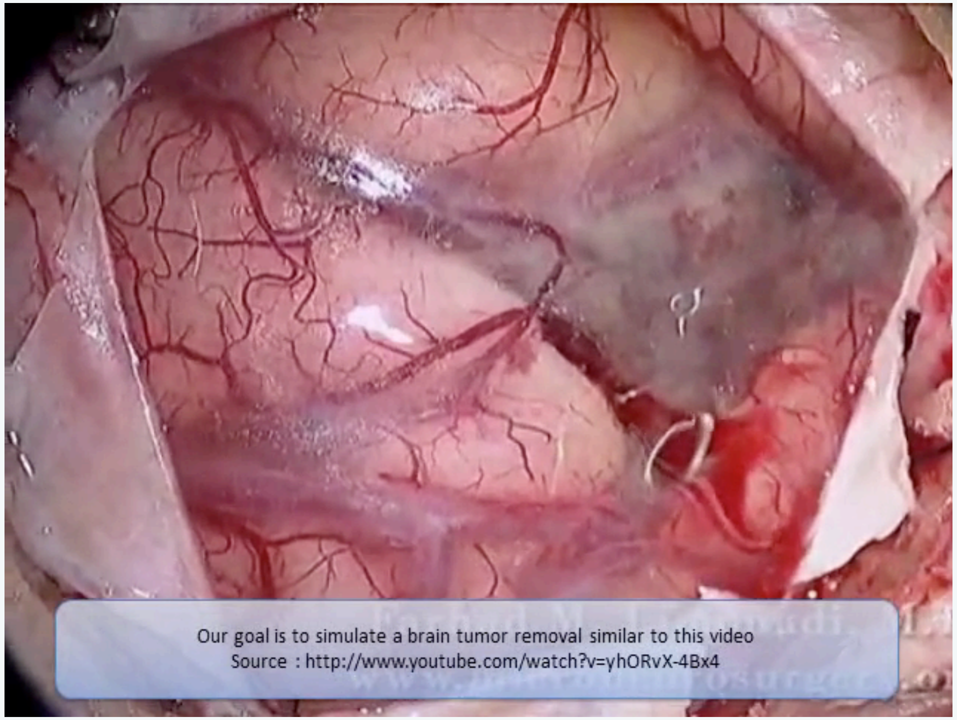


Immersed collocation



Real-time cutting, MEDIA2014, IEEE2017

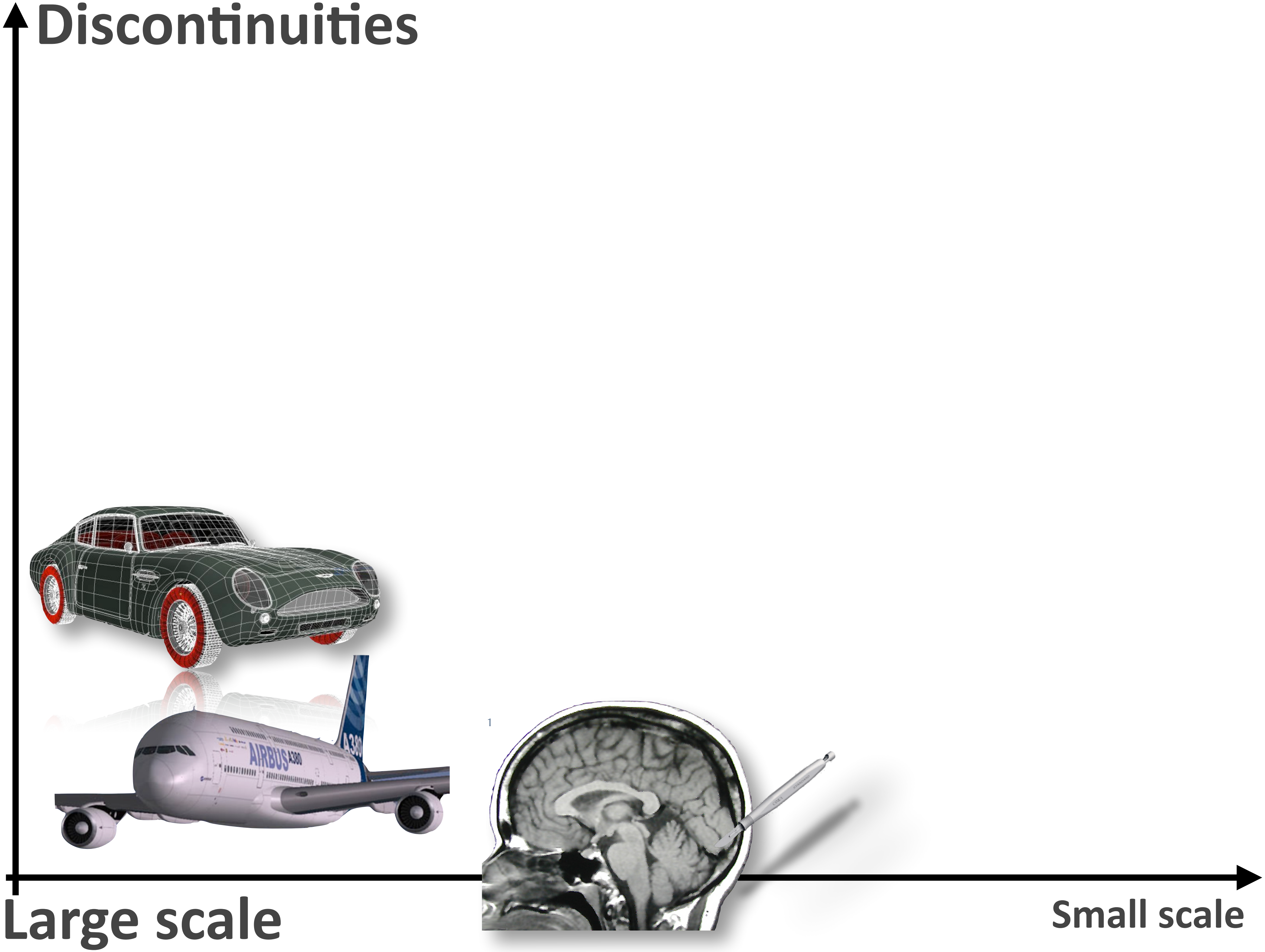
Interface problems are frequent in nature and engineering

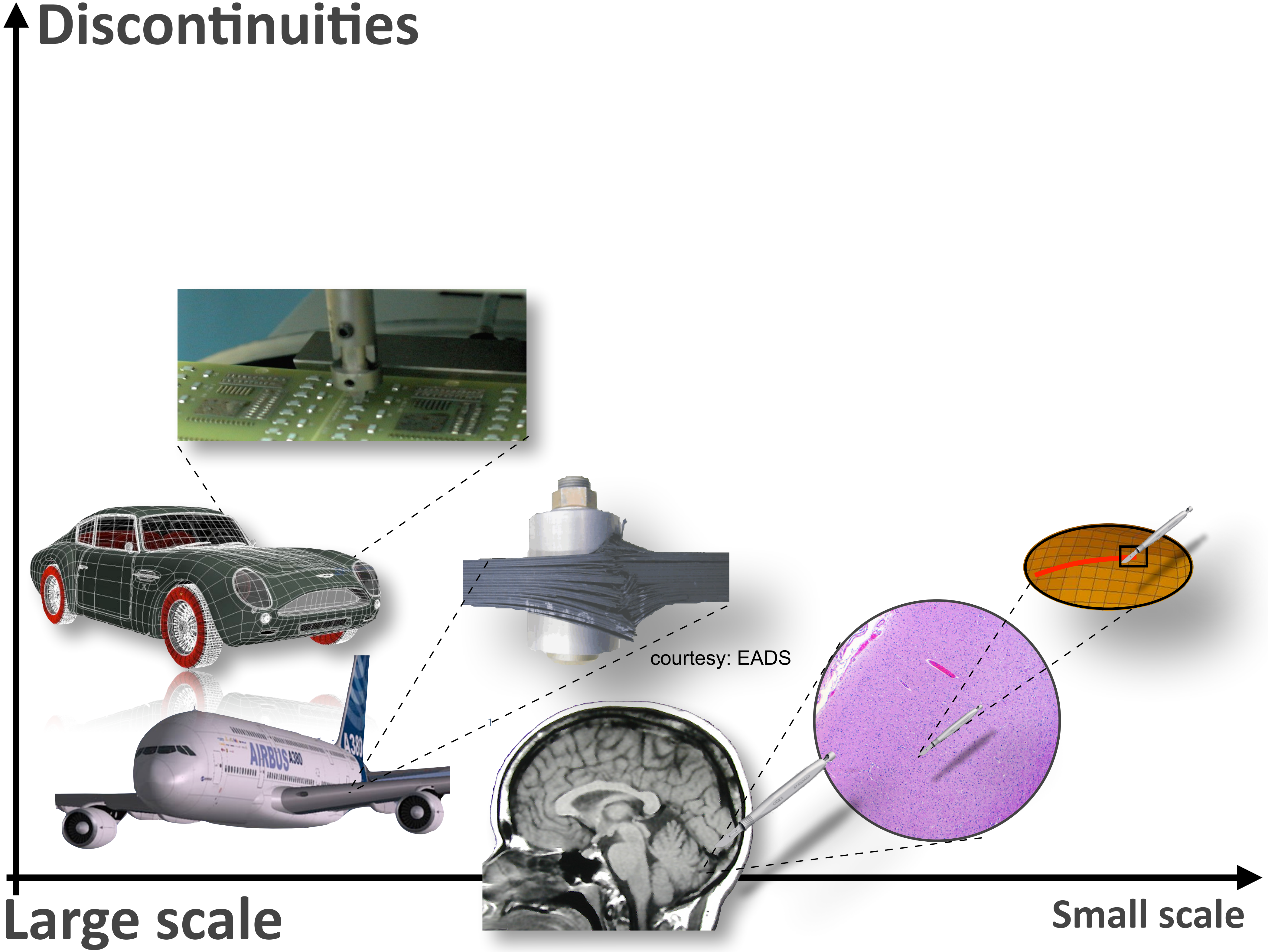
Discontinuities

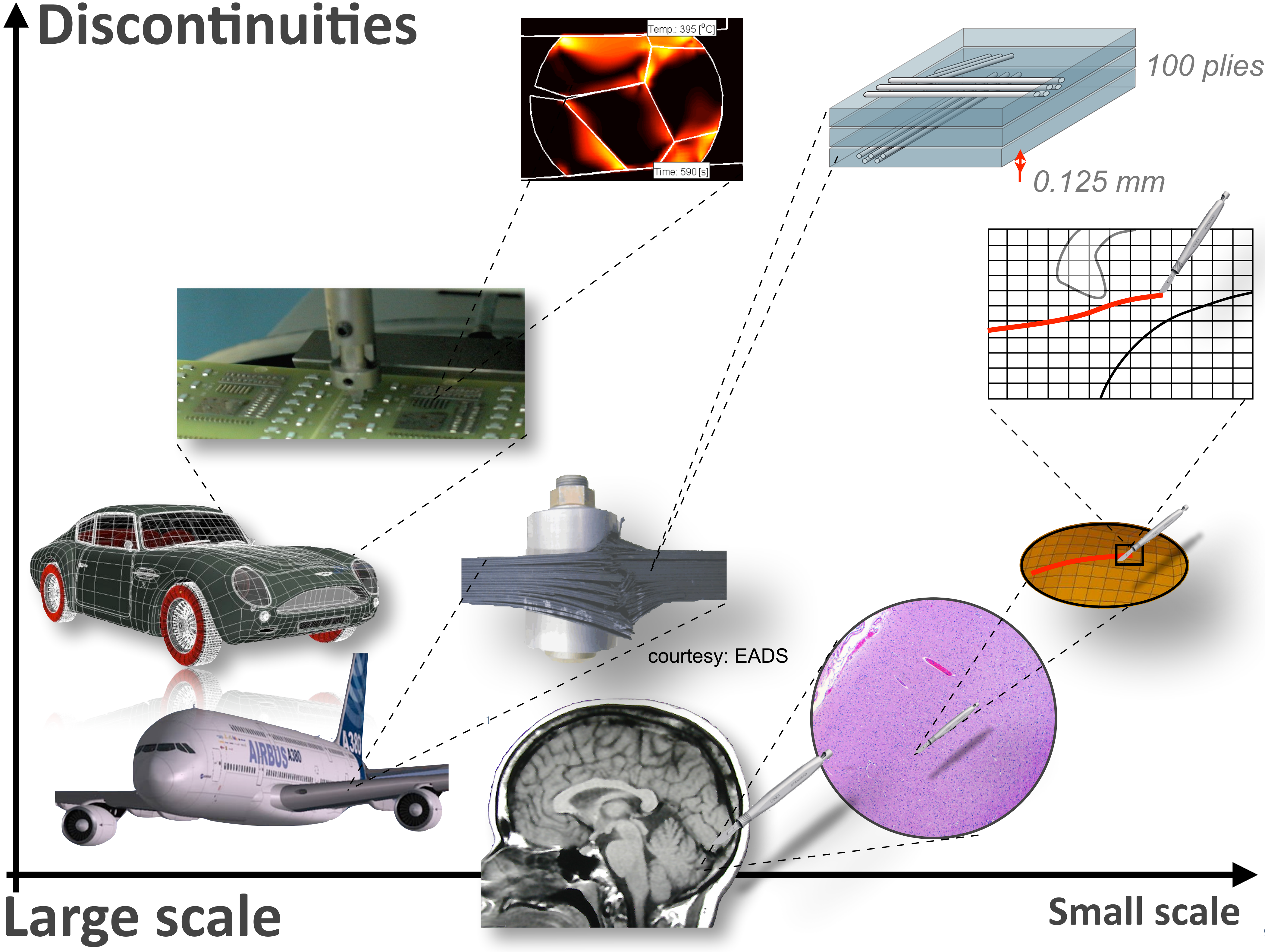
1

Large scale

Small scale


Discontinuities
AIRBUS A380
A380
Large scale
Small scale

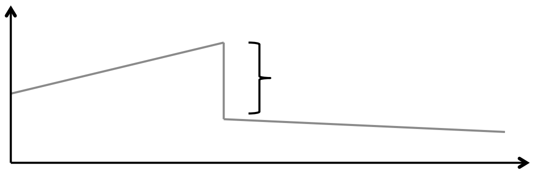

Discontinuities
courtesy: EADS
Large scale
Small scale


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

Classification of discontinuities

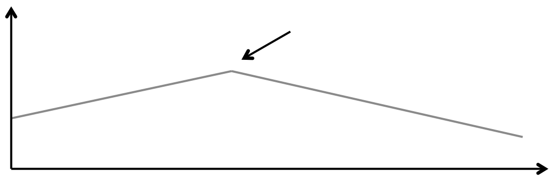
Strong discontinuities

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



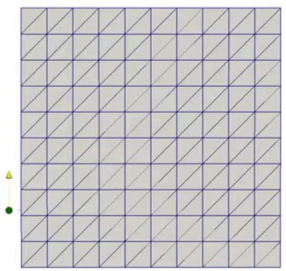
Weak discontinuities

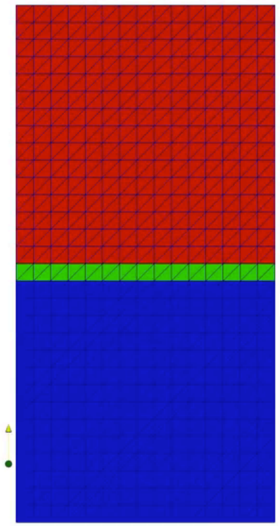
- The first derivative of the solution is discontinuous, e.g. discontinuities in the strain field through a material interface.

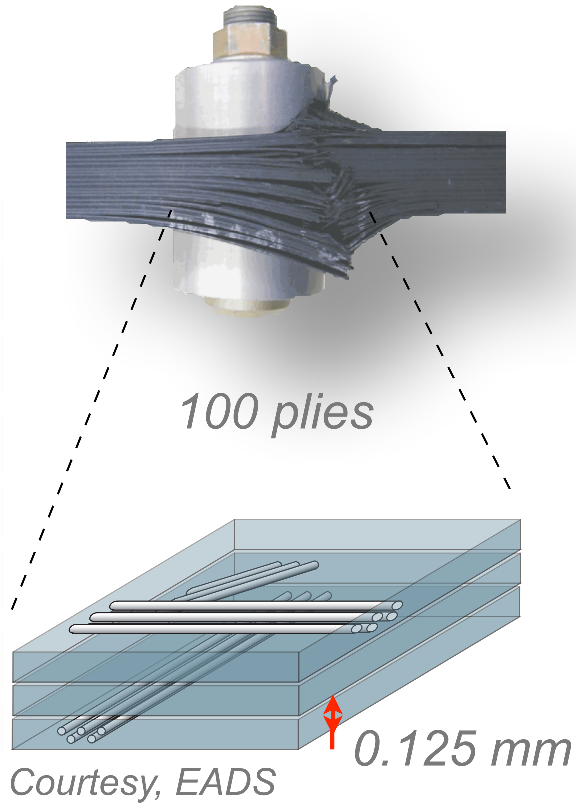


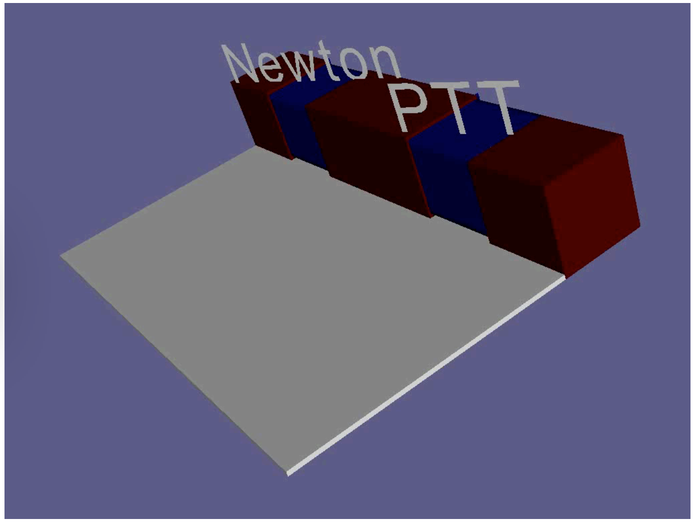
Interfaces in practical engineering simulations

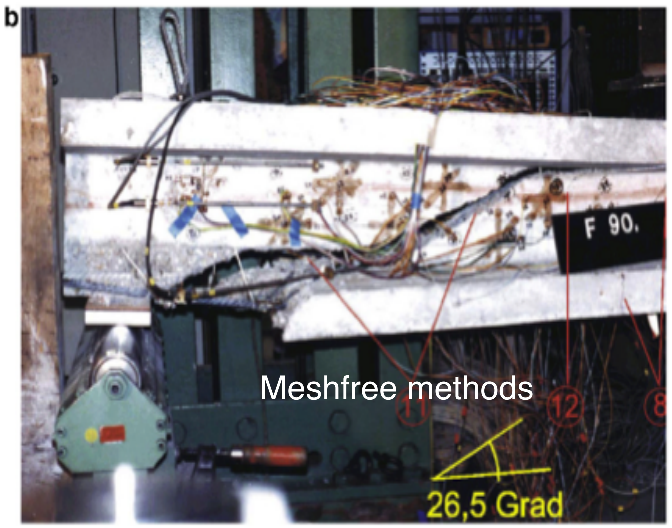
Interfaces between phases

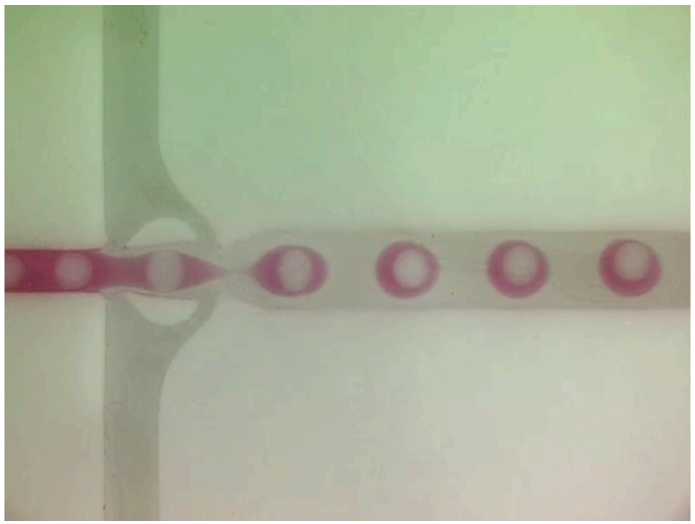






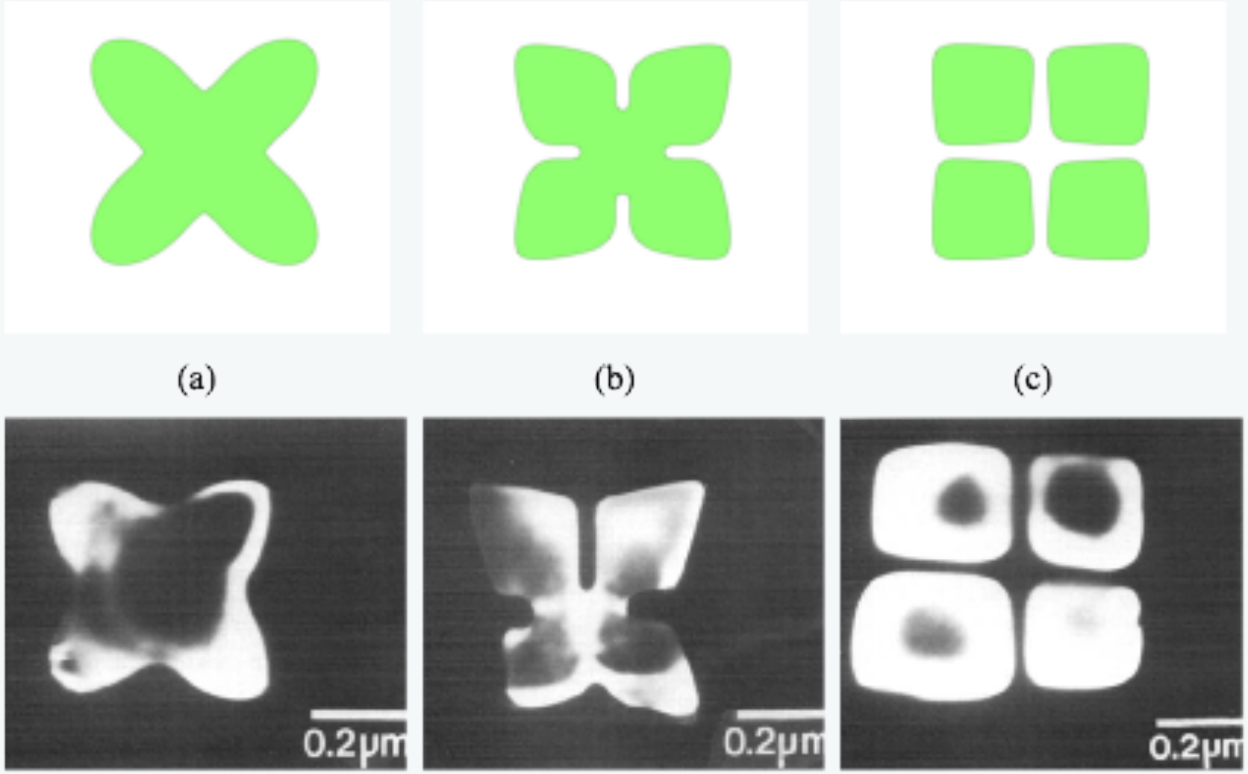






CMECH 2007, EFM2008 CAS 2009, with Timon Rabczuk and Goangseup Zi

Equilibrium of nano-inhomogeneities



(a) (b) (c)

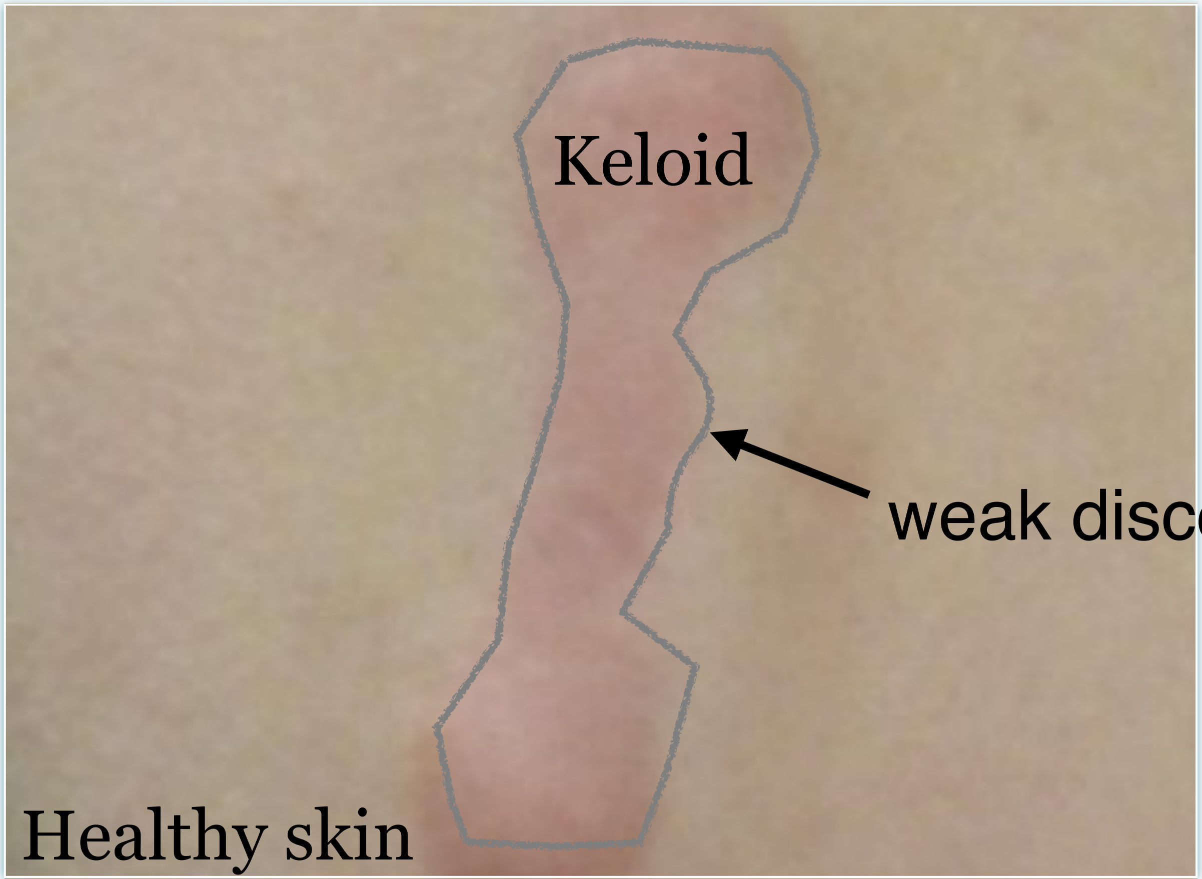
(d) (e) (f)

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

Keloids

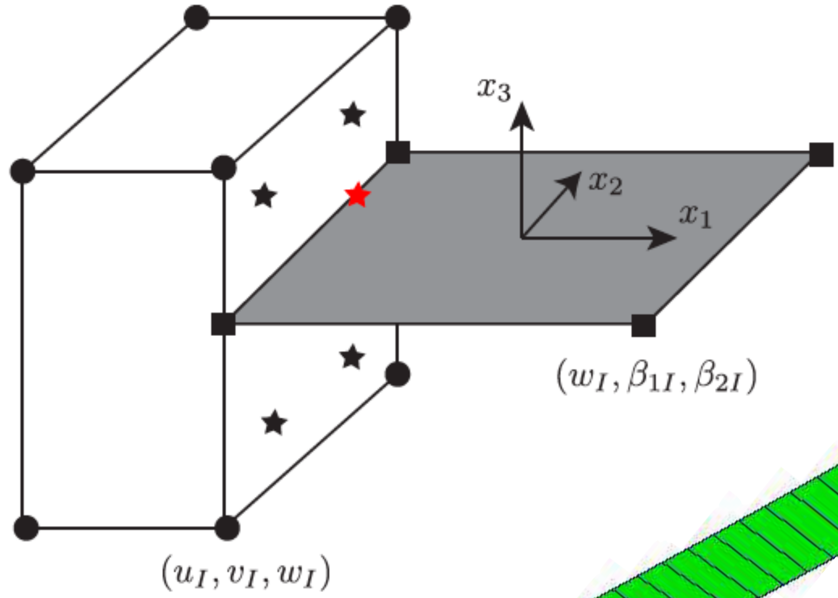
Keloids

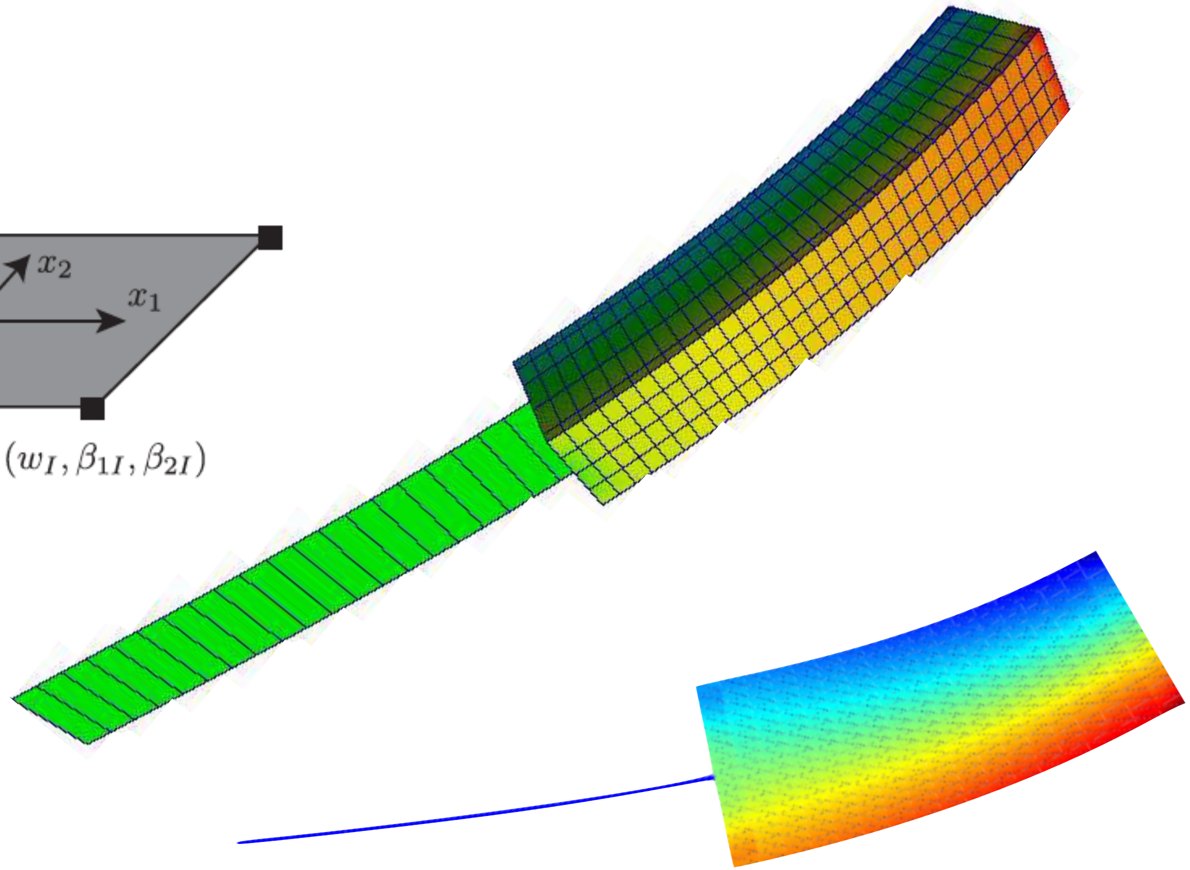
Keloids



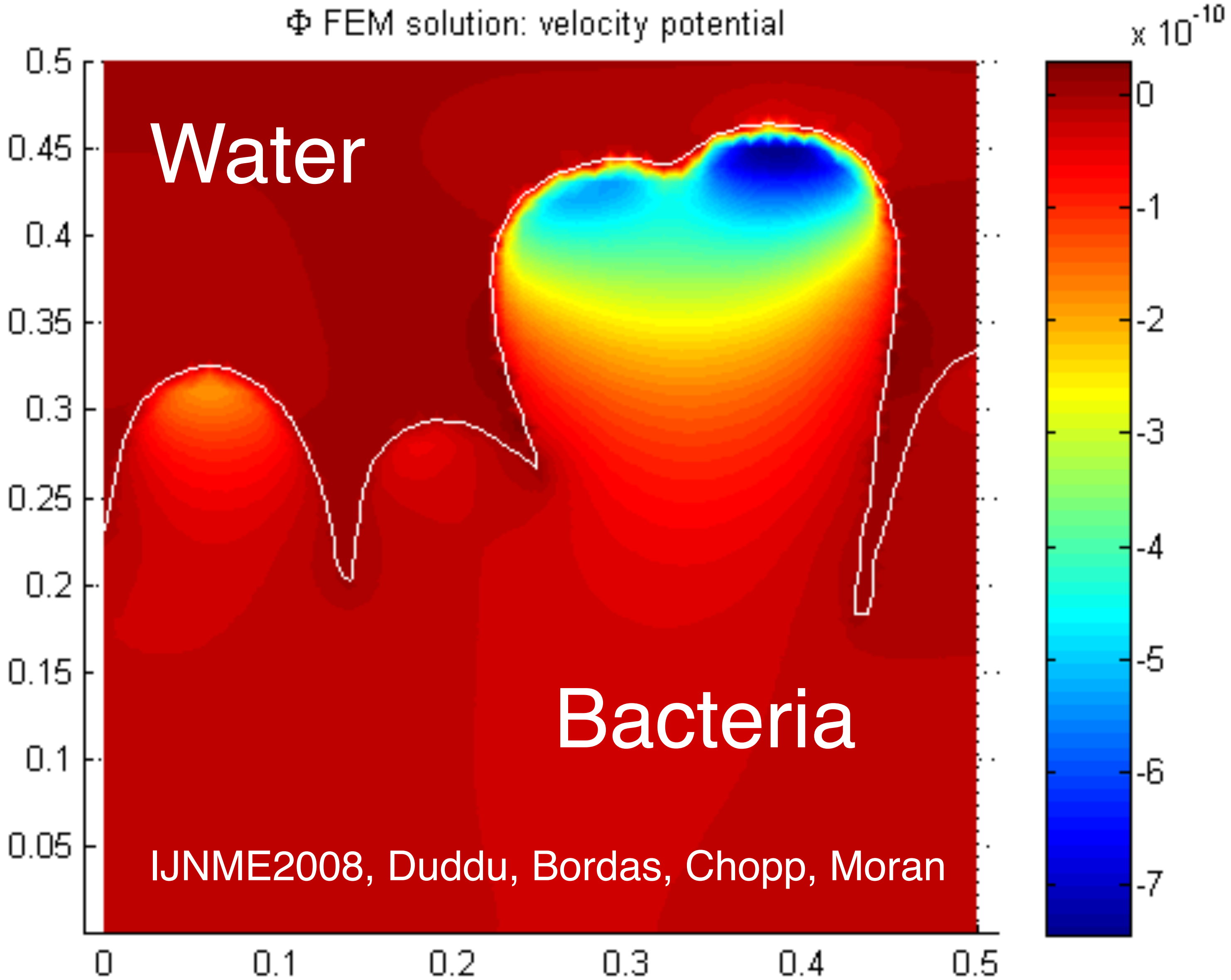
weak discontinuity

Example: interfaces between different kinematics





Example: Microbial biofilms



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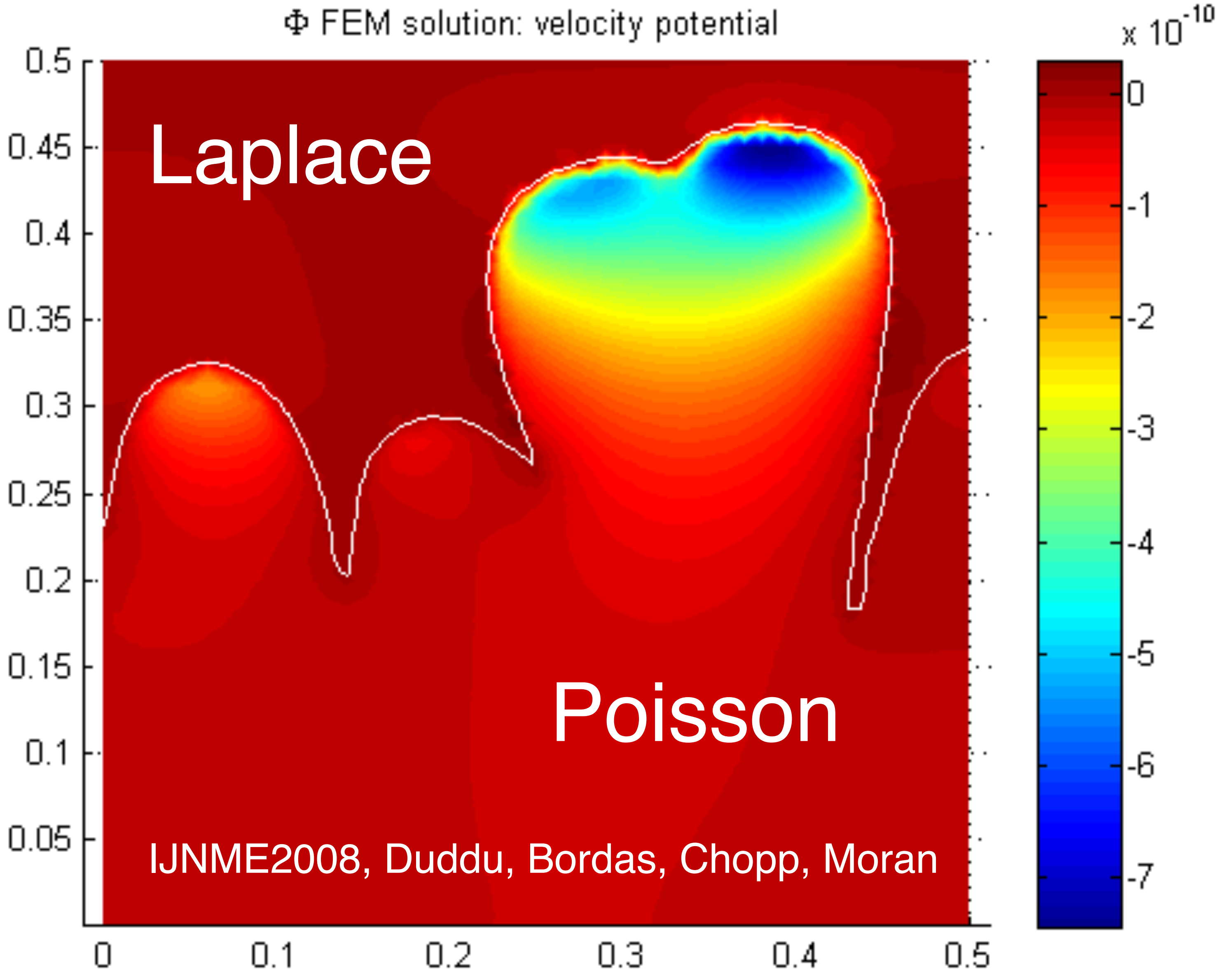
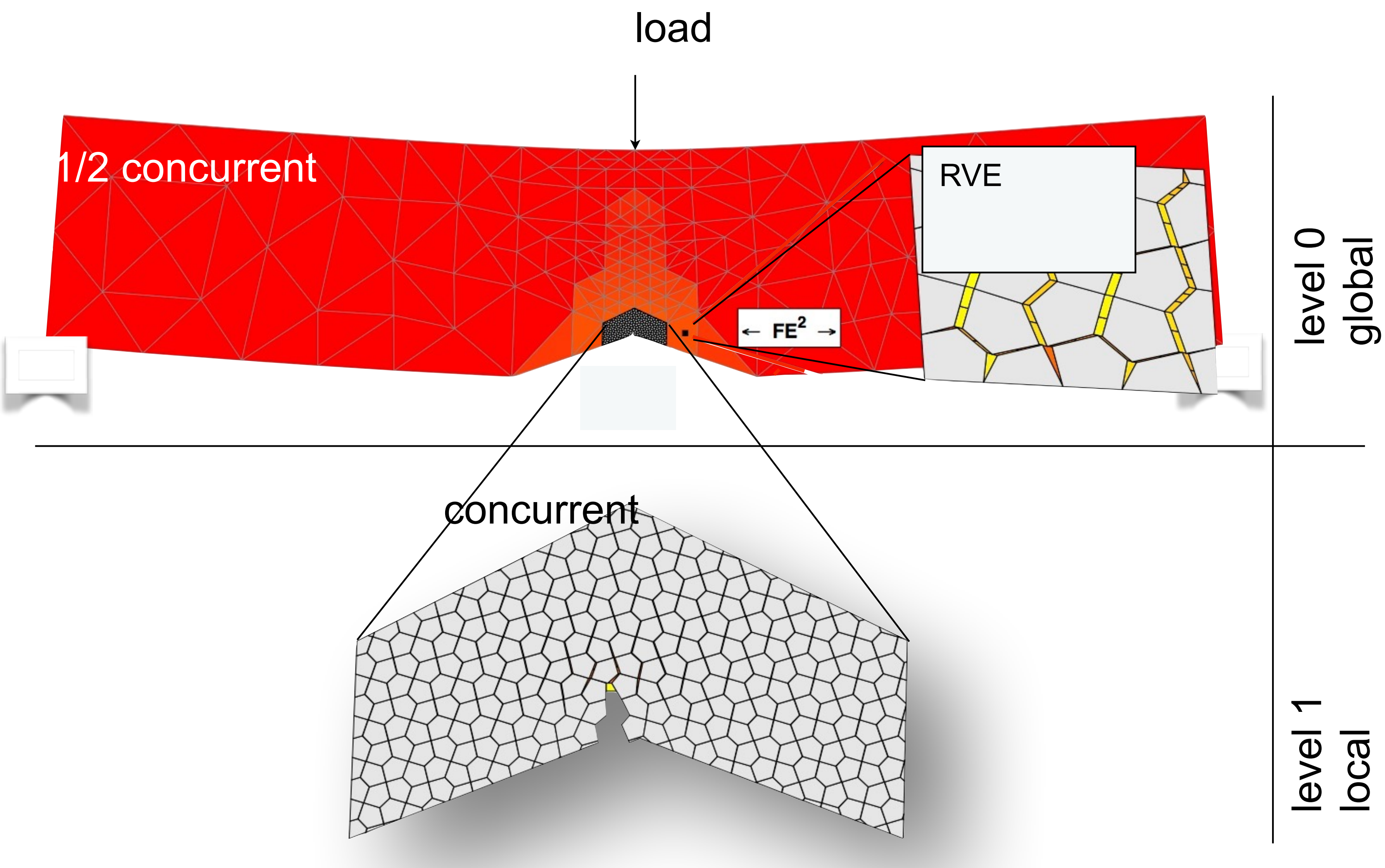
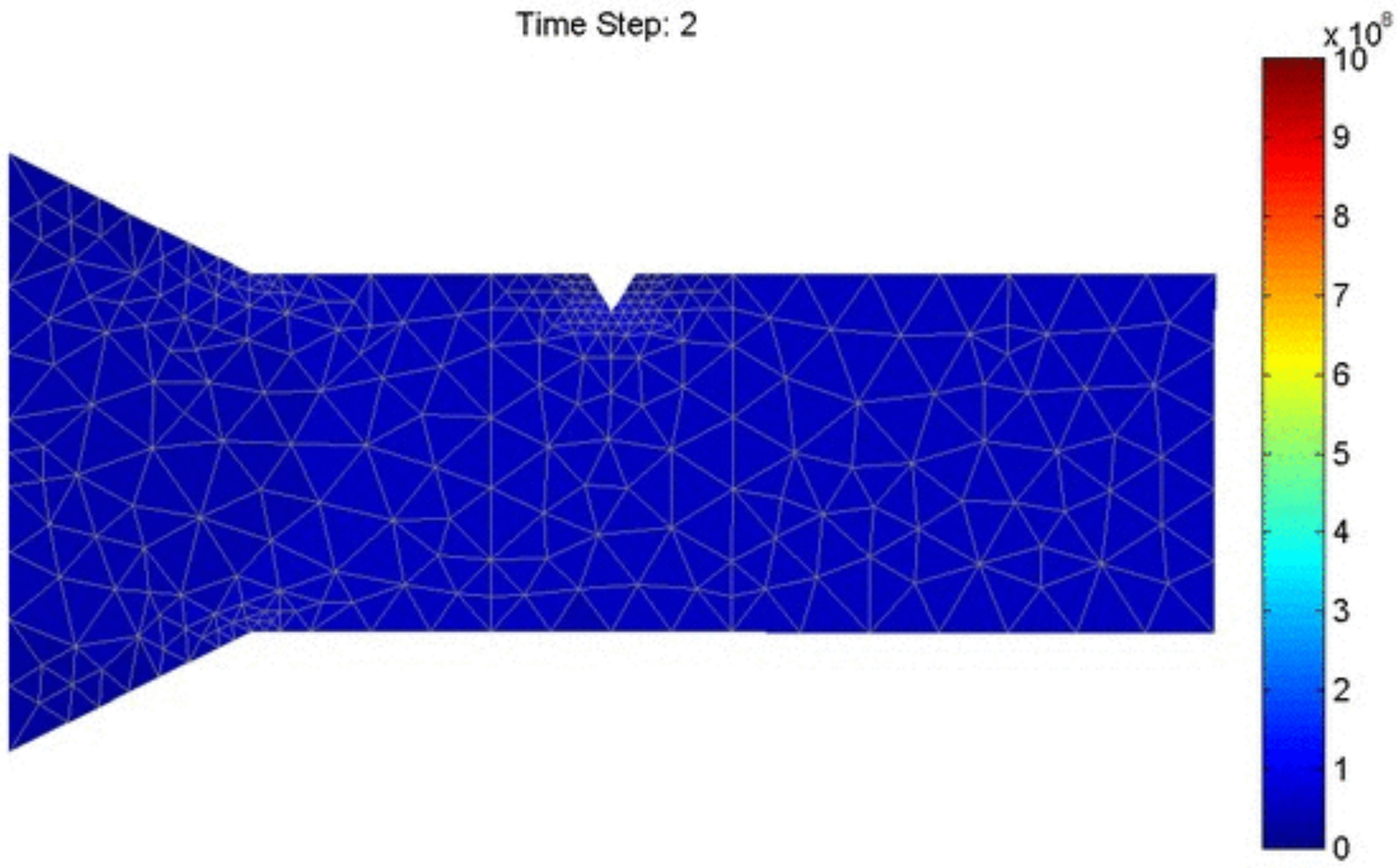


Example: Micro-continuum interfaces



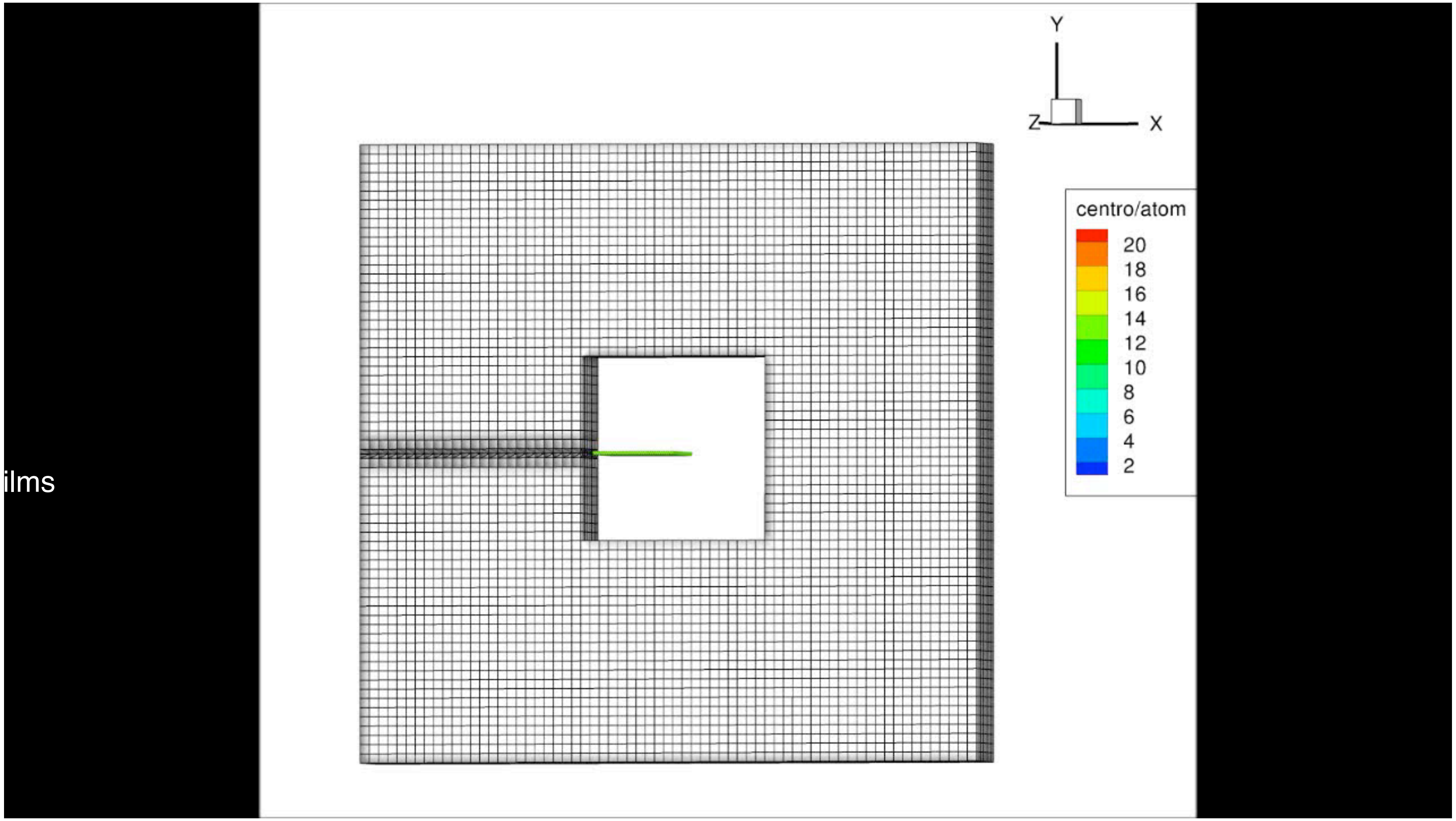
PhilMag15, Akbari
CMAME13,CMECH16, Goury
NMPDES13,CMAME15, Chi

Example: Micro-continuum interfaces

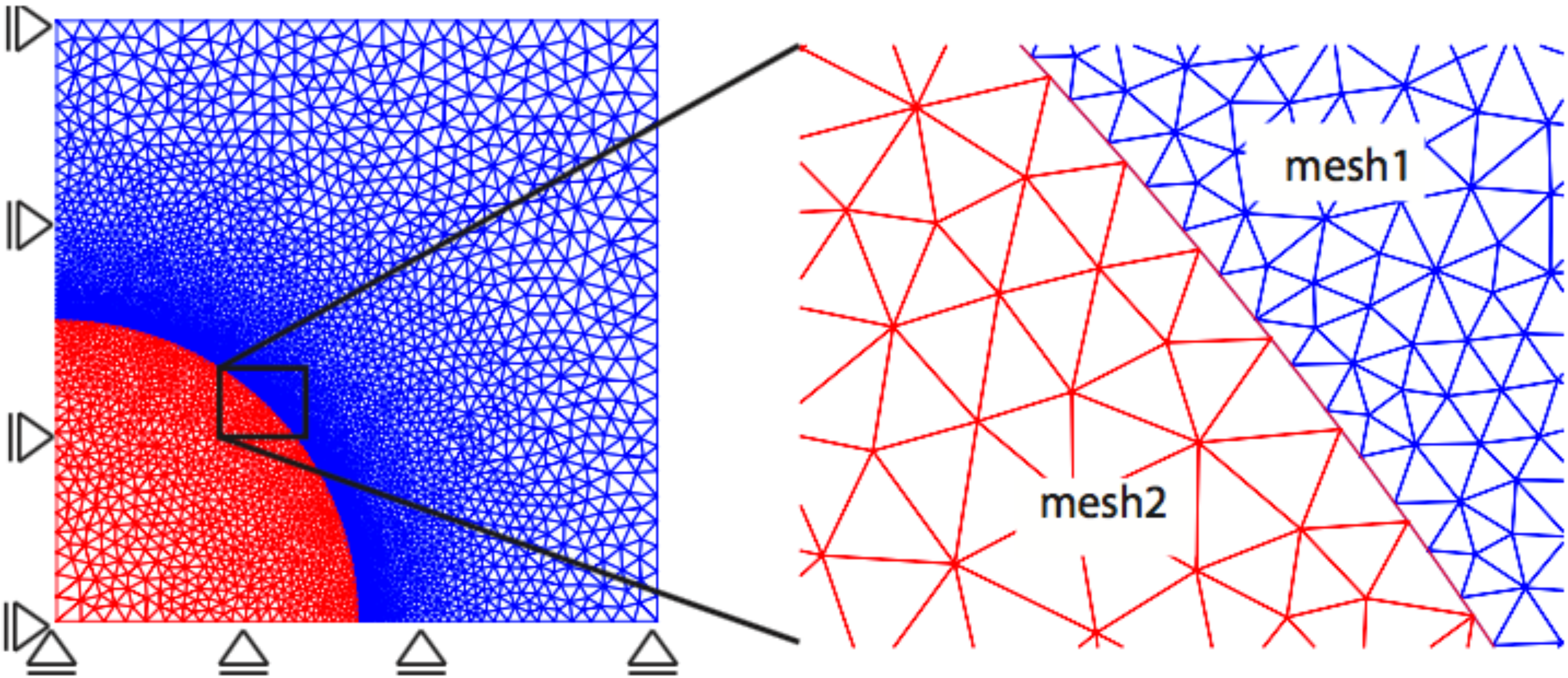


Example: Continuum molecular dynamics coupling

CMECH14, IJMSE13 Talebi

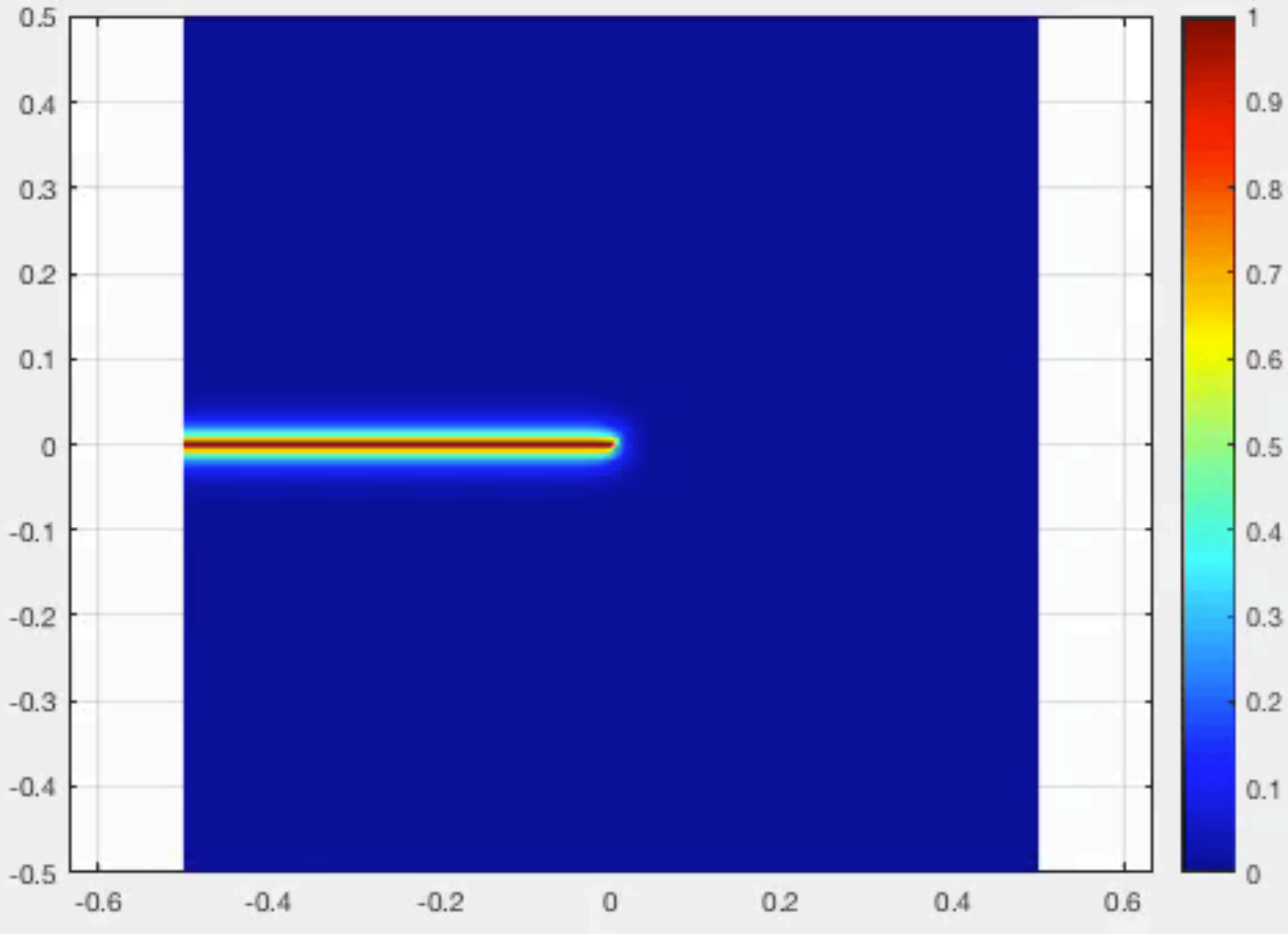


Example: non-matching meshes/discretisation interfaces



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 are also interfaces



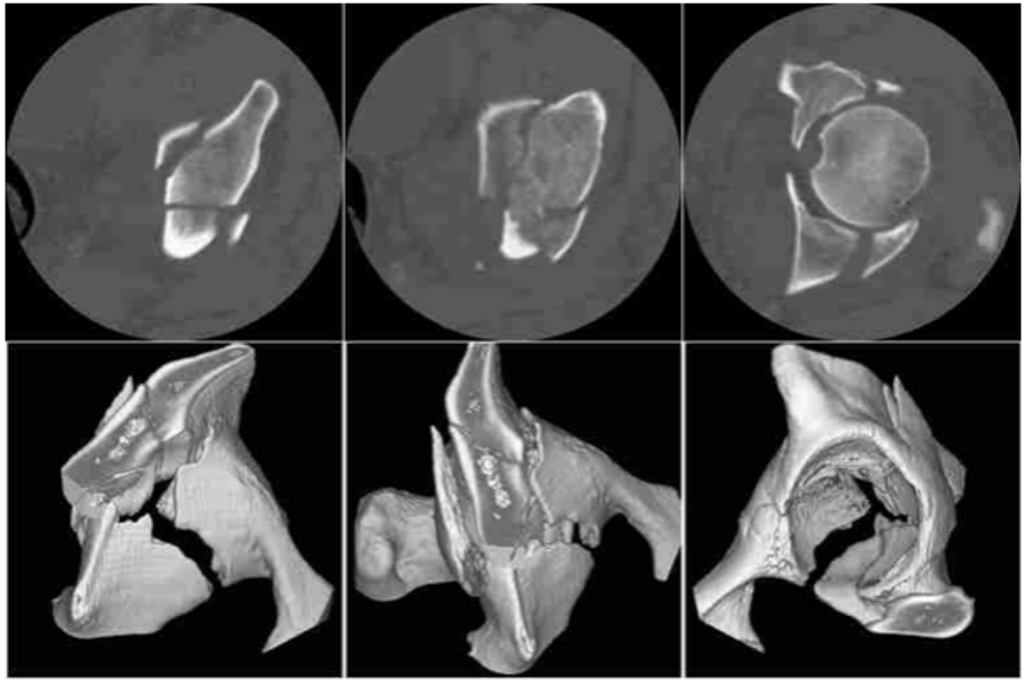
2017 Nguyen-Vinh Phu

Shuttle crash, 2003

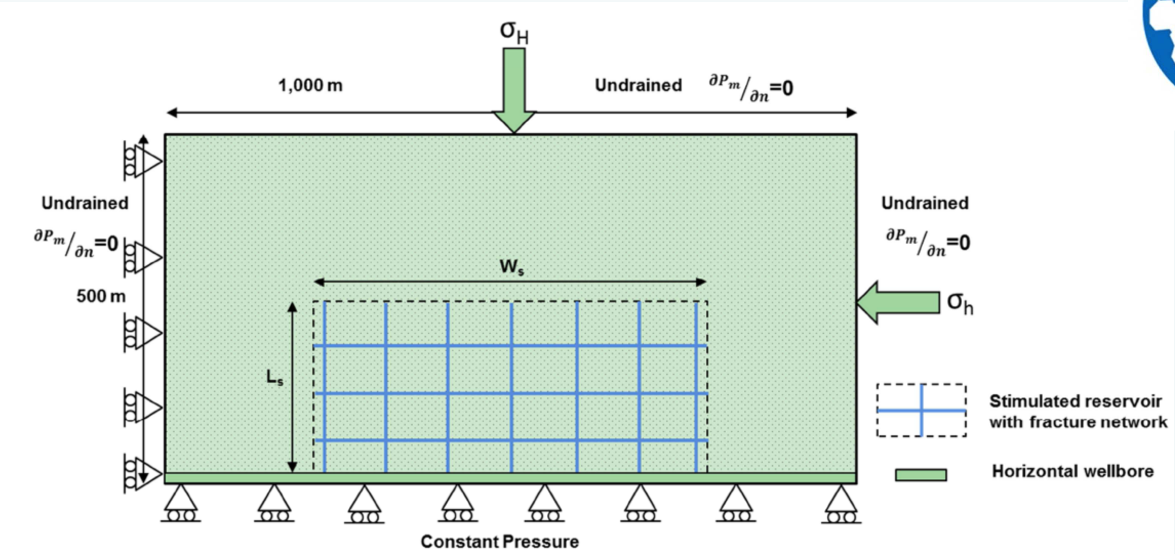
Landslide, Colorado

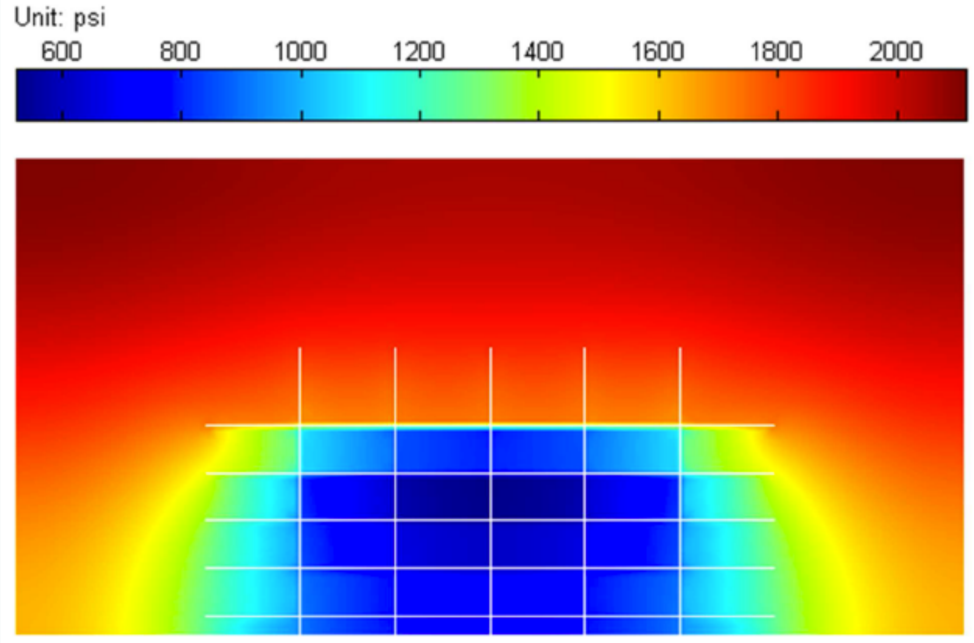
Taiwan earthquake, 2003

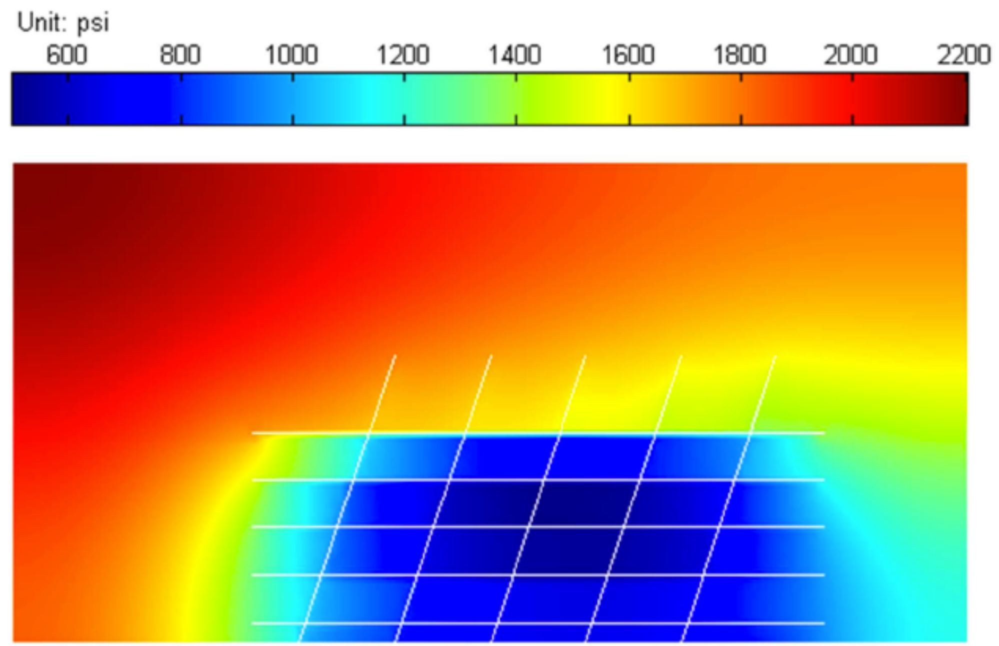
Fragmentation of concrete

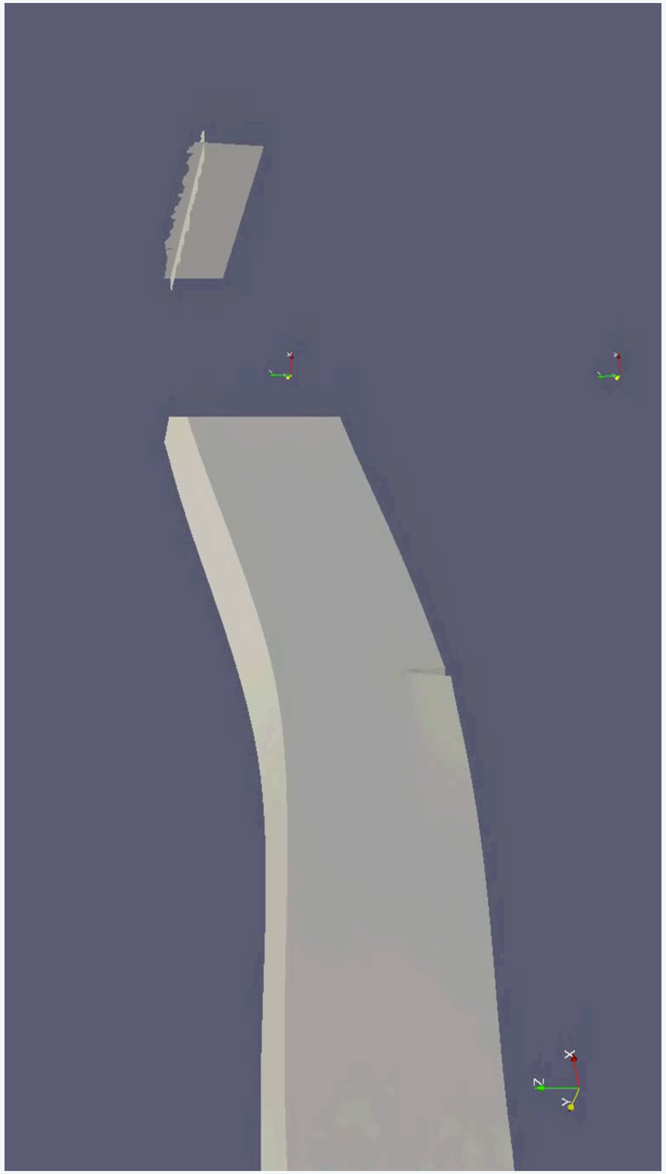
Oil extraction from shale -

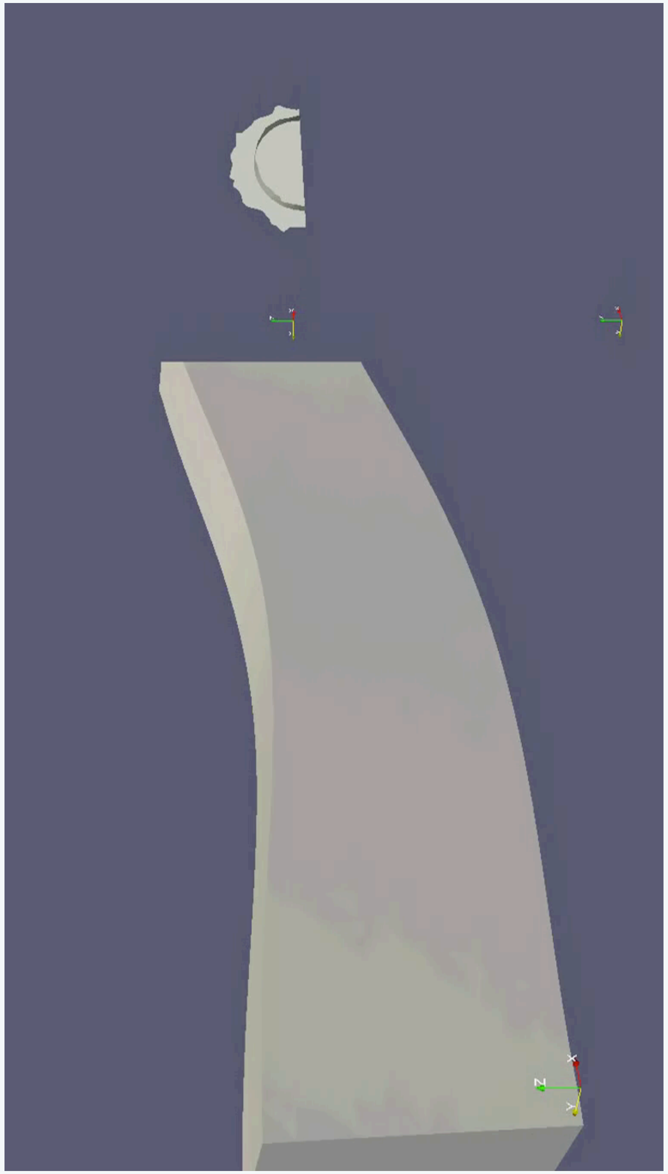




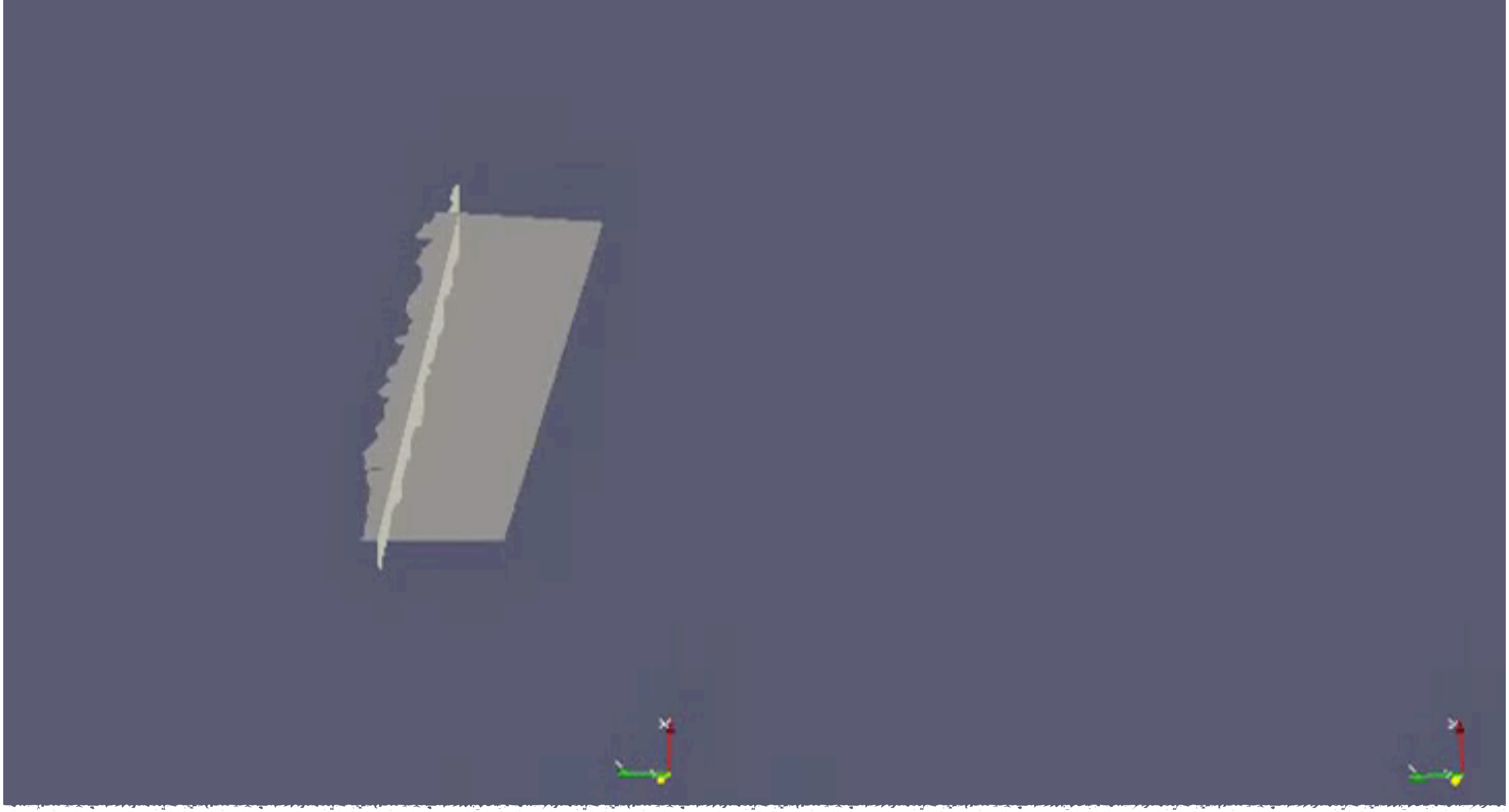


Fracture of homogeneous materials

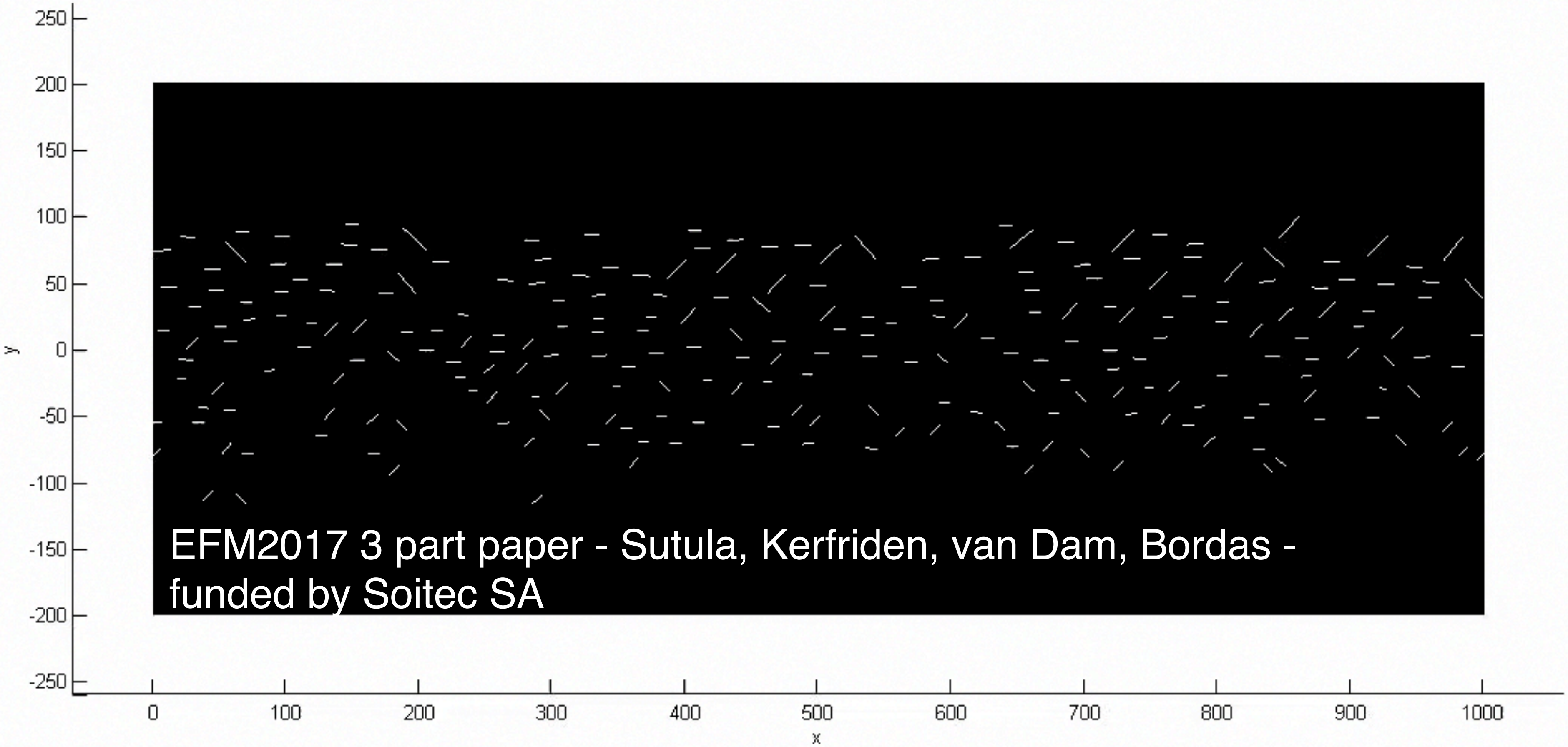




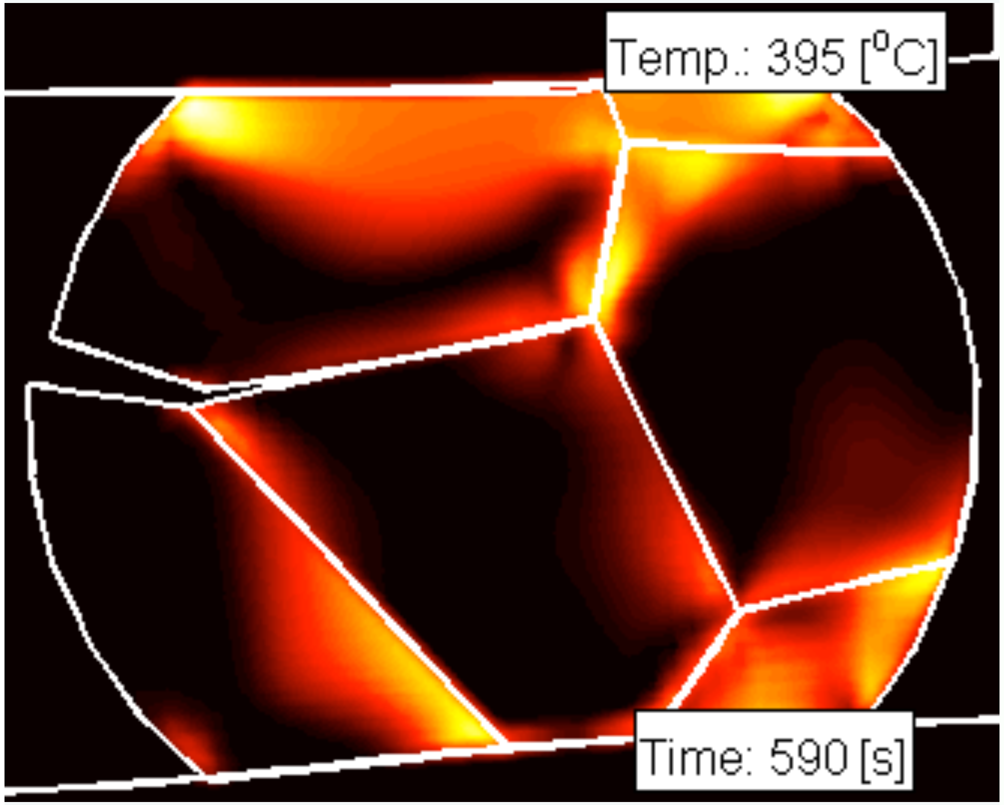
Agathos, Chatzi, Ventura, Talaslidis, SPAB: IJNME, CMAME2016, IJNME2017 CMECH17

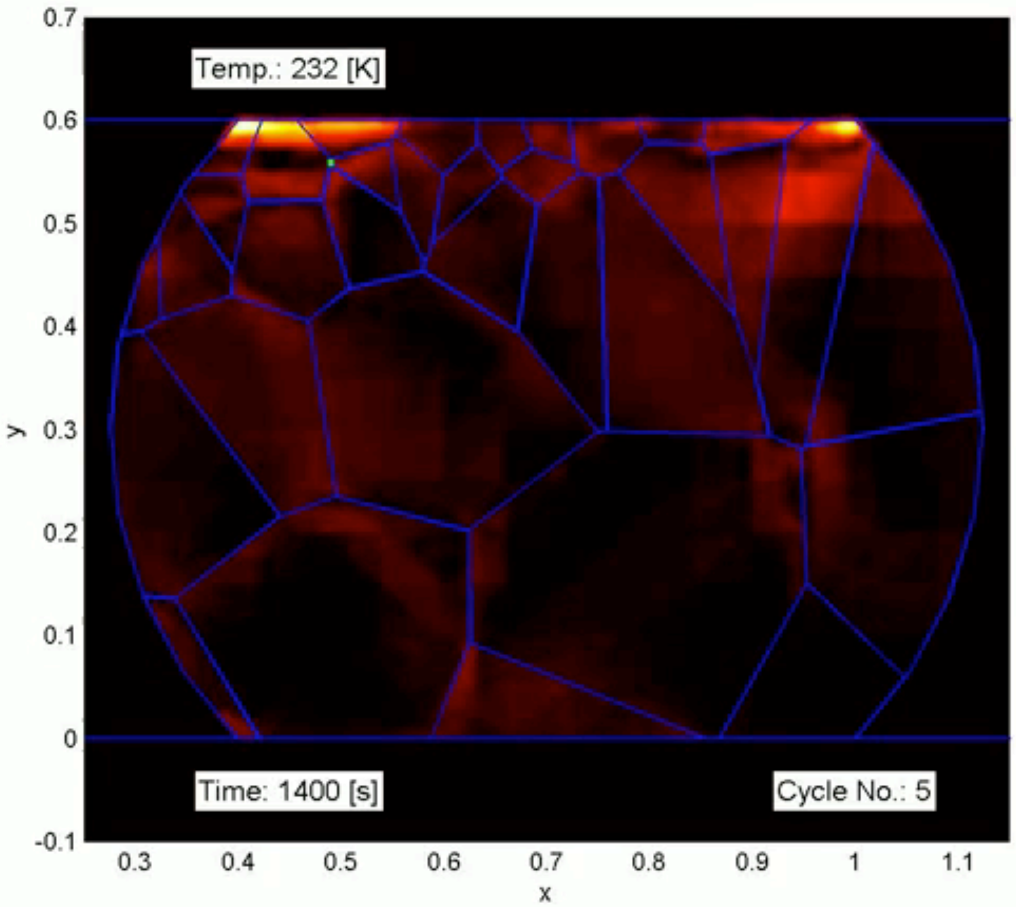


Energy-minimal multi-crack growth 300 cracks growing in Si due to H+ bombardment (SmartCut TM)



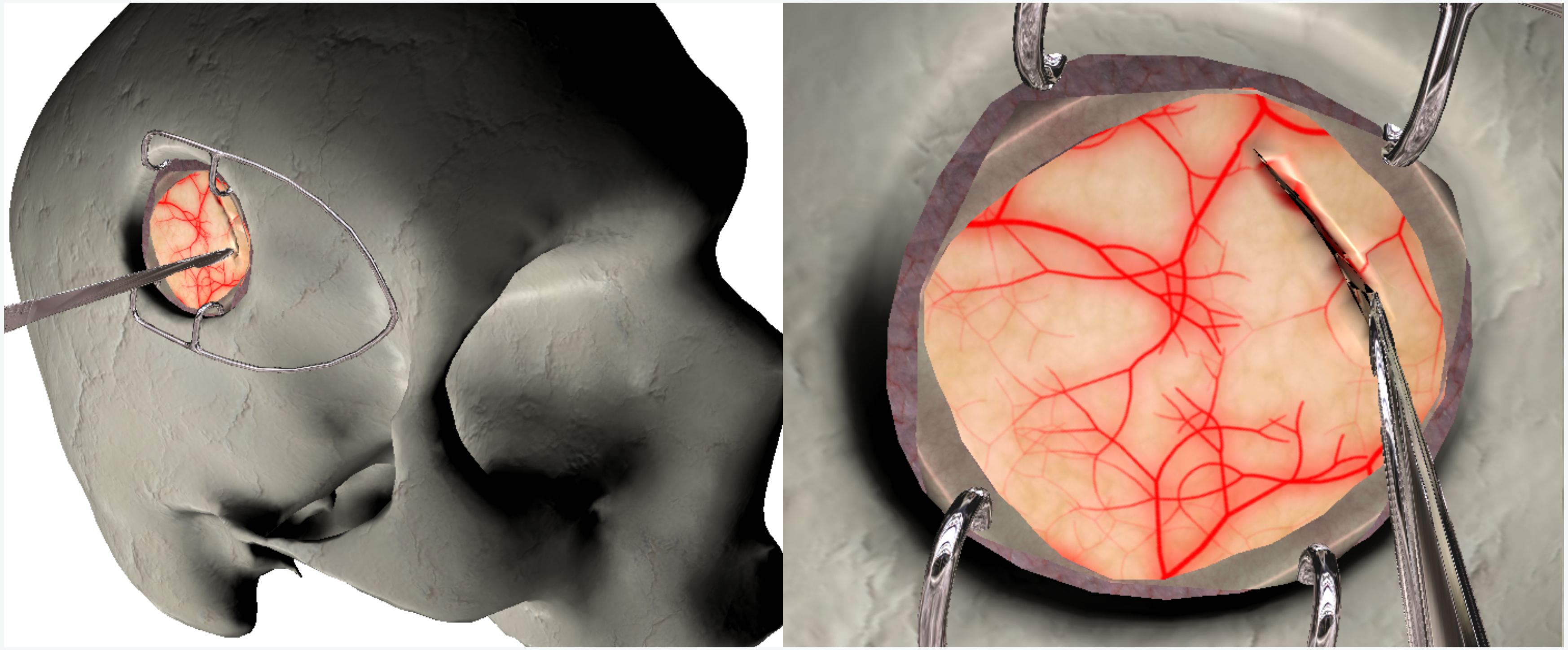
Polycrystalline failure (SnAgCu vs. SnPb)





IJNME2011, CMS2012, Menk & SPAB funded by Bosch GmbH

Cutting in soft tissue



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

Outline

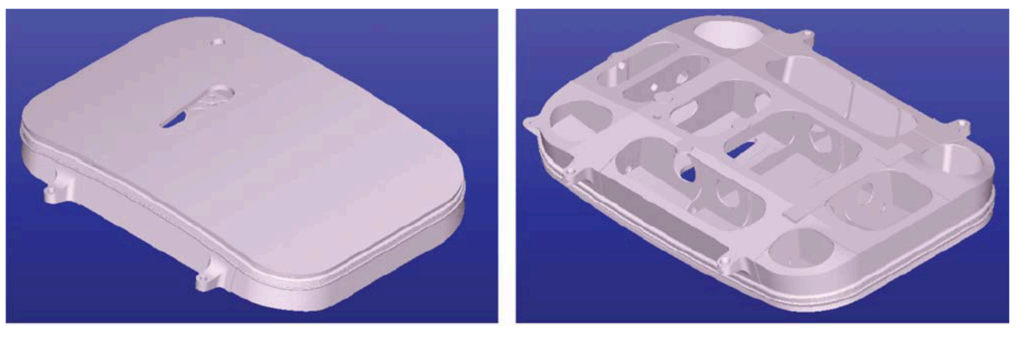
Part I. Computational approaches for industrial-scale fracture mechanics simulations and surgical simulation

- **Adaptive partition of unity enrichment**
- (Multi-scale fracture)
- Adaptivity in IGA through Geometry-Independent Field approximaTion

Part II. Model Selection and Uncertainties in surgical simulation (quick introduction)

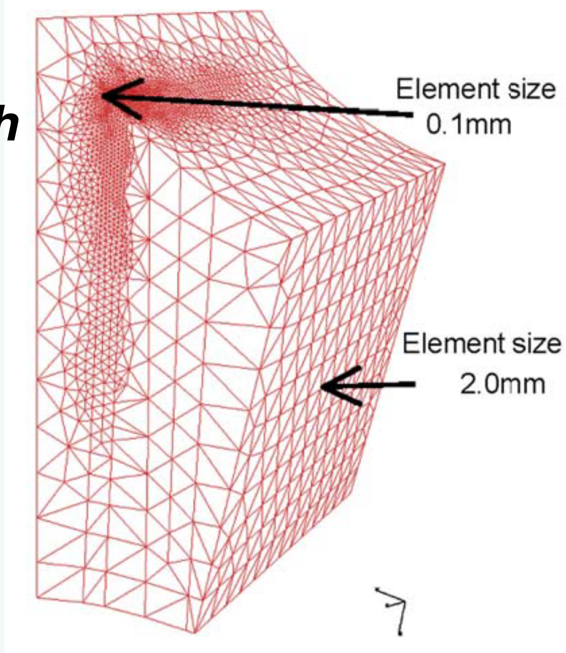
Fracture of 'homogeneous' materials

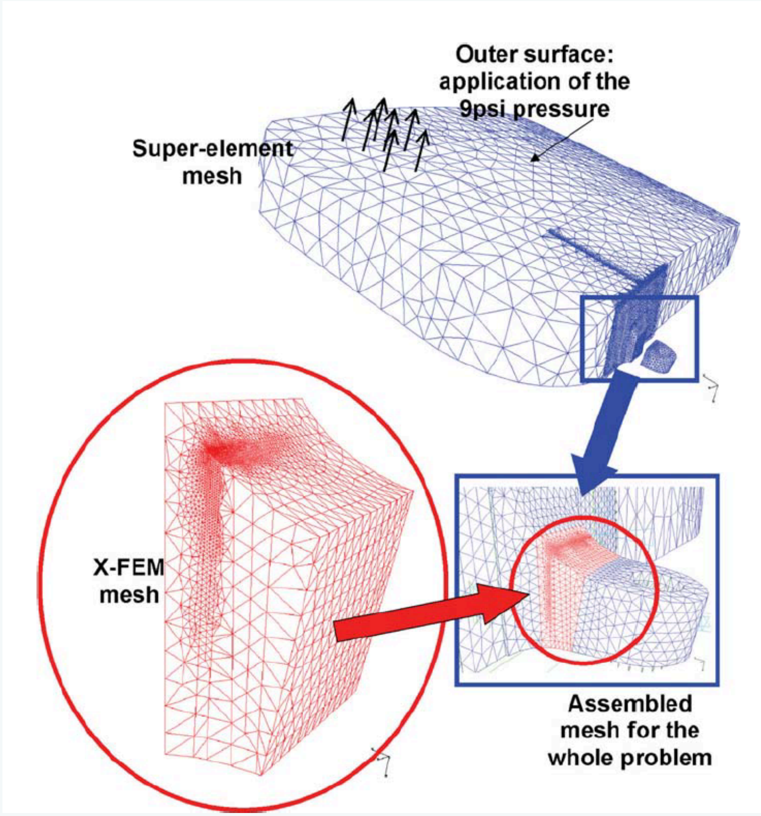
Question: when should a structure be inspected for flaws?



(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

Two issues in Computational Fracture

- Choice of the Model
- Choice of the Discretisation Scheme

Model Choice

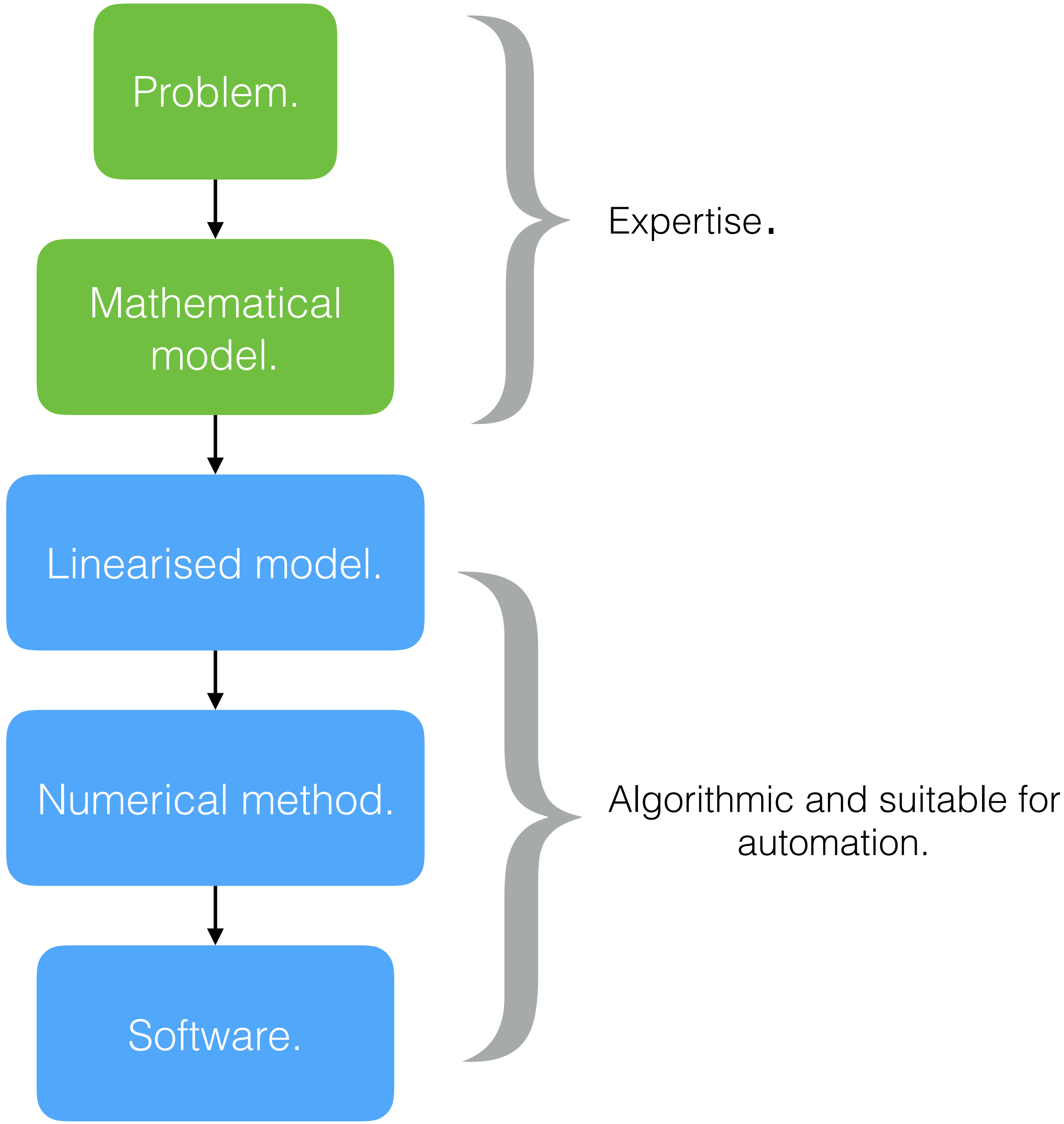
- Small scale yielding? Linear elastic fracture?
- Elastic-Plastic fracture mechanics?
- Damage models (local? non-local? gradient?)
- Multi-scale? (concurrent? semi-concurrent? adaptive?)

Discretisation Choice

- Finite element method (remeshing?)
- Boundary element method (non-linearities?)
- Scaled boundary finite elements (SBFEM) - see Plenary by Chongmin Song :)
- Extended finite element methods (multi-crack?)
- Meshfree methods (cost? stability? robustness?)
- Cracking particle methods (Rabczuk and Belytschko)

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

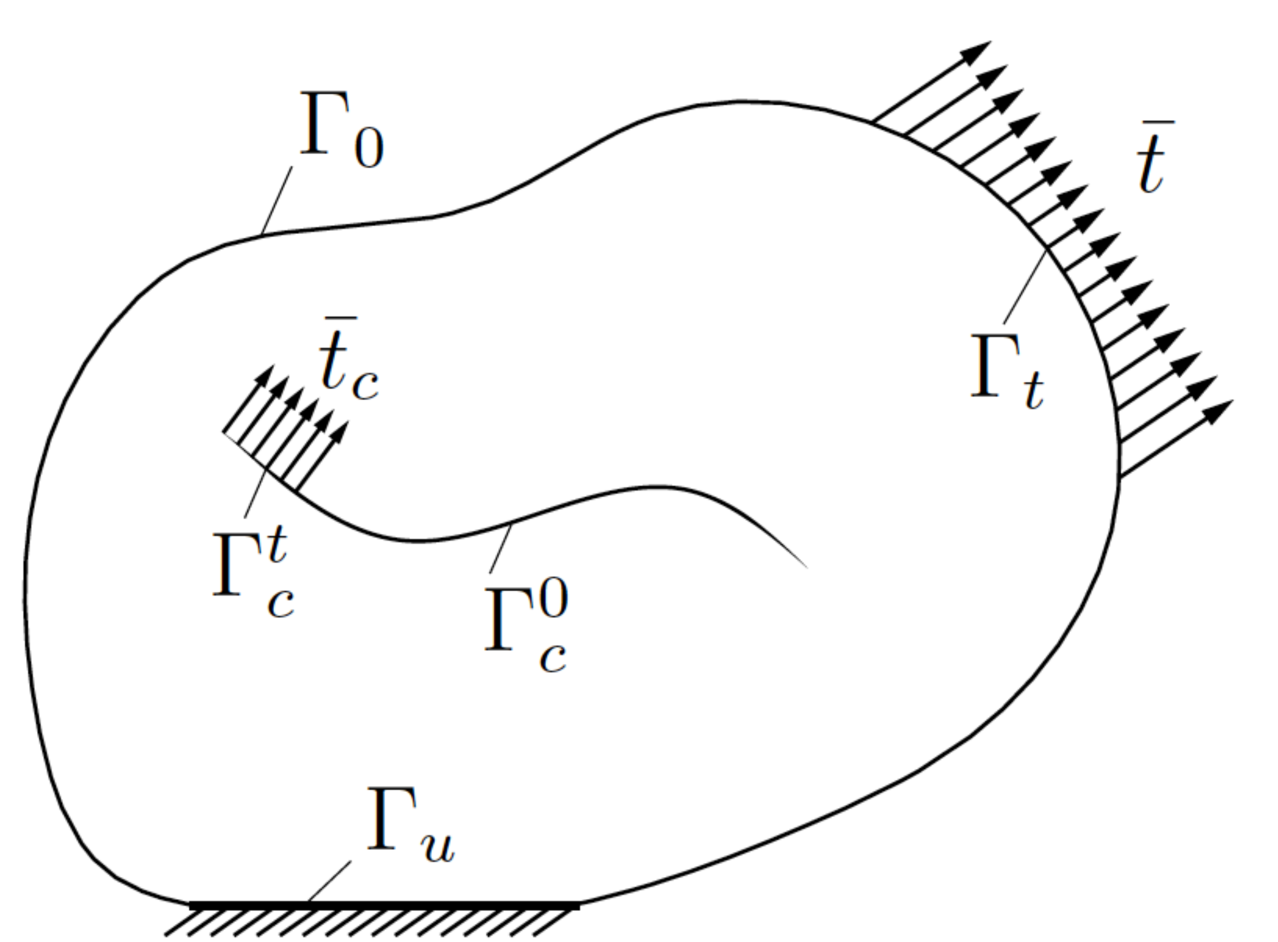
- Key idea: implement high-level description of finite element models in the Unified Form Language.
- Let algorithms take over the tedious/difficult work of linearisation and transforming maths into lower-level languages.
- Not a toy; scales to huge problems with billions of unknowns on Top100 supercomputers.


Problem.
Mathematical model.
Linearised model.
Numerical method.
Software.
Expertise.
Algorithmic and suitable for automation.

What is a crack?

a 1D line in 2D space

a 2D surface in 3D space



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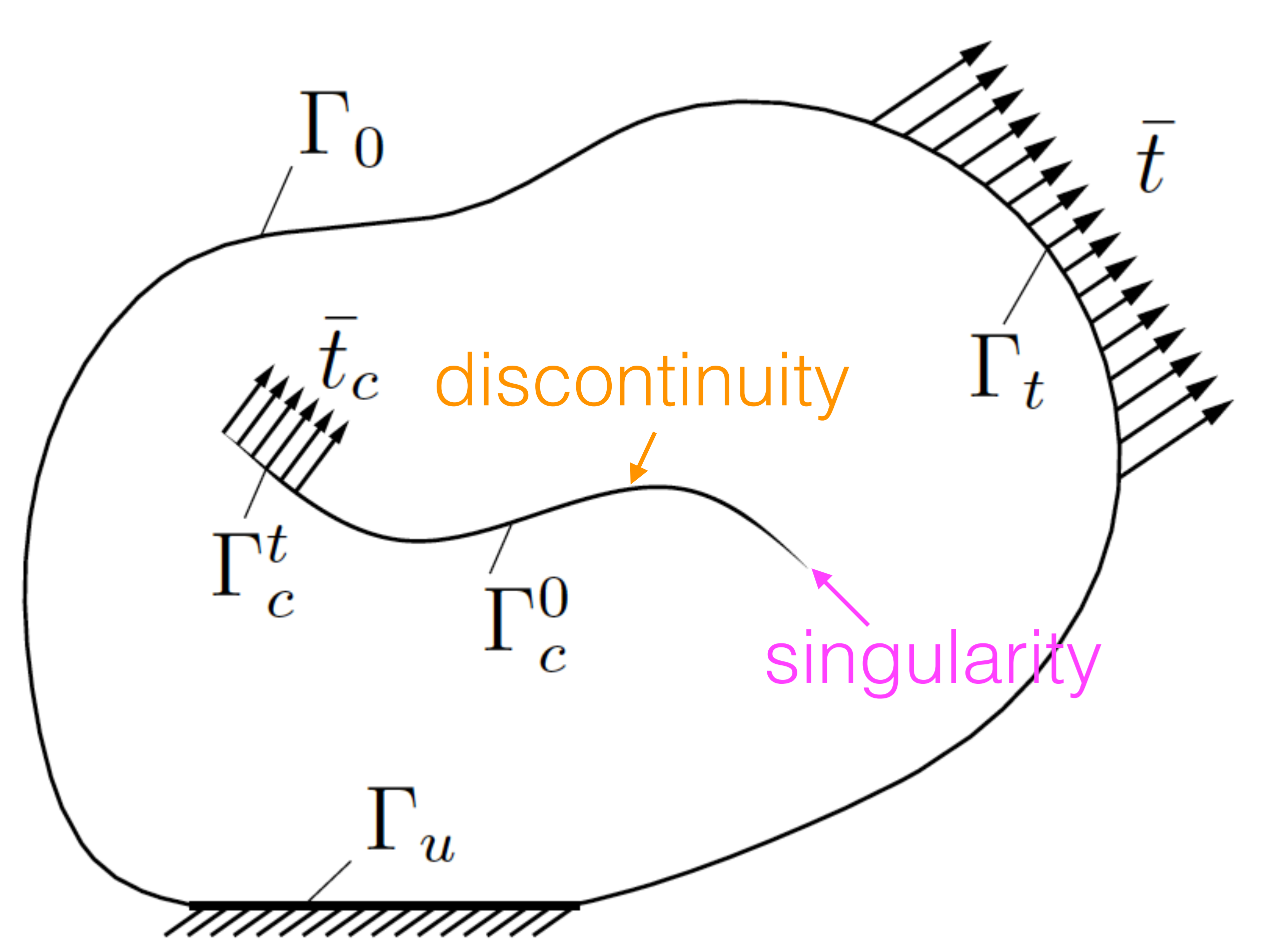
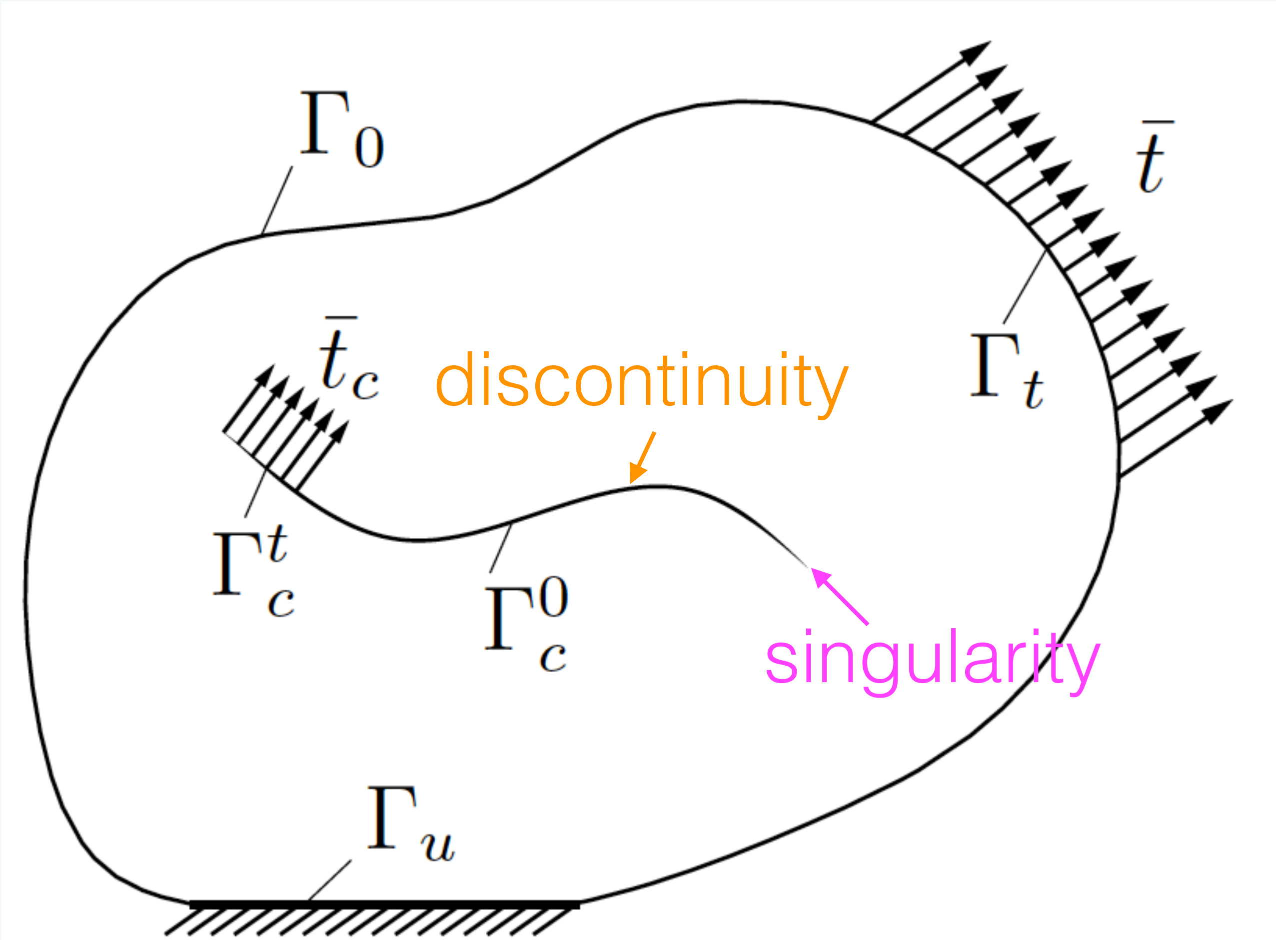
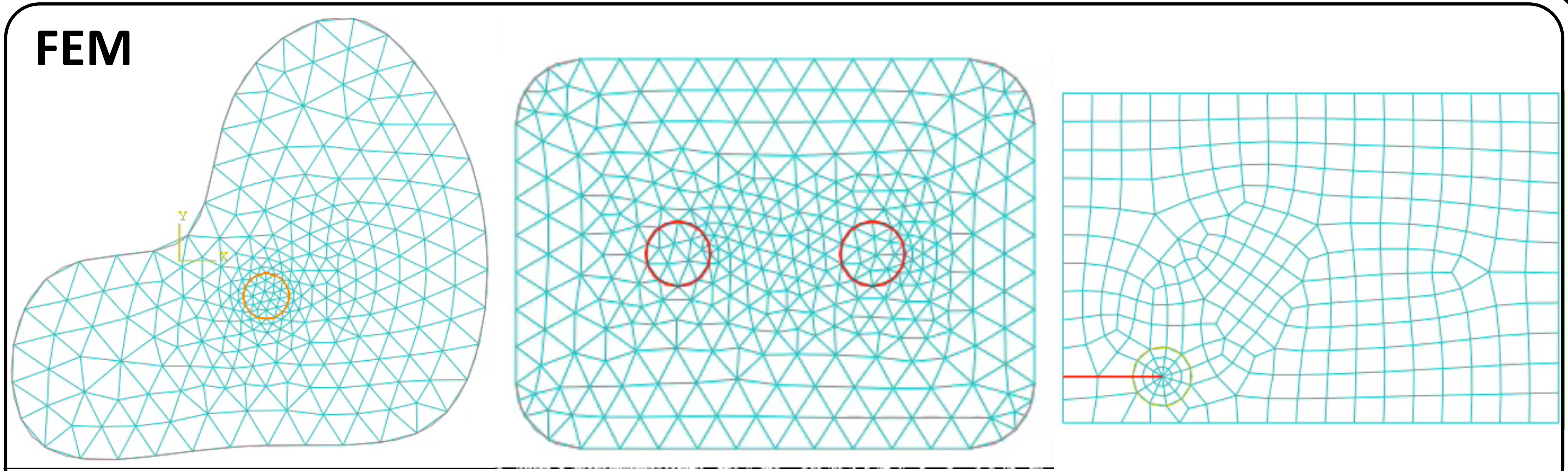


Finite elements for evolving discontinuities & singularities

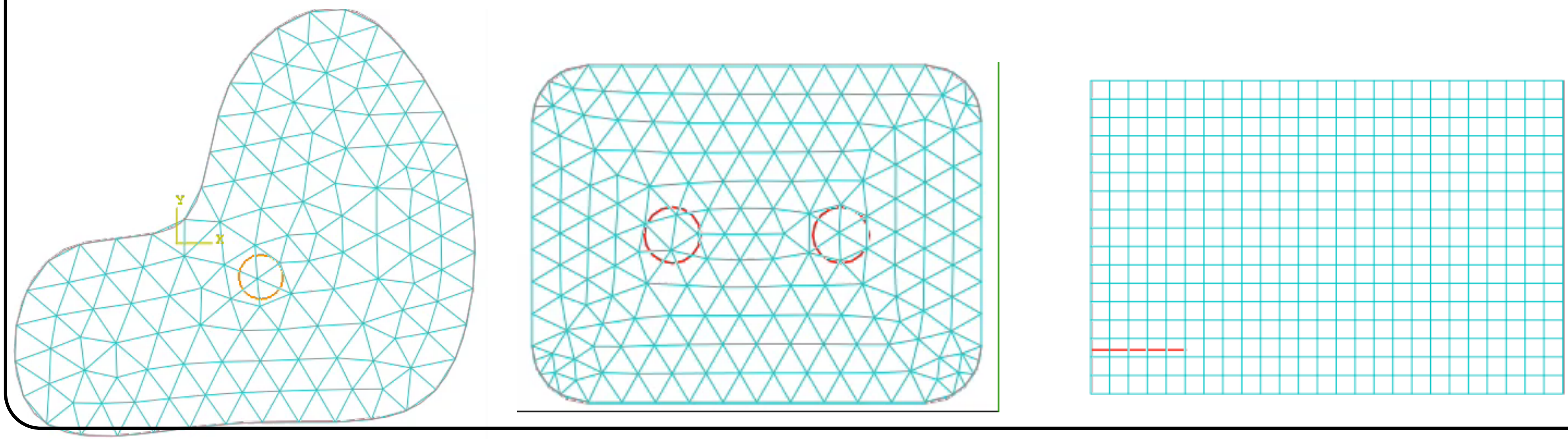


Free boundary problems

FEM



XFEM



One can show. 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

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

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

Dependson
- 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. Partition of Unity.
1995.

One can show . if $v_h = I_h u$ Lagrange approximation of u. ⑥

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Babuška, 1994. Partition of Unity.
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(C: Cea's Constant)

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

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• <u>Depends on</u> (C):
  - Physical Constants in Ω
  - Geometry of Ω
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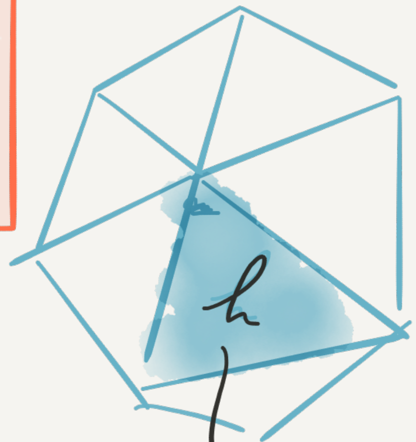
  - Degree of polynomial approx.



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

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

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(C: Cea's Constant)

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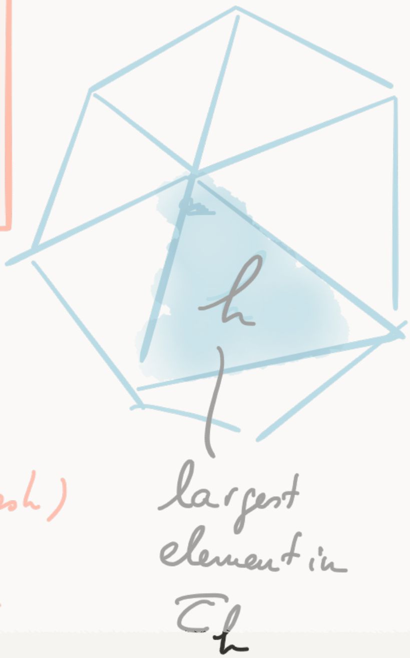
- <u>Depends on</u> (C):
  - Physical Constants in Ω
  - geometry of Ω
  - Quality of elements in $\mathcal{T}_h$ (mesh)
  - Degree of polynomial approx.



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

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

Why PUM?

Babuška 1994 → 1996 ...

- A priori error estimate:

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

- p: polynomial order
- $\|\cdot\|_m$: $H^m(\Omega)$ — measure of the error
- C, h: see (6)
- r: smoothness of u

Elasticity / Fracture

- $m = 1$
- r : small ⇒ u "not so smooth" → only a "few" ∂. of u are smooth

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

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

Why PUM? Babuška 1994 → 1996 ...

- A priori error estimate:

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

m: measure of the error, $H^m(\Omega)$

C, h: see ⑥

p: polynomial order

r: smoothness of u

Elasticity / Fracture

- $m = 1$, r : small → only a "few" ∂. of u are smooth

⇒ u "not so smooth".

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

($p+1-1 = p$, $r-1$; $\|u\|_{H^r(\Omega)}$: LARGE.)

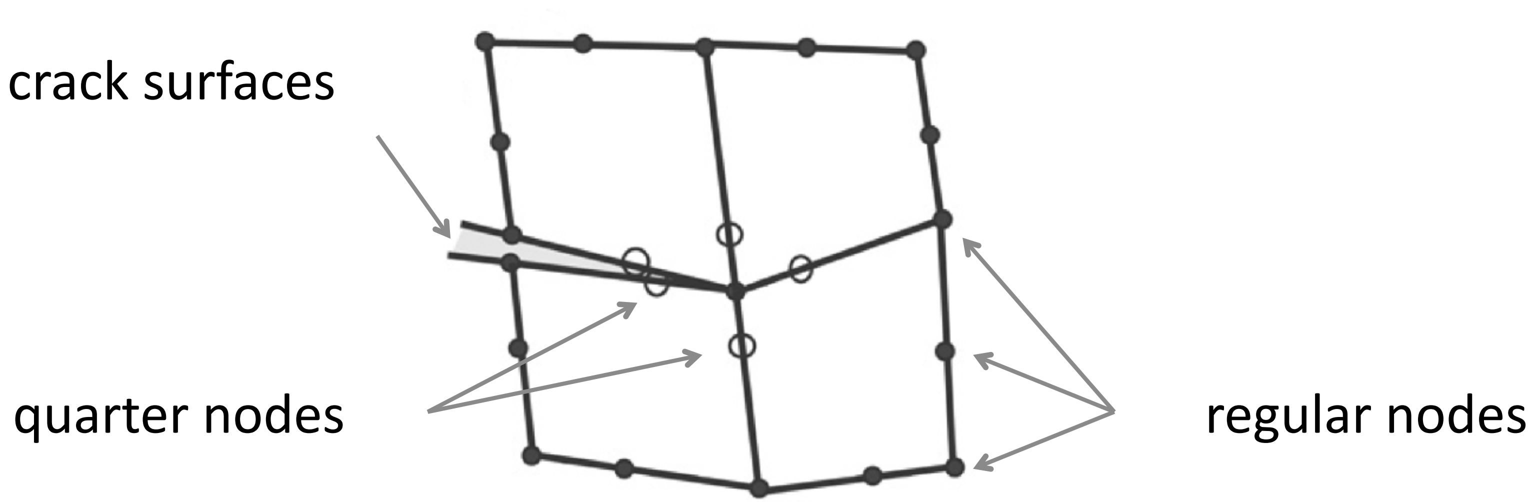
$$\leq C\, h^{\min(p,\, r-1)} \|u\|_{H^r(\Omega)}$$

h: mesh refinement; $r-1$: "small".

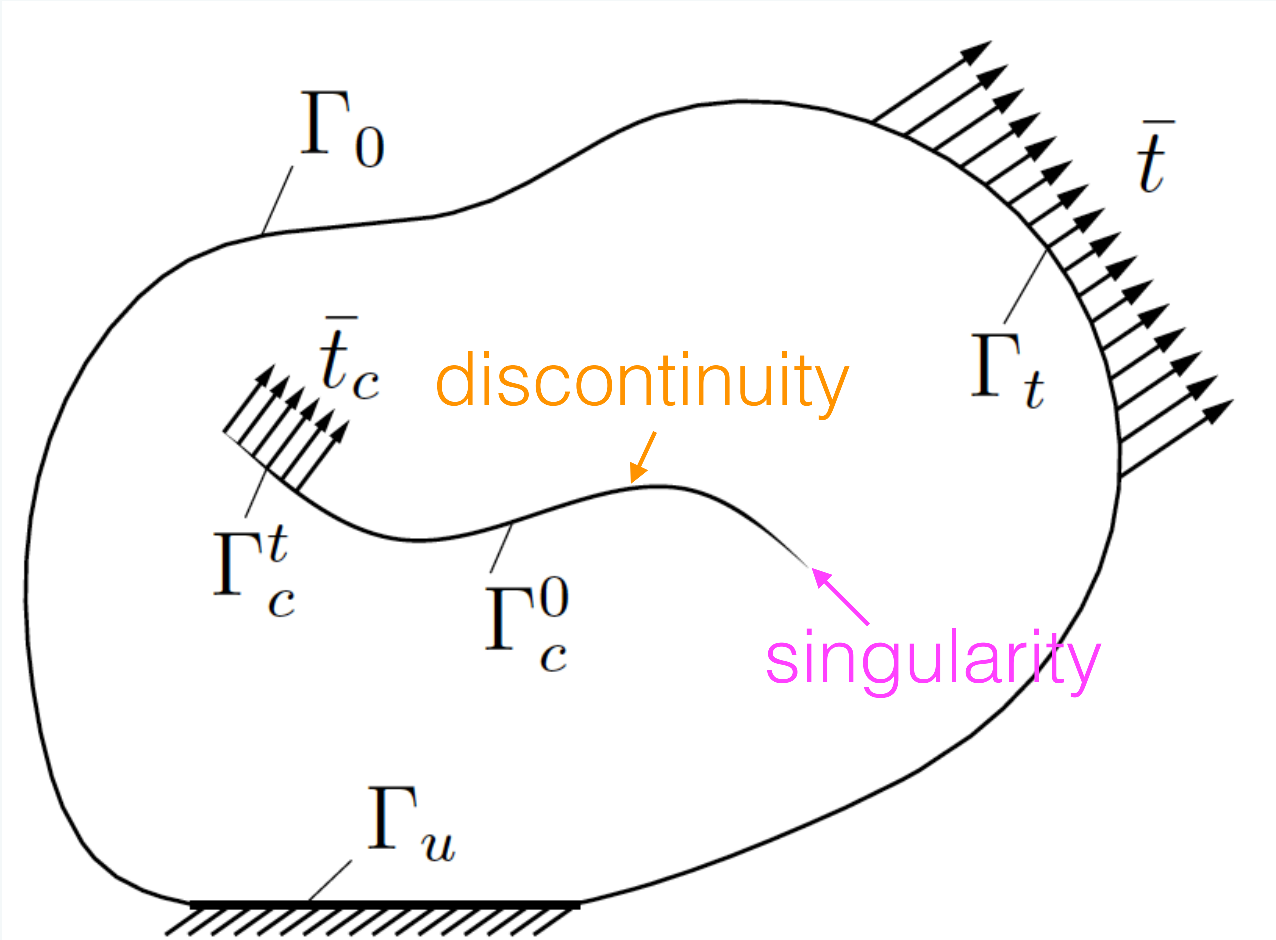
Singular elements (Barsoum, 1974)

For simulating the crack tip singular field in LEFM

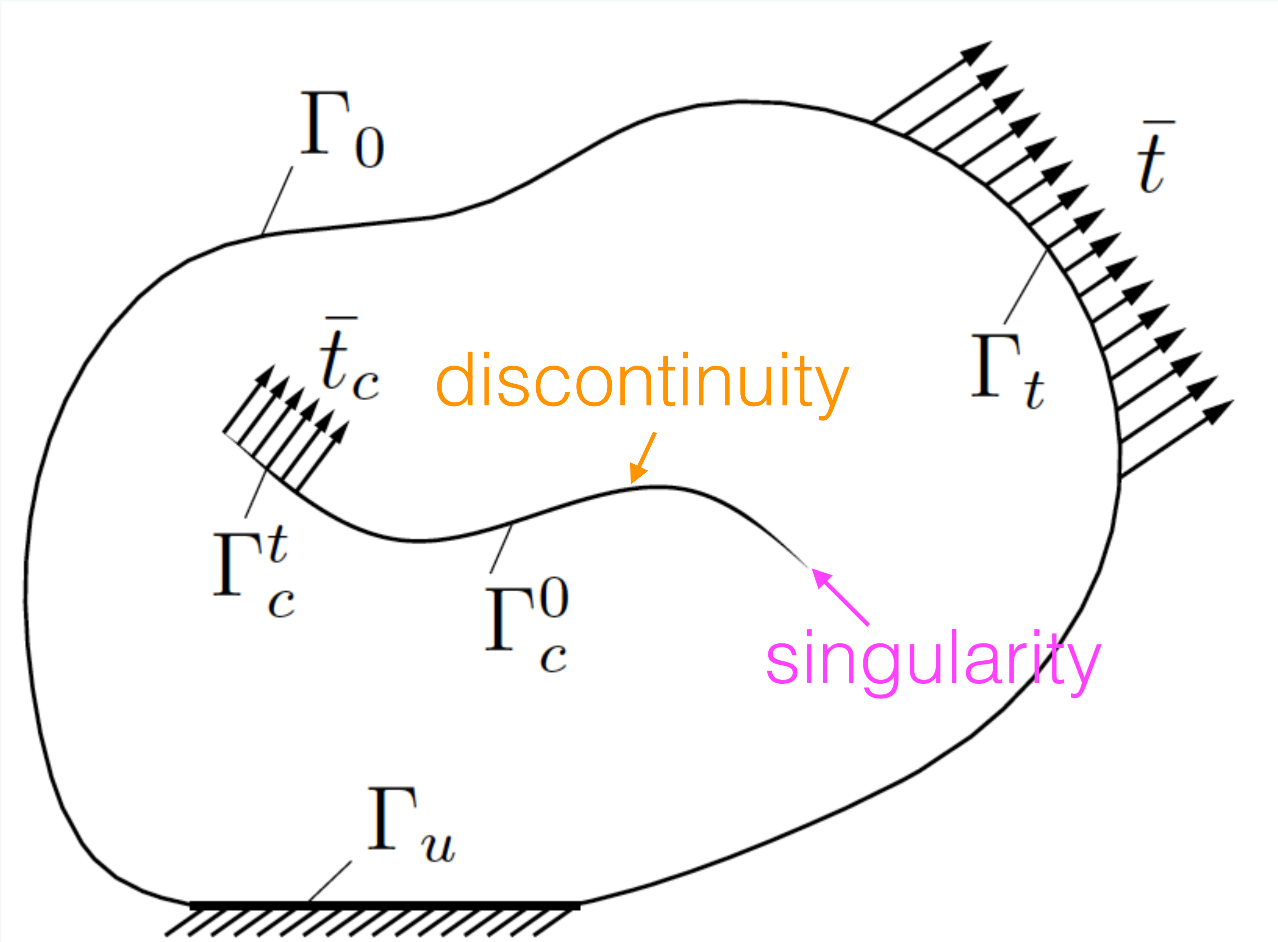
- A simple way how to introduce a singularity of $1/\sqrt{r}$ in isoperimetric finite elements is by displacing the mid-side nodes of two adjacent edges to one quarter of the element edge length from the node where the singularity is desired.



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



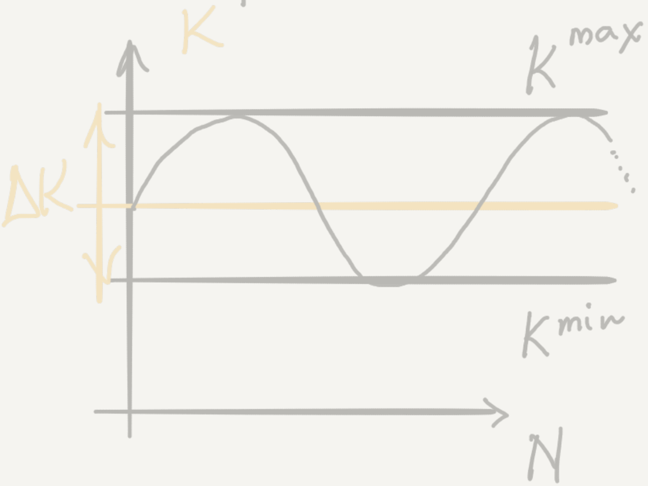
Computational fracture (LEFM) requires highly accurate solutions…



COMPUTATIONAL FRACTURE

Fracture (1)

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



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

Δa: amount of crack growth for ΔN cycles

ΔN: number of cycles

ΔK: Stress Intensity factor amplitude

C, m are empirical coefficients

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

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

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

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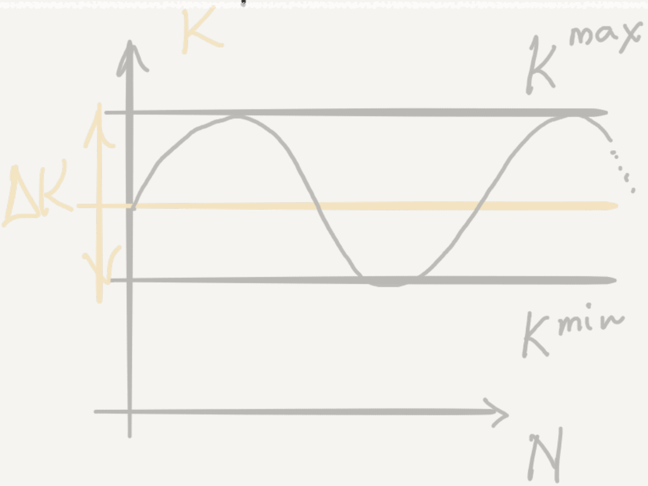

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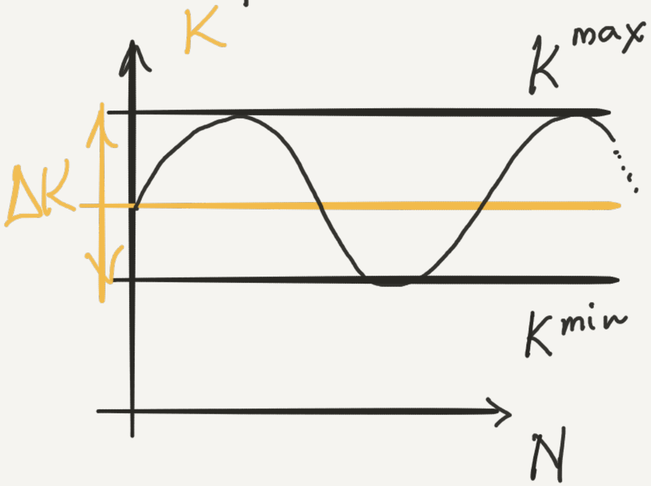

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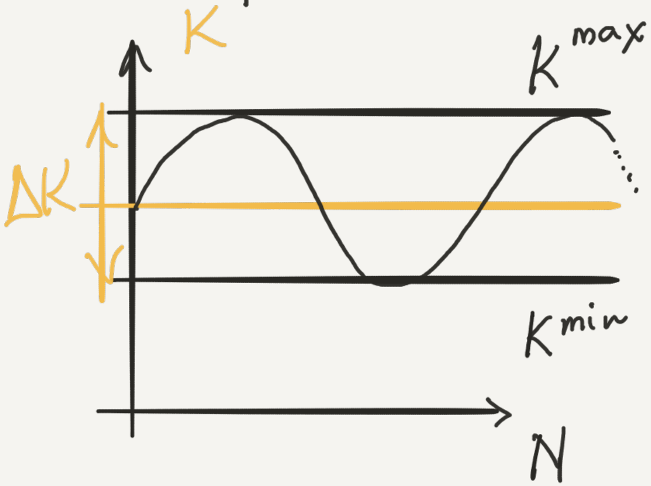

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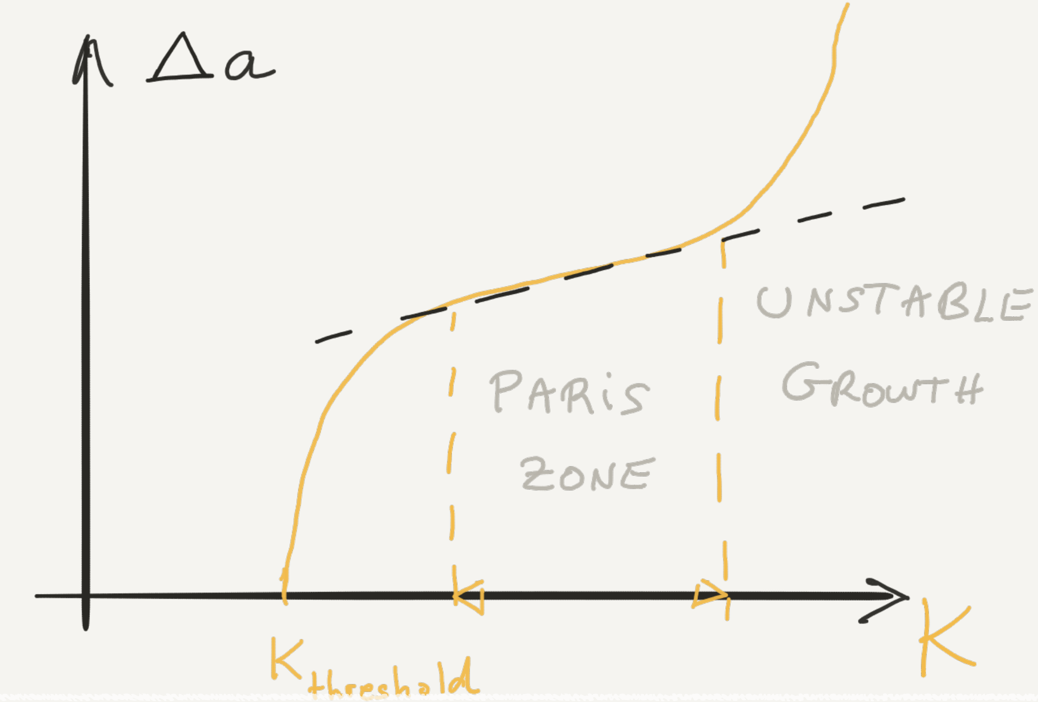


NO GROWTH

Fracture ②

Numerically Computed

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

$3 \leq m \leq 5$ Paris Exponent

Assume error ε_K on K

$\frac{\varepsilon_K}{K} << 1$ (ε)

Increment in each advance assuming an error ε_K is committed

$$\Delta a^\varepsilon = C \left(K + \varepsilon_K \right)^m \Delta N$$

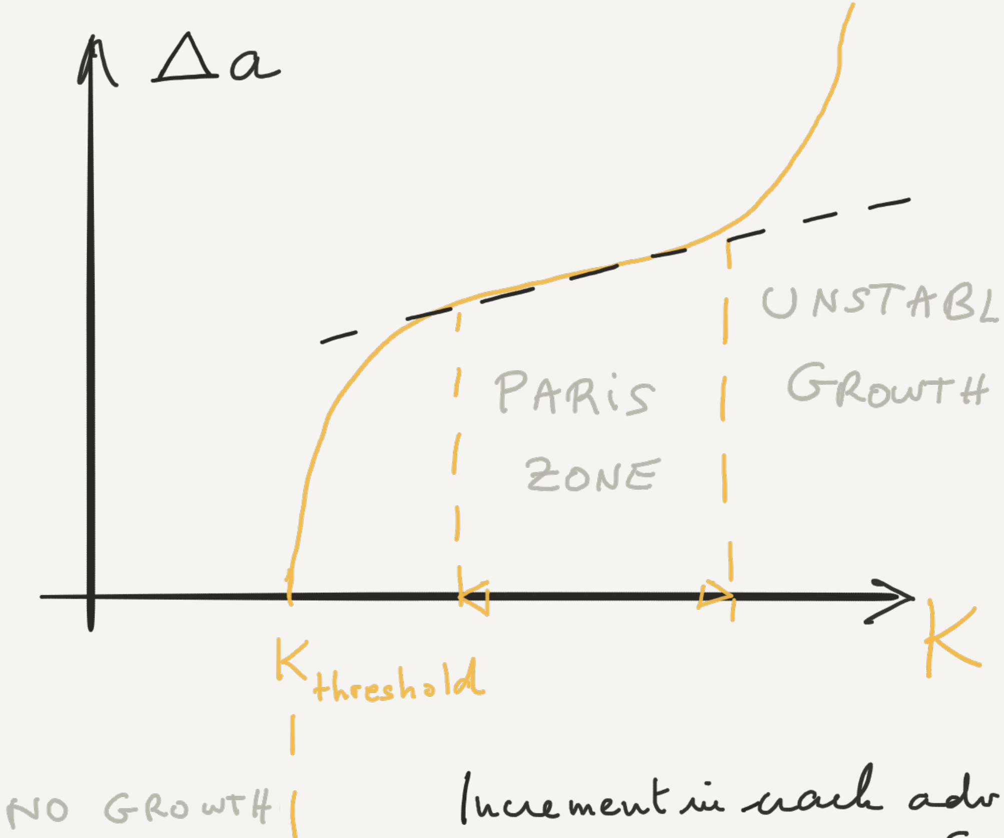
$$\Delta a^\varepsilon = C \; K \left(1 + \frac{\varepsilon_K}{K} \right)^m \Delta N$$

$$\Delta a^\varepsilon \simeq C \; K^m \left(1 + m \, \varepsilon \right) \Delta N$$

$$\Delta a^\varepsilon \simeq \Delta a \left(1 + m\varepsilon \right)$$

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

Fracture ②



Numerically Computed (K)

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

$3 \leq m \leq 5$ Paris Exponent

Assume error ε_K on K

$$\frac{\varepsilon_K}{K} \ll 1 \quad (\varepsilon)$$

Increment in each advance assuming an error ε_K is committed

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

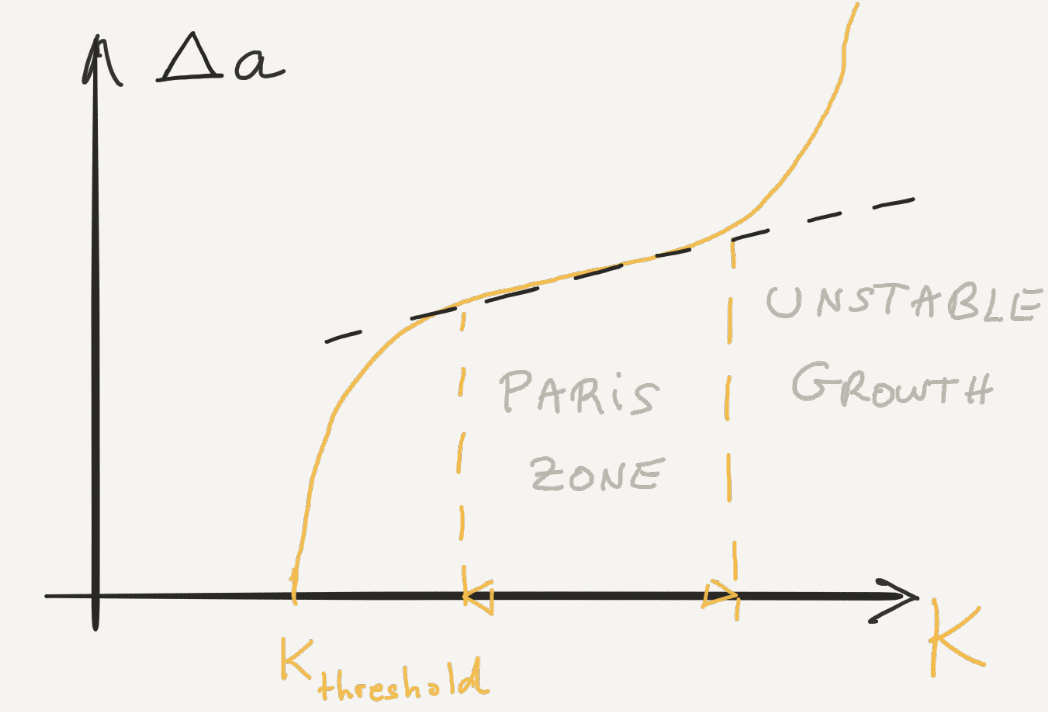
$$\Delta a^{\varepsilon} = C\,K\left(1 + \frac{\varepsilon_K}{K}\right)^m \Delta N$$

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

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

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

Fracture ②



NO GROWTH

Numerically Computed

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

$3 \leq m \leq 5$ Paris Exponent

Assume error ε_K on K

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

Increment in each advance assuming an error ε_K is committed

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

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

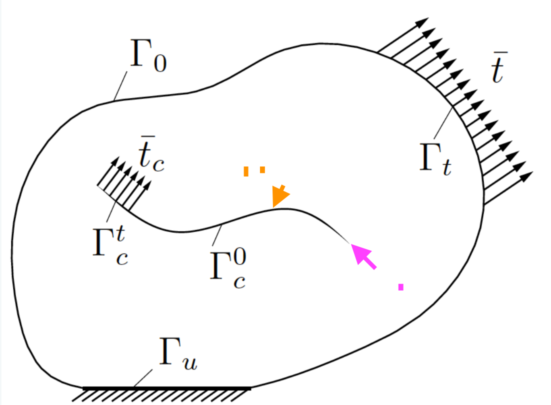
The idea of Partition of Unity Enrichment (PUFEM, GFEM, XFEM, hp clouds, enriched IGA, enriched meshfree methods, enriched BEM…)

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

Singularities?

Discontinuities?

Boundary layers?

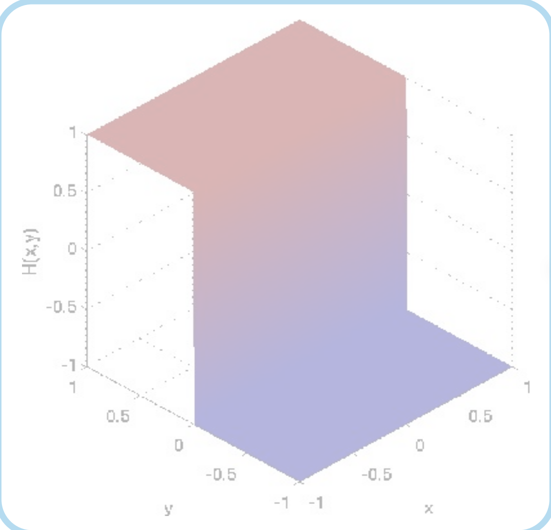


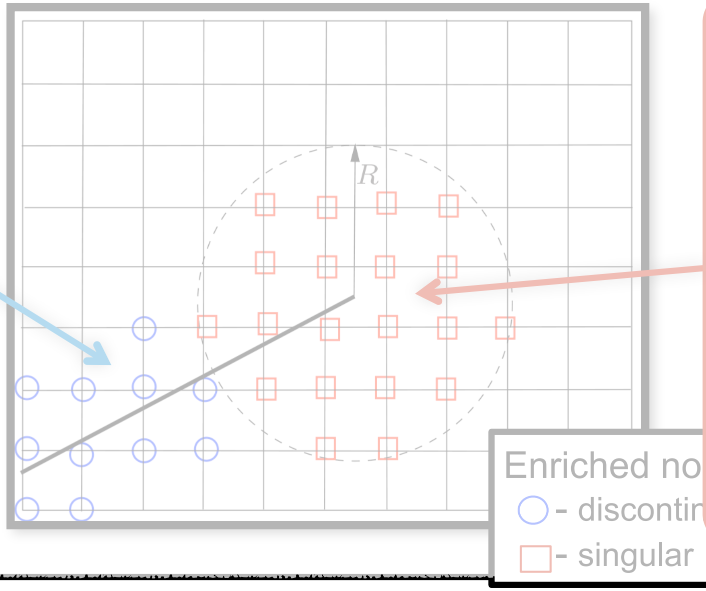
Formulation for crack growth:

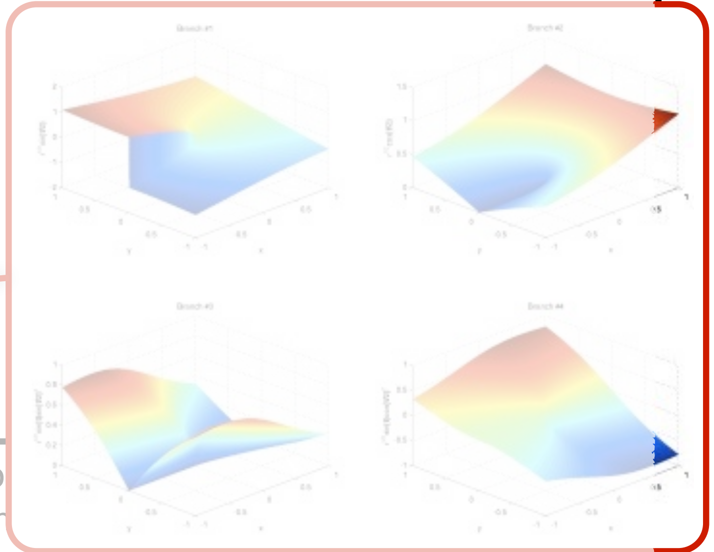
$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I\in\mathcal{N}_I} N_I(\mathbf{x})\mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J\in\mathcal{N}_J} N_J(\mathbf{x})H(\mathbf{x})\mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K\in\mathcal{N}_K} N_K(\mathbf{x})\sum_{\alpha=1}^{4}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

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

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







GFEM/XFEM

Formulation for crack growth:

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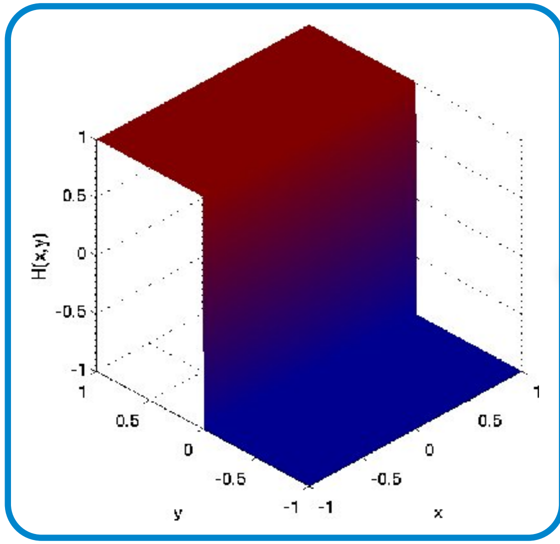

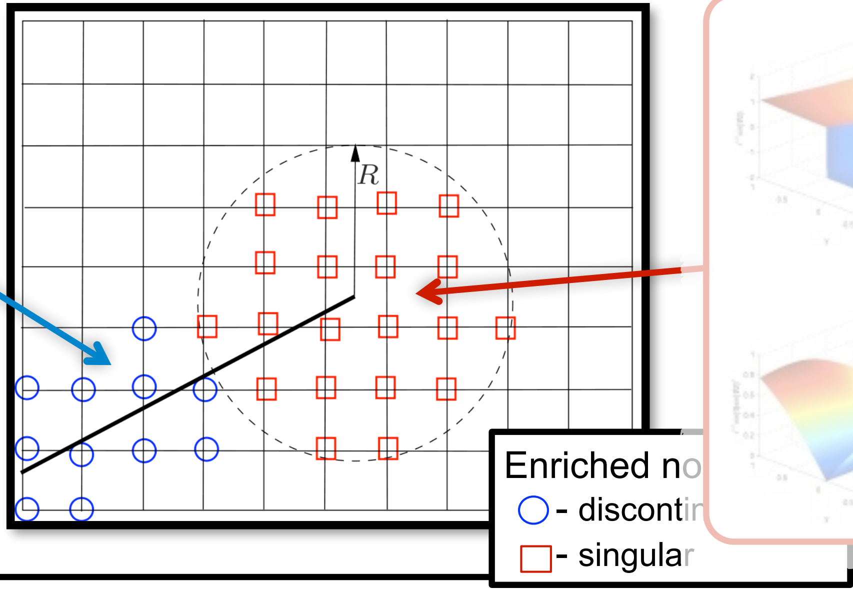

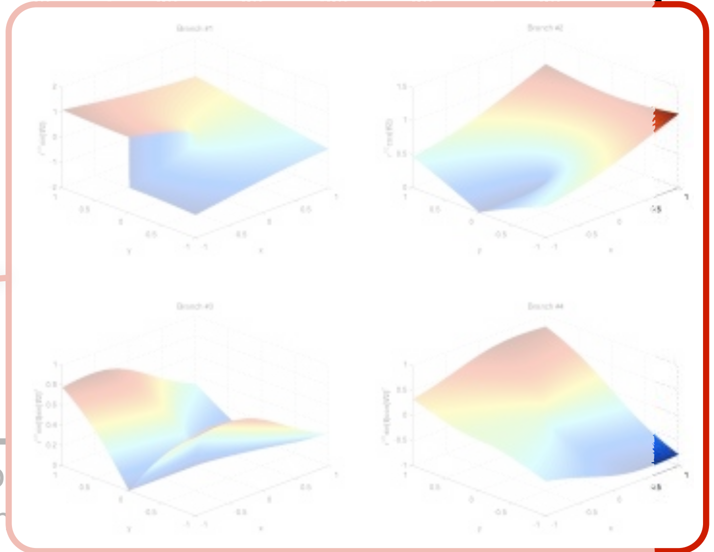

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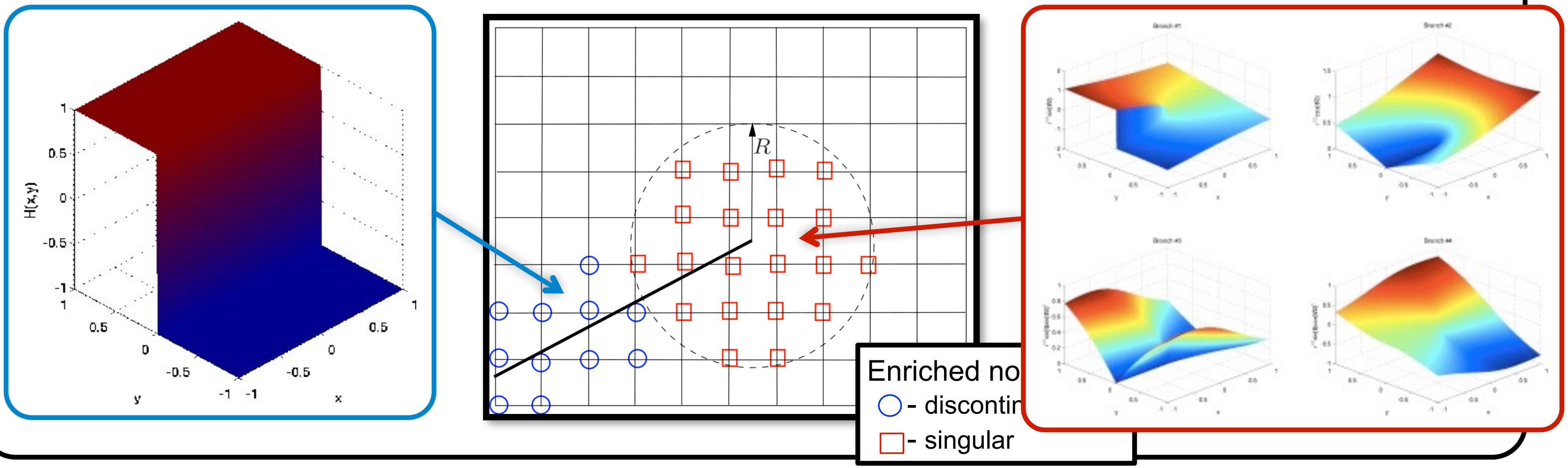
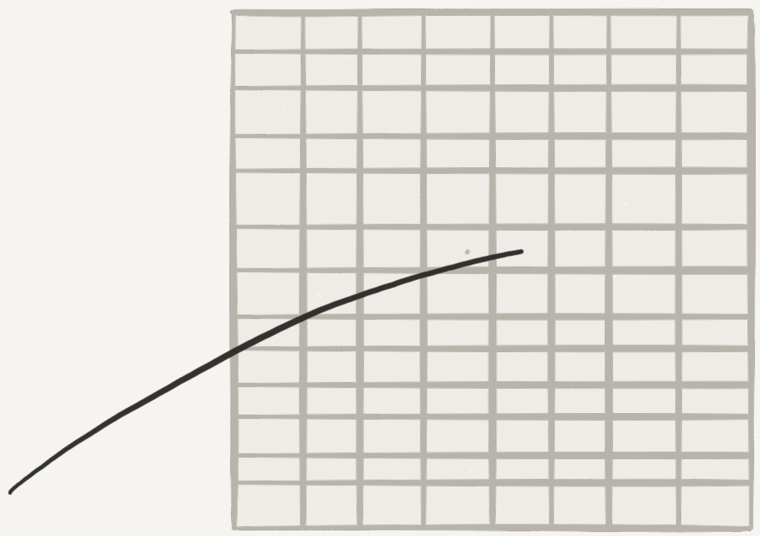
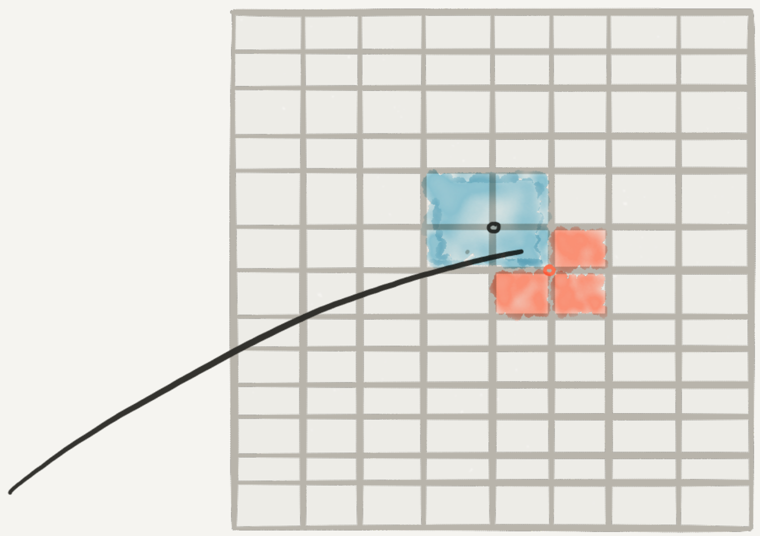
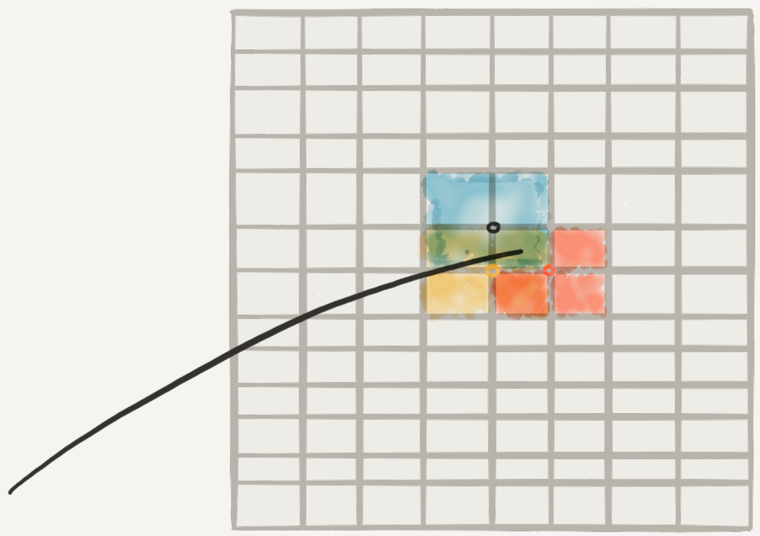
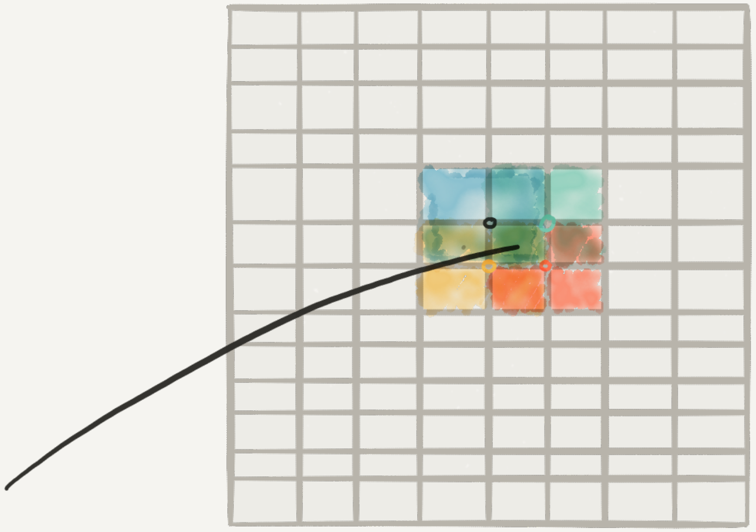


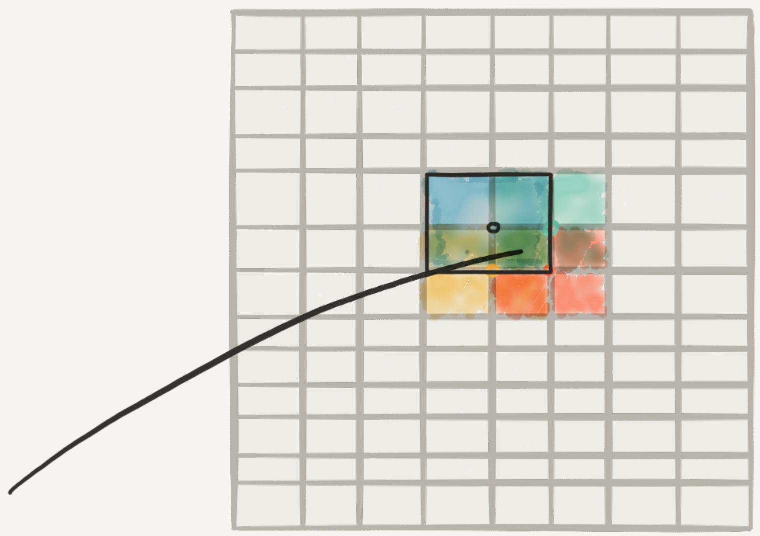


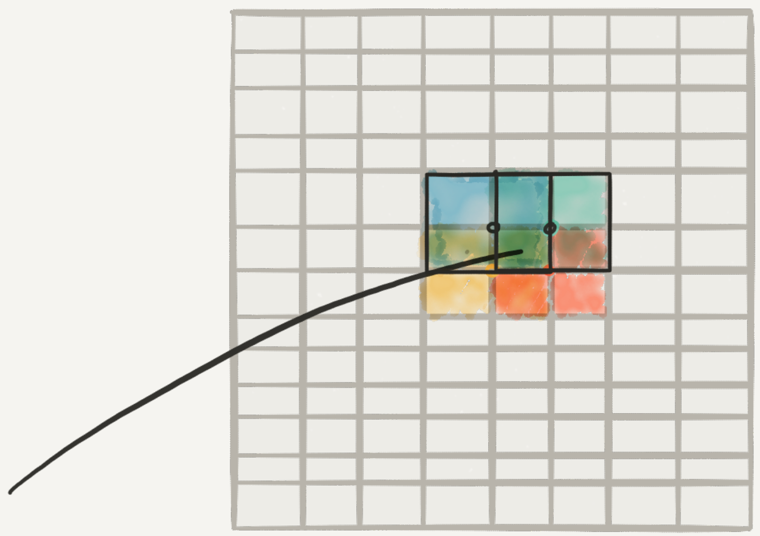
Nodes whose support contain the tip (front) are enriched by near-tip branch functions

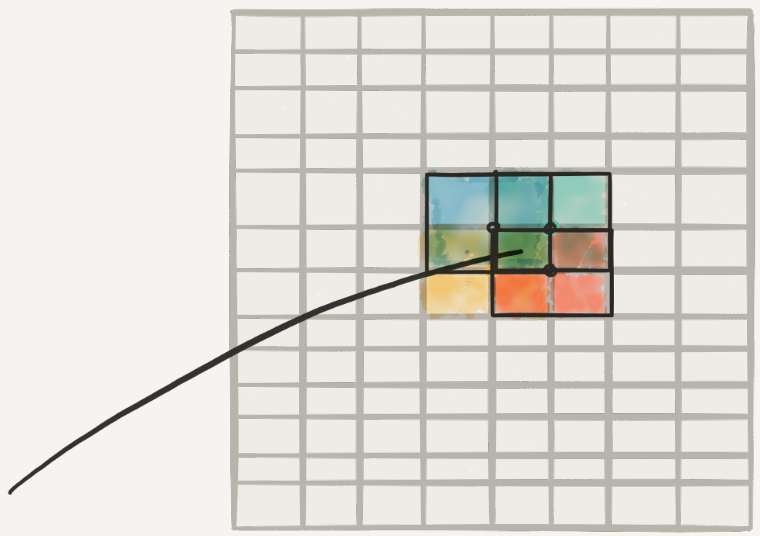


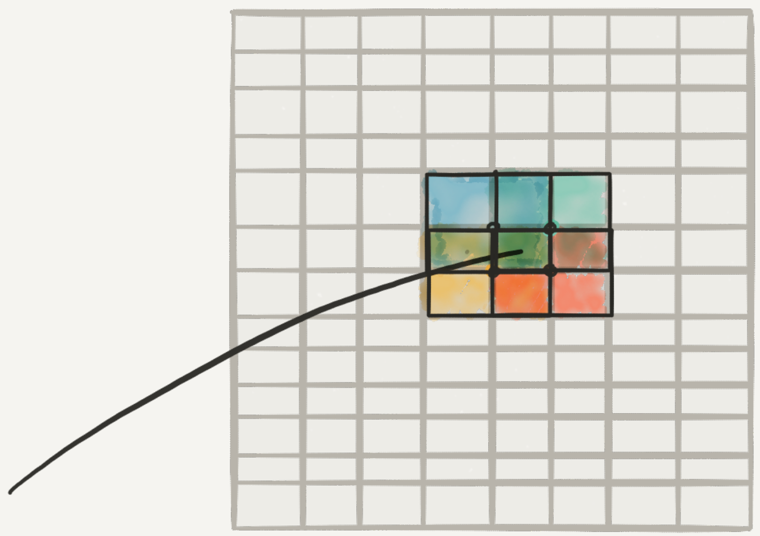




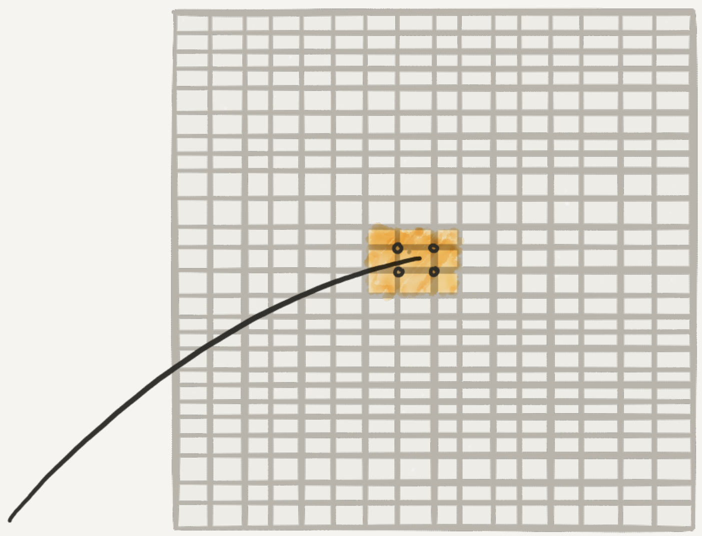




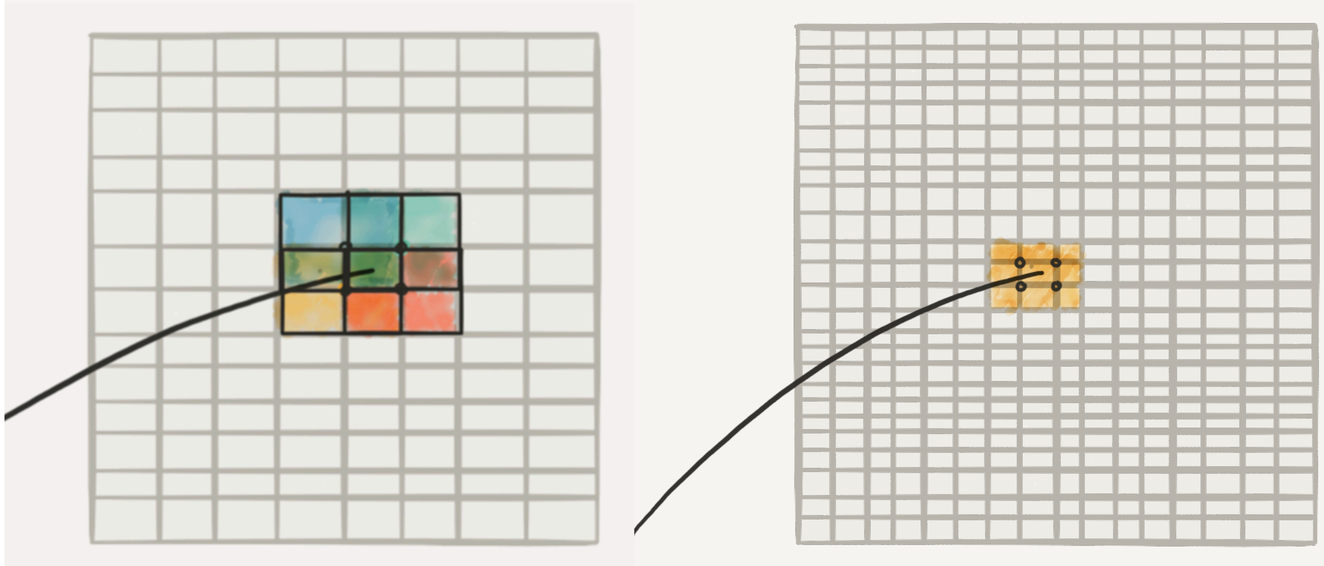




The enriched area is composed here of 9 elements

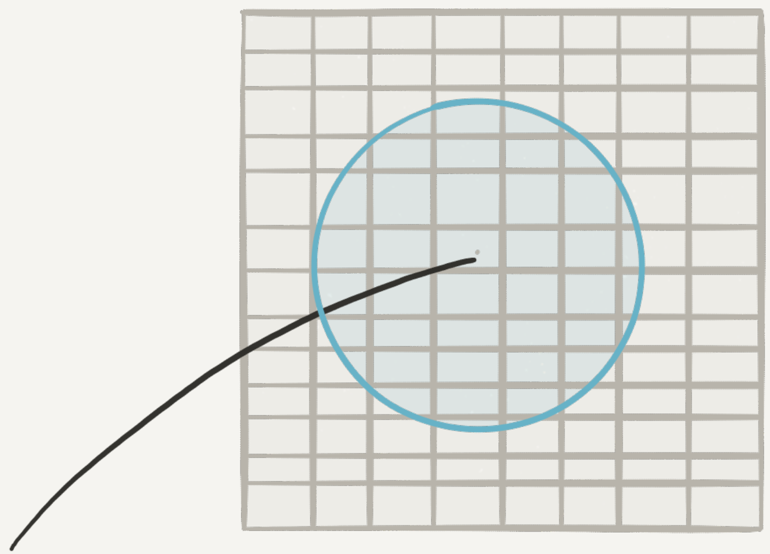


Assume we refine the mesh
The enriched area is still made up of 9 elements
But those elements represent a smaller portion of the entire domain

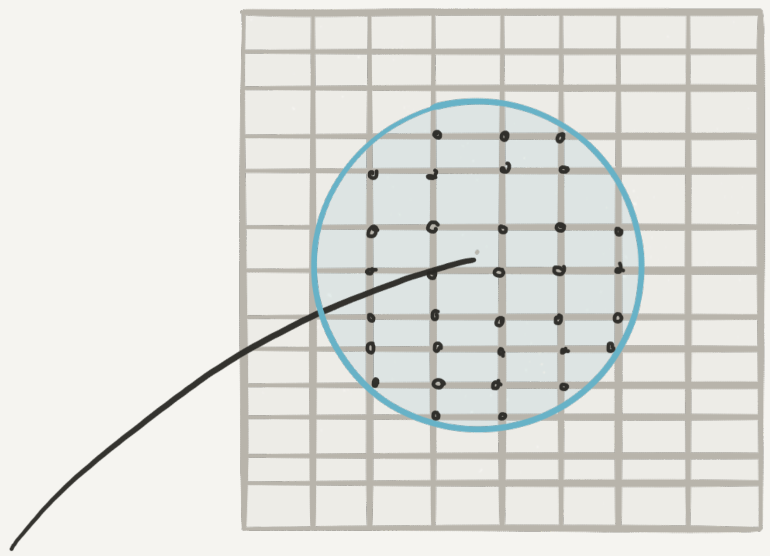


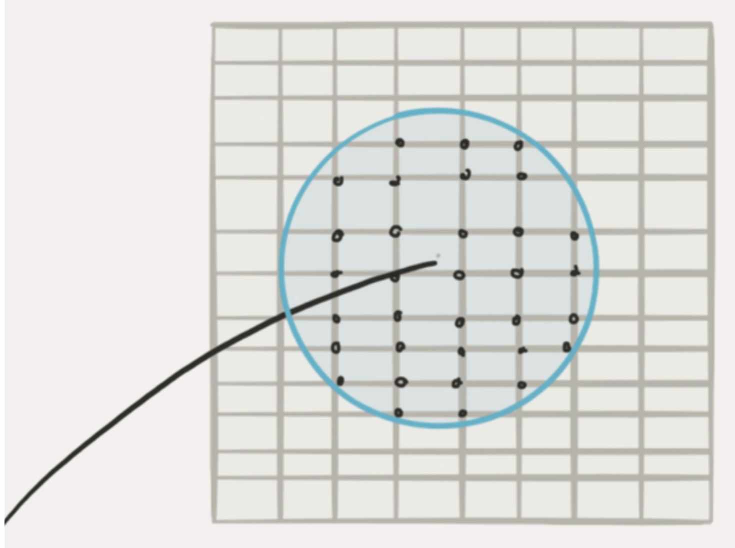
By refining the mesh, the influence of the enrichment zone on the convergence of the method tends to zero

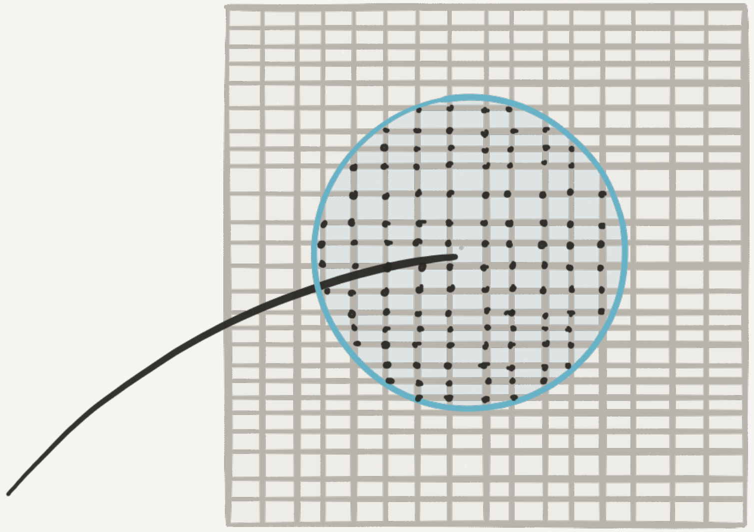
With topological enrichment, we lose the benefit of enrichment



Enriching an area independent of the mesh size
(geometrical enrichment versus topological enrichment)



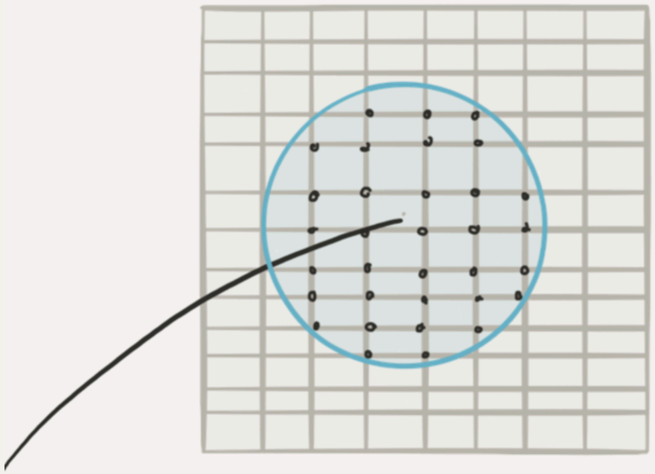


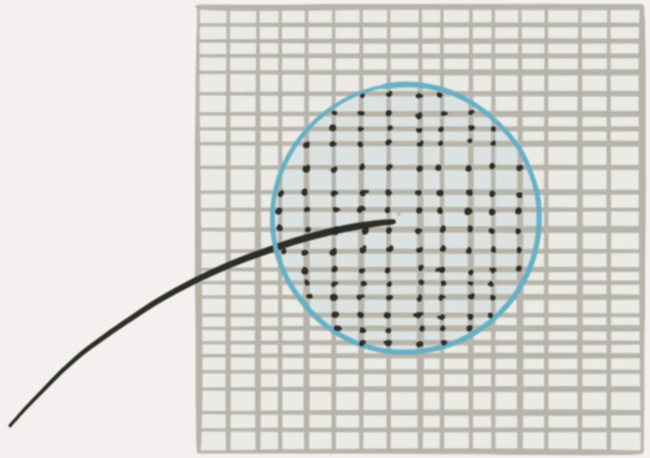


Geometrical enrichment ensures that as the mesh is refined, the enriched area remains constant (more nodes become enriched)

This ensures that 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 and Agathos 2016, 2017)
- ☑ 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)

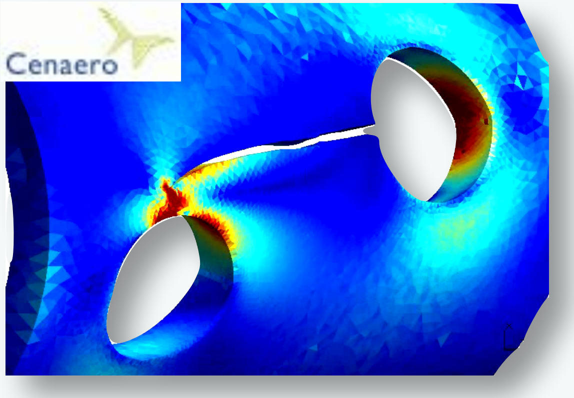
Summary

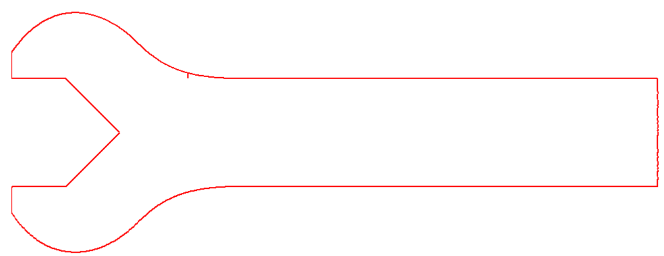
Fracture of homogeneous materials

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

- 3D fracture requires **accurate** stress intensity factors (SIFs)
  - ☐ Error at each step ~ (Error on SIF)^4
  - ☐ Standard enrichment => oscillations along the front
  - ☐ **Need higher order enrichment or "large" enrichment radii**
- 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)**

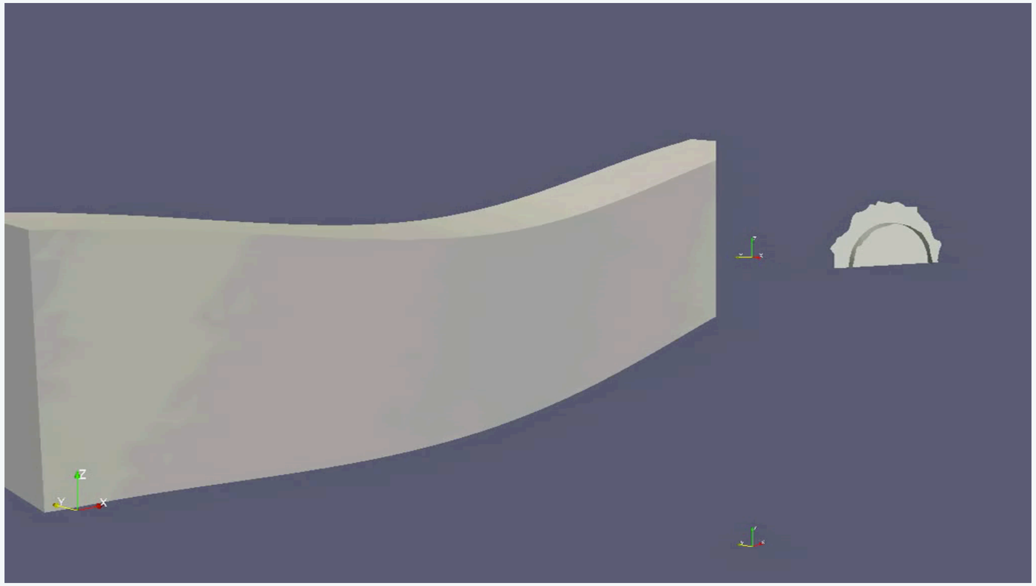
Question: How to control accuracy and simplify/avoid meshing and avoid conditioning issues?





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

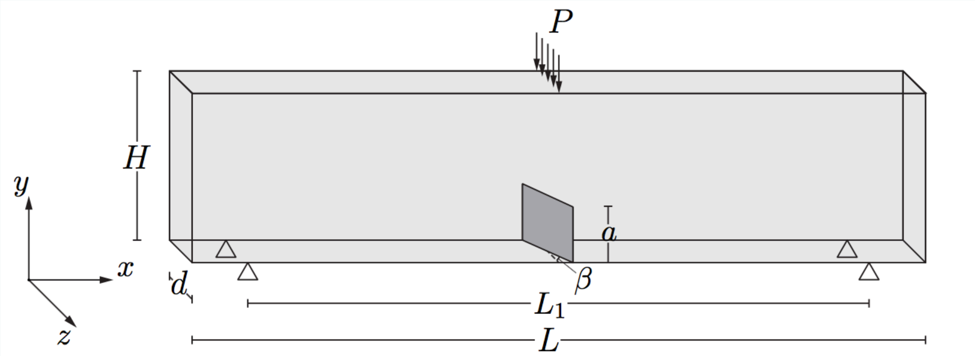
How to avoid meshing completely for crack propagation simulations?

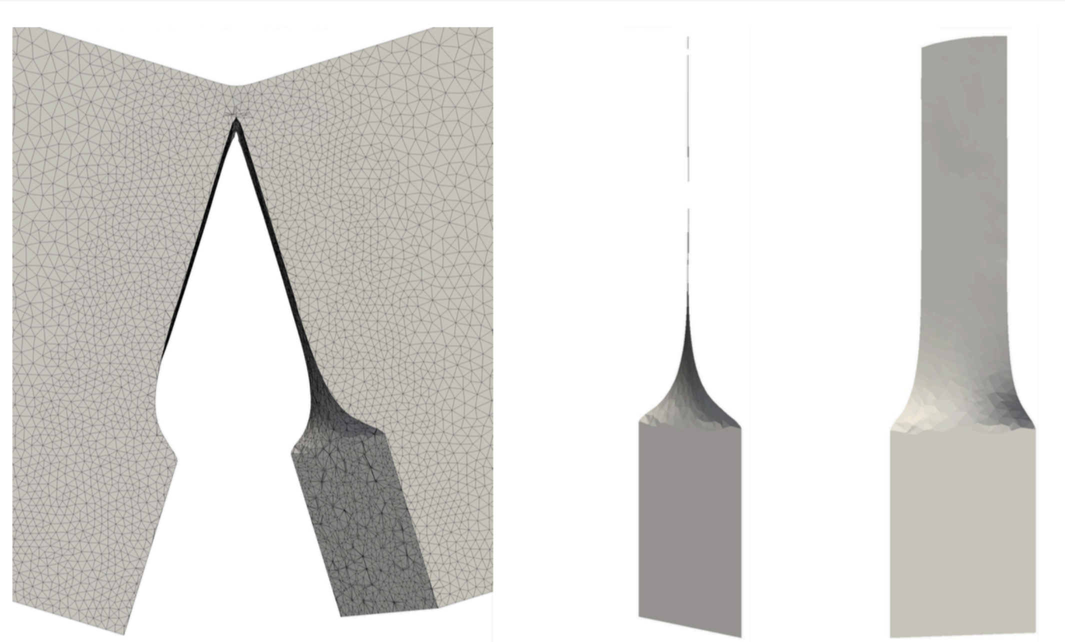


K. Agathos et al. IJNME 2016, CMAME 2016, IJNME 2017, CMAME 2017 with Eleni Chatzi and Giulio Ventura

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?

3D Orthogonalised Cut-off XFEM (Agathos)

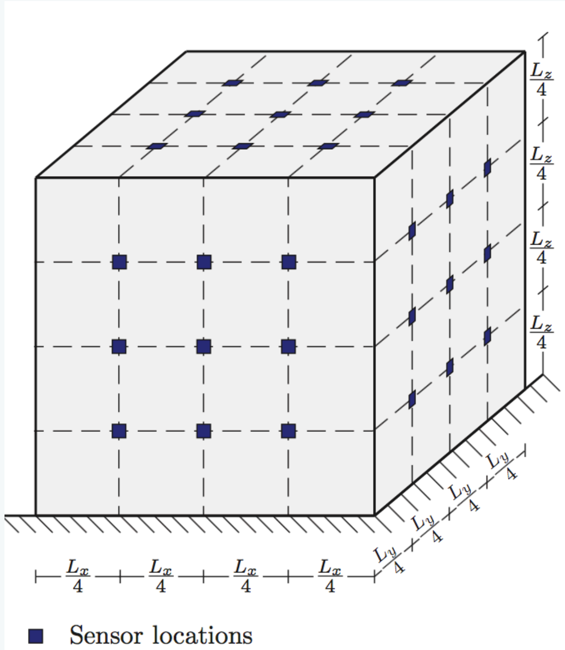


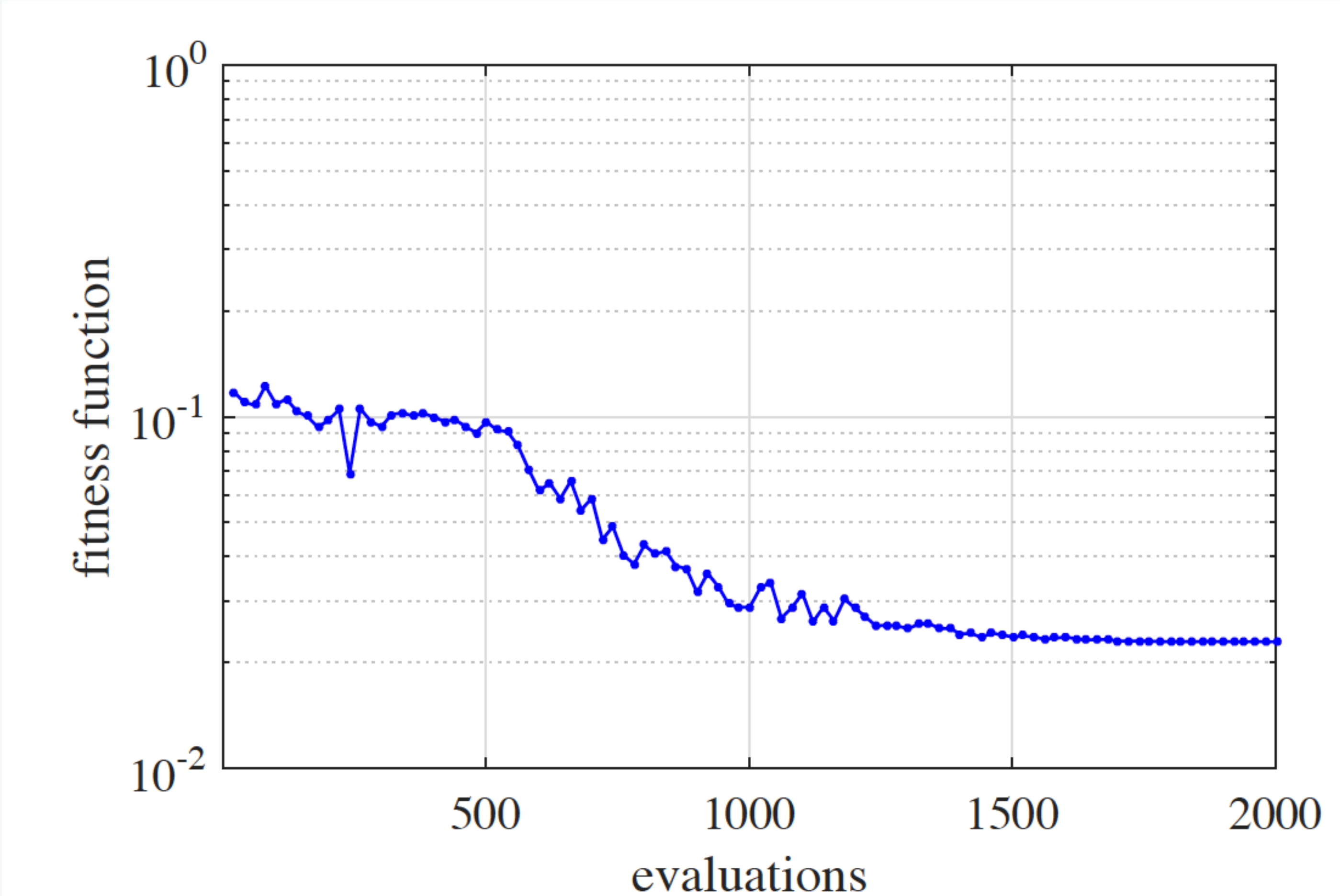


- ☑ A novel form of fixed volume enrichment
- ☑ Orthogonalisation of enrichment functions
- ☑ **Same conditioning as FEM**.
- ☑ Enables the use of higher order terms in fracture mechanics
- ☑ Equivalent accuracy to XFEM with geo. enrichment + optimal convergence

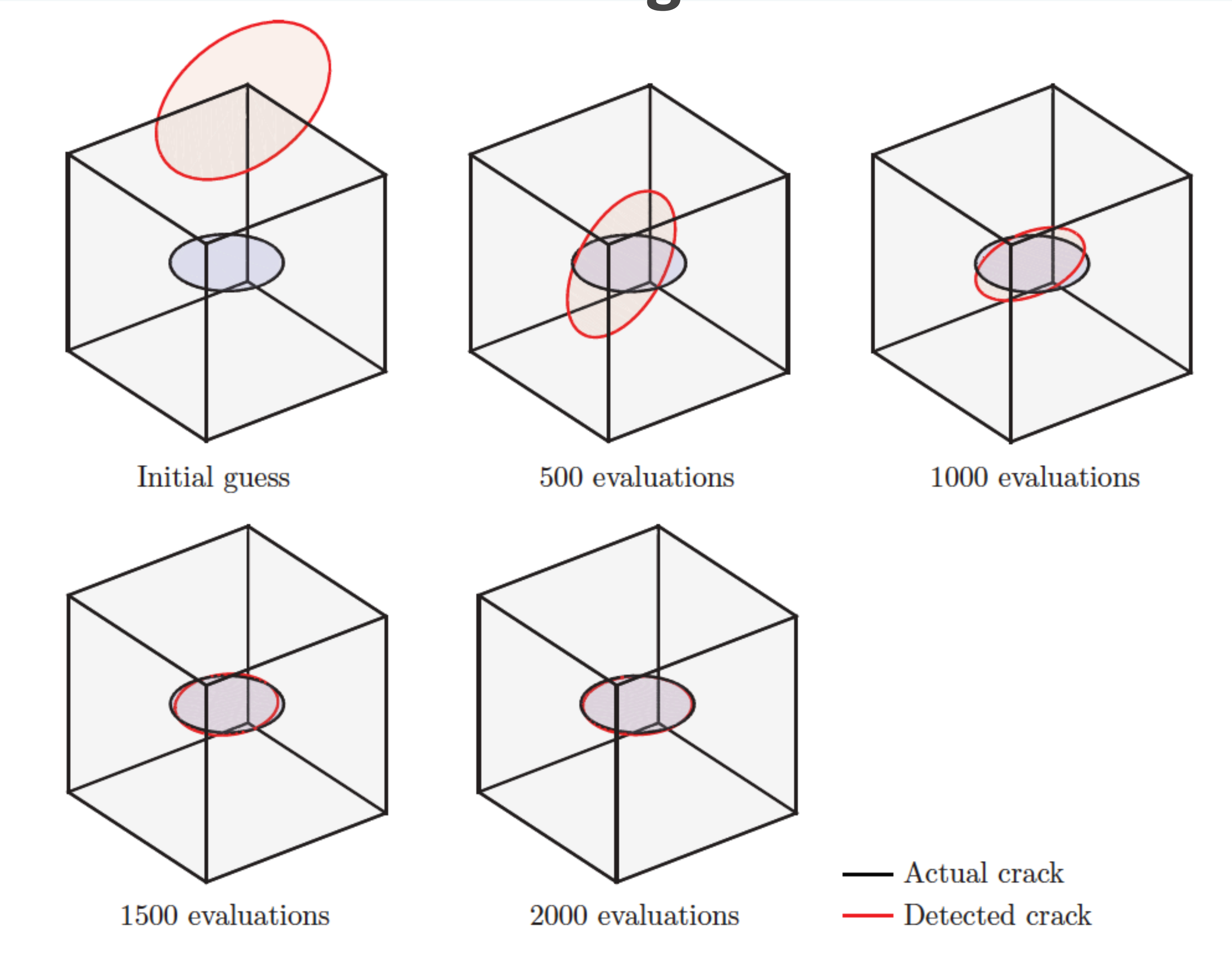
Conclusion: we can now add arbitrary numbers of enrichments and enrich over 'large' volumes of the domain.

Flaw identification





Convergence



The methodology is described in detail in these 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, 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.

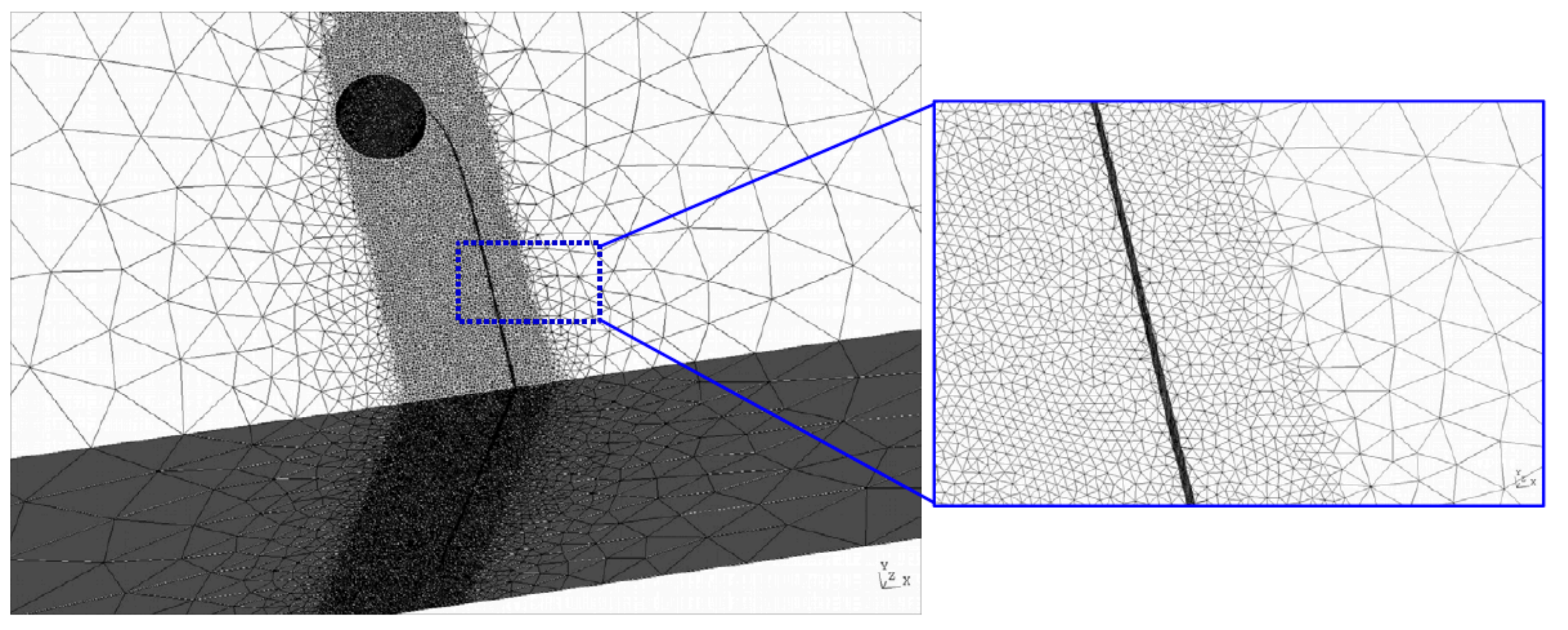
https://orbilu.uni.lu/bitstream/10993/22331/2/paper.pdf

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

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

Refine along the "expected" crack path…

(Goal oriented) adaptive computational fracture use h-refinement

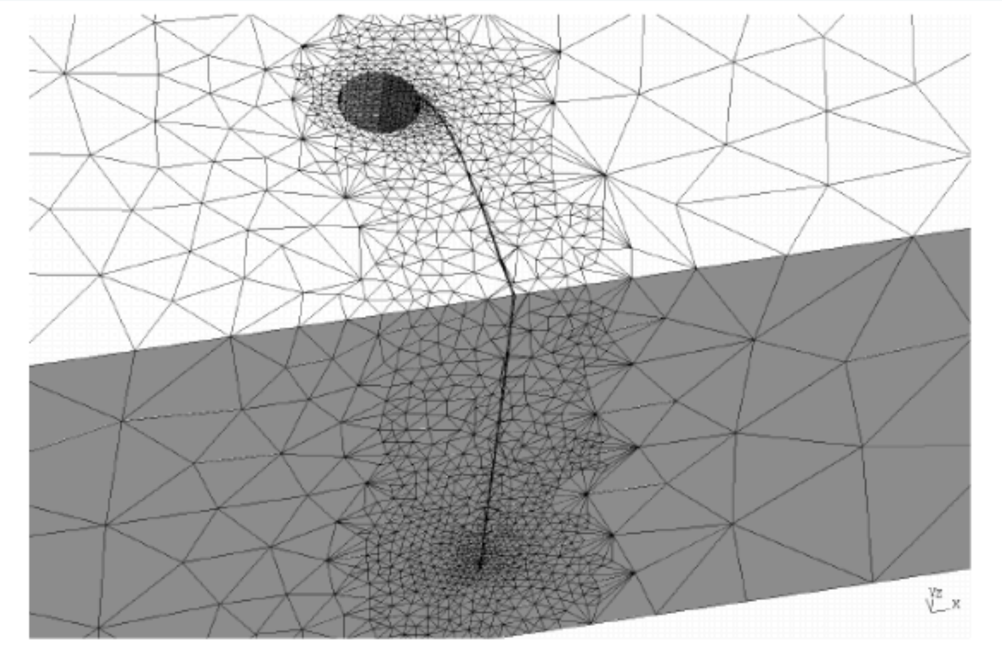


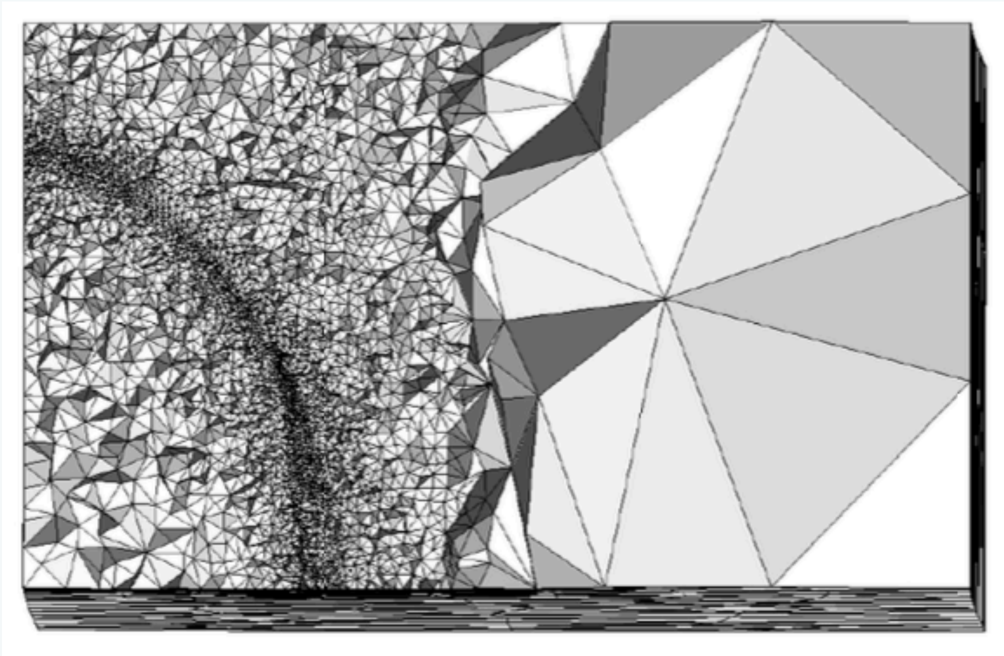
Before: mesh "finely" in the region where the crack is "expected" to propagate

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.

Much better… adapt the discretisation locally

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.

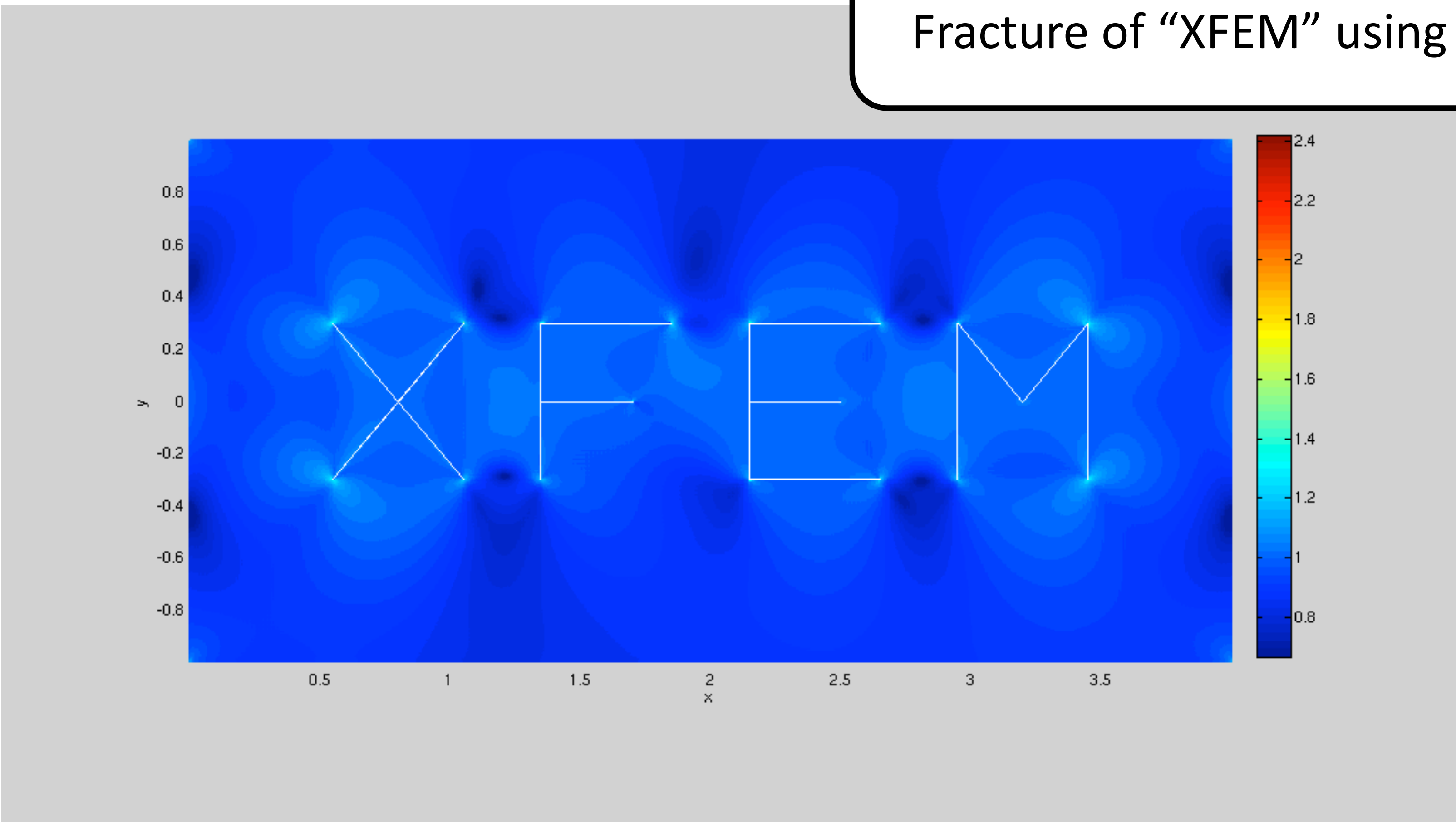
Partial Conclusions

- 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 interfaces?….

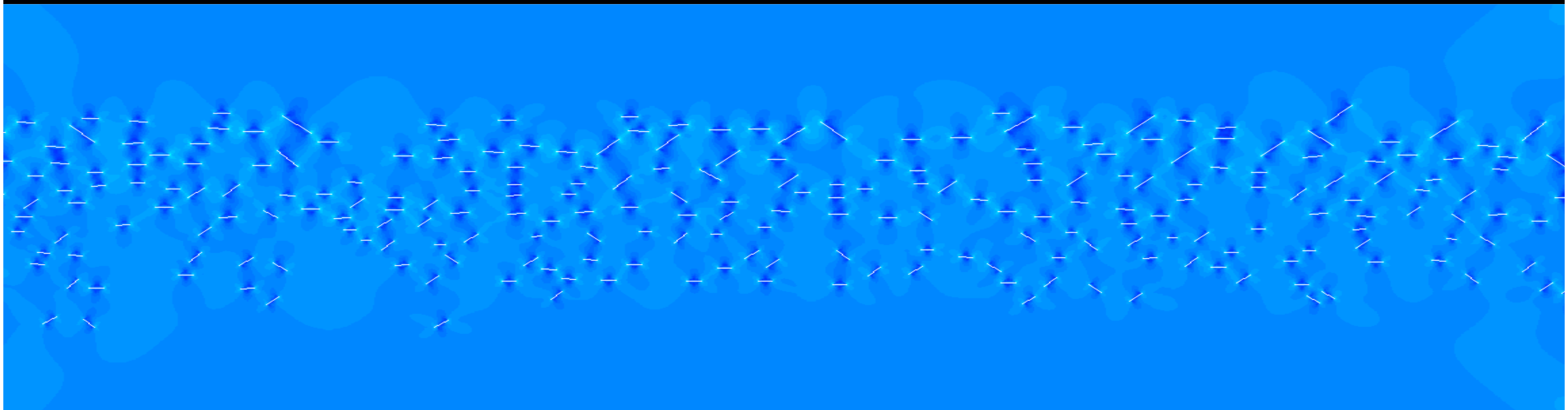
Extended Finite Element Method (XFEM)

Fracture of "XFEM" using XFEM



Case study II. Plate with 300 cracks vertical extension BCs

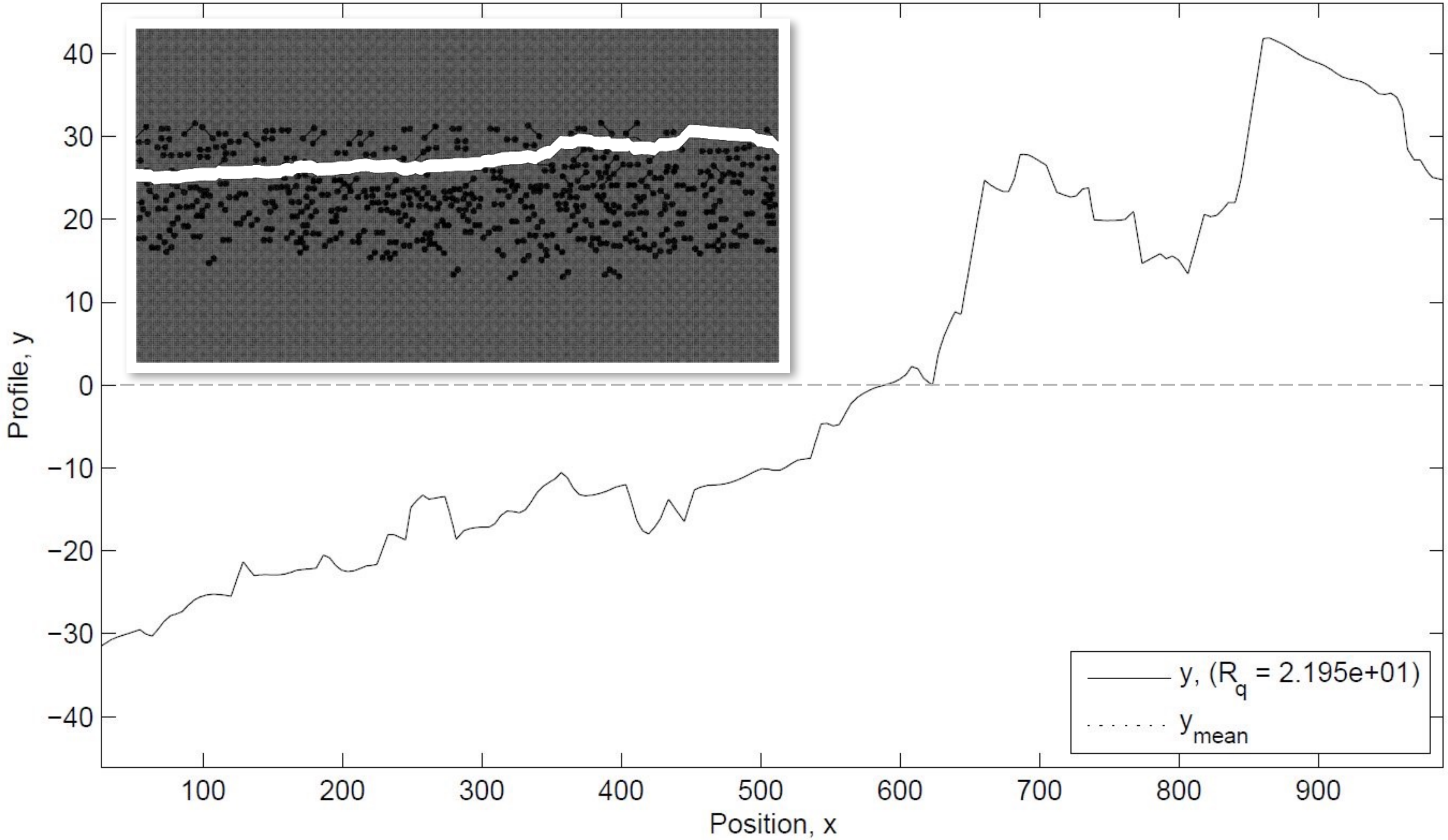
Energy-minimal crack growth using XFEM



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

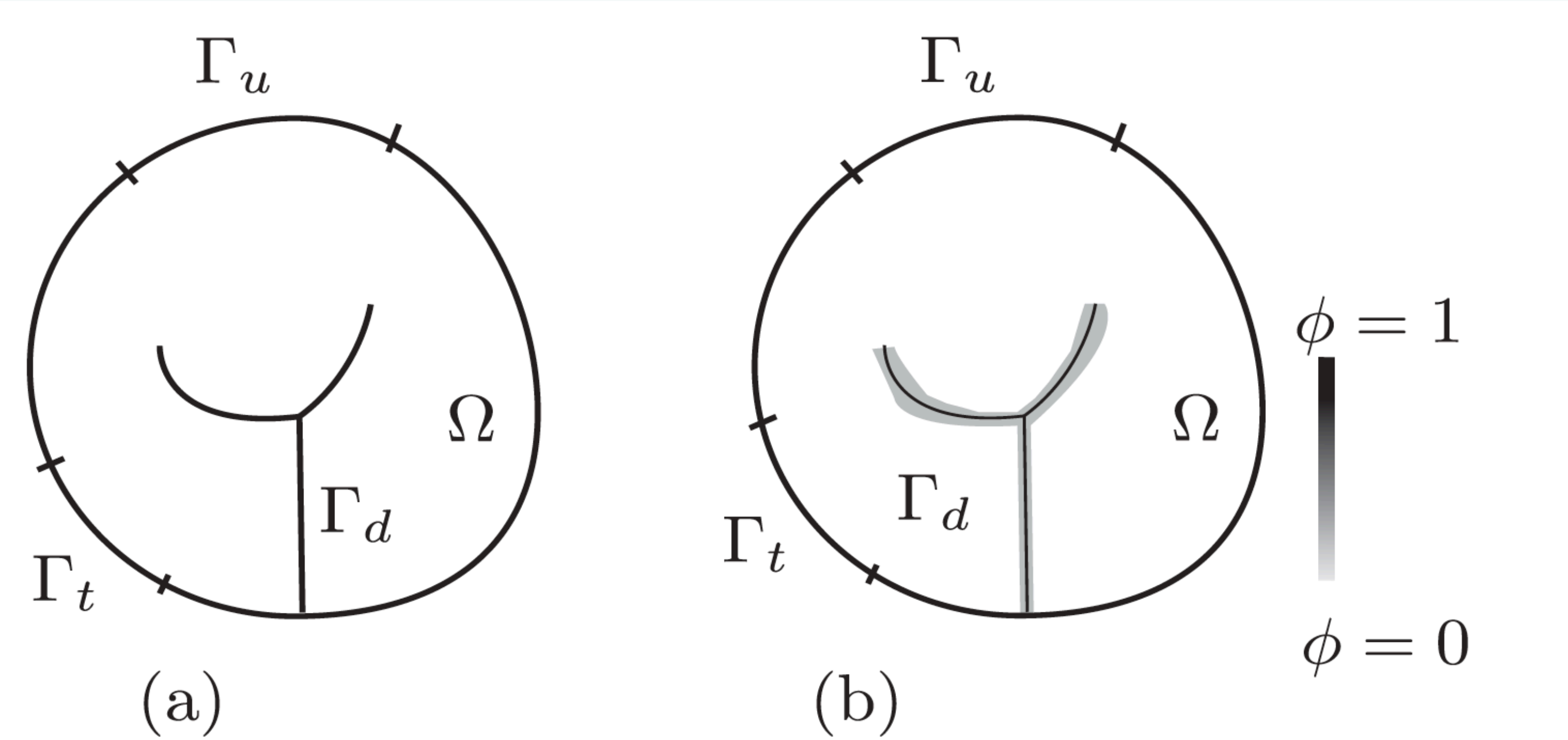
Vertical extension of a plate with 300 cracks

Post-split roughness



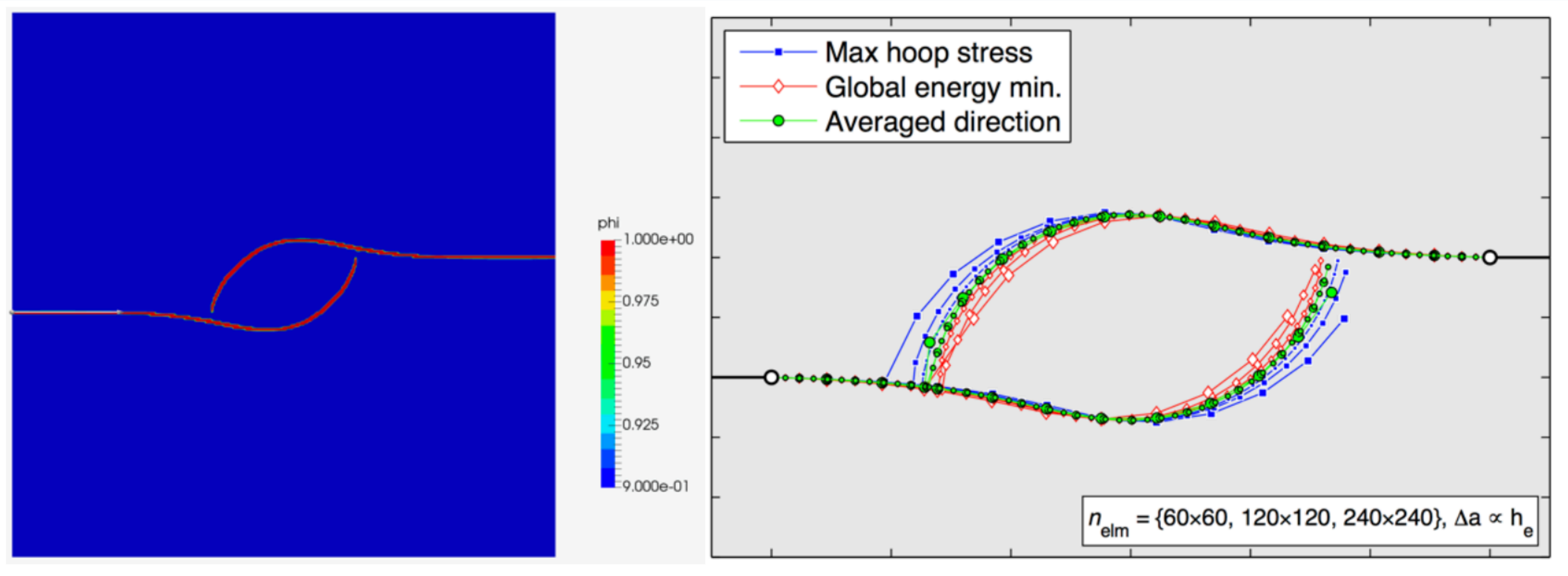
More cracks?... 3D? ...

Phase field/thick level sets



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

Energy minimal XFEM vs. Phase field



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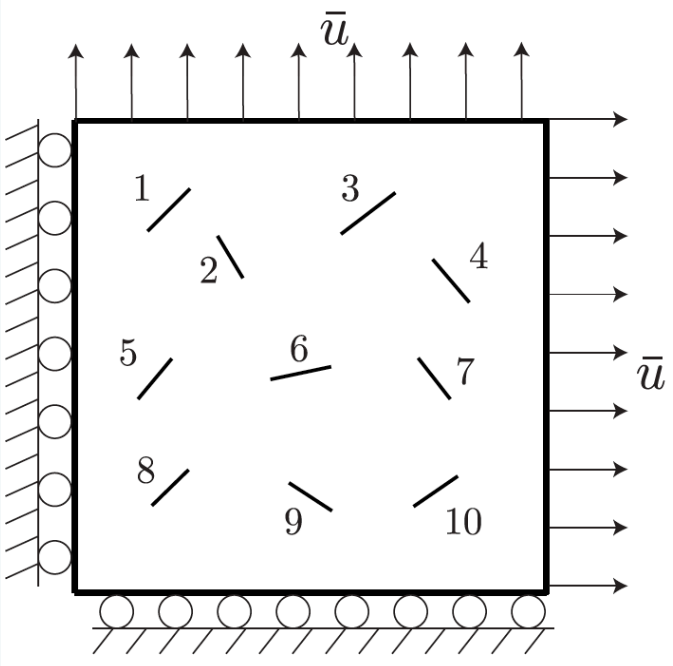

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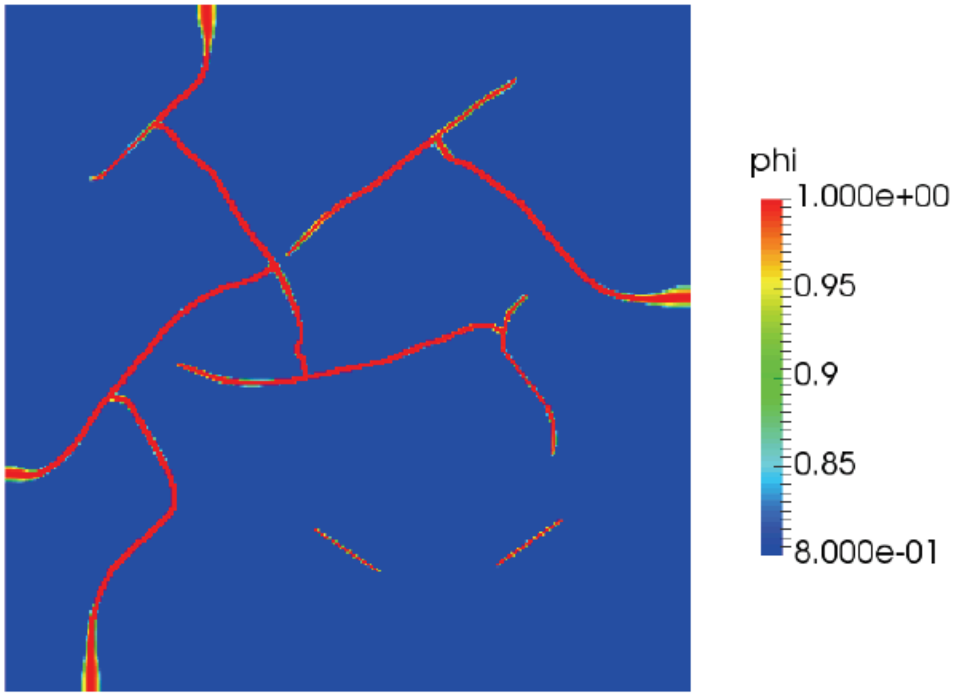

phi
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0.9
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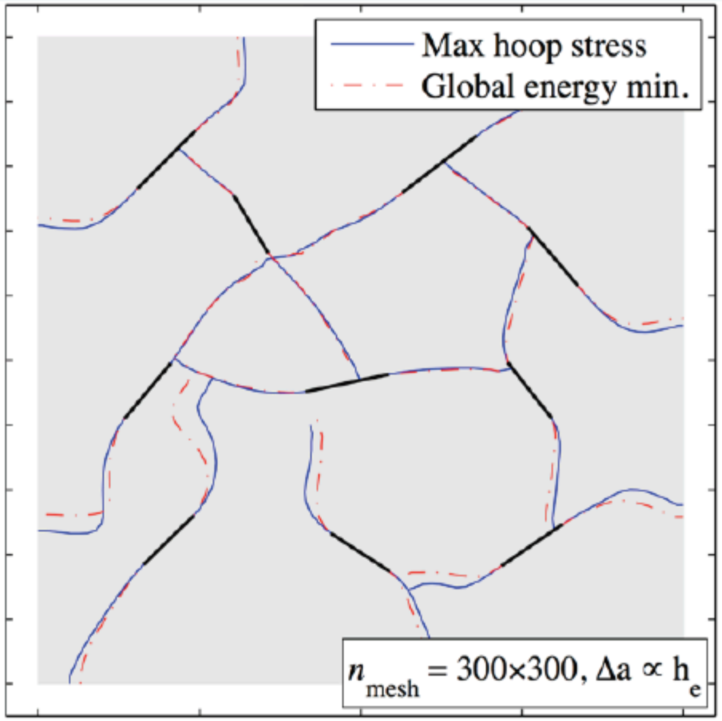
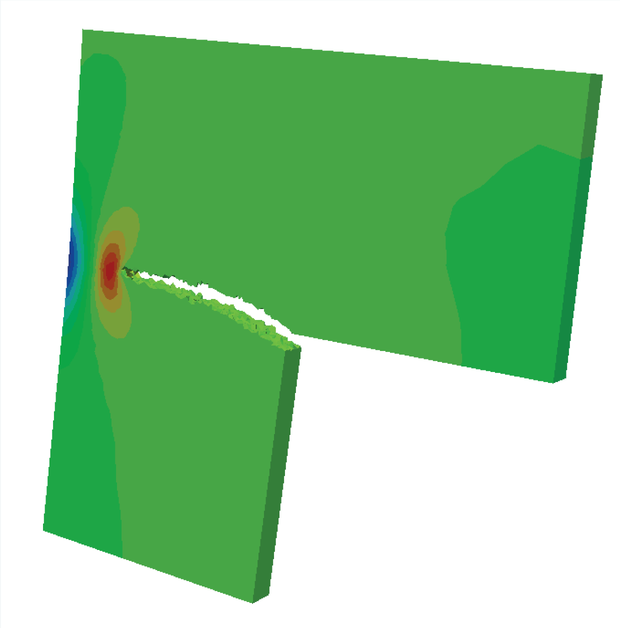
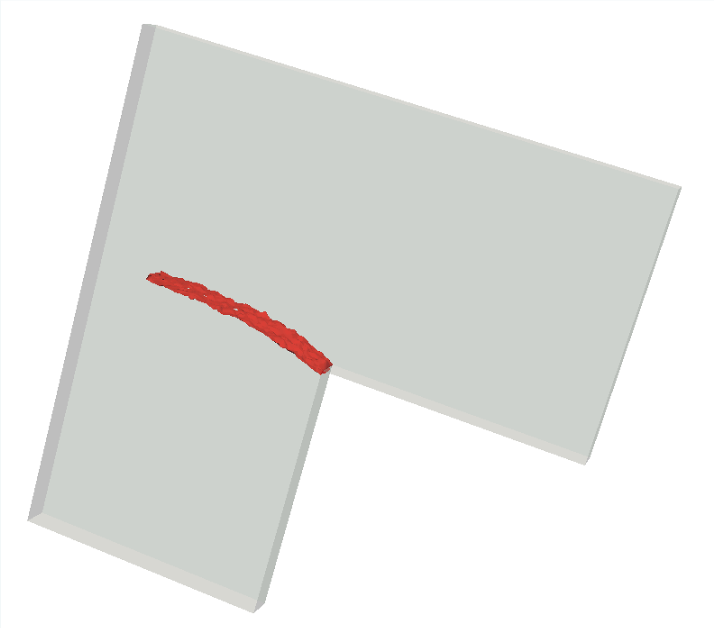
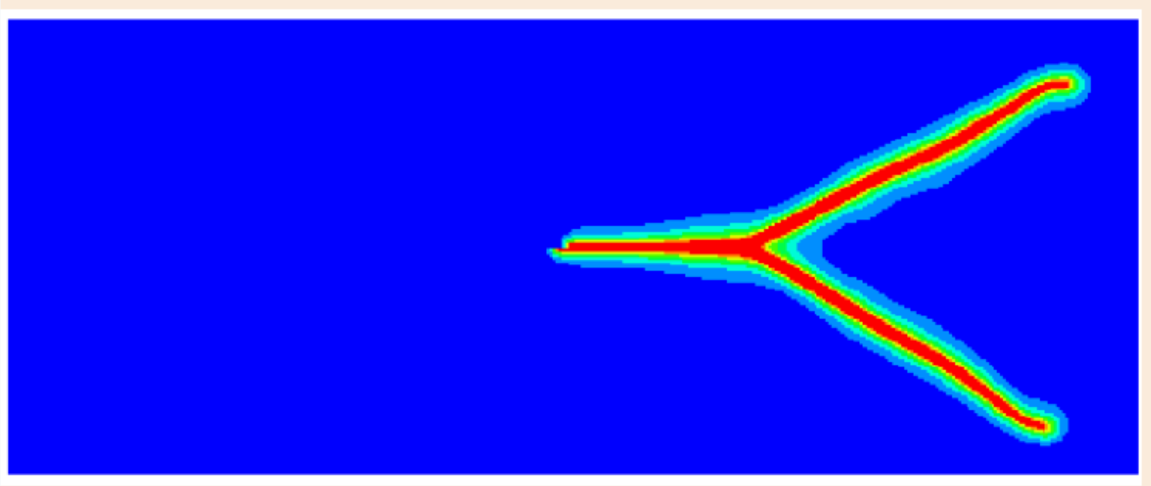
8.000e-01



Max hoop stress
Global energy min.
$n_{mesh} = 300\times300$, $\Delta a \propto h_e$







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Outline

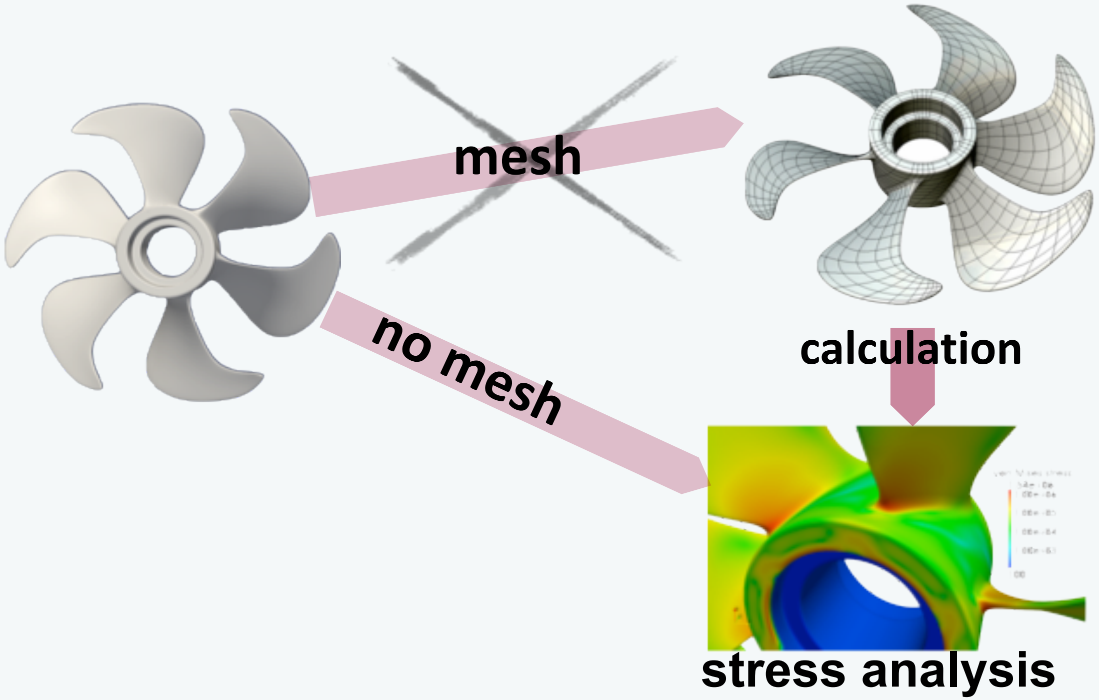
Part I. Computational approaches for industrial-scale fracture mechanics simulations and surgical simulation

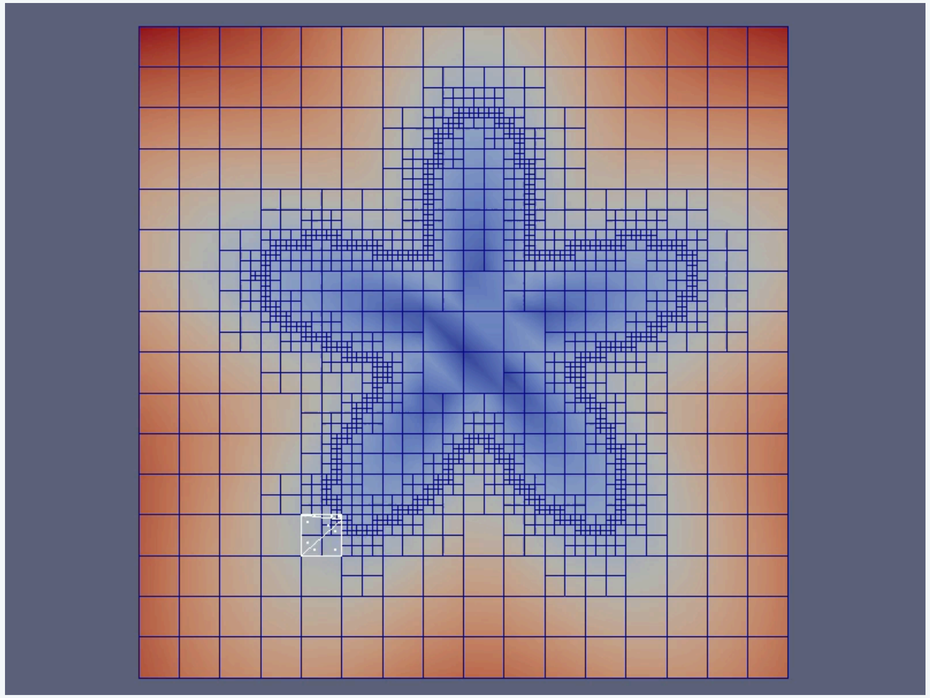
- Adaptive partition of unity enrichment
- (Multi-scale fracture)
- **Adaptivity in IGA through Geometry-Independent Field approximaTion**

Part II. Model Selection and Uncertainties in surgical simulation (quick introduction)

Handling (complex) interfaces numerically

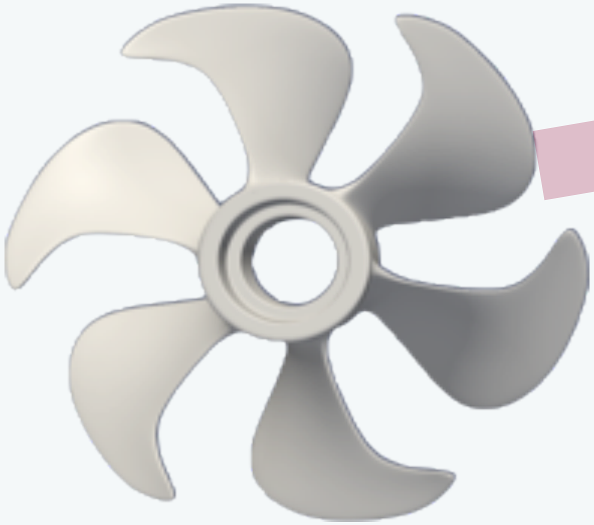
Coupling, or decoupling?



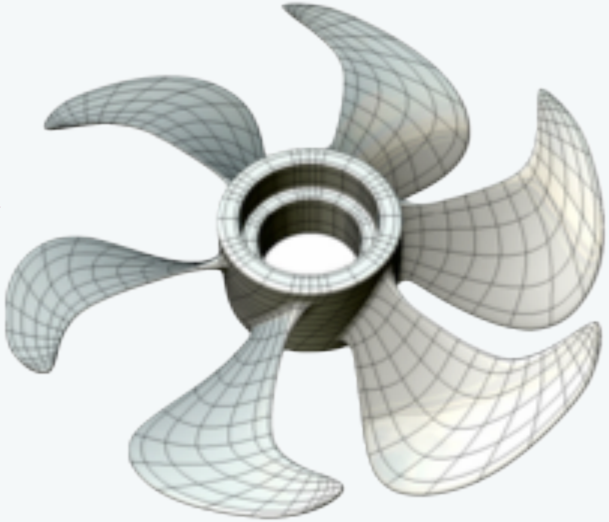


Question: When are we better off coupling/decoupling the geometry from the field approximation?

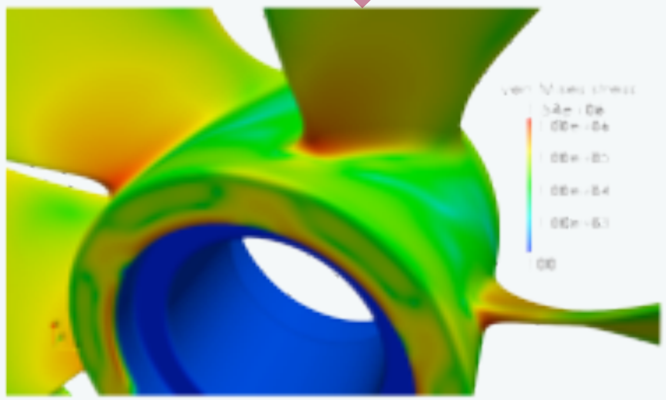
Isogeometric analysis



mesh

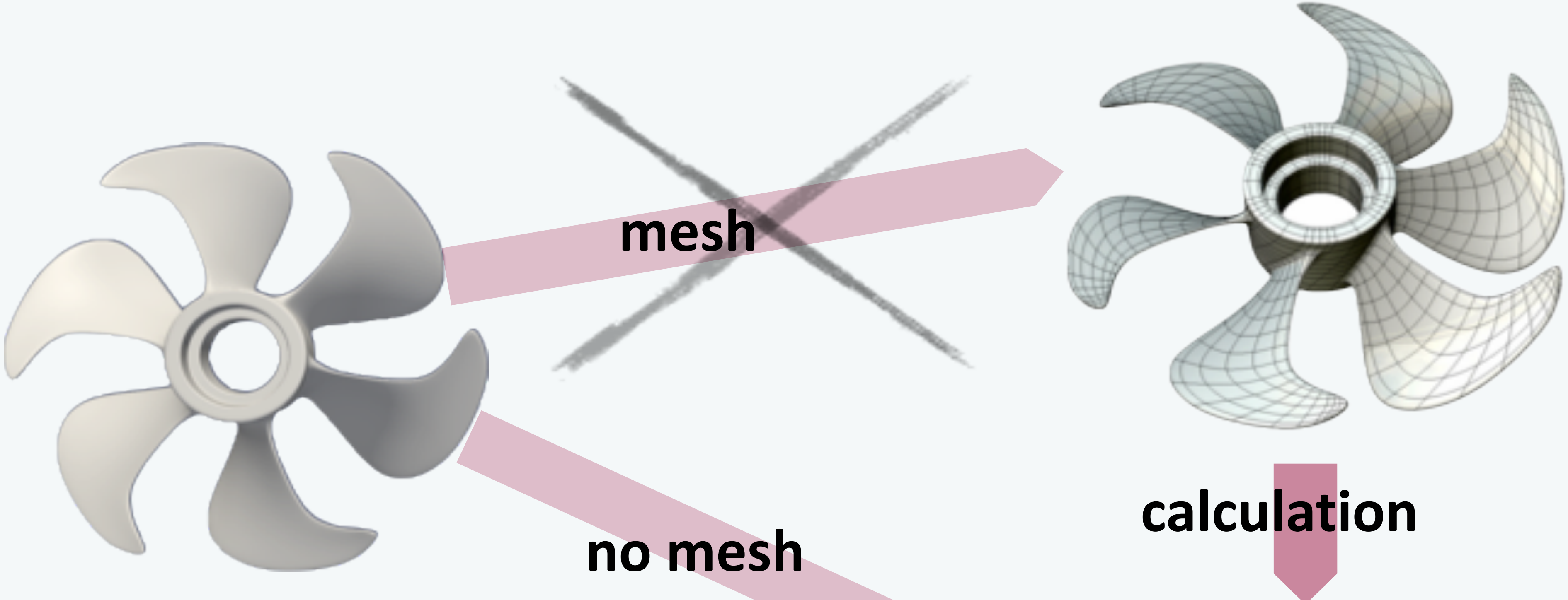


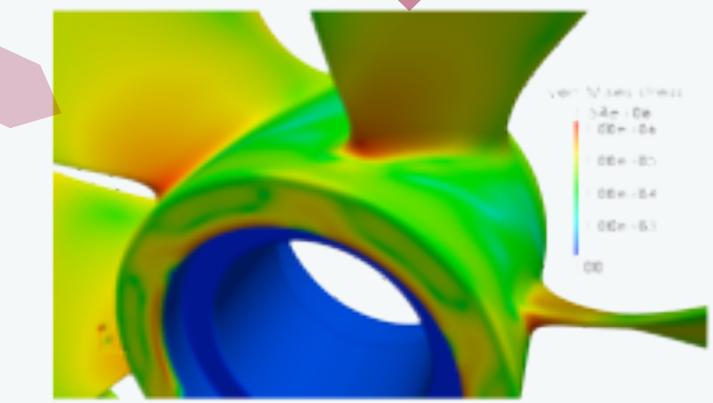
calculation



stress analysis

Isogeometric analysis

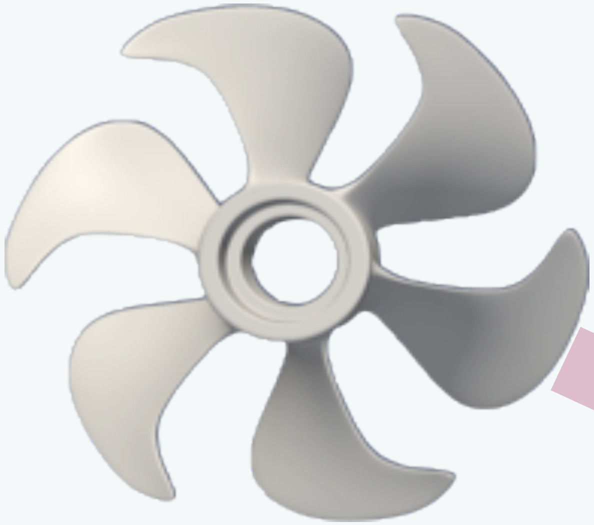




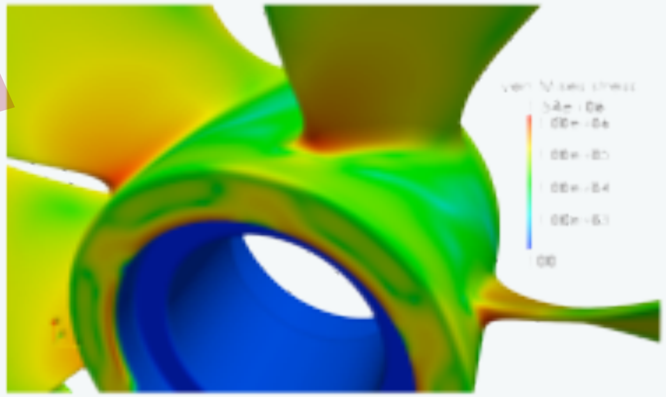
stress analysis

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



direct calculation

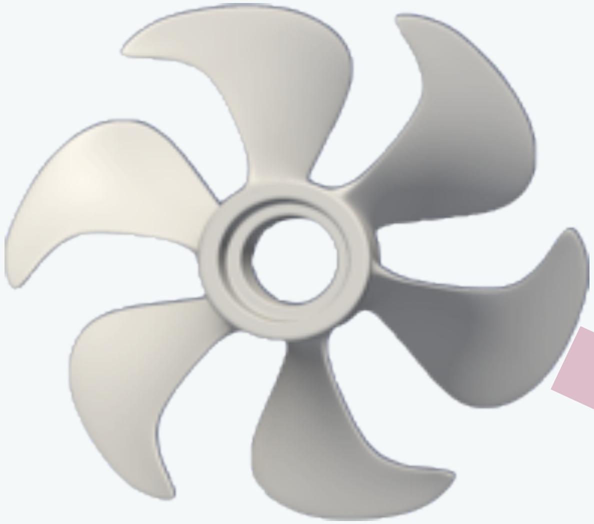


stress analysis

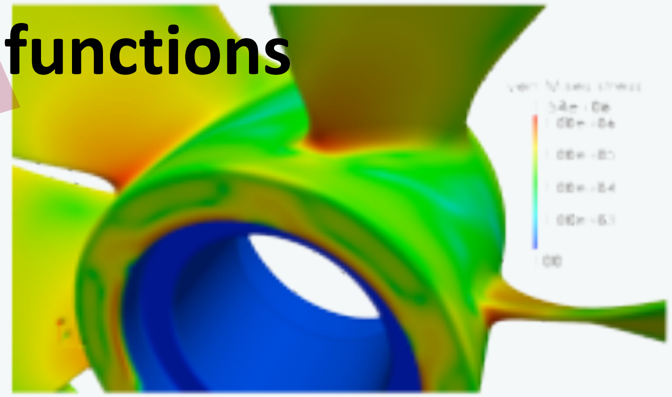
Idea: Hughes et al. 2005. Do not discard geometric information by creating a mesh. Use the CAD information to solve the finite element problem.

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.

Isogeometric analysis: limitations

Geometry

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

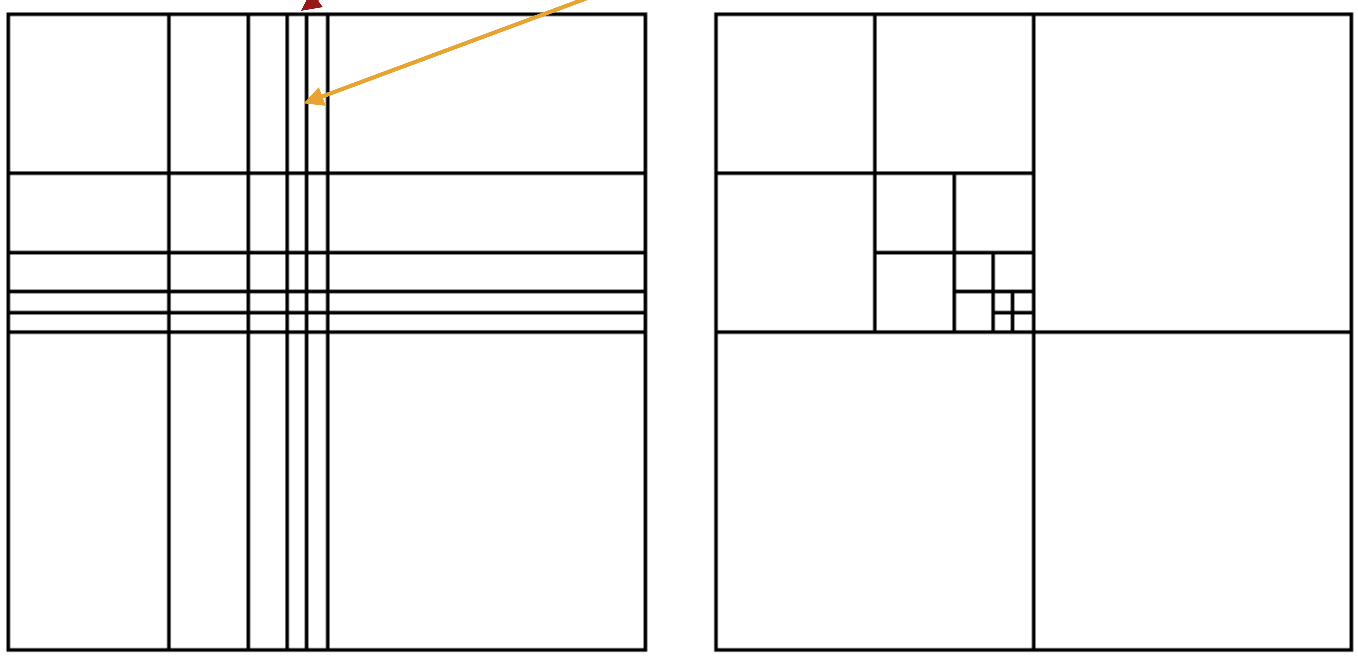
Adaptivity

- [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 IGA

Using NURBS,

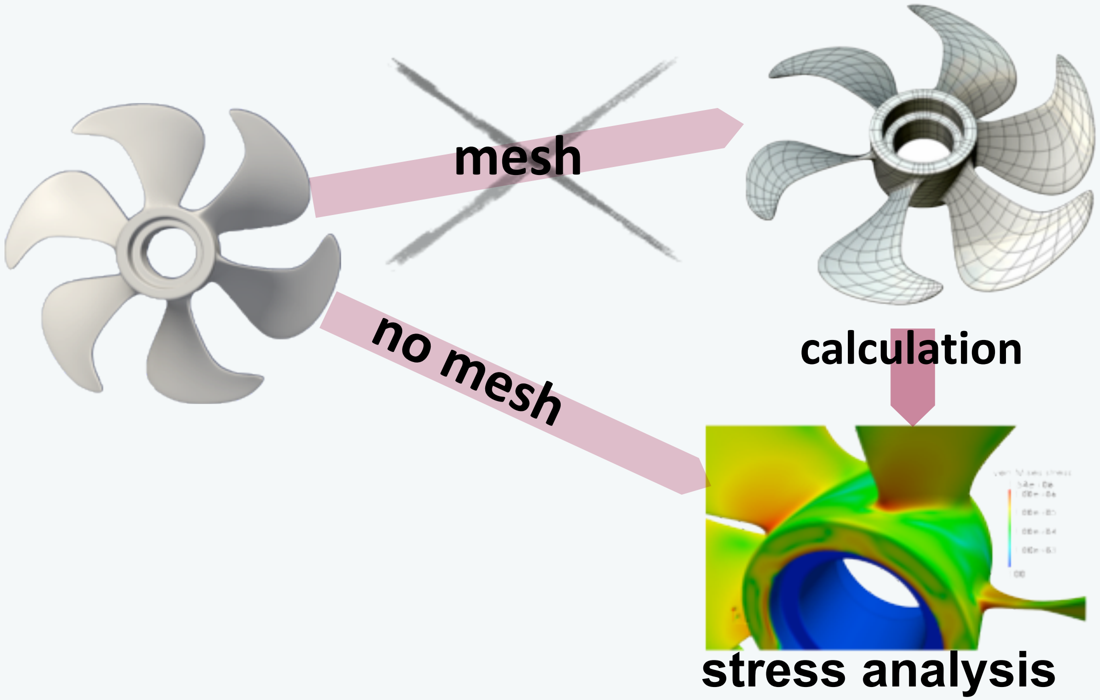
Refinement in one direction forces refinement in the other



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

Handling (complex) interfaces numerically

Coupling



Question: How can we fully benefit from the "IGA" concept?

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

Handling (complex) interfaces numerically

Coupling geometry and field approximation

Question: How can we fully benefit from the "IGA" concept?

☑ Refine the field independently from the geometry

Isogeometric Finite Elements

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

Geometry Independent Field approximaTion (GIFT)

☑ Super/Sub-geometric

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

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

Handling (complex) interfaces numerically

Coupling geometry and field approximation

Question: How can we fully benefit from the "IGA" concept?

☑ Refine the field independently from the geometry

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

Permalink: http://hdl.handle.net/10993/31469 **See Keynote presentation by Elena Atroshchenko yesterday**

Parallel Session 2B.2: Numerical Methods and High Performance Computing (14:45 — 17:40)

Location: Board Room 1, Sai Gon-Phu Quoc Resort

Time	Content (Title)	Speaker	Affiliation
Session Chairs: Jaehong Lee & Seiya Hagihar			
14:45 — 15:15	Geometry Independent Field approximation (GIFT): pairing CAD geometry with PHT-splines field	Elena Atroshchenko (Keynote)	University of Chile, Santiago, 8370448, Chile

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

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

Geometry Independent Field approximaTion (GIFT)

Conclusions

- Tight link between CAD and analysis
- The same basis functions, which are used in CAD to represent the geometry, are used in the IGA as shape functions to 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…)

Outline

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- (Multi-scale fracture)
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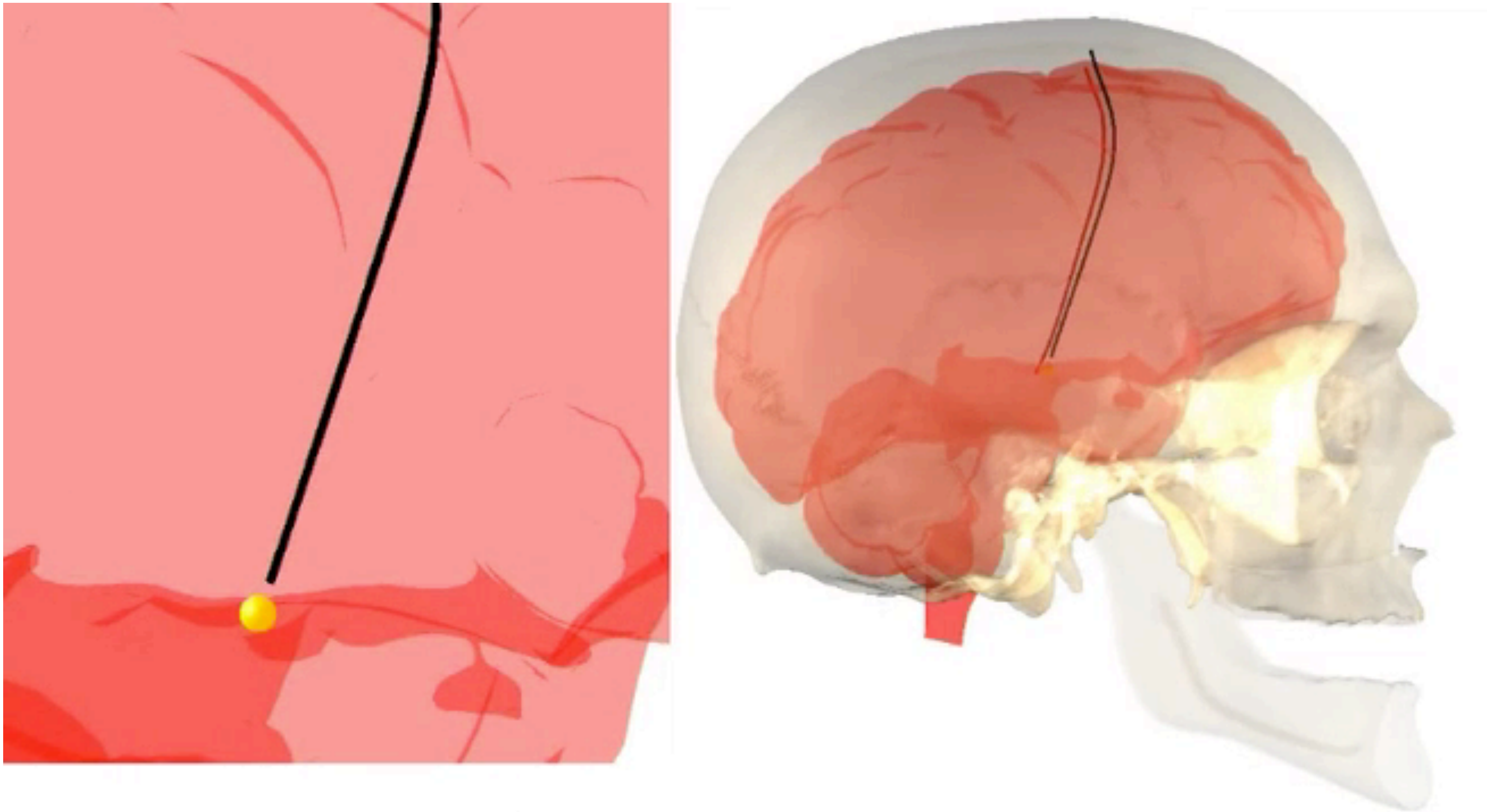
Part II. Model Selection and Uncertainties in surgical simulation (quick introduction)

Part II. Controlling modelling errors

Forward and Inverse

Uncertainty Quantification

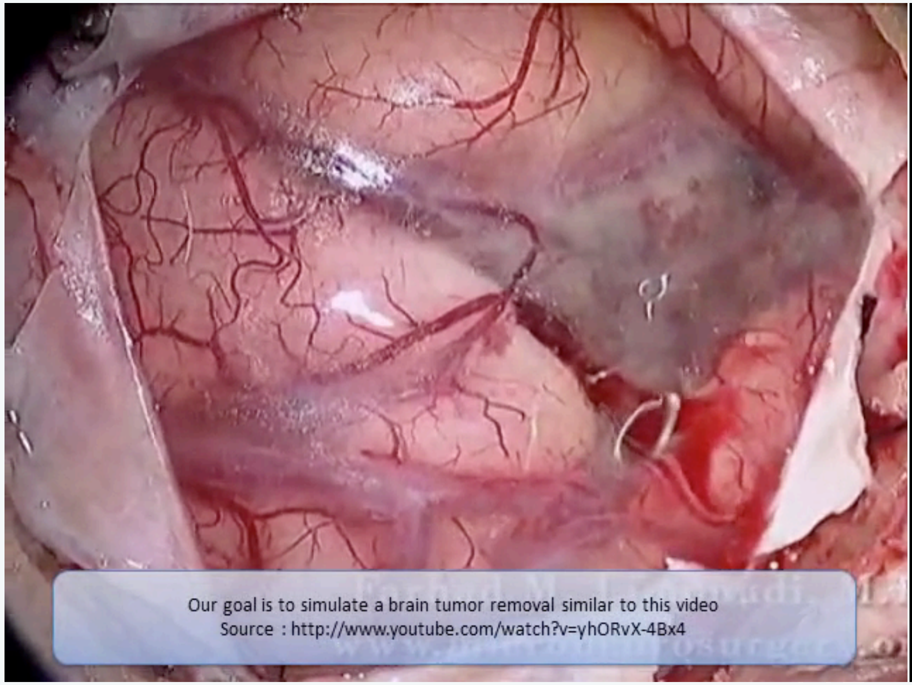


Deep-brain stimulation

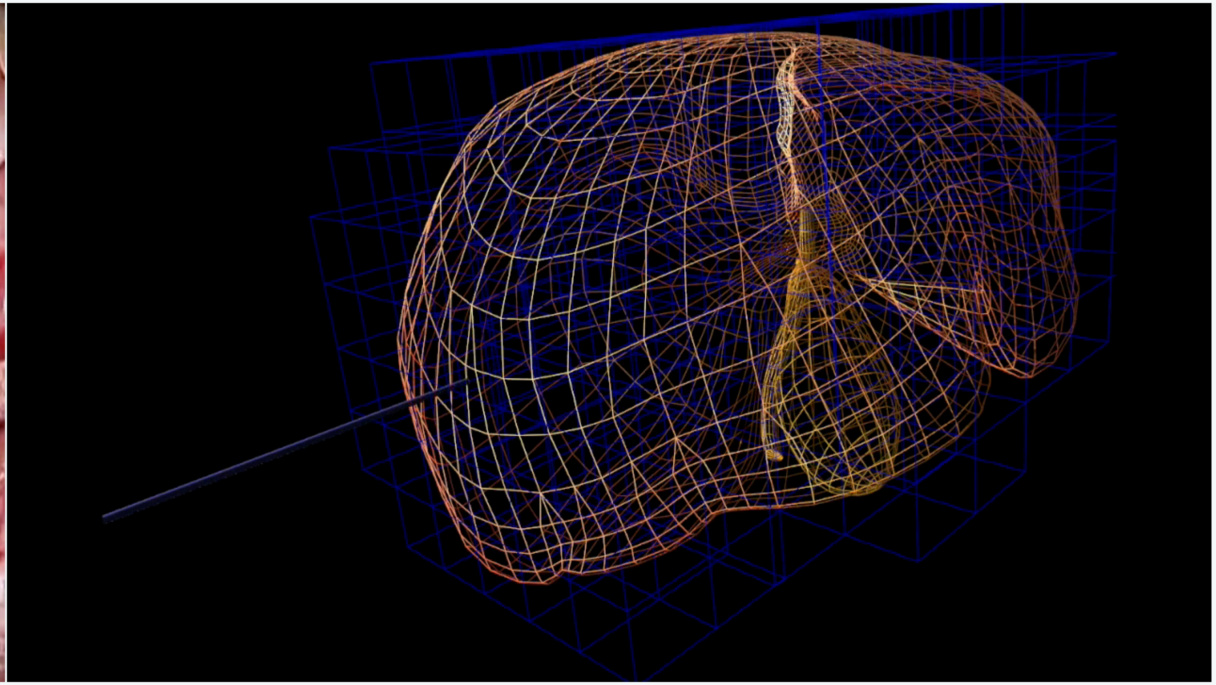
Courtesy Alexandre Bilger, post-doc in the Legato team, PhD thesis, Inria, 2014

Interfaces in surgical simulation

Cutting and Needle Insertion



H. Courtecuisse et al. Medical Image Analysis, 2014

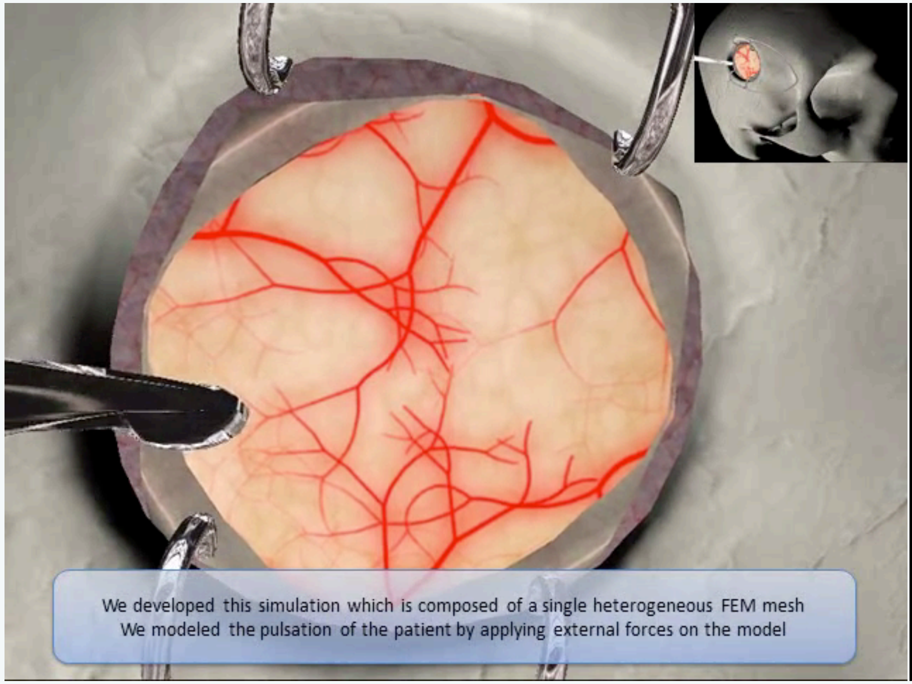


P.H. Bui et al. IEEE T. Biomed Eng. 2017 & Frontiers in Surgery, 2017

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

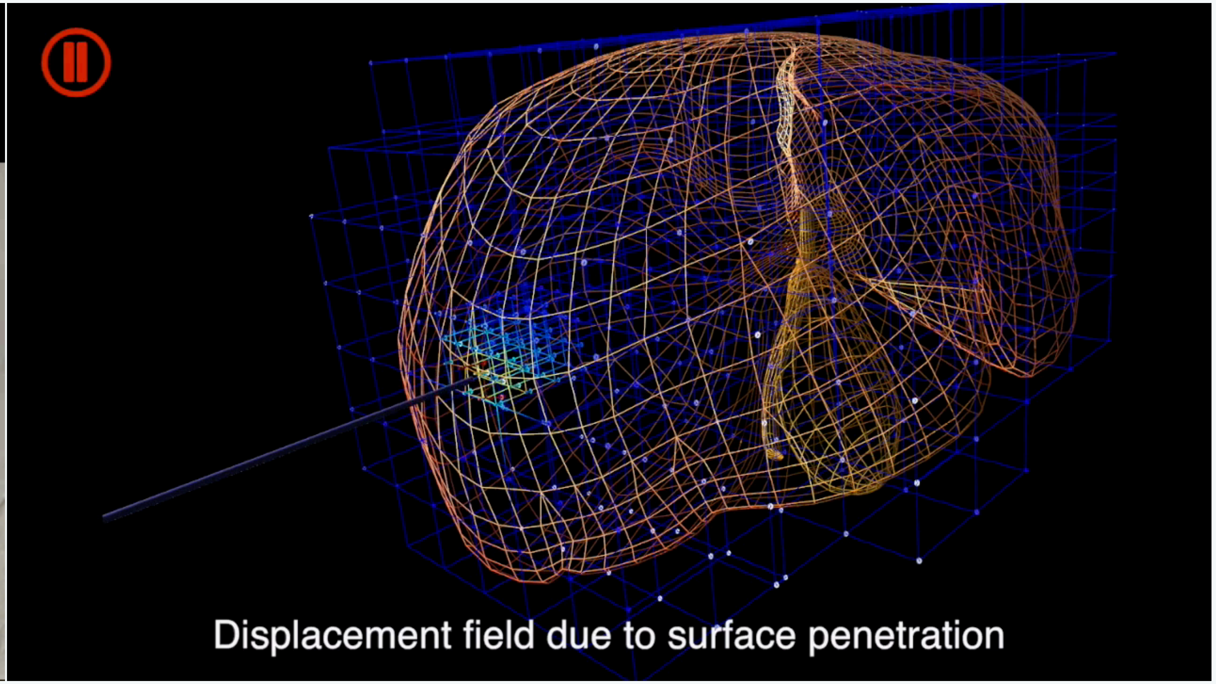
Interfaces in surgical simulation

Real-time adaptive methods for 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?

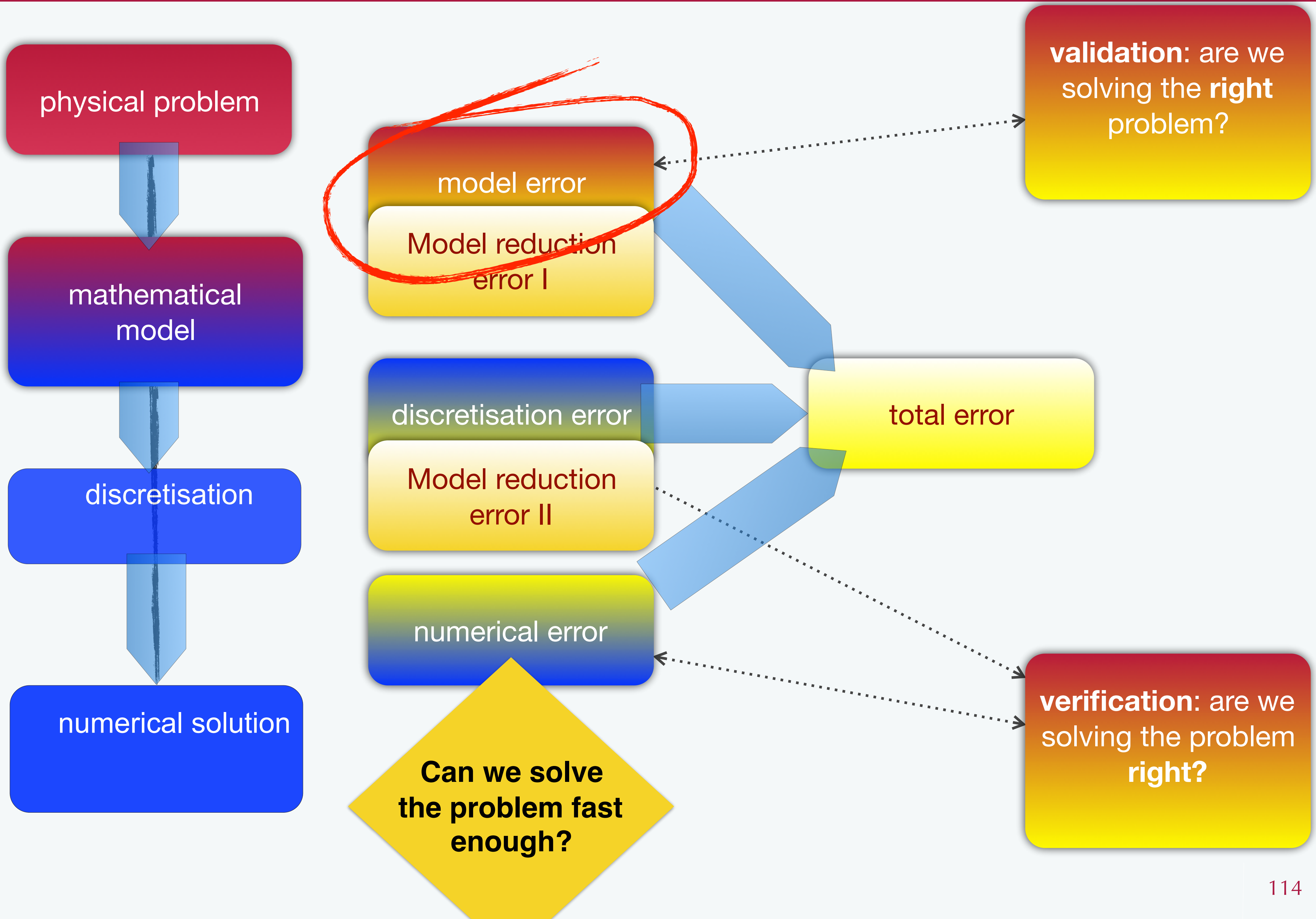


P.H. Bui et al. IEEE T. Biomed Eng. 2017 & Frontiers in Surgery, 2017

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

Modelling and simulation

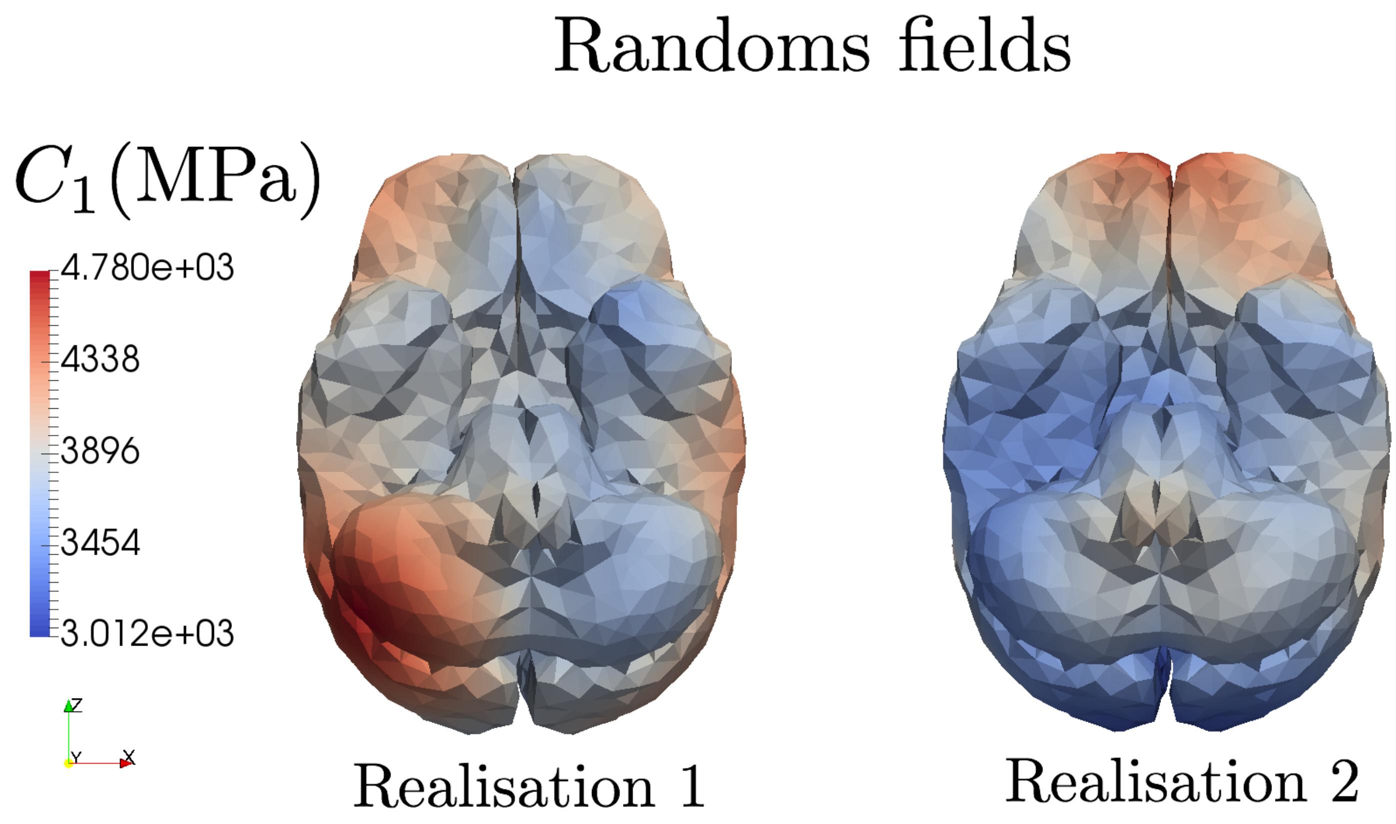


Questions asked

- What is the influence of uncertainties in material parameters?
- What probability distributions are suitable for material parameters?
- What is the best model given experimental data?
- Can we update models and parameters in a patient specific way using (real-time) experimental data?

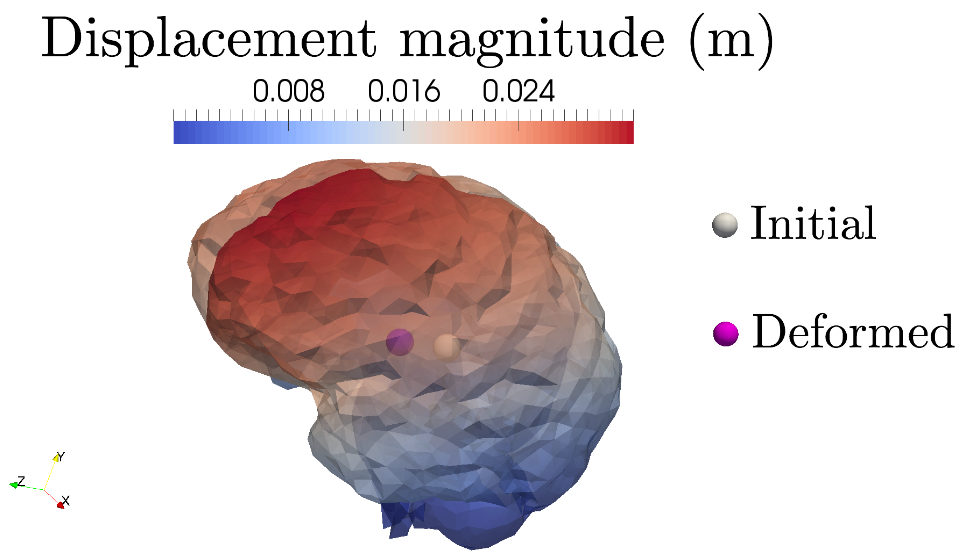
Random Fields

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

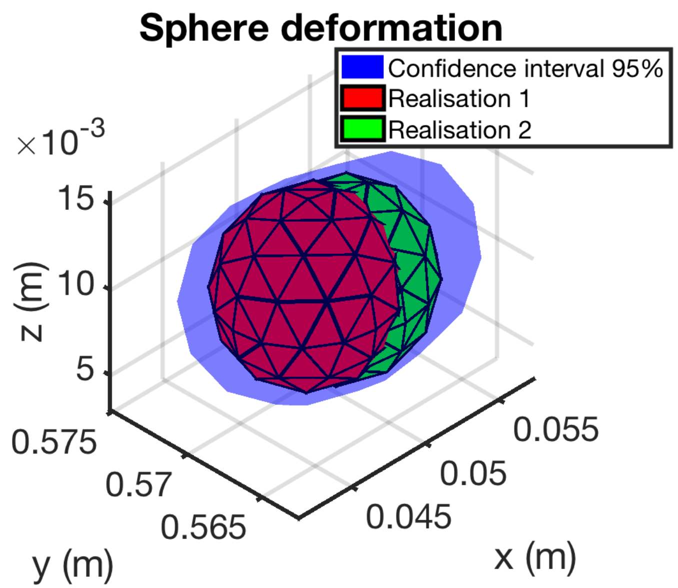


Two realisations of RF, with a log-normal distribution, for the parameter C_1 (in MPa).

Stochastic FE analysis of brain deformation
Numerical results (8 RV, Holzapfel model)



Brain deformation with random parameters
1 MC realisation.



Confidence interval 95%
MC simulations.

Numerical results: convergence

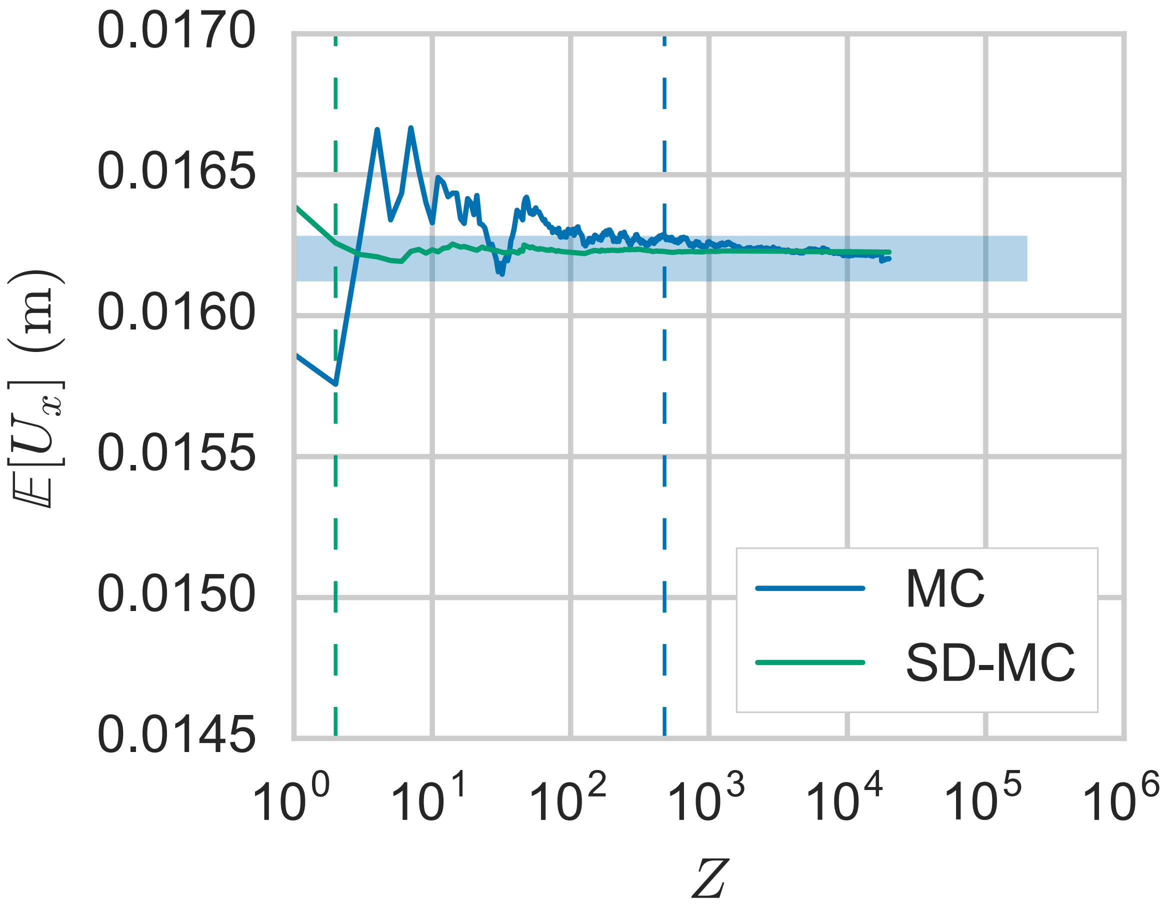
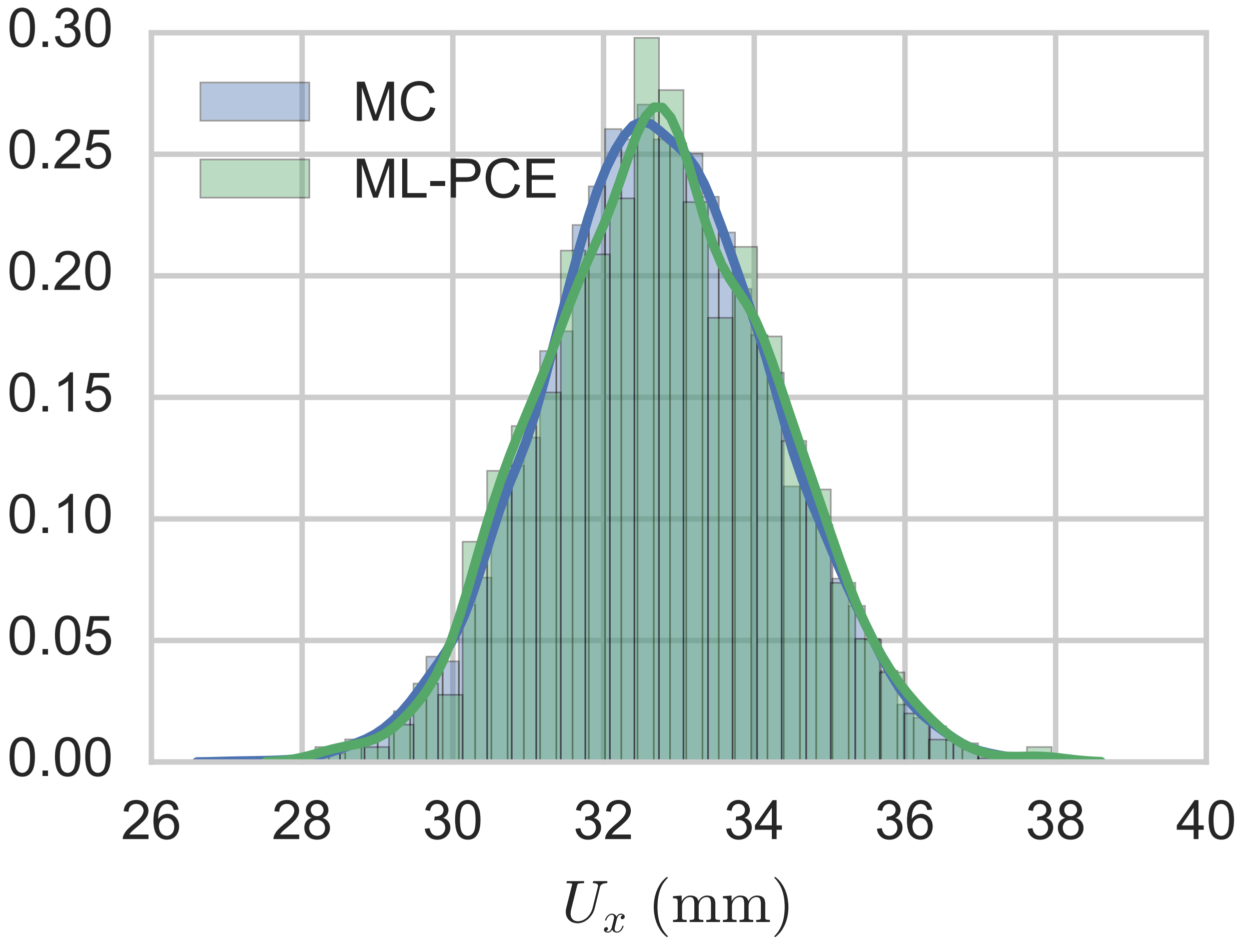


Fig. Center of the sphere: expected value of the displacement in the x direction as a function of Z.

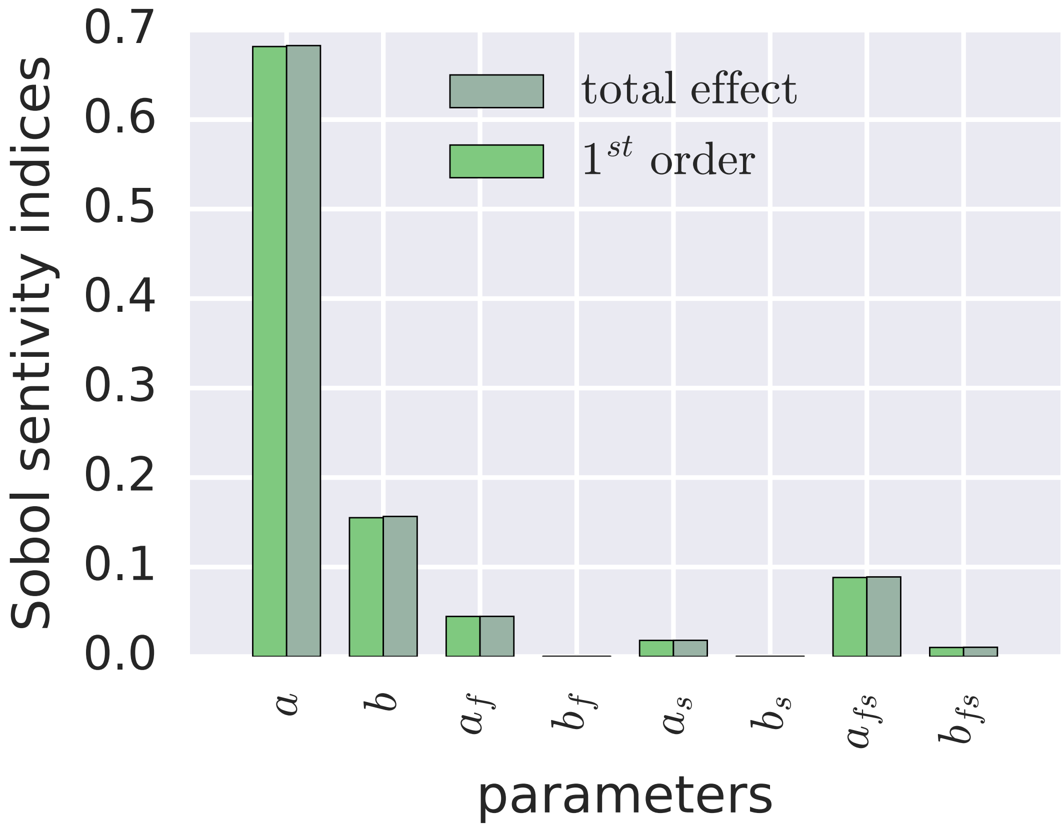
Numerical results (8 RV, Holzapfel model)
ML Monte-Carlo technique: ML-PCE



Histogram (MC and MC-PCE methods).

Global sensitivity analysis

- Sobol sensitivity indices [Sobol 2015, Saltelli 2002]

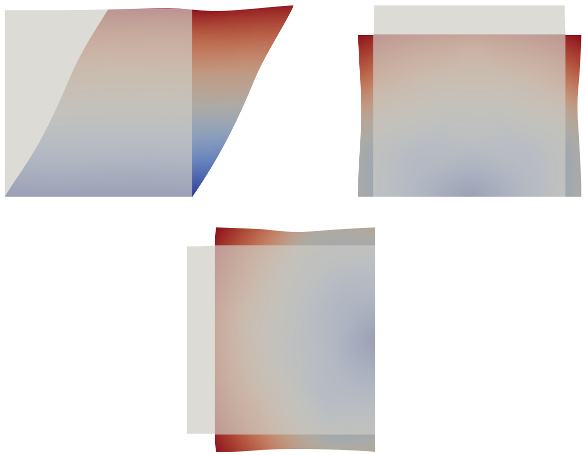


Quantity of interest: displacement magnitude of the target.

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

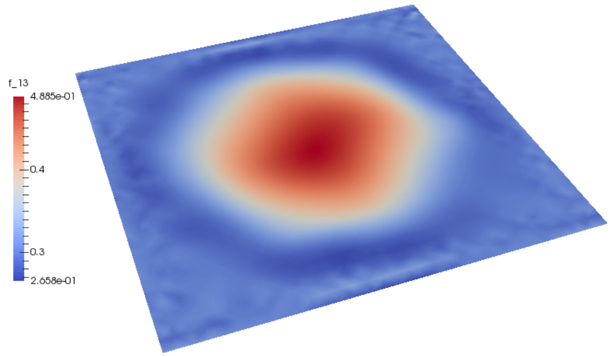
Q: Which parameters am I most uncertain about?

Bayesian testbed for characterising hyperelastic materials

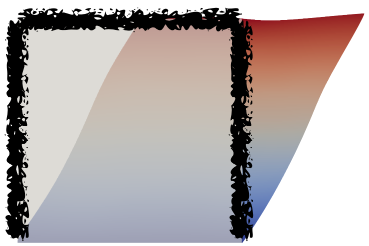


Experimental results

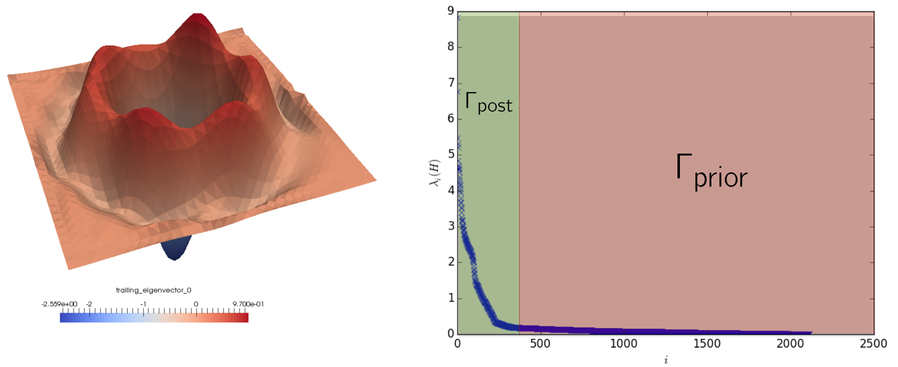
$$\pi_{\text{posterior}}(x \mid y) \propto \pi_{\text{likelihood}}(y \mid x)\pi_{\text{prior}}(x)$$



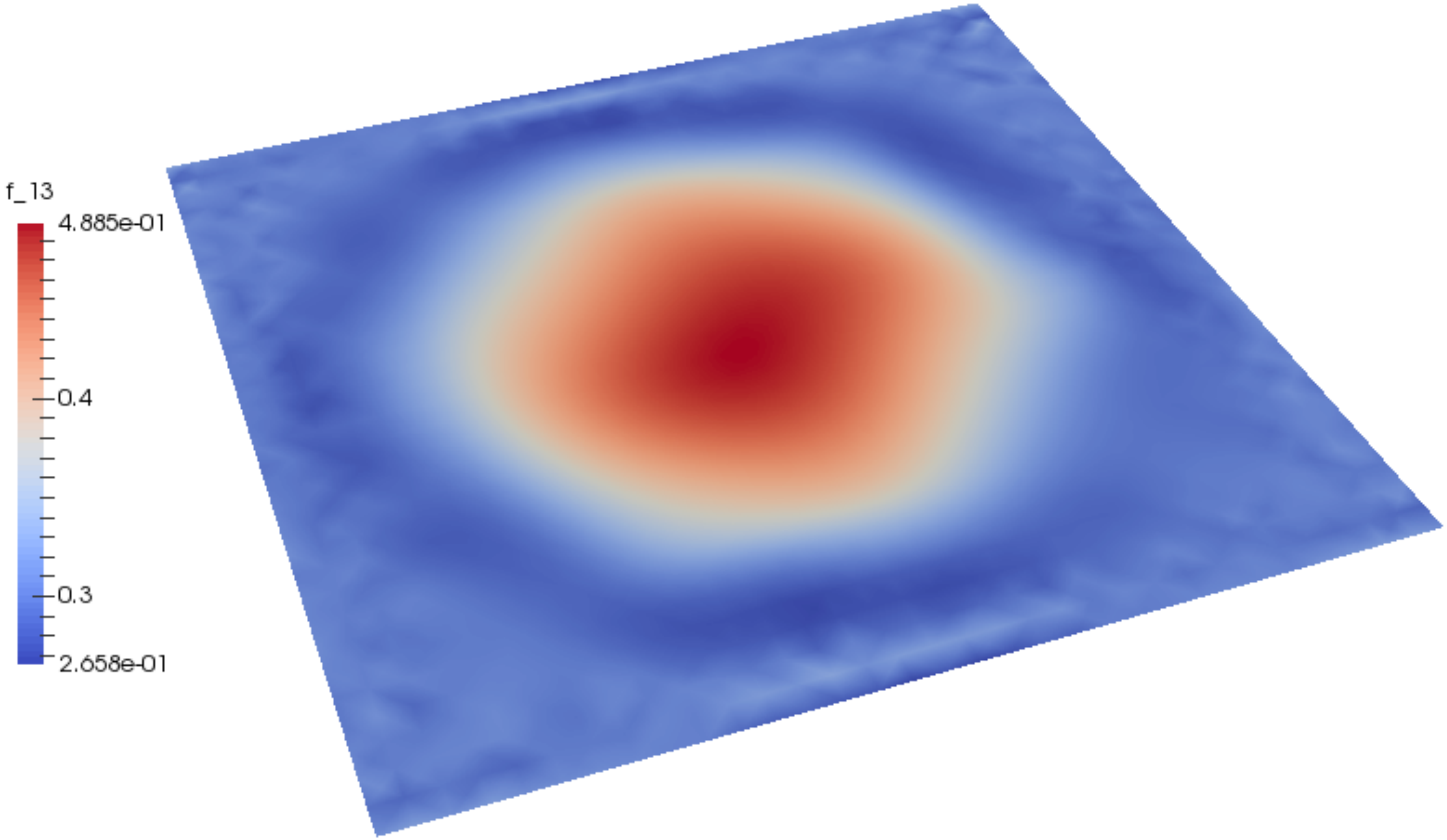
Parameter recovery



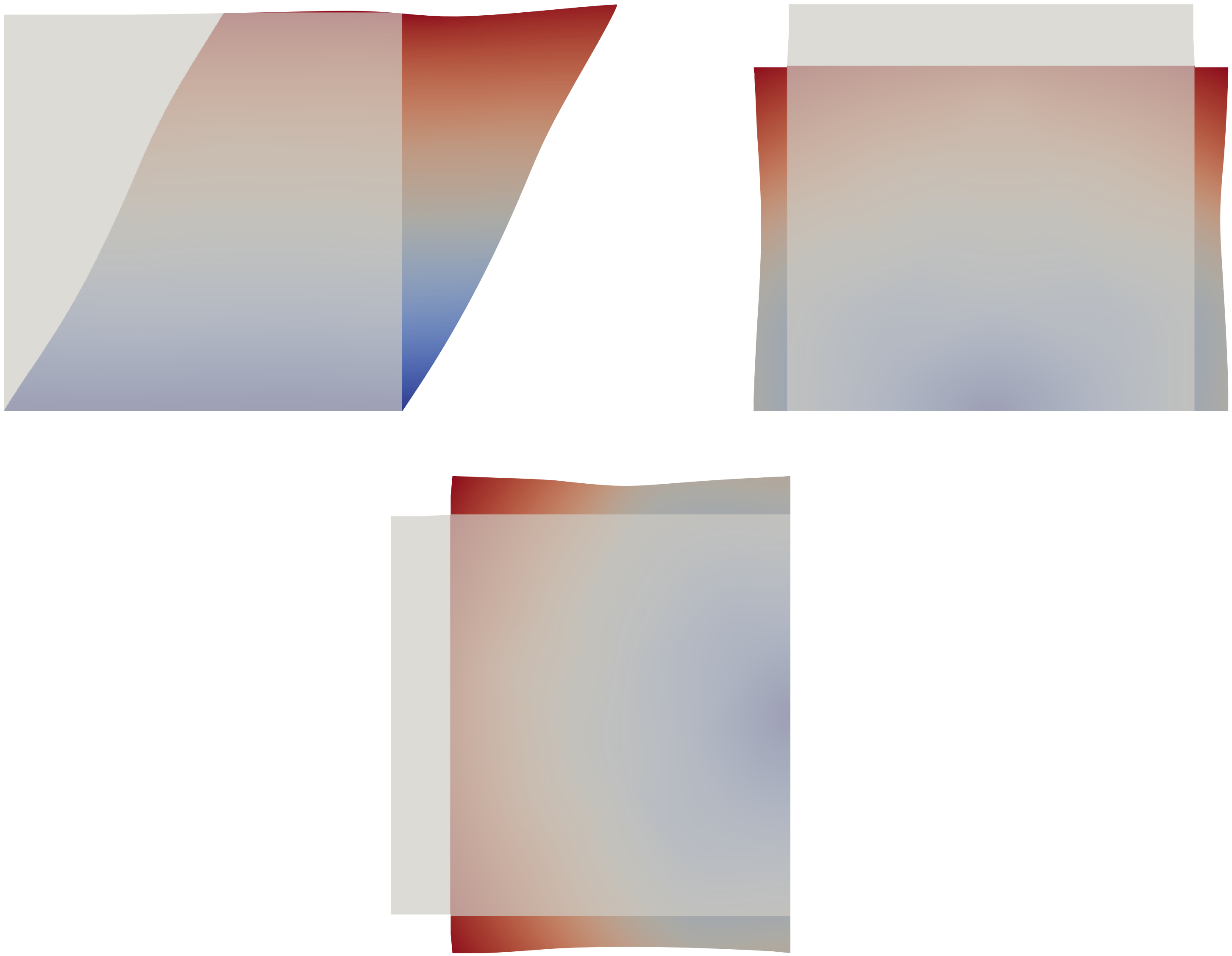
Uncertain and partial data

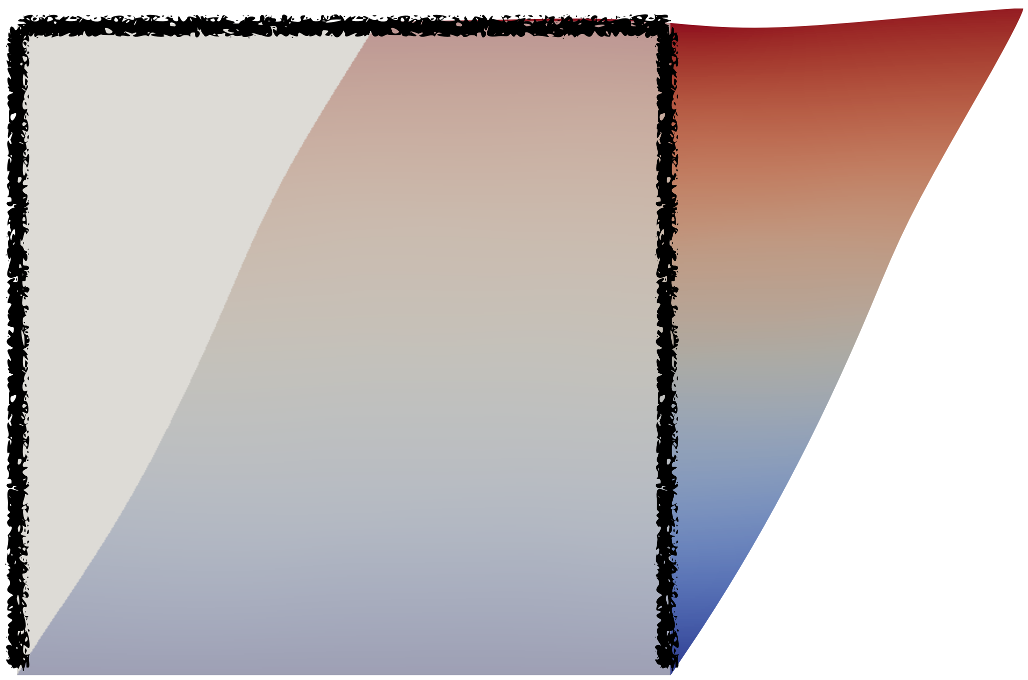


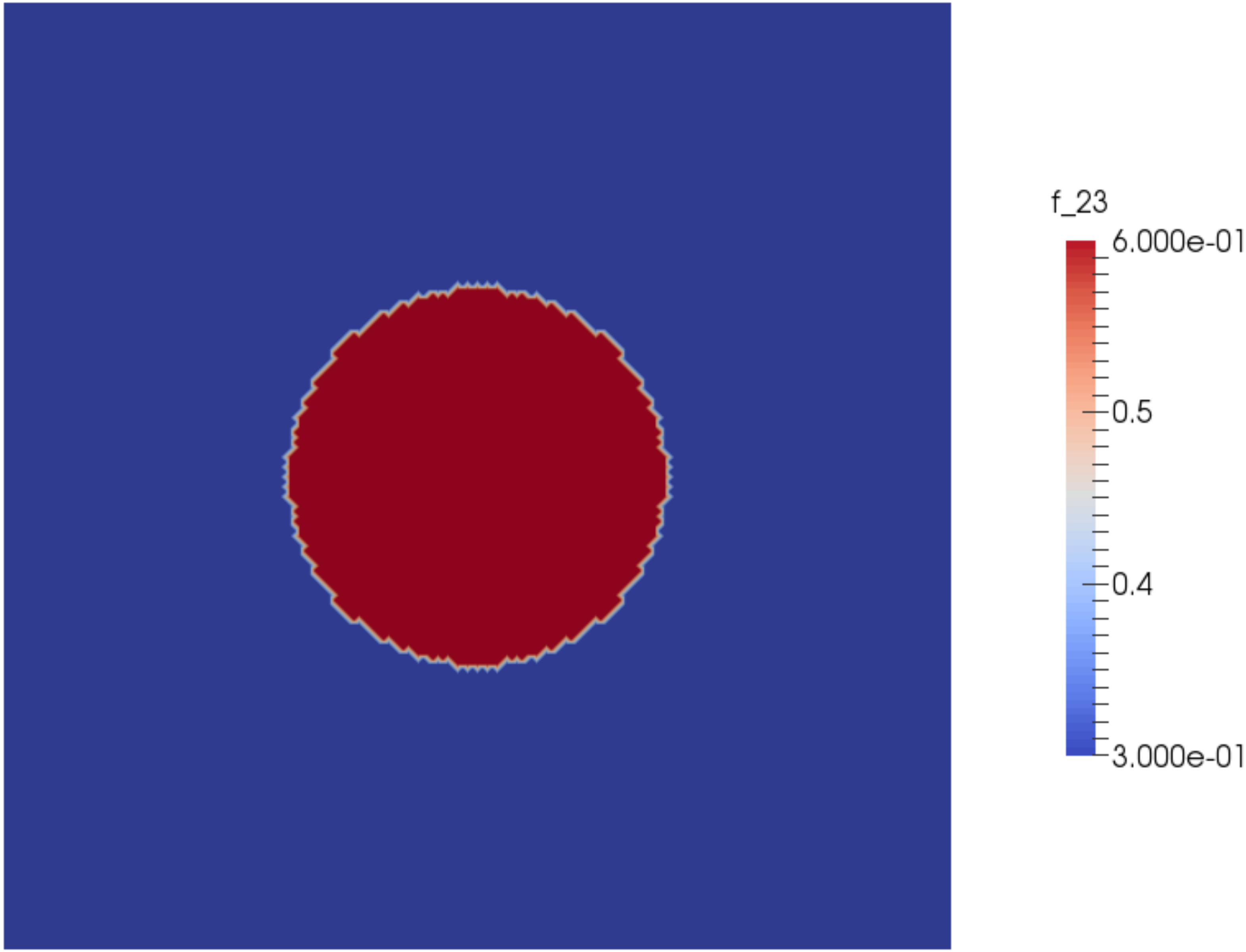
Quantification of uncertainty



X_{map}



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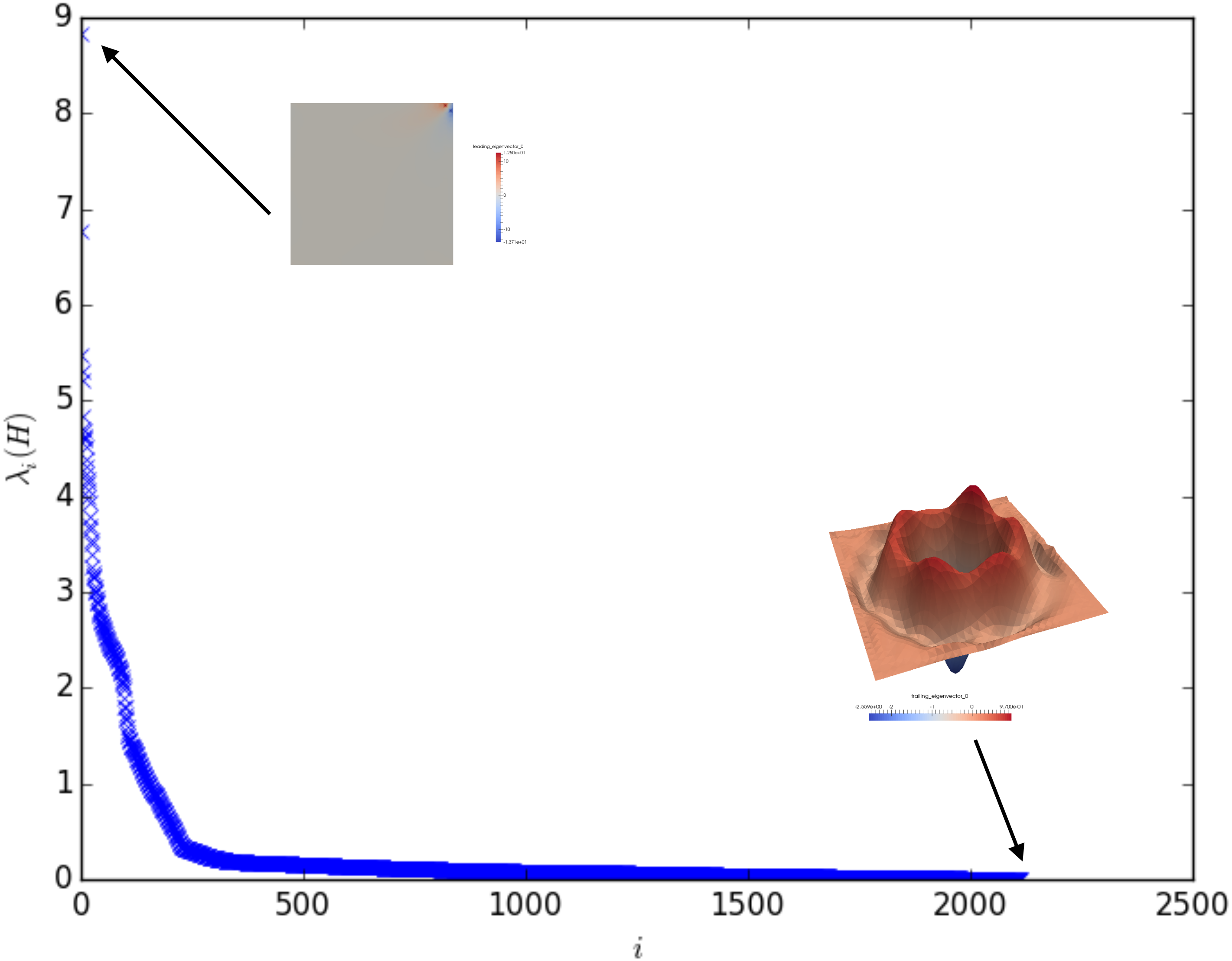

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2500
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leading_eigenvector_0
trailing_eigenvector_0

Bayes Theorem

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

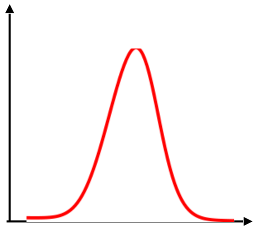
Goal: Given the observations, find the posterior distribution of the unknown parameters.

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

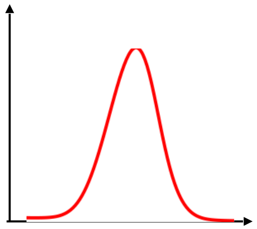
- Key idea: implement high-level description of finite element models in the Unified Form Language.

- Let algorithms take over the tedious/difficult work of linearisation and transforming maths into lower-level languages.

Prior
Knowledge



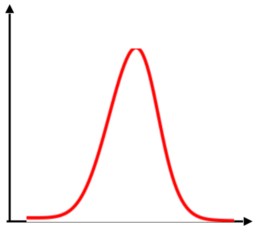
Prior Knowledge



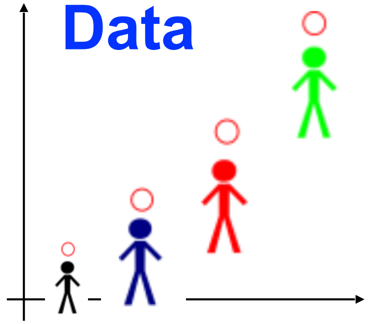
Hypothesis

model is Neo-Hookean viscous

Prior Knowledge

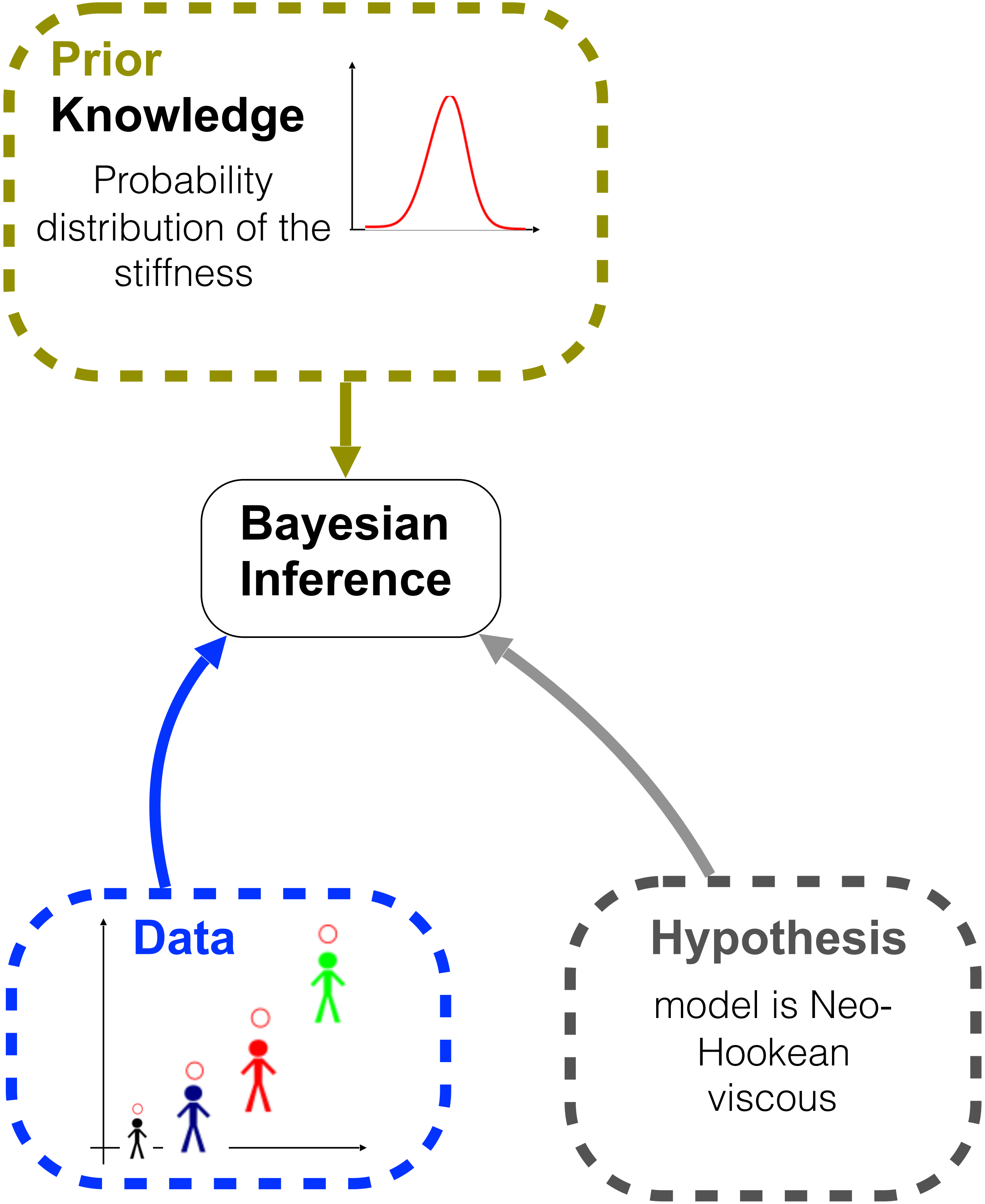


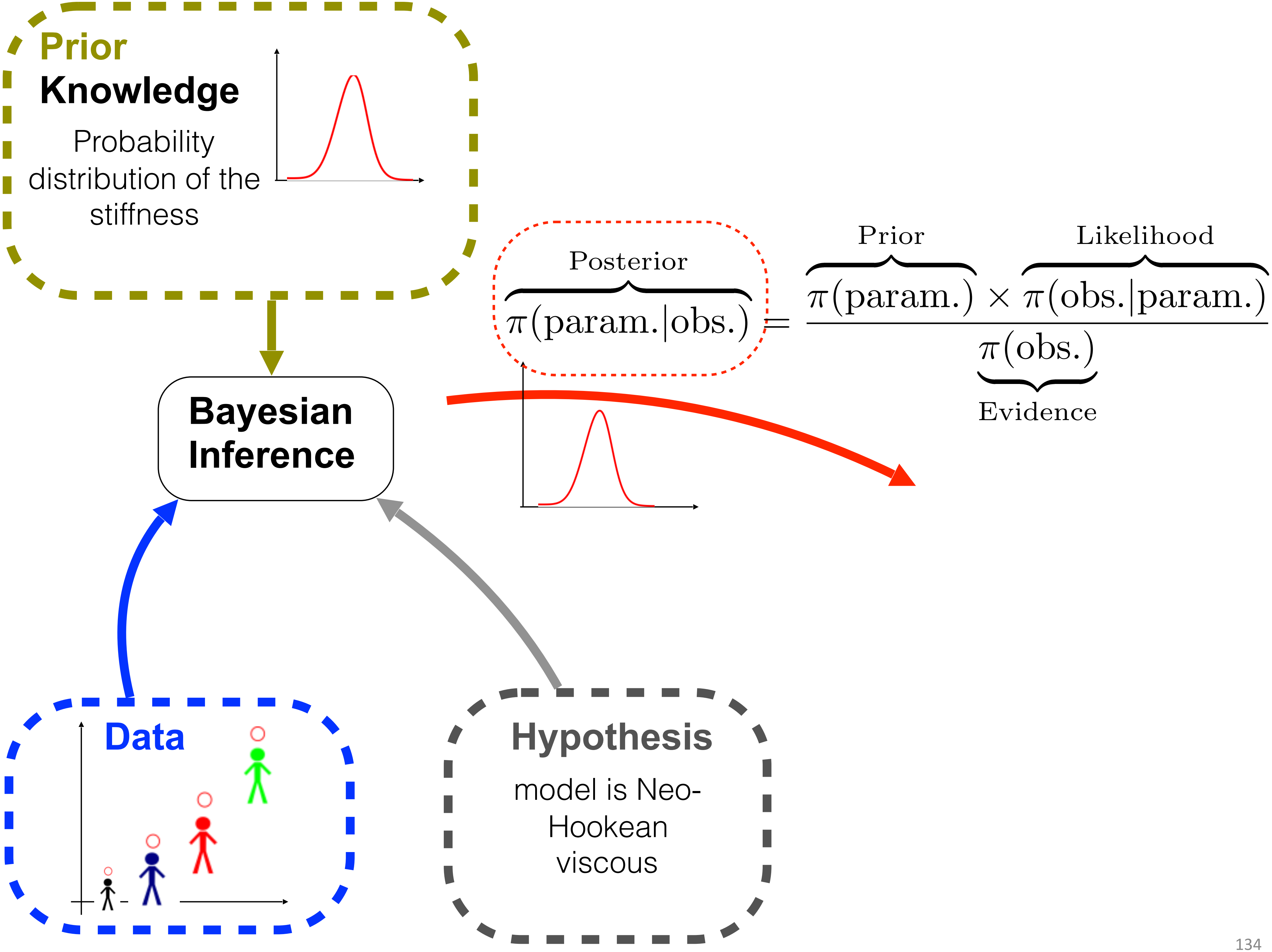
Data

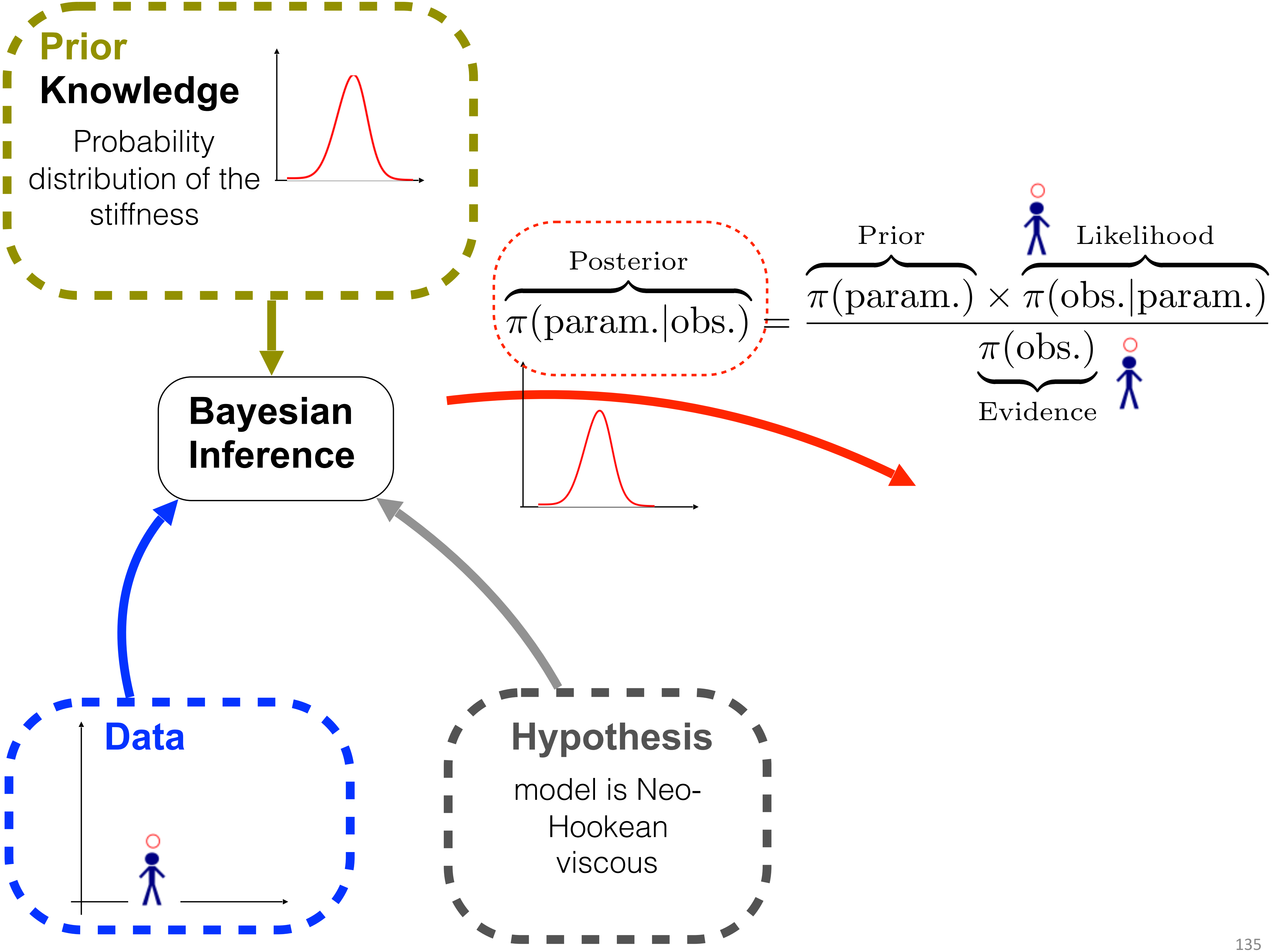


Hypothesis

model is Neo-Hookean viscous


Prior
Knowledge
Probability distribution of the stiffness
Bayesian Inference
Data
Hypothesis
model is Neo-Hookean viscous


Prior Knowledge
Probability distribution of the stiffness
Bayesian Inference
Data
Hypothesis
model is Neo-Hookean viscous
$\overbrace{\pi(\text{param.}|\text{obs.})}^{\text{Posterior}} = \frac{\overbrace{\pi(\text{param.})}^{\text{Prior}} \times \overbrace{\pi(\text{obs.}|\text{param.})}^{\text{Likelihood}}}{\underbrace{\pi(\text{obs.})}_{\text{Evidence}}}$


Prior
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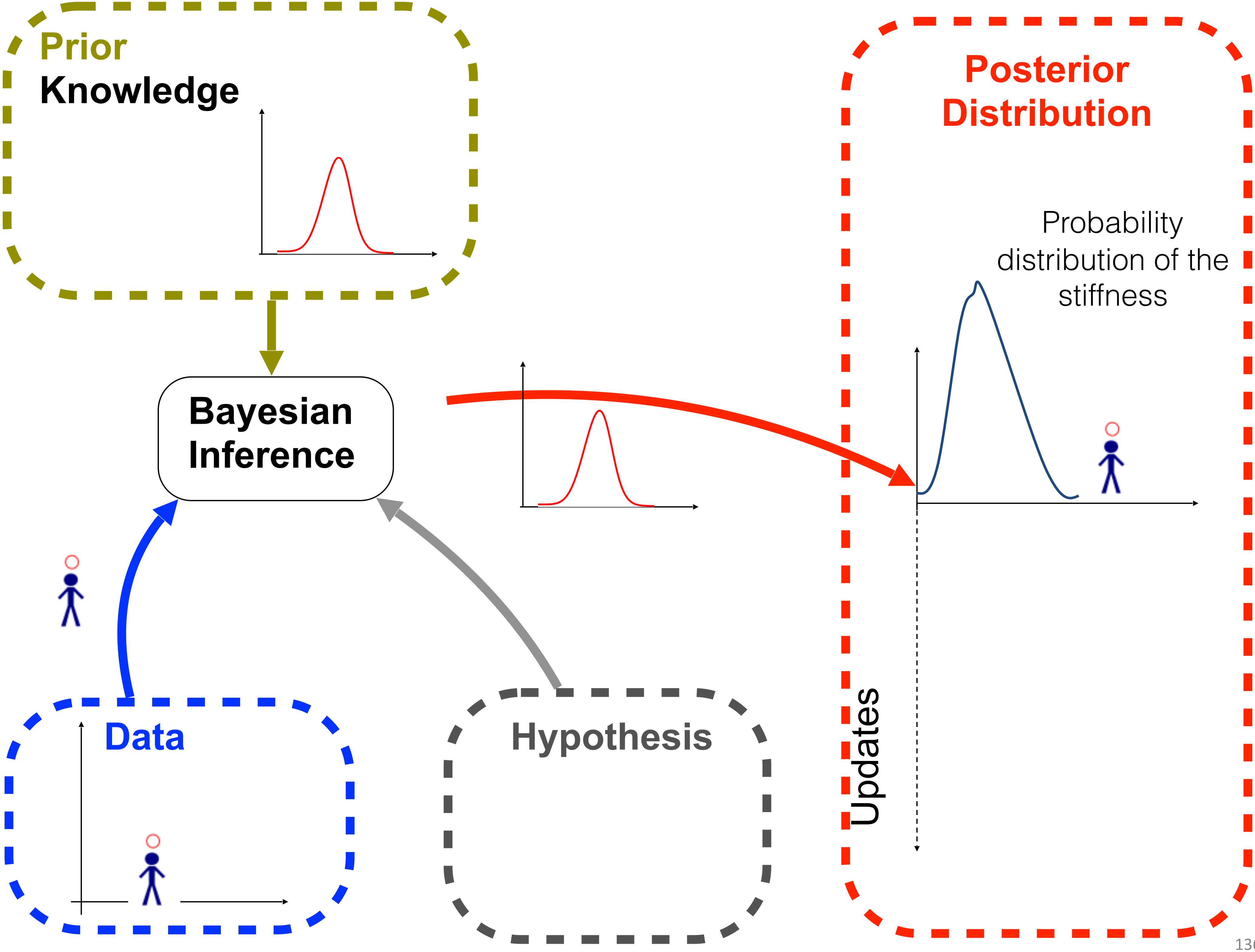
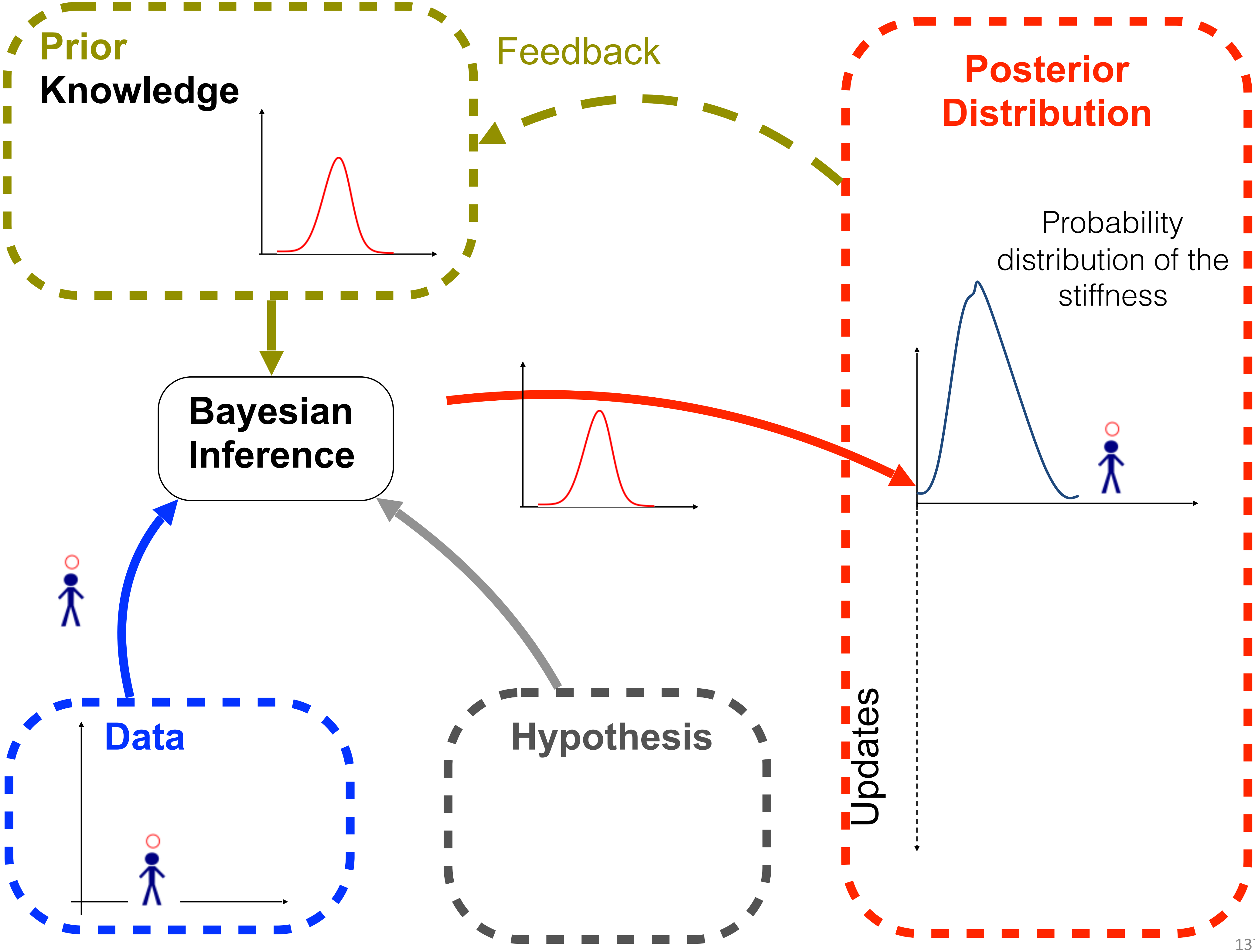
Probability distribution of the stiffness
Bayesian Inference
Posterior
Prior
Likelihood
$\pi(\text{param.}|\text{obs.}) = \frac{\pi(\text{param.}) \times \pi(\text{obs.}|\text{param.})}{\pi(\text{obs.})}$
Evidence
Data
Hypothesis
model is Neo-Hookean viscous



Prior
Knowledge
Bayesian
Inference
Data
Hypothesis
Posterior
Distribution
Probability
distribution of the
stiffness
Updates


Prior
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Feedback
Posterior
Distribution
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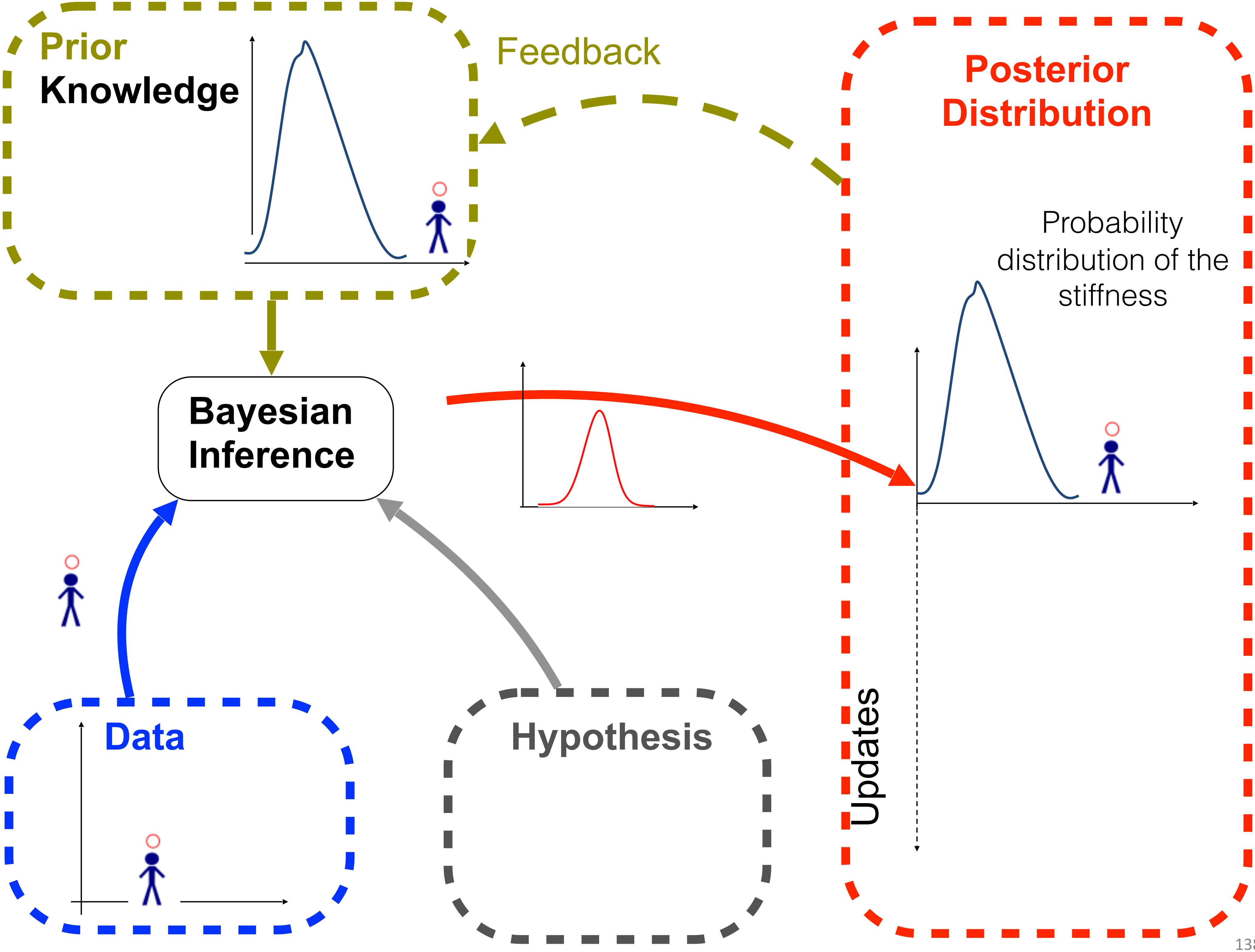
Bayesian
Inference
Data
Hypothesis
Updates



Prior
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Distribution
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distribution of the
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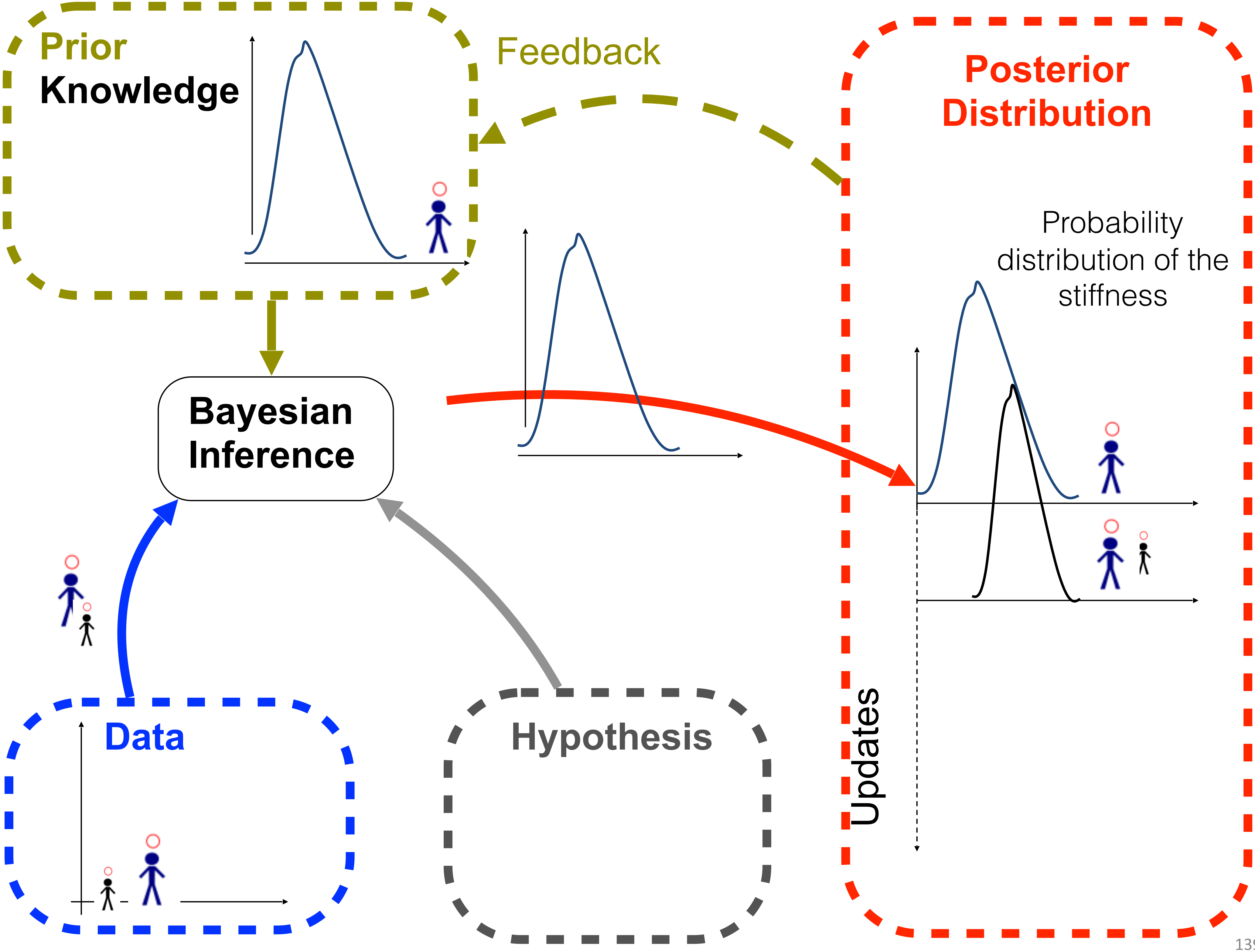
Updates
Data
Hypothesis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Inference
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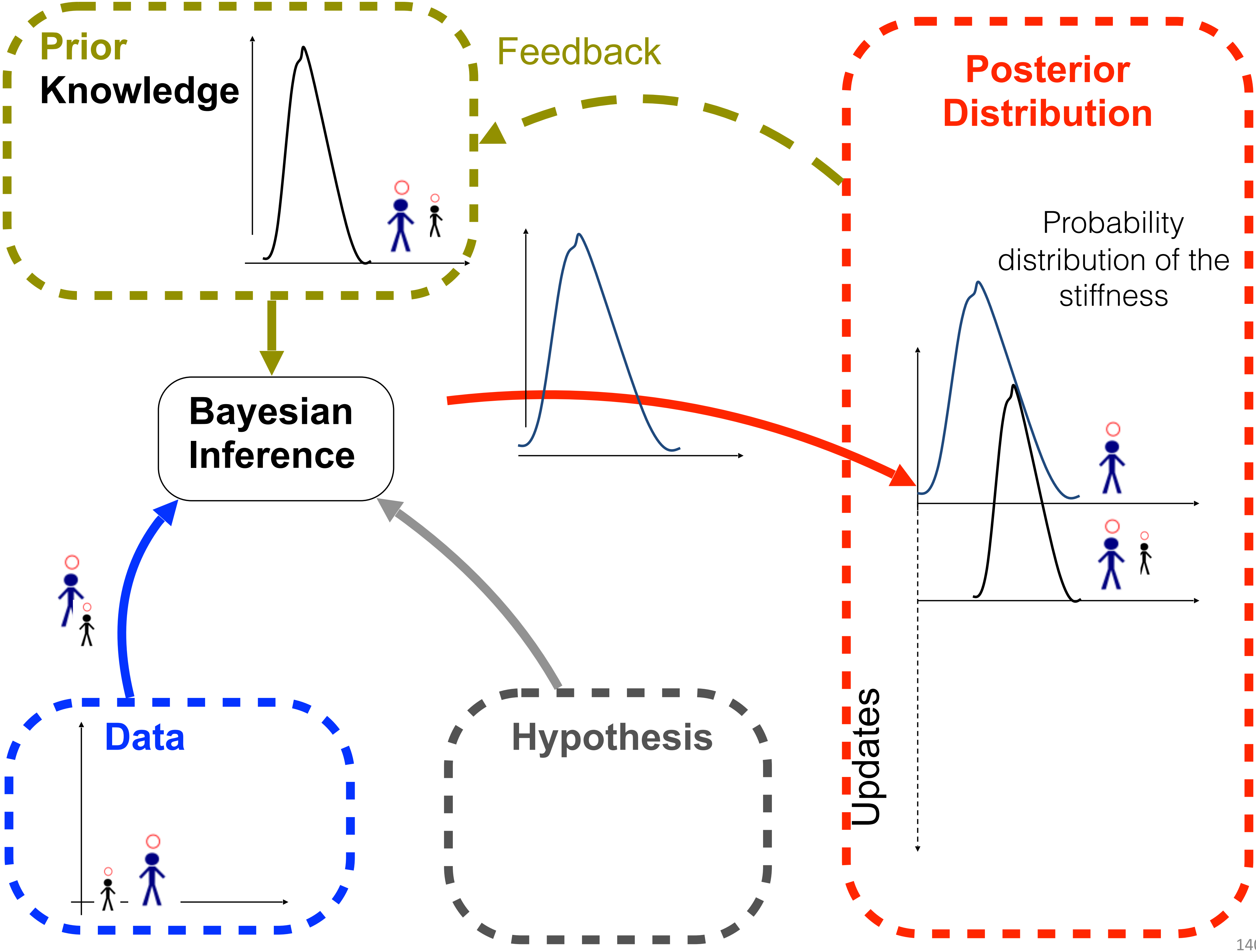
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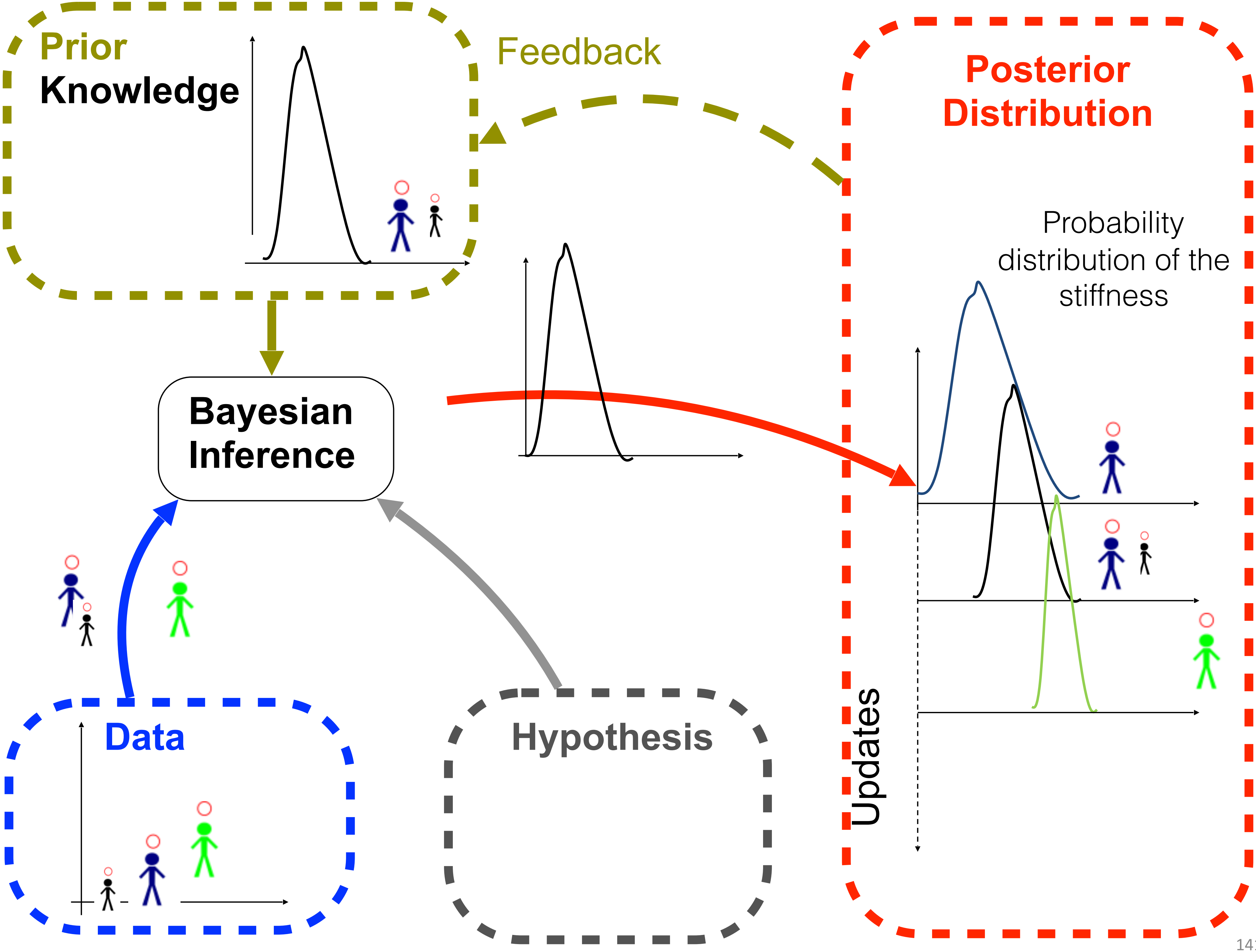
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Probability distribution of the stiffness
Bayesian
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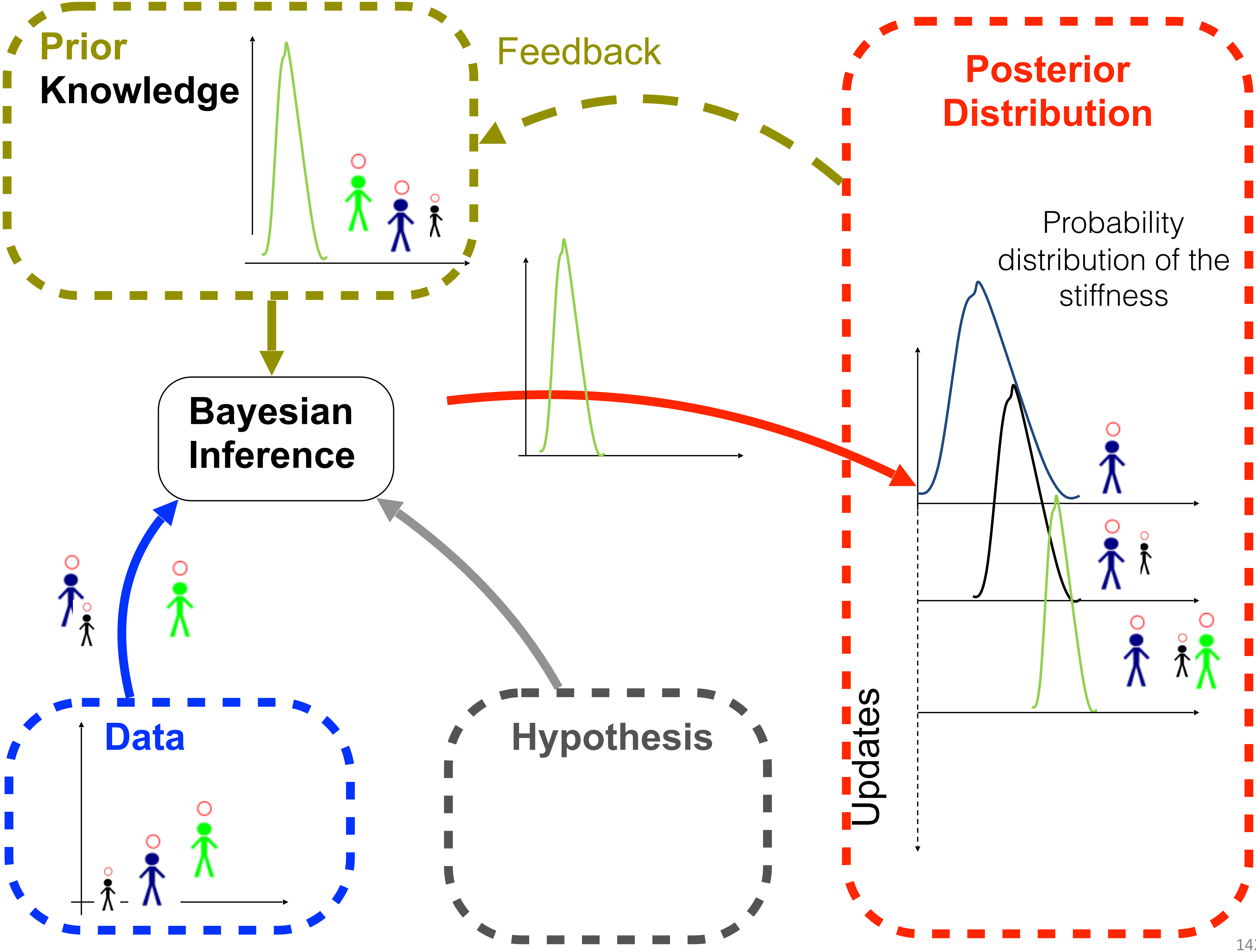
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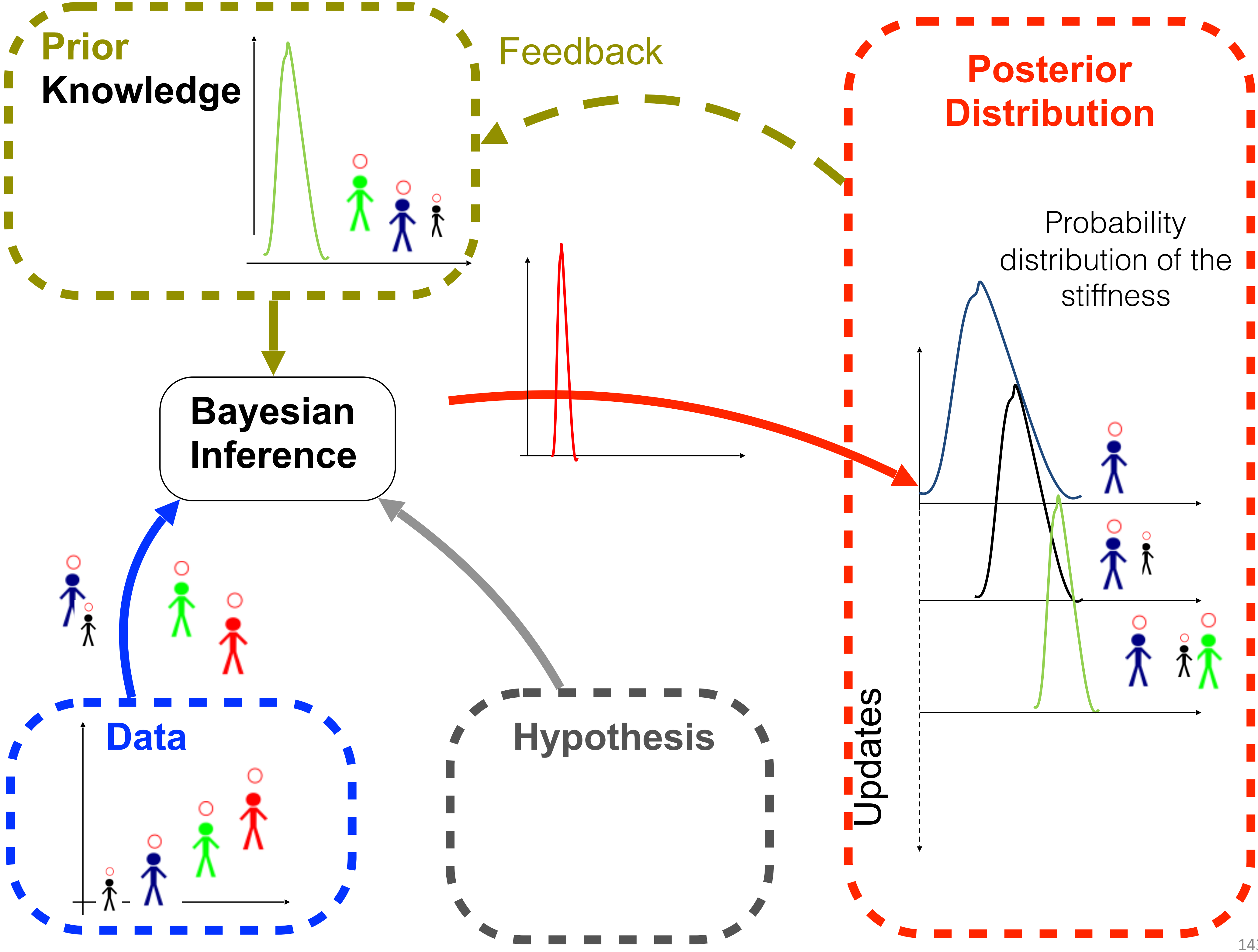
Distribution
Probability distribution of the stiffness
Bayesian
Inference
Data
Hypothesis
Updates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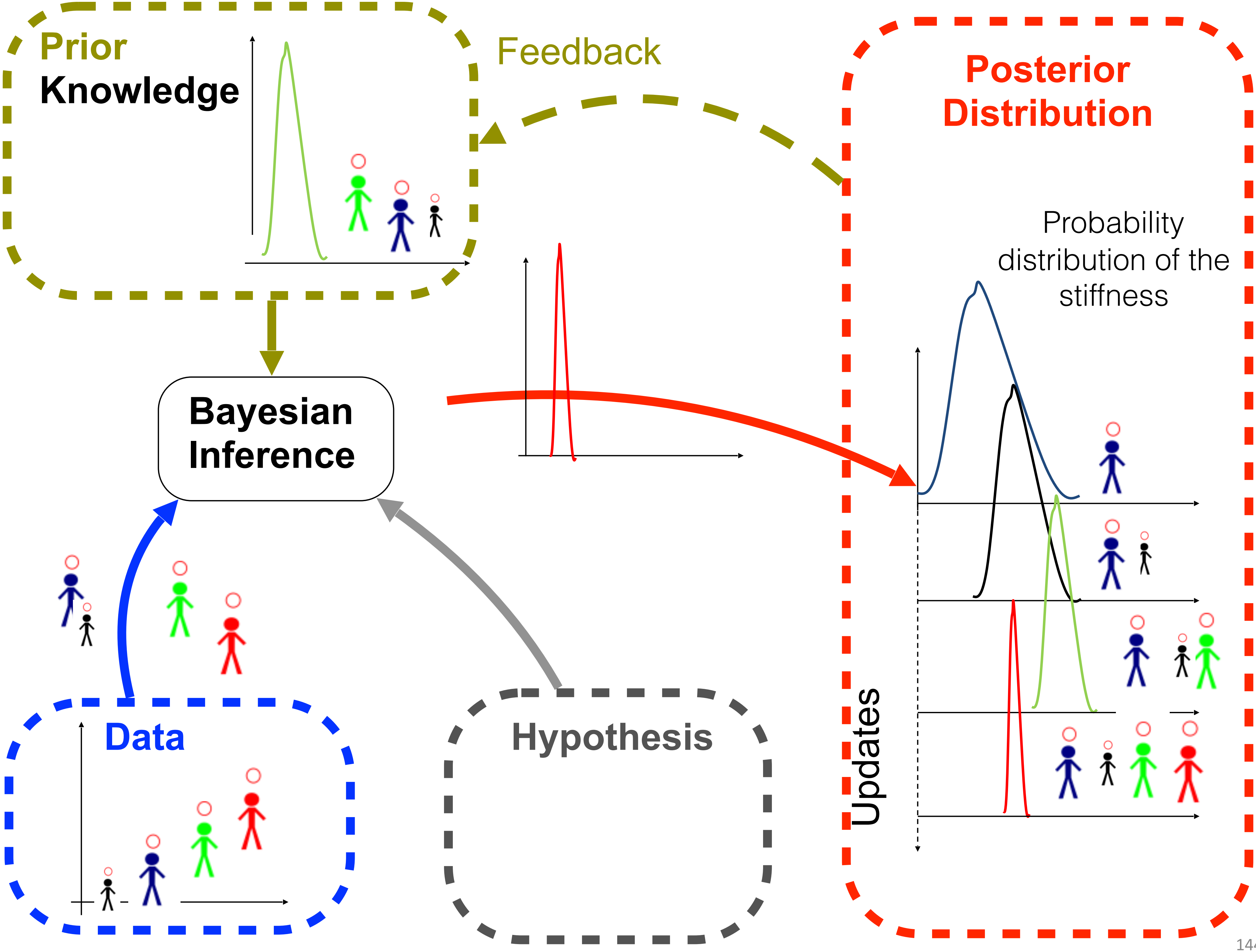
stiffness
Bayesian
Inference
Updates
Data
Hypothesis



Prior
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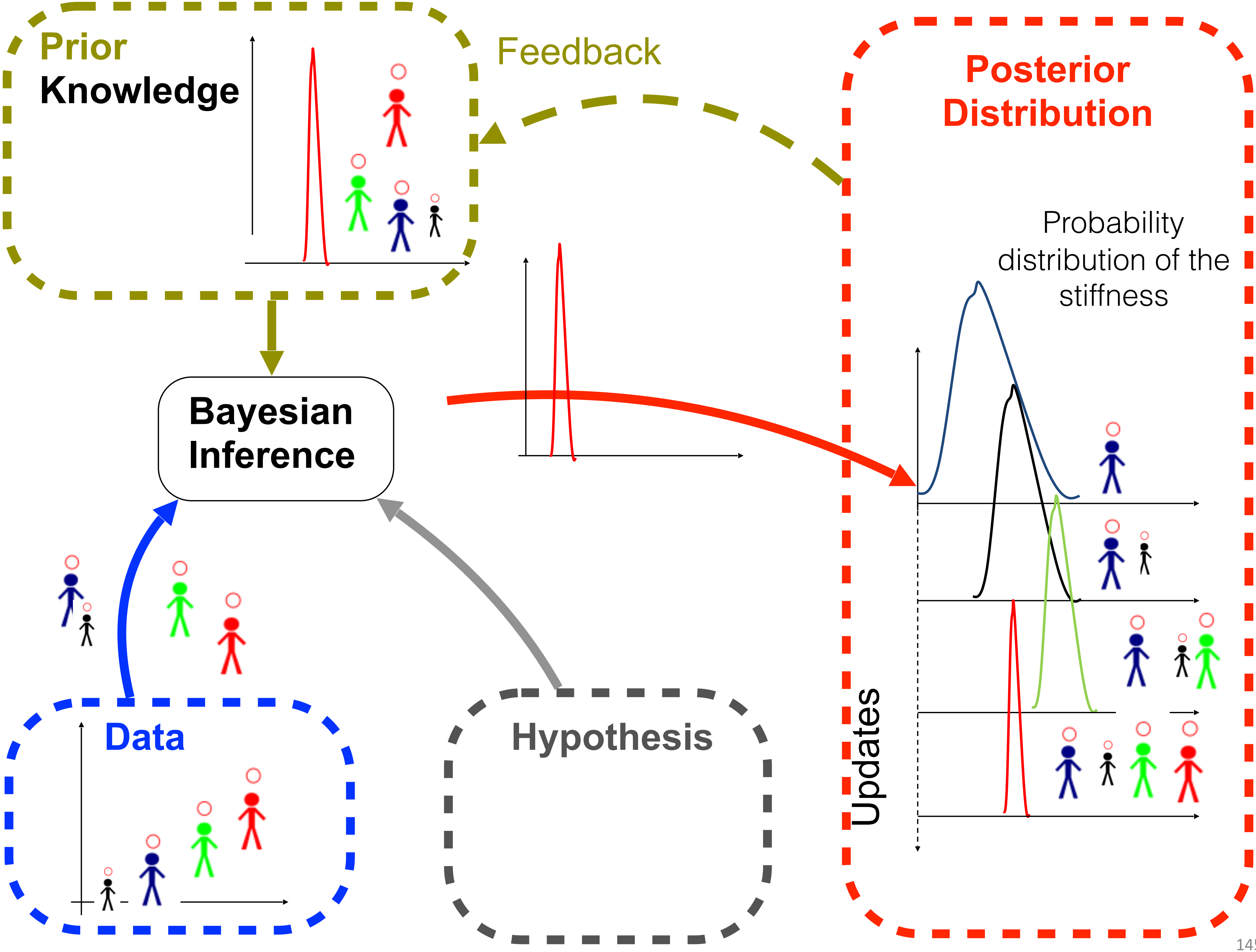
Posterior
Distribution
Probability distribution of the stiffness
Bayesian
Inference
Updates
Data
Hypothesis



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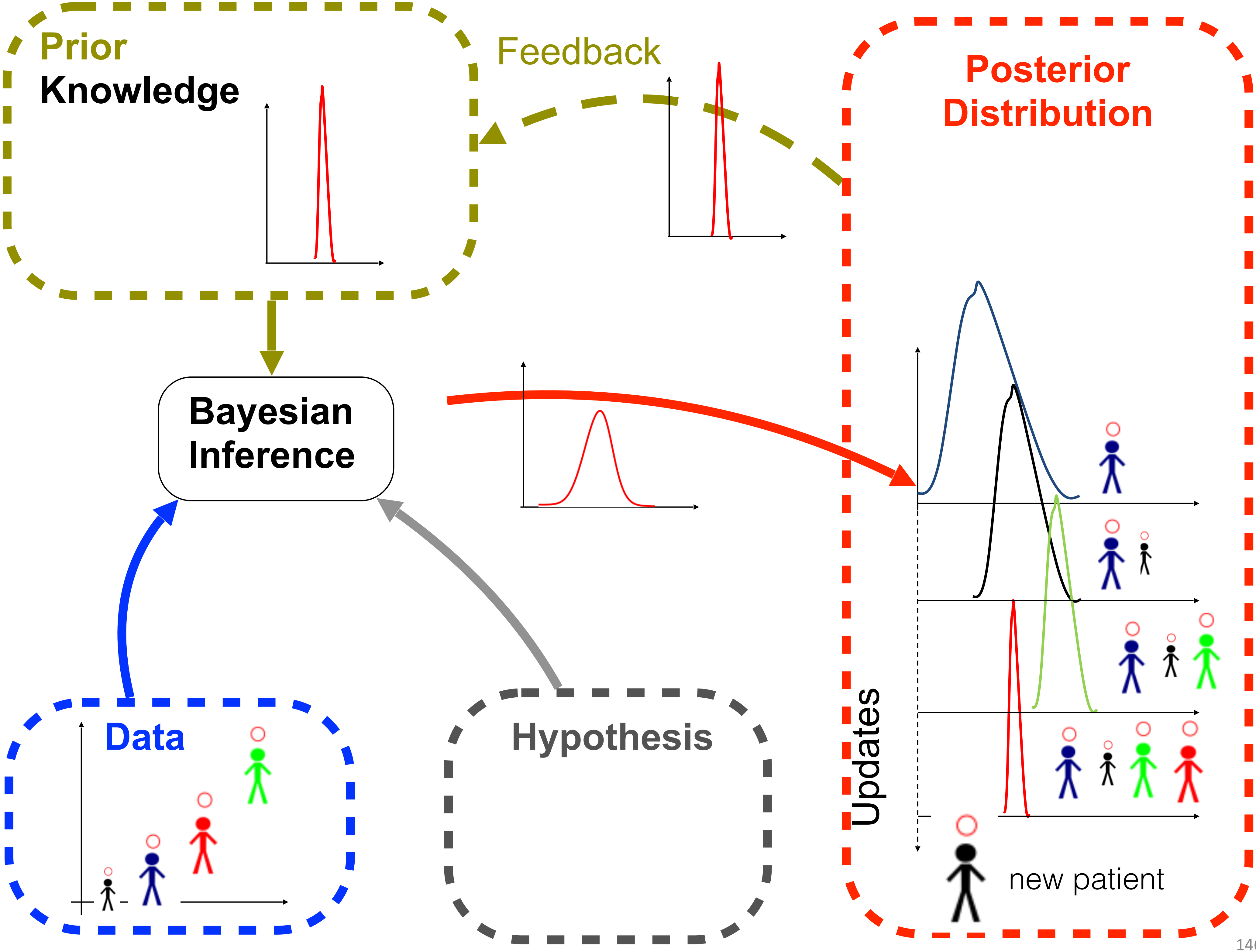
Probability
distribution of the
stiffness
Bayesian
Inference
Data
Hypothesis
Updates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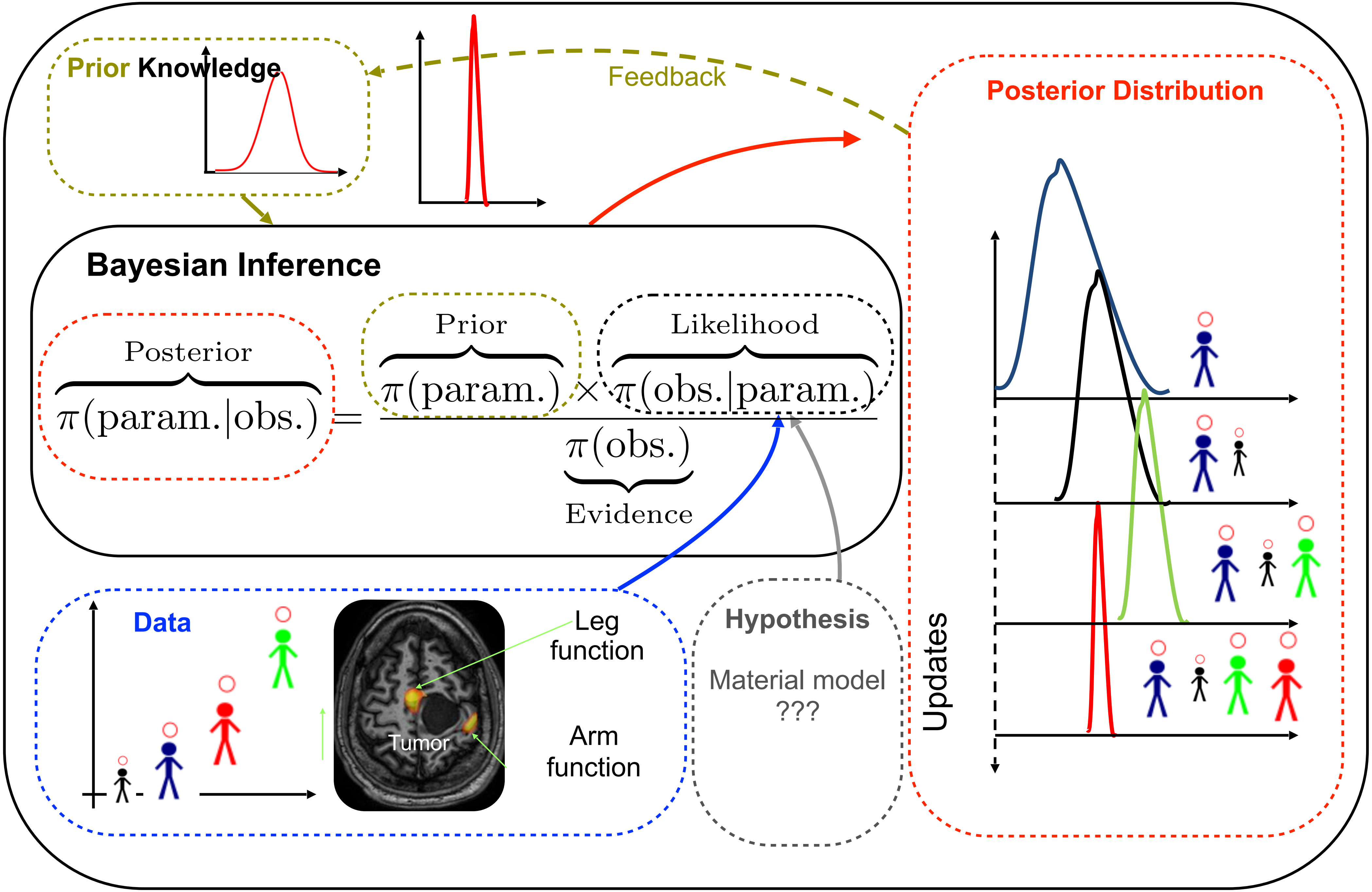
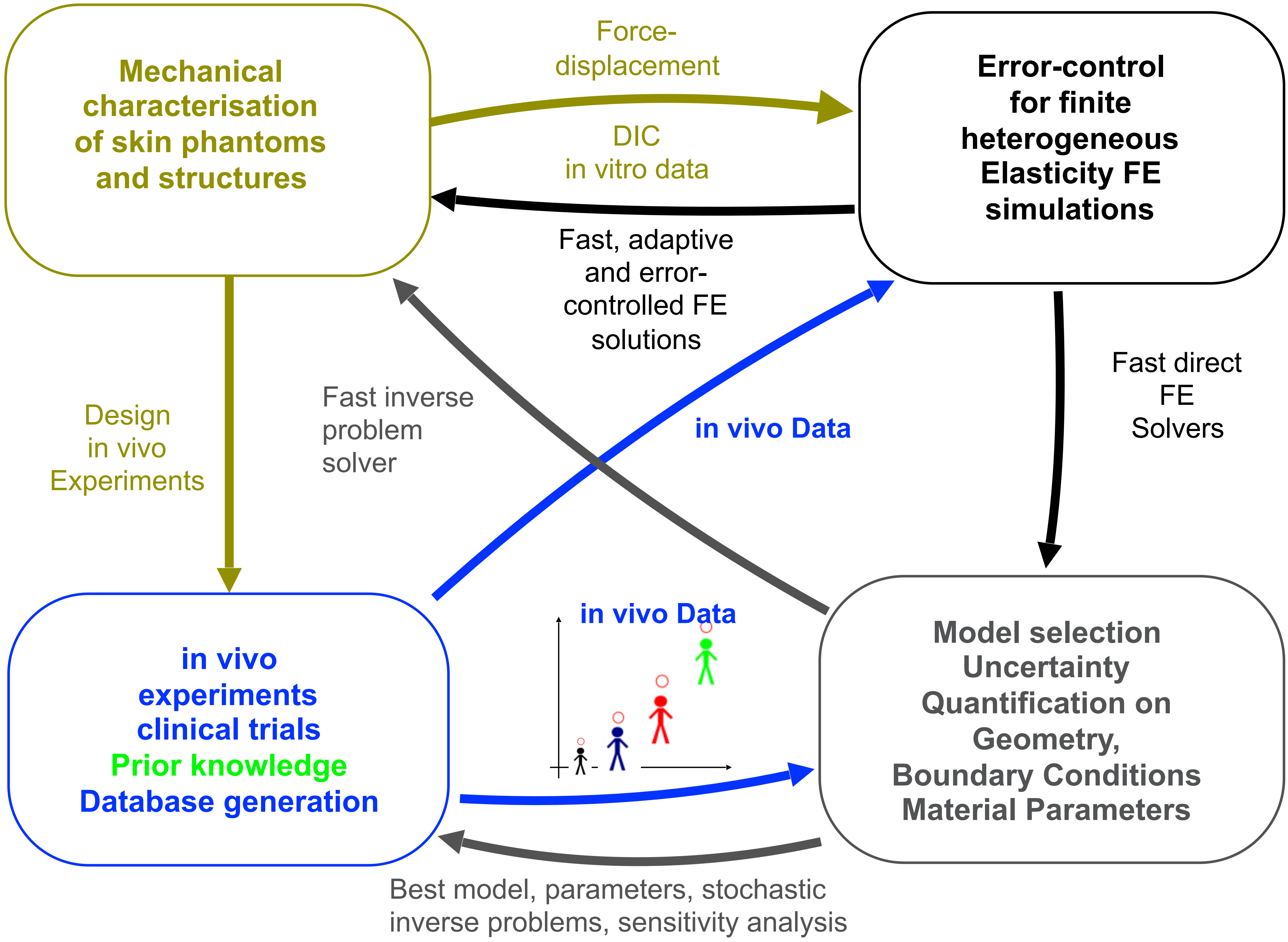
Distribution
Bayesian
Inference
Data
Hypothesis
Updates
new patient



Prior Knowledge
Feedback
Posterior Distribution
Bayesian Inference
Posterior
Prior
Likelihood
$\pi(\text{param.}|\text{obs.}) = \frac{\pi(\text{param.}) \times \pi(\text{obs.}|\text{param.})}{\pi(\text{obs.})}$
Evidence
Data
Tumor
Leg function
Arm function
Hypothesis
Material model ???
Updates



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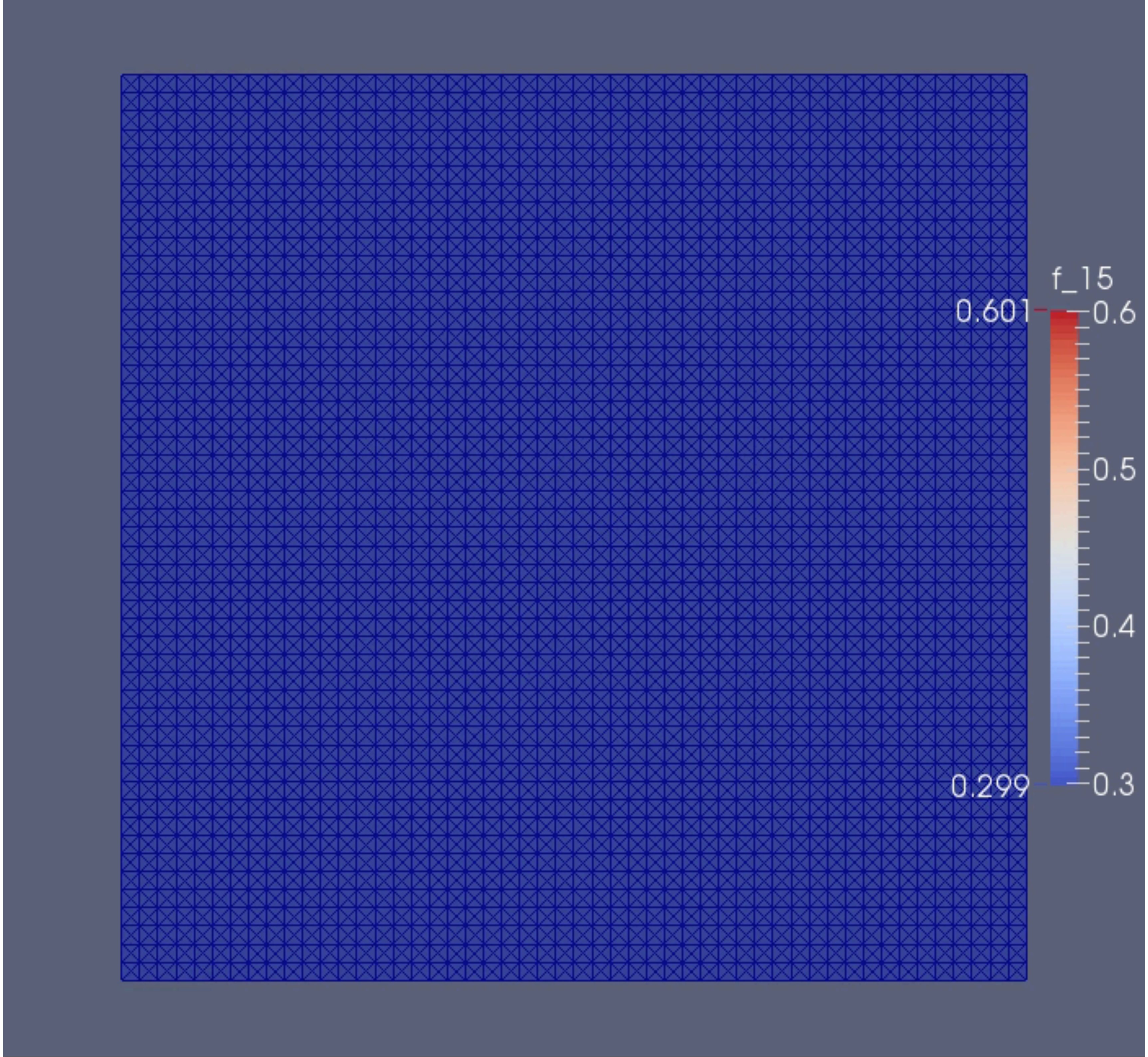
Force-displacement
Error-control for finite heterogeneous Elasticity FE simulations
DIC
in vitro data
Fast, adaptive and error-controlled FE solutions
Design in vivo Experiments
Fast inverse problem solver
in vivo Data
Fast direct FE Solvers
in vivo Data
in vivo experiments
clinical trials
Prior knowledge
Database generation
Model selection
Uncertainty Quantification on Geometry, Boundary Conditions Material Parameters
Best model, parameters, stochastic inverse problems, sensitivity analysis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Surgical planning
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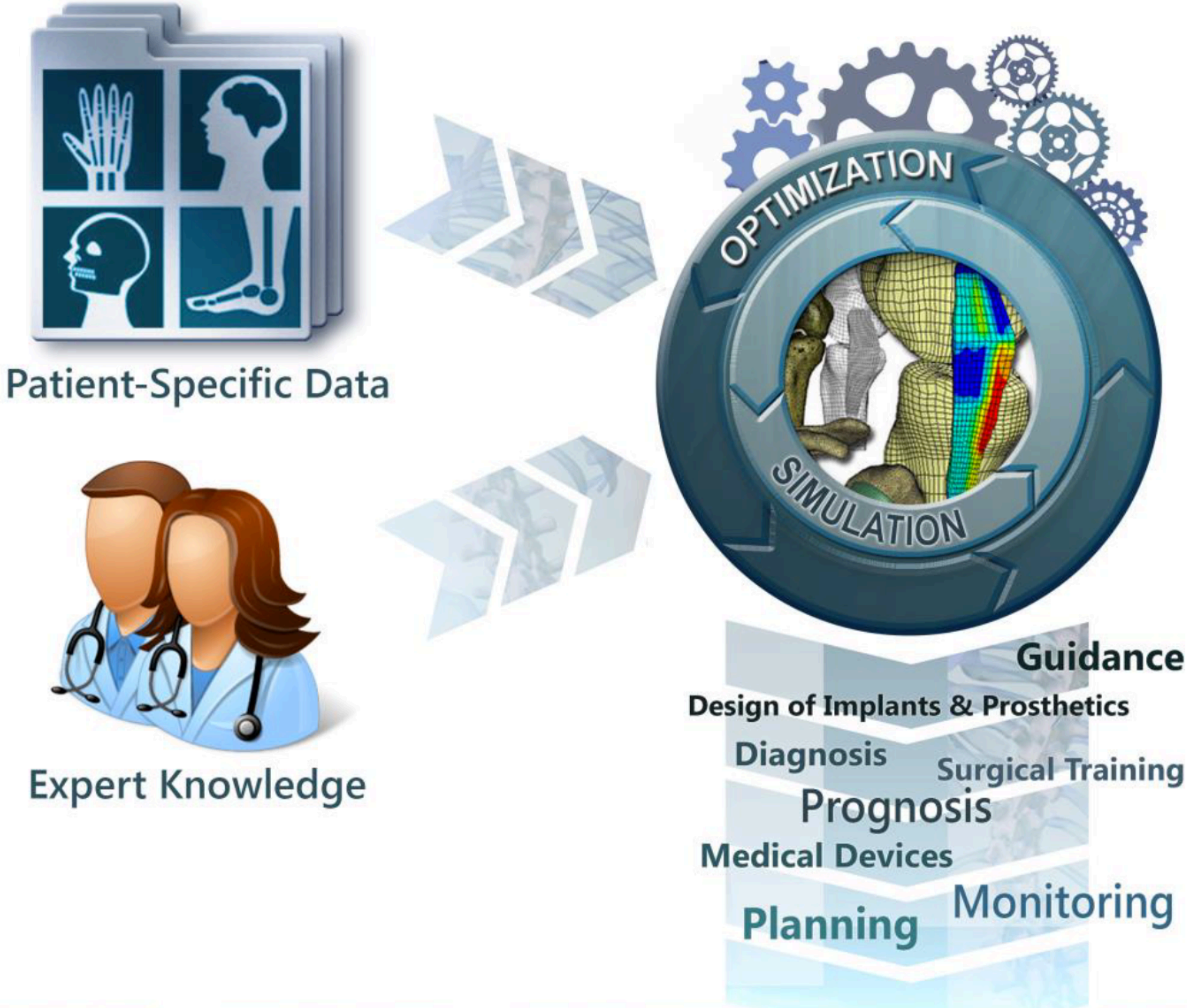
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Diagnosis
Surgical Training
Prognosis
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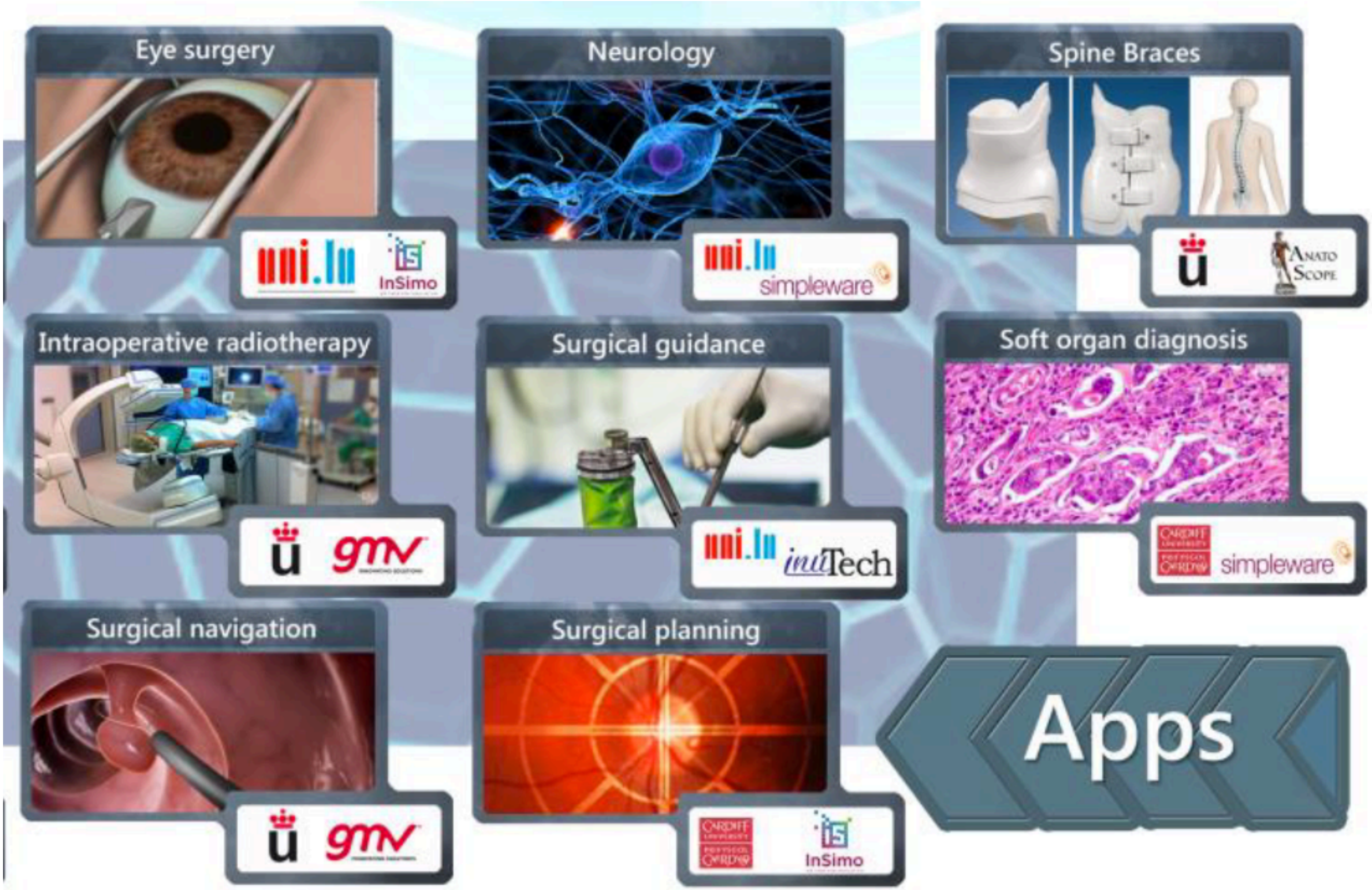
Planning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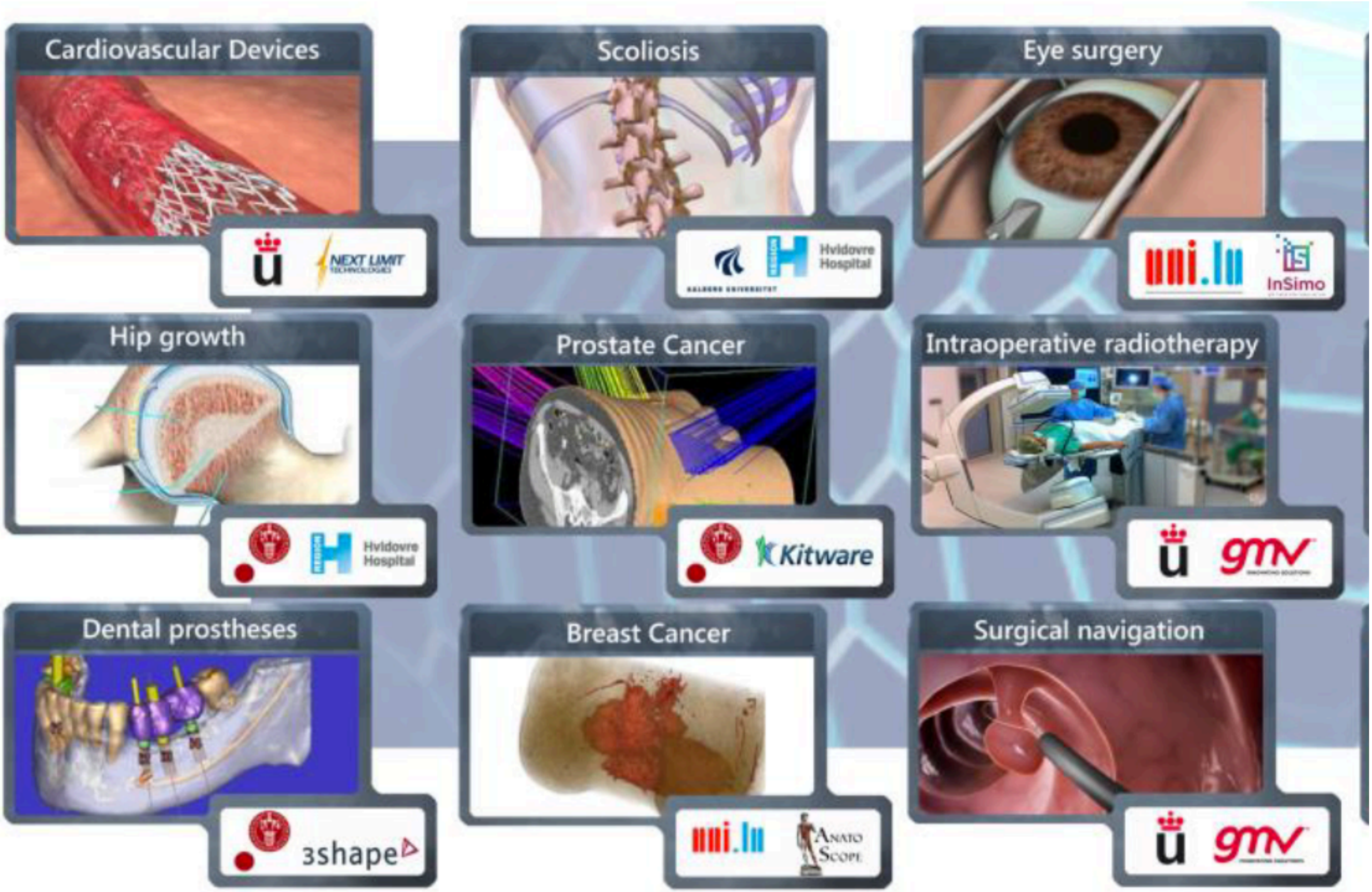
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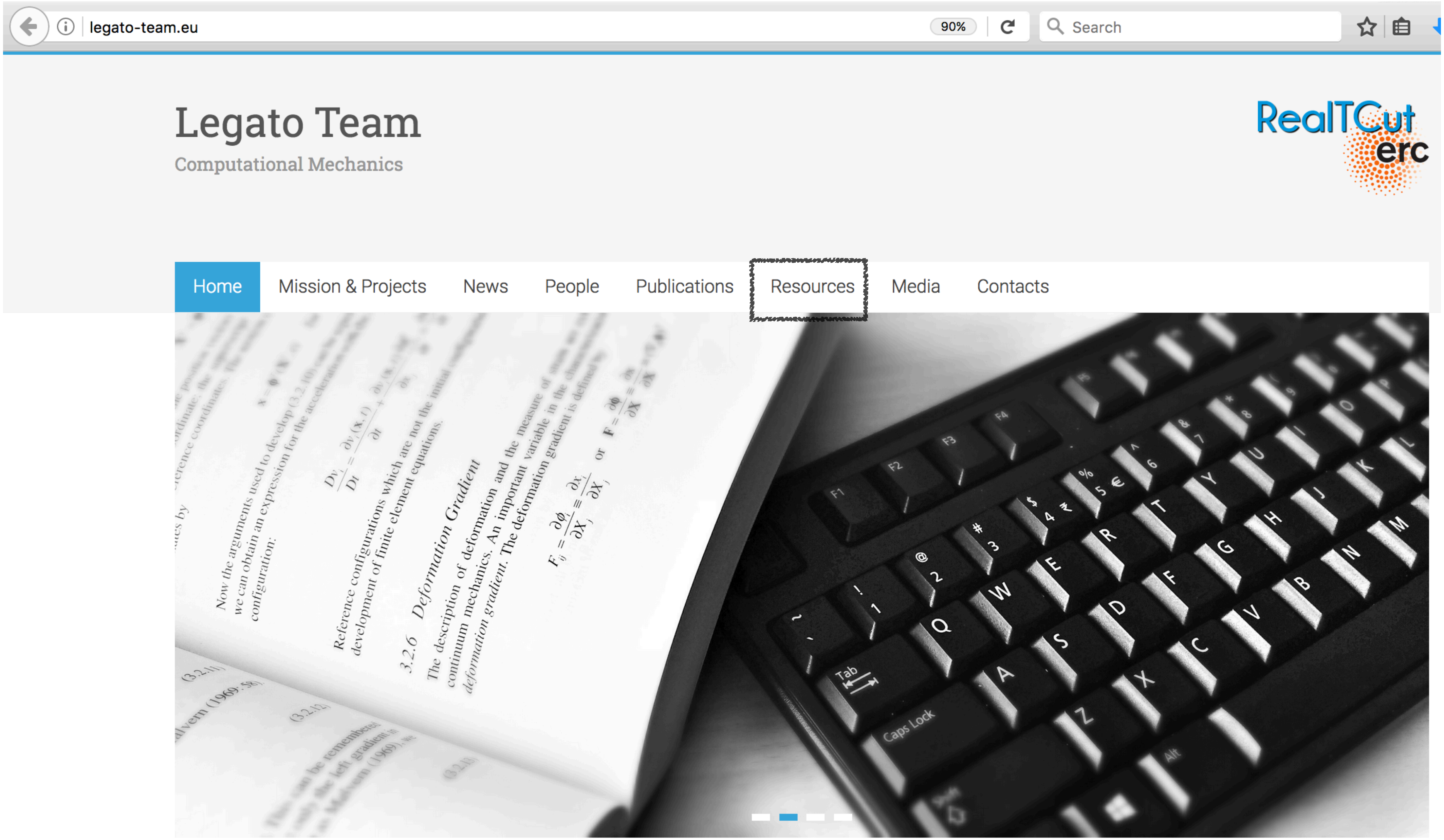
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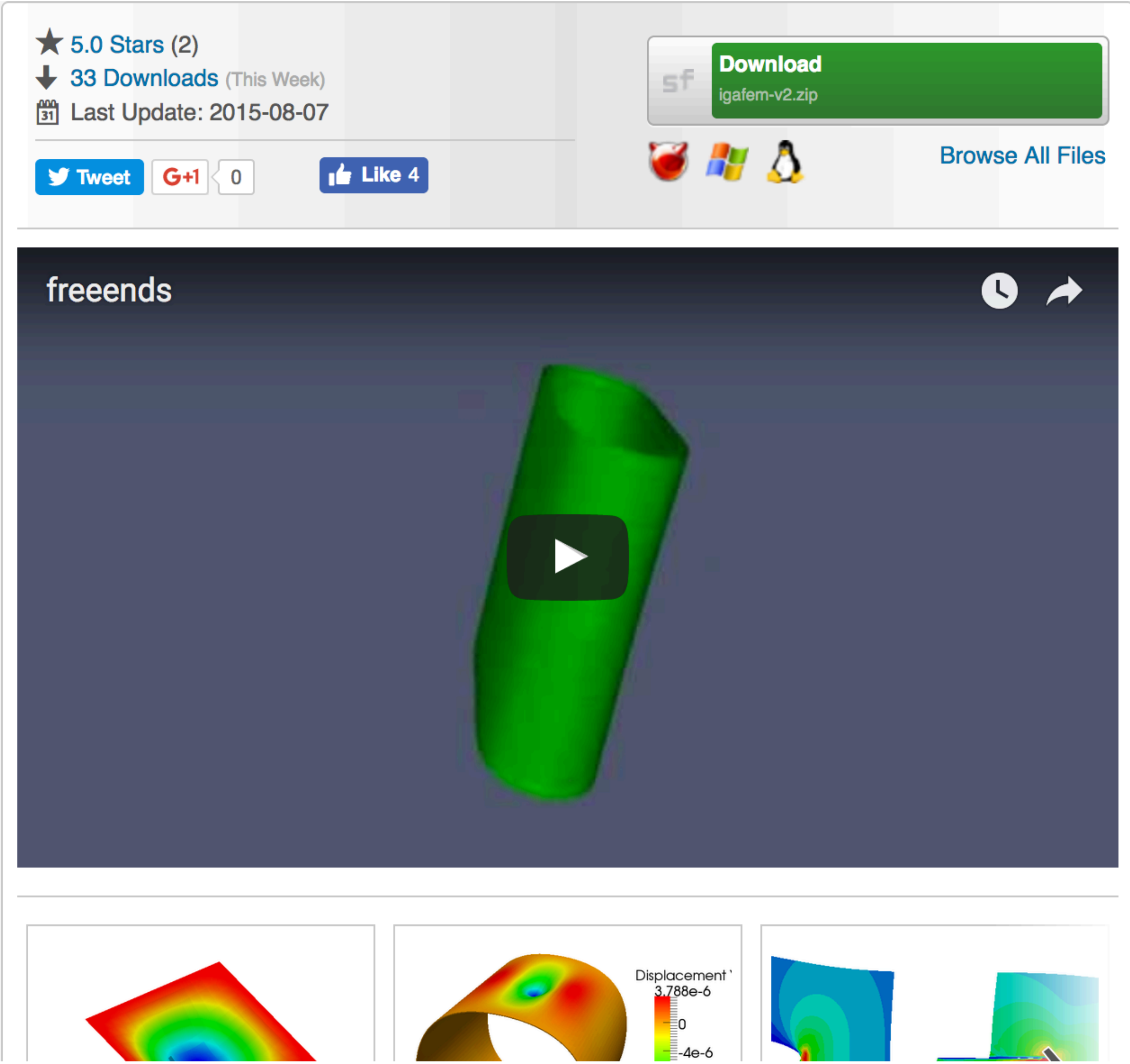
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