Computed in Luxembourg

Computational Sciences Luxembourg

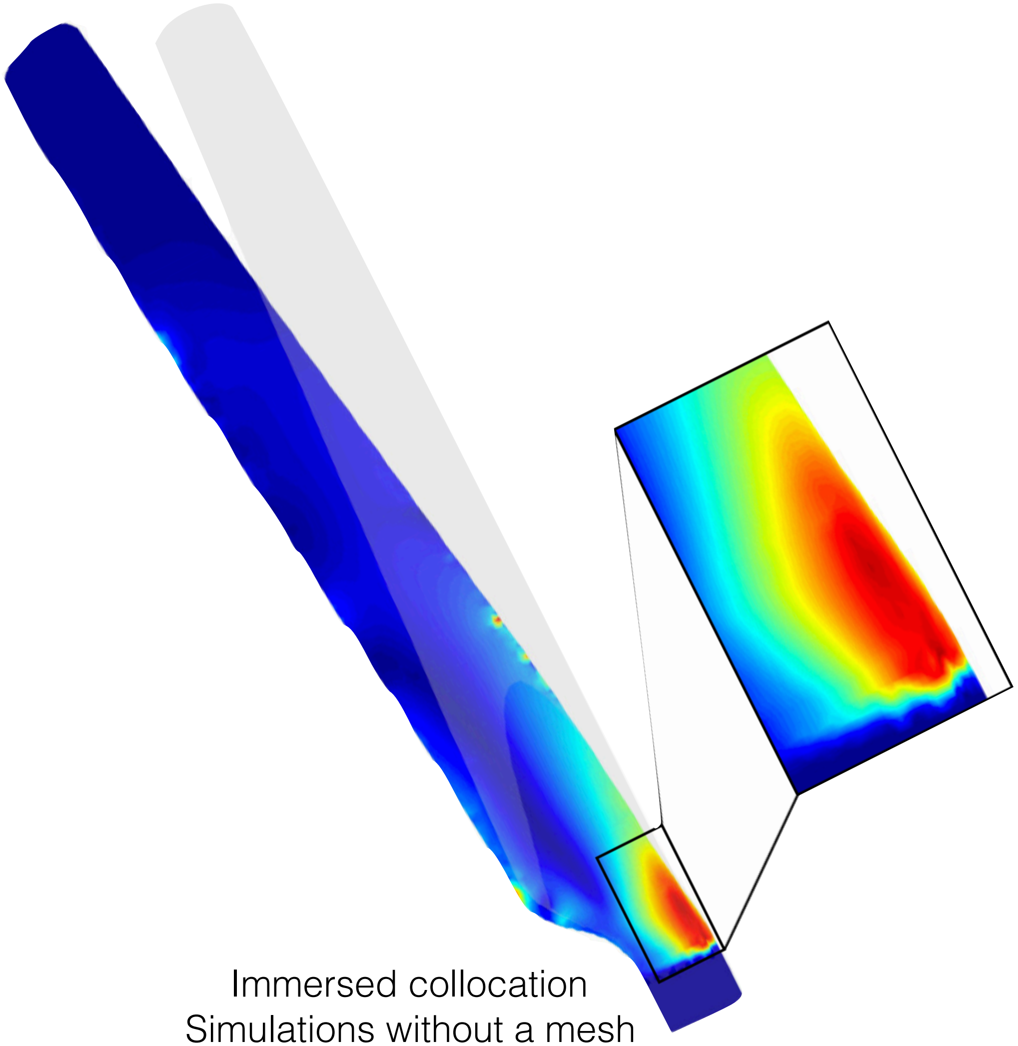
UNIVERSITÉ DU LUXEMBOURG

Computational Sciences and the Transition to Data-Driven Modelling and Simulation

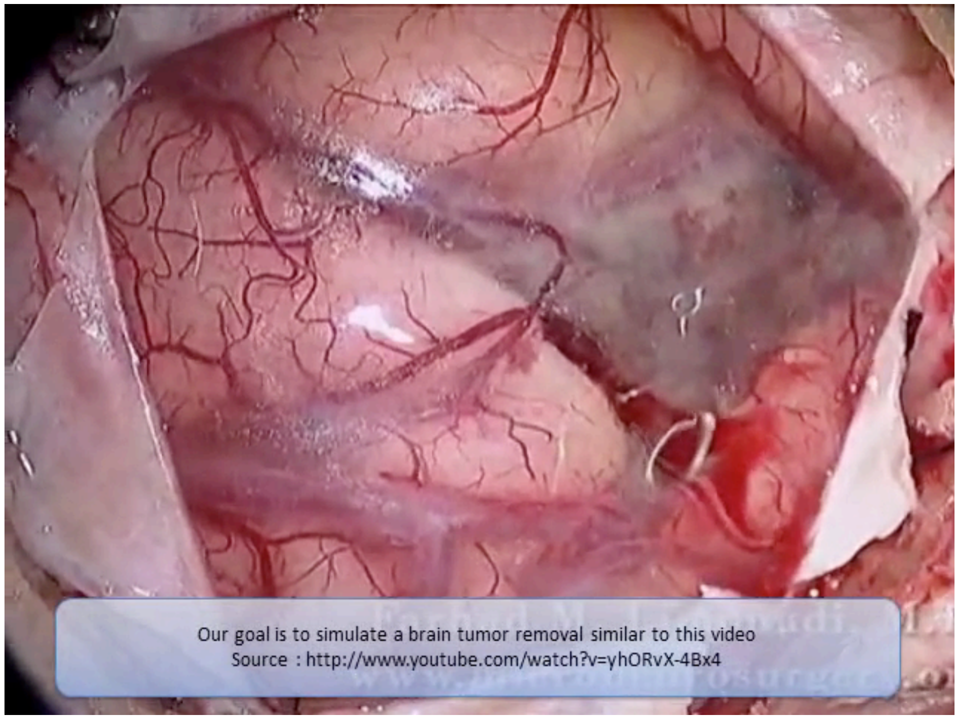
Case studies in Engineering & Personalised Medicine

UNIVERSITÉ DU LUXEMBOURG

50 ans Inria, Nancy, France, 20171220



Immersed collocation
Simulations without a mesh



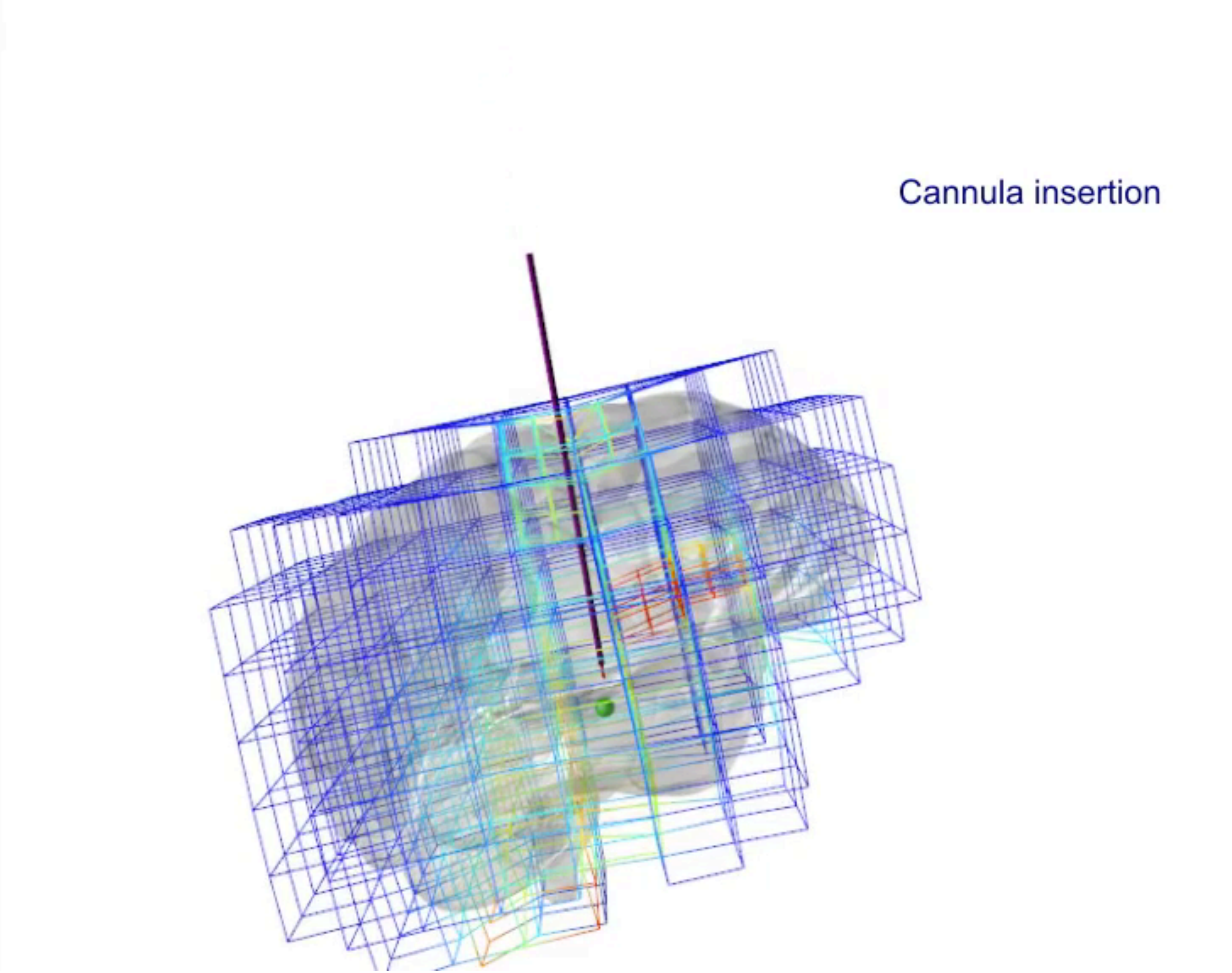
Real-time cutting, MEDIA2014, IEEE2017

Engineering

Personalised medicine

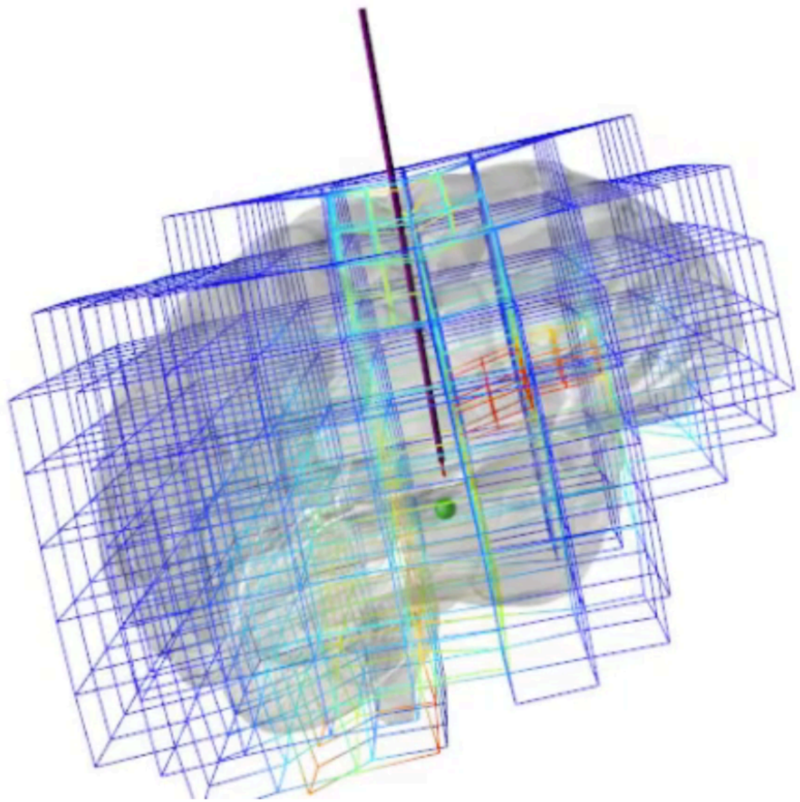
erc

RealTCut



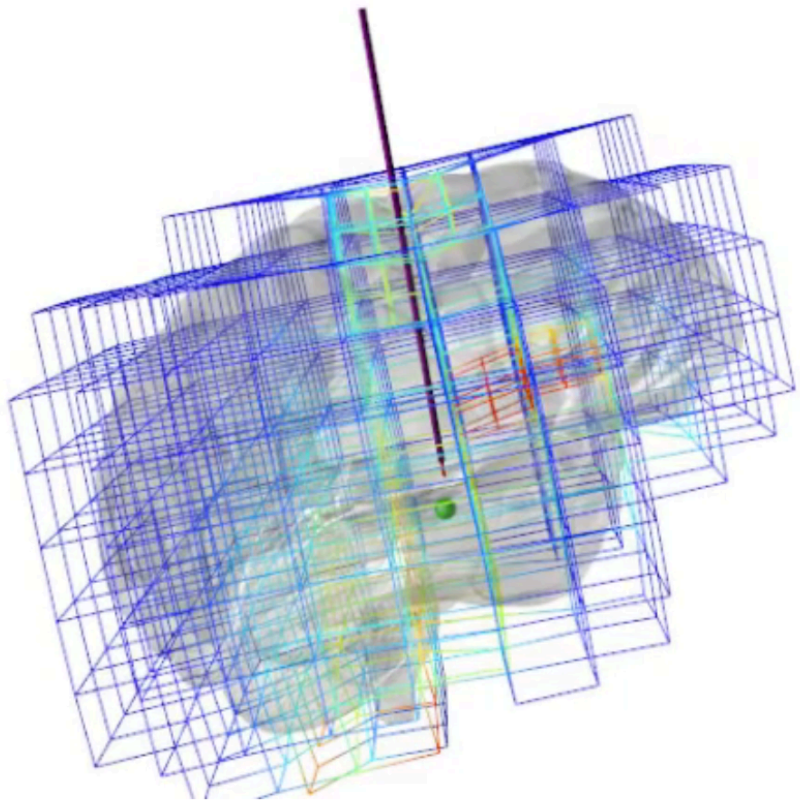
RealTCut

CHALLENGE: everything happens close to the needle… focus the computational expense



RealTCut

CHALLENGE: everything happens close to the needle… focus the computational expense



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

erc
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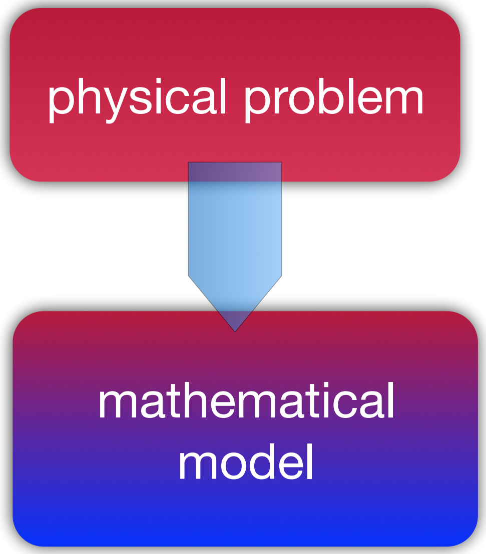
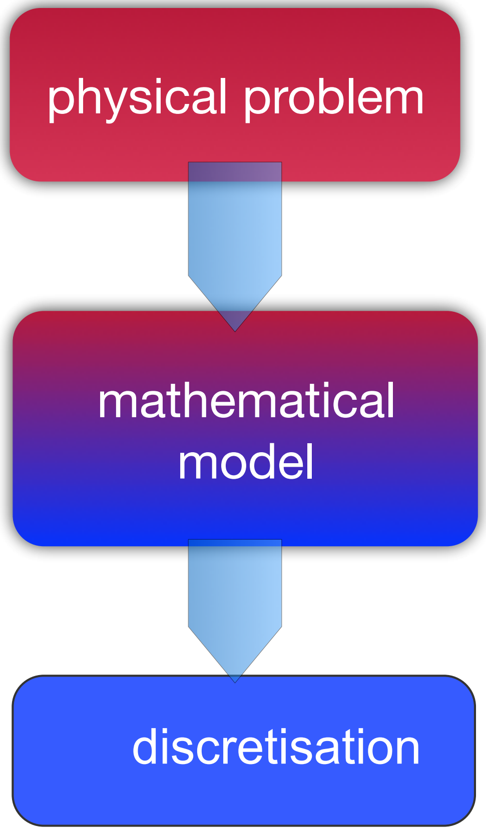
Quantify the quality of the simulation

physical problem

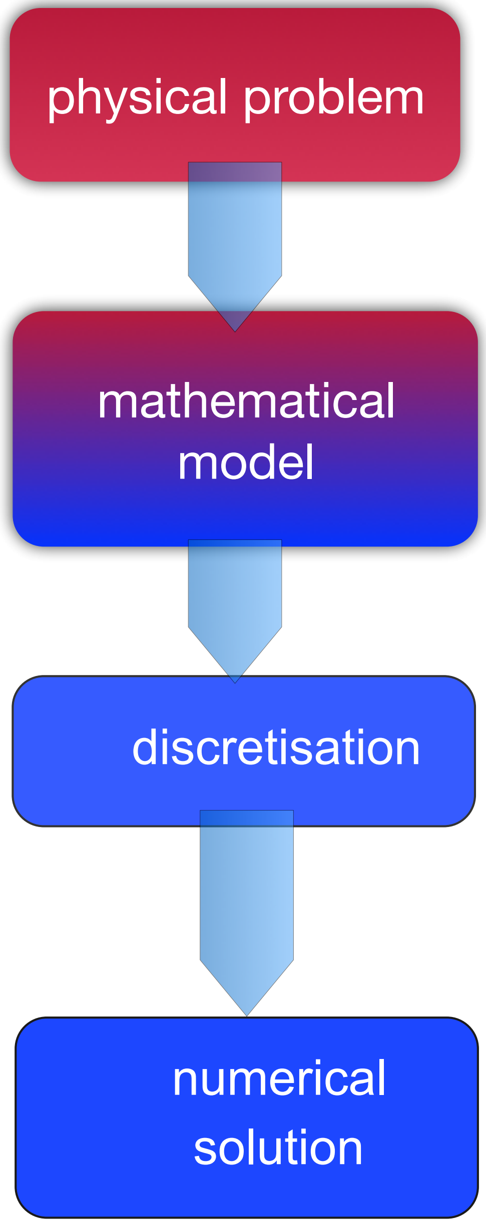
Quantify the quality of the simulation



Quantify the quality of the simulation



Quantify the quality of the simulation



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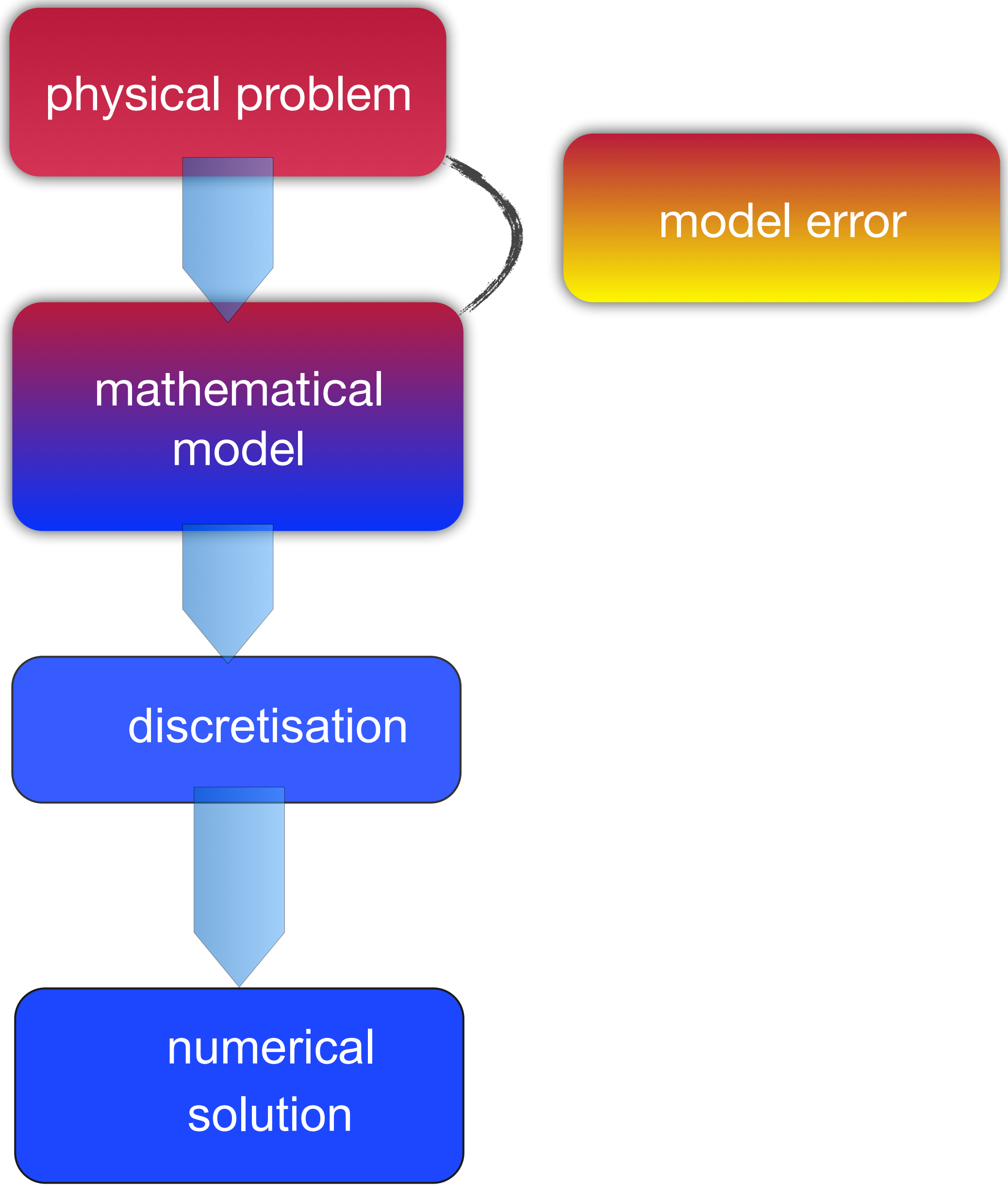
Quantify the quality of the simulation



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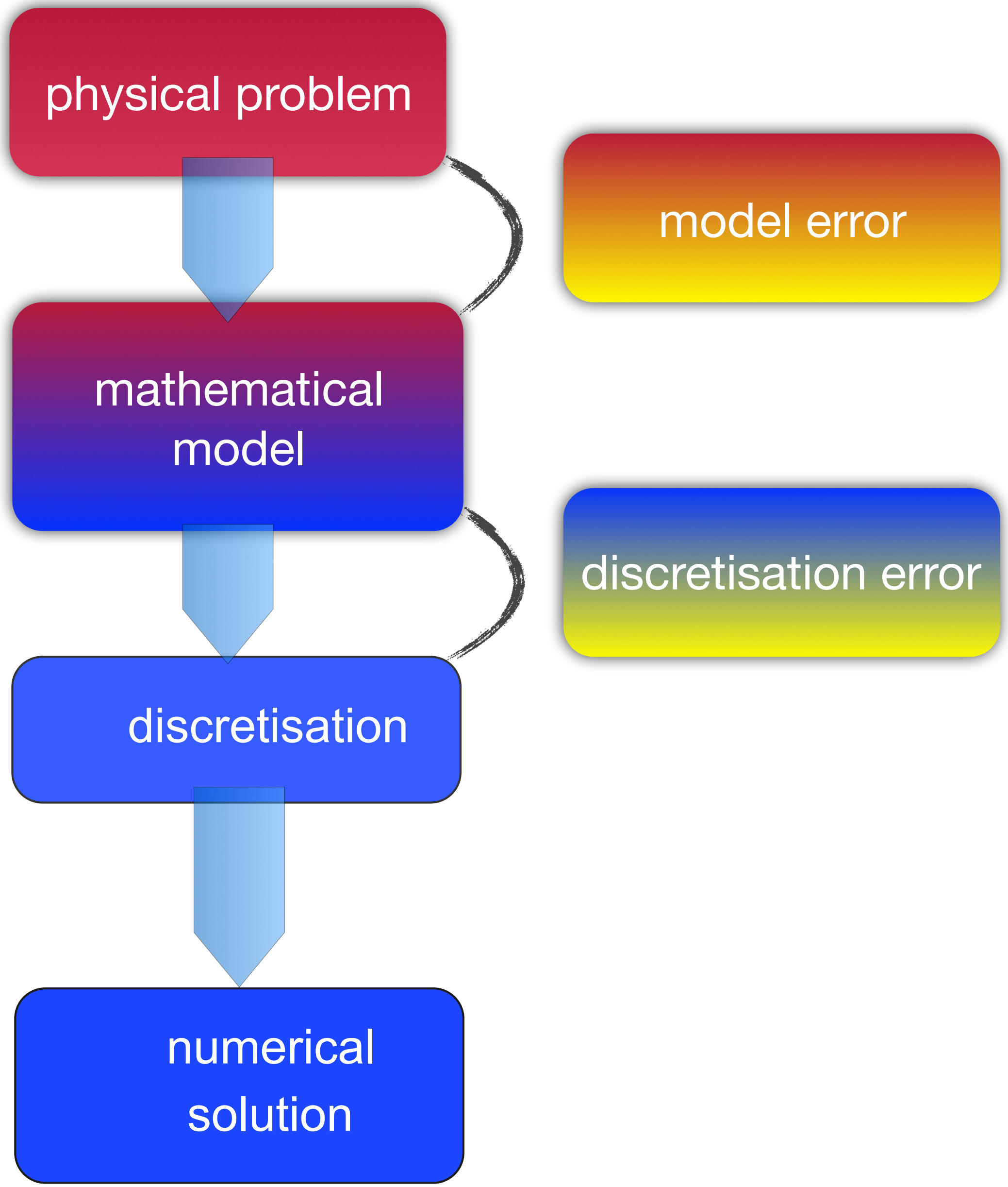

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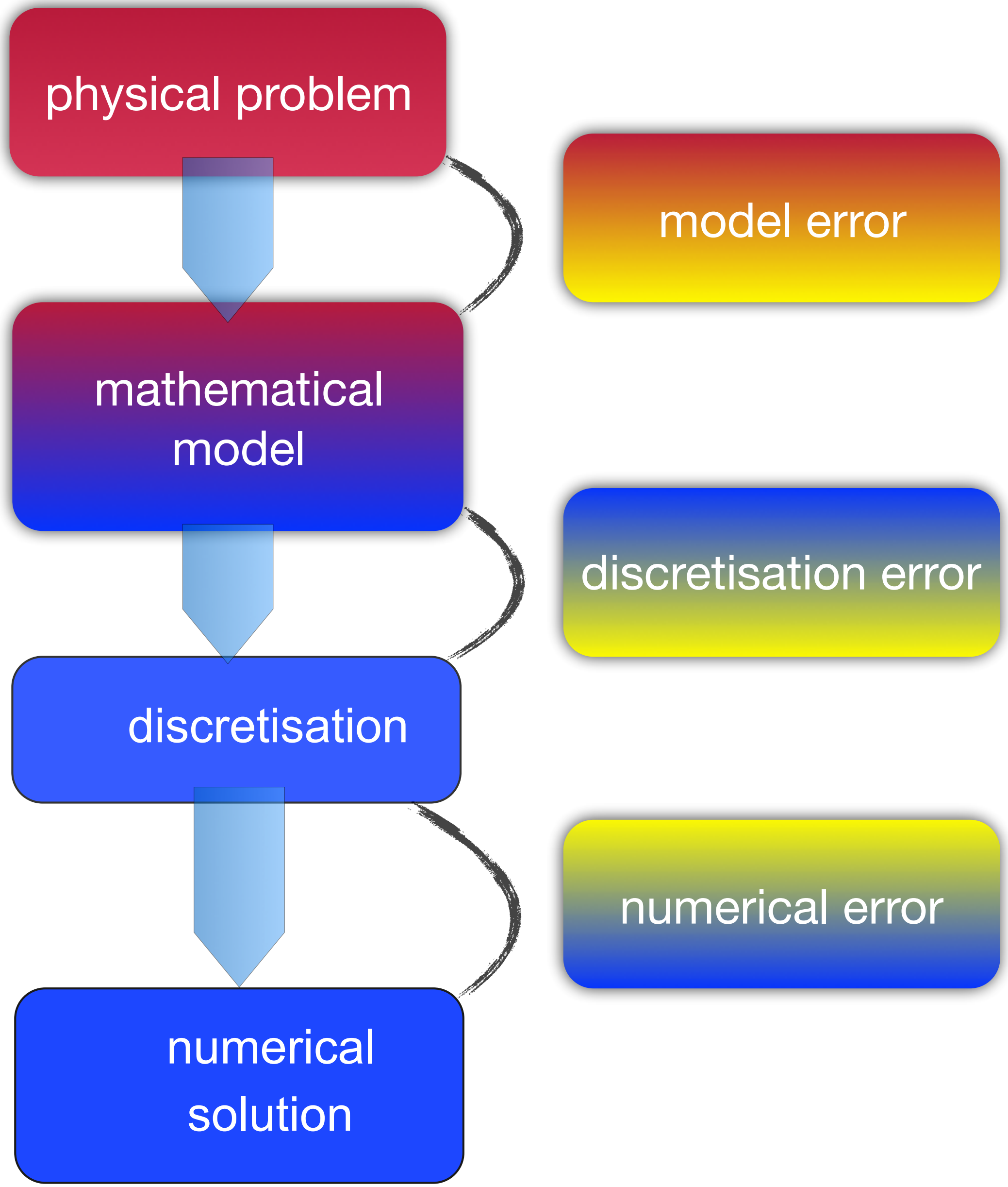
Quantify the quality of the simulation



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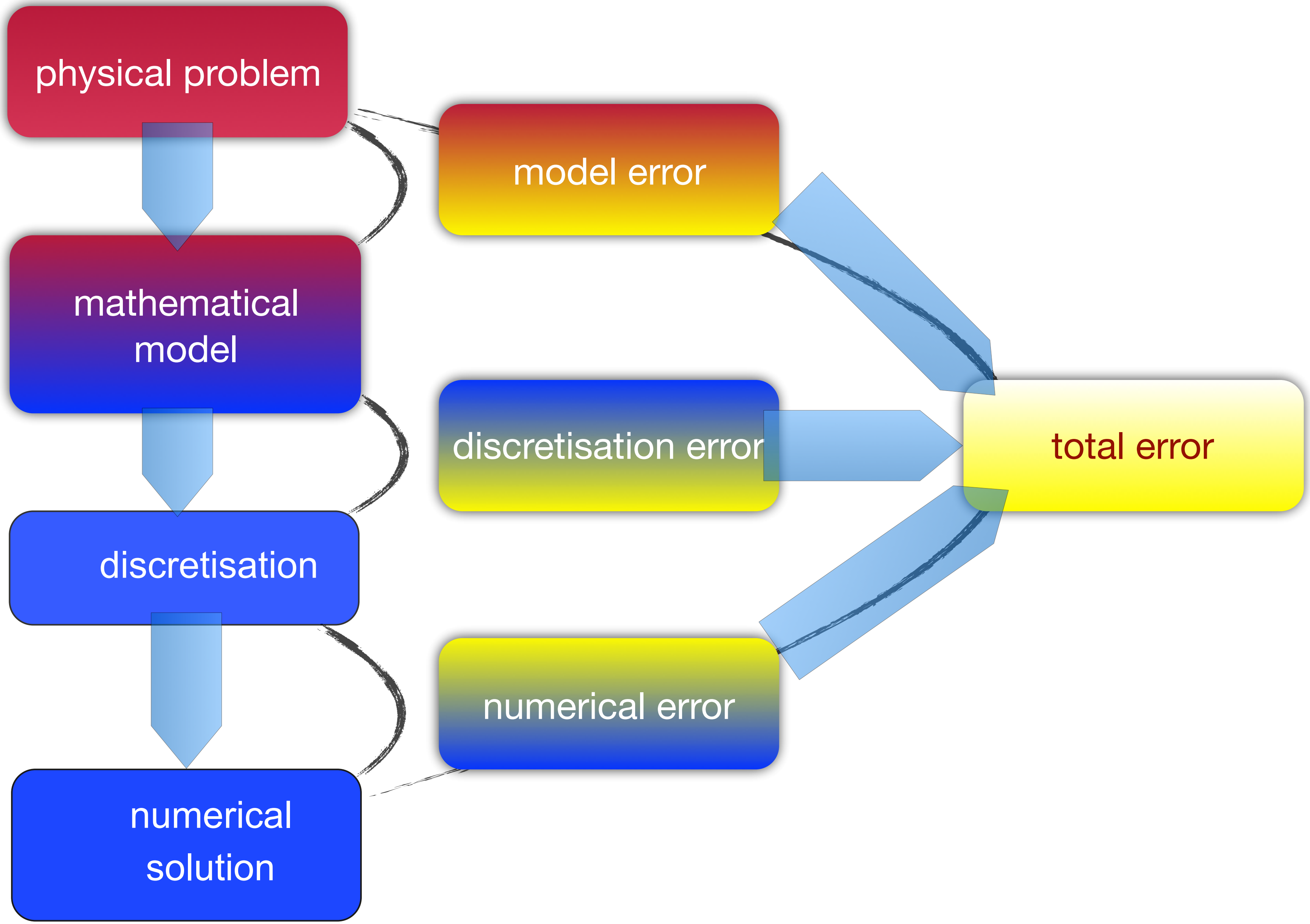
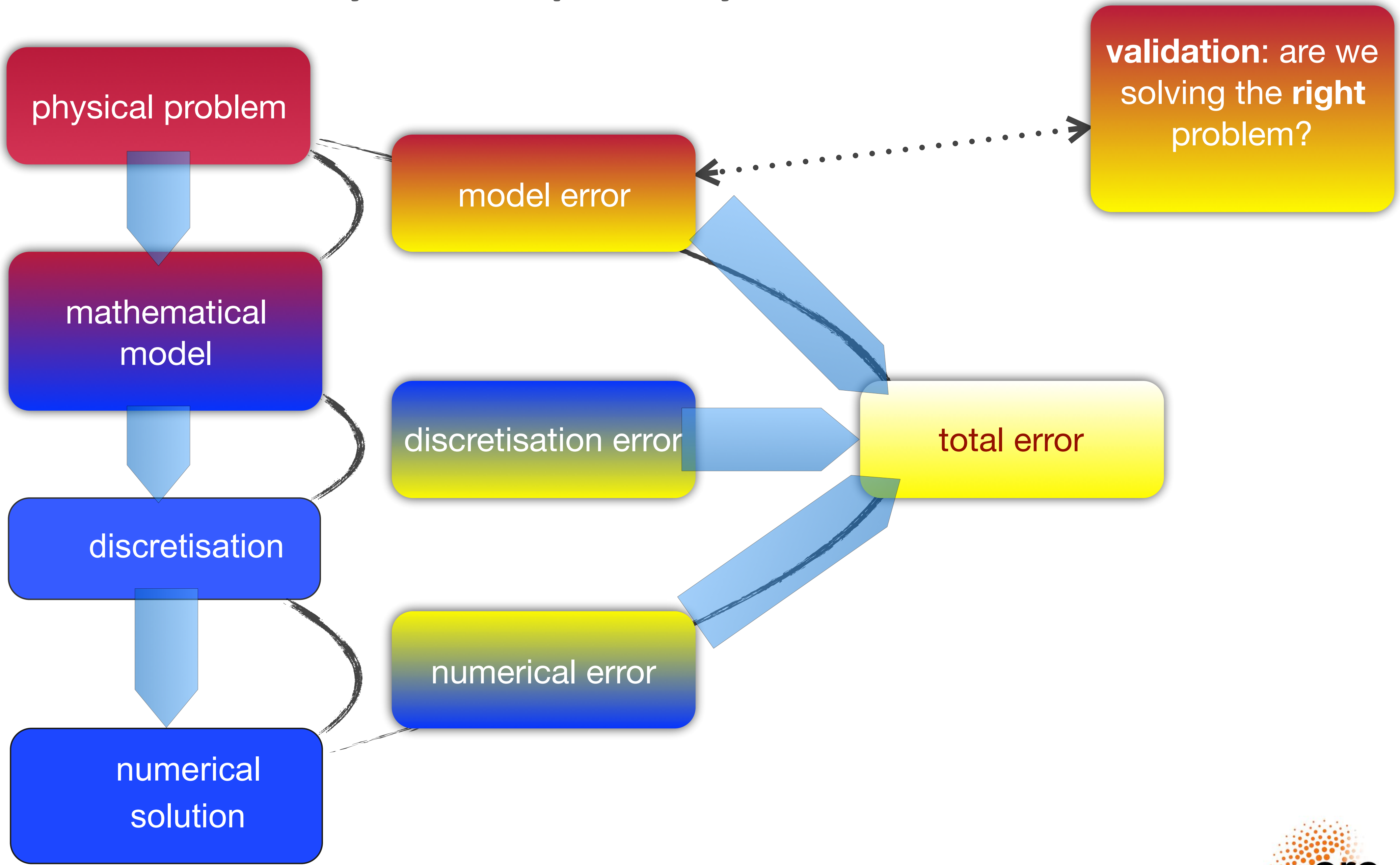
Quantify the quality of the simulation



Quantify the quality of the simulation



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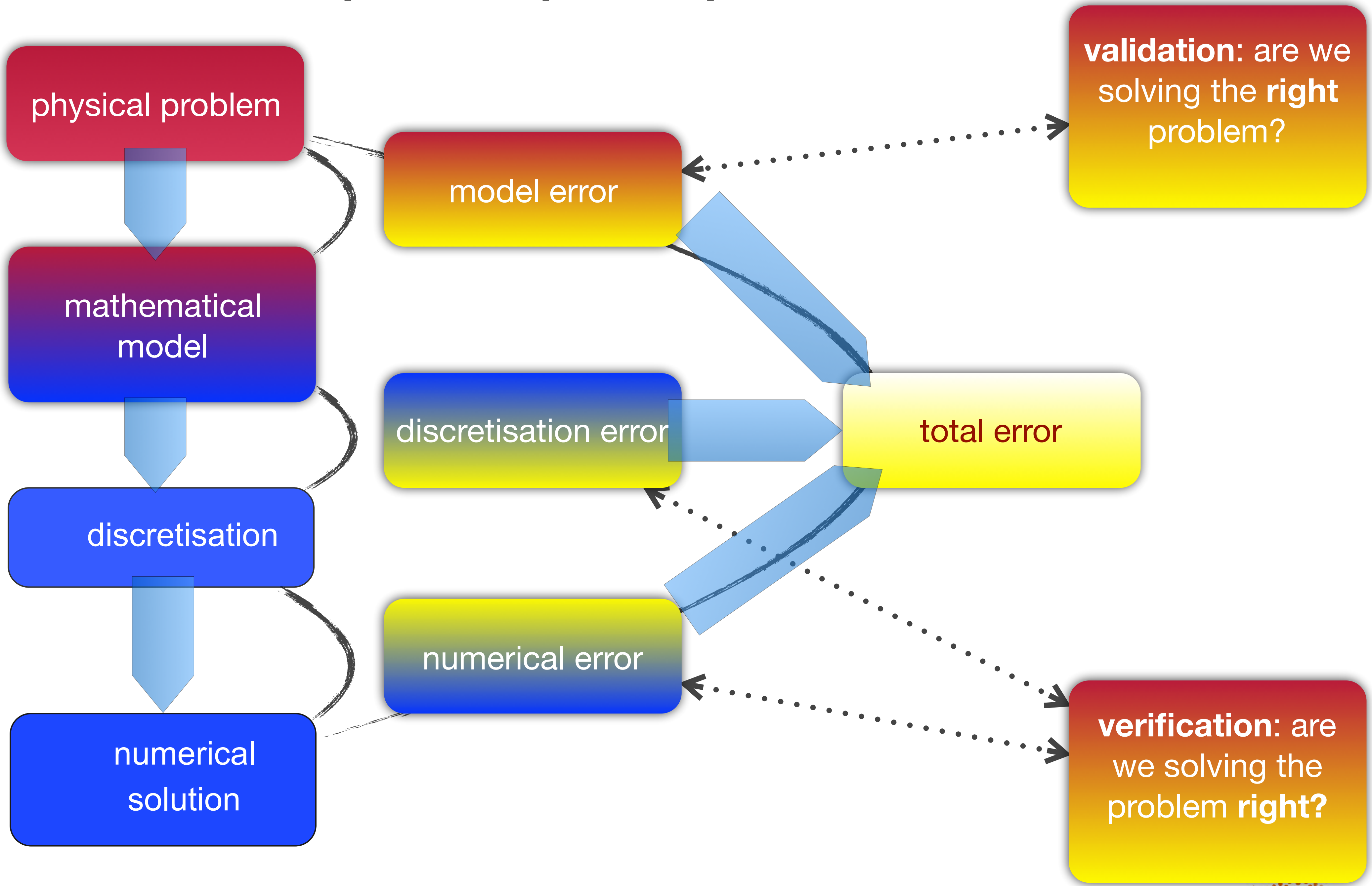
Quantify the quality of the simulation



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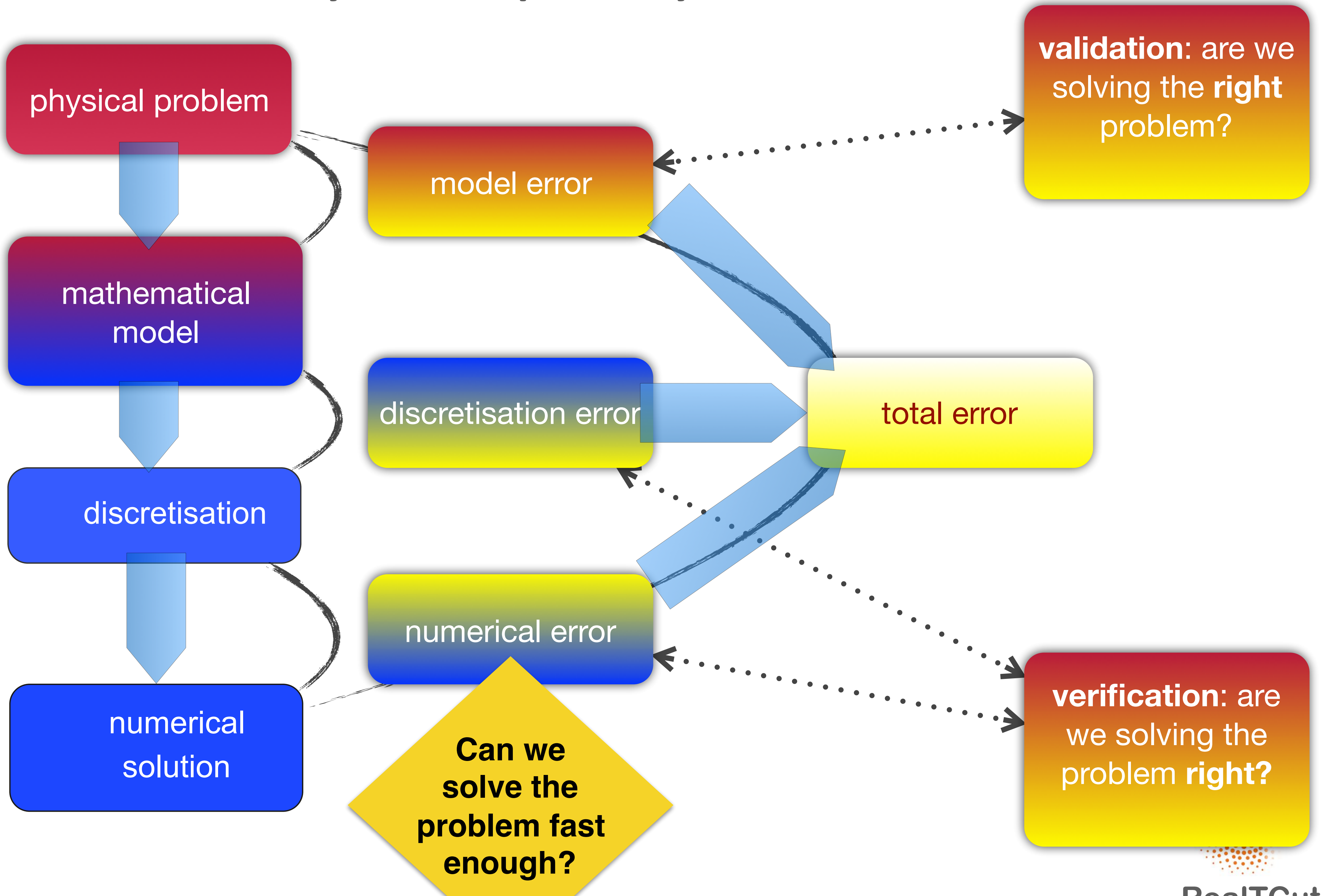
Quantify the quality of the simulation

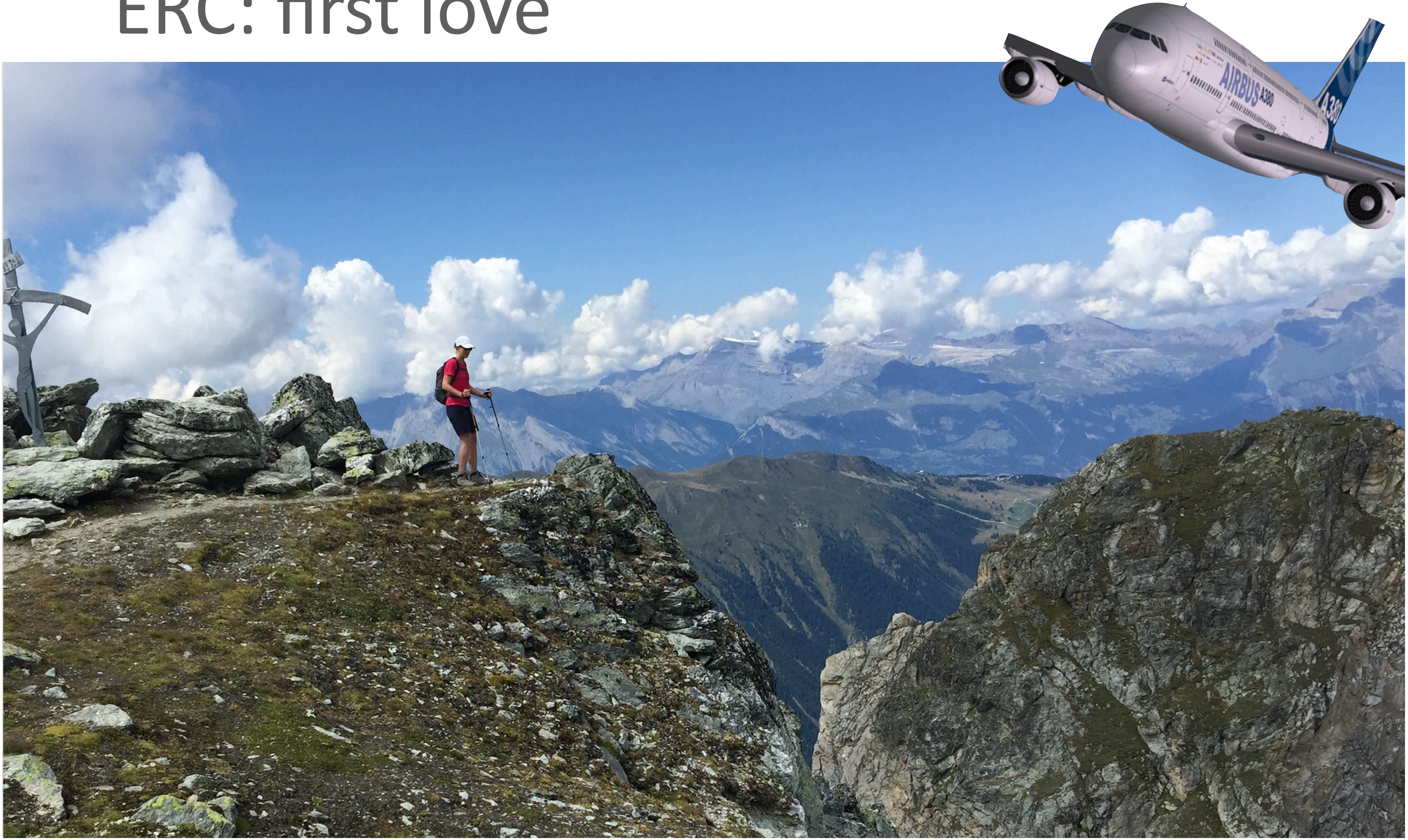


ERC: first love

erc

RealTCut

ERC: first love



erc

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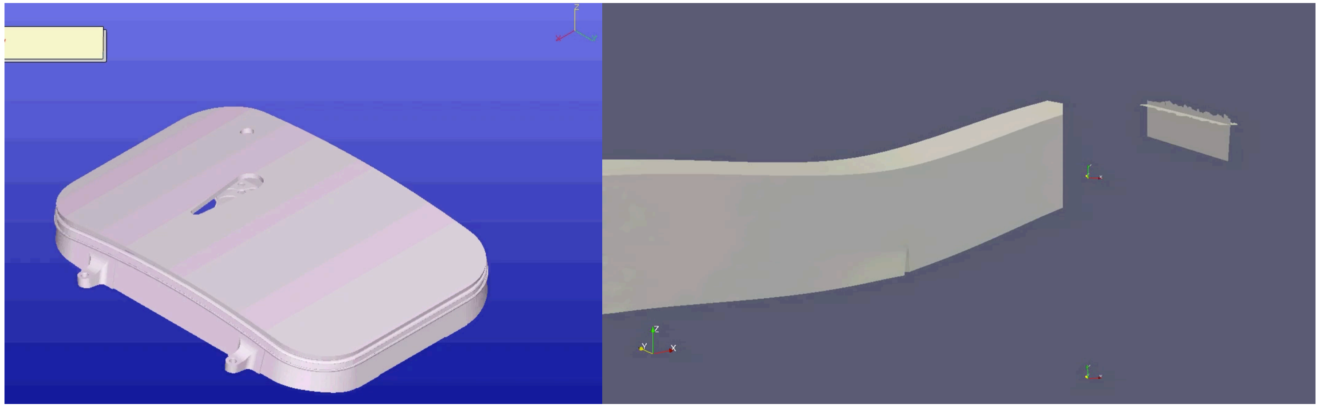
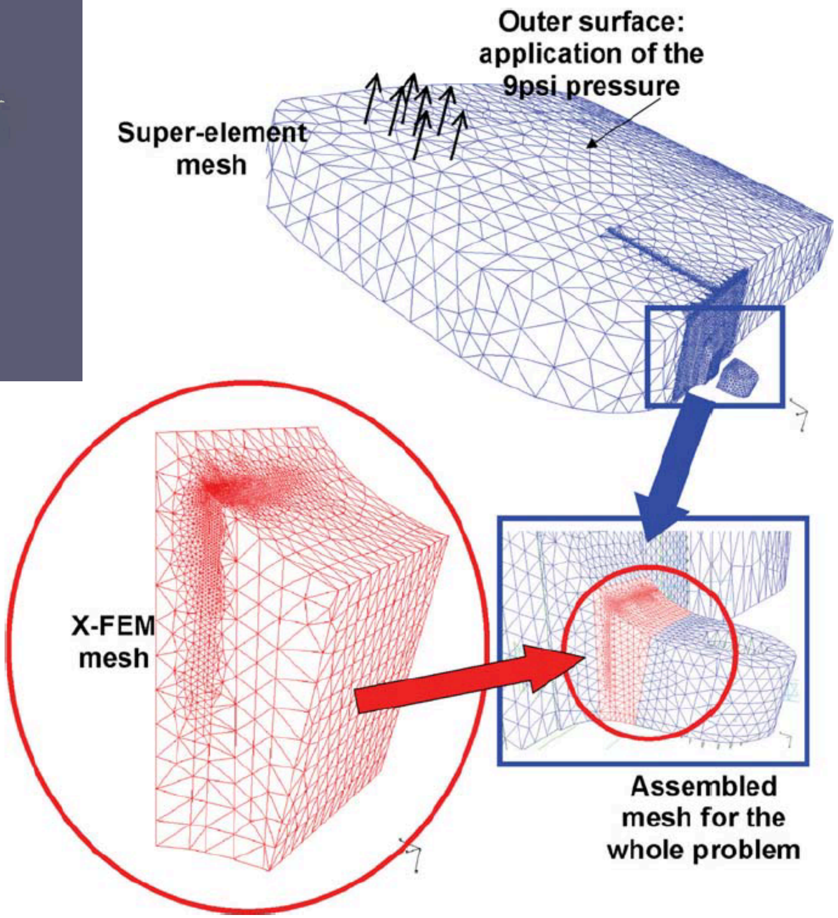
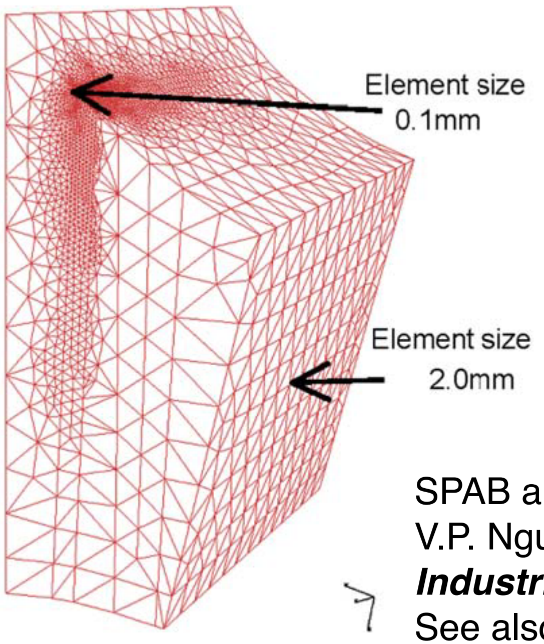
1999-2003 Damage Tolerance Assessment of Aerospace Structures PhD

How often should we inspect a structure for flaws?





ad hoc mesh refinement



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

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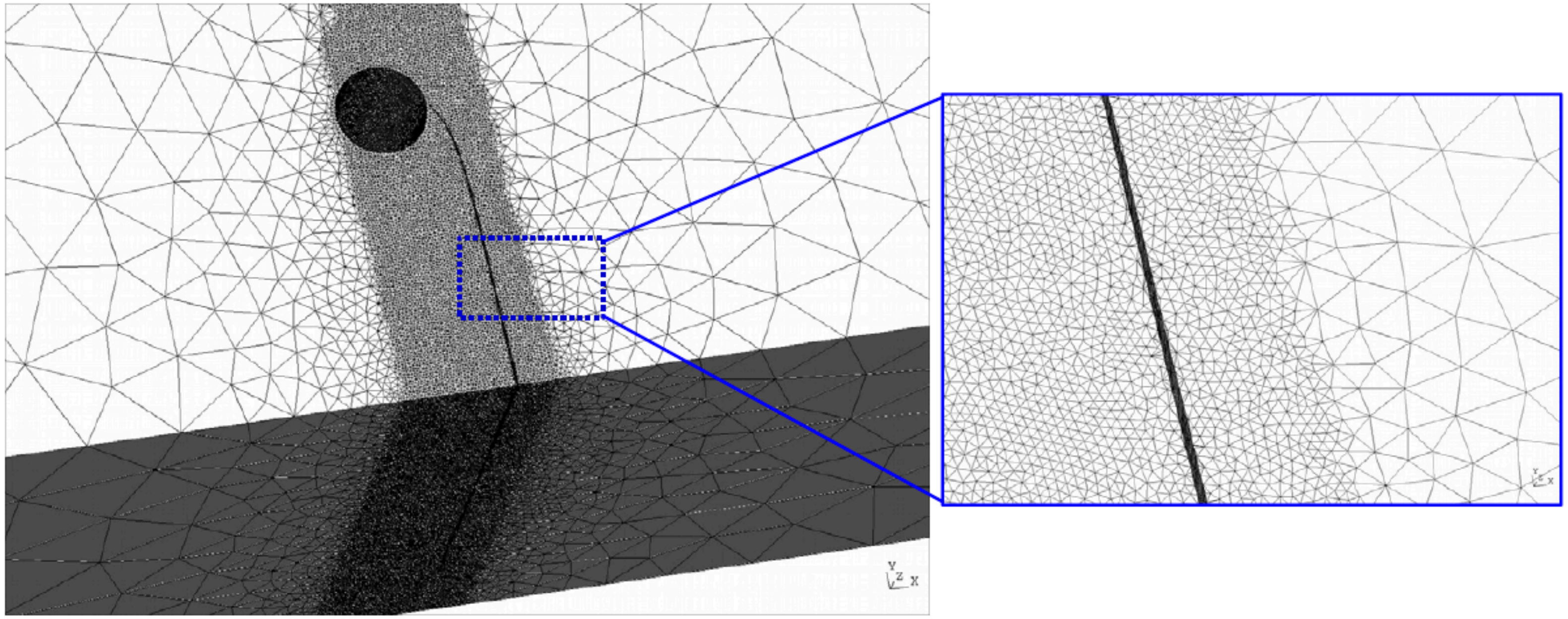
Refine along the "expected" crack path…



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.

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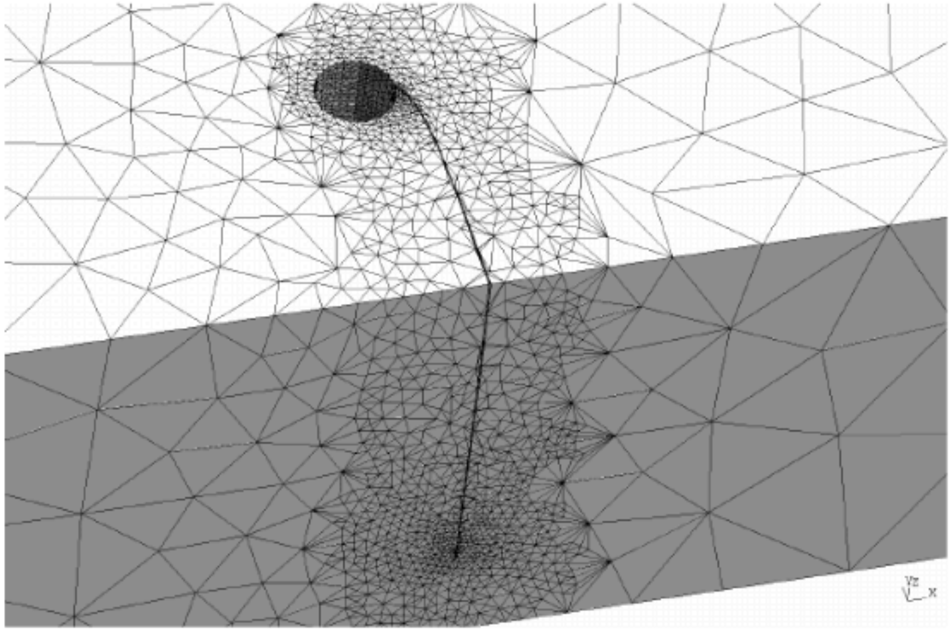
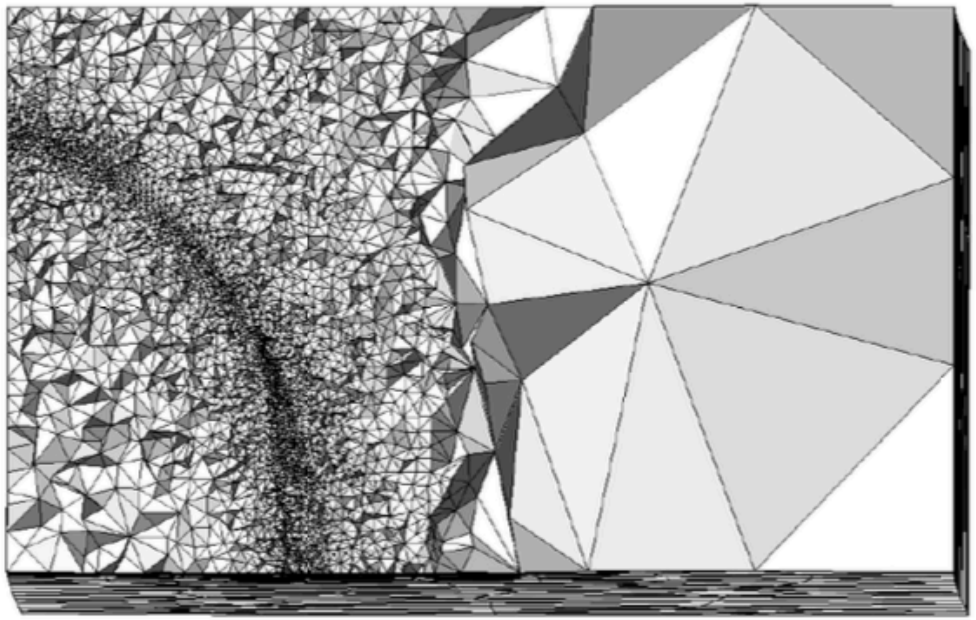
Much better… adapt the discretisation locally





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.

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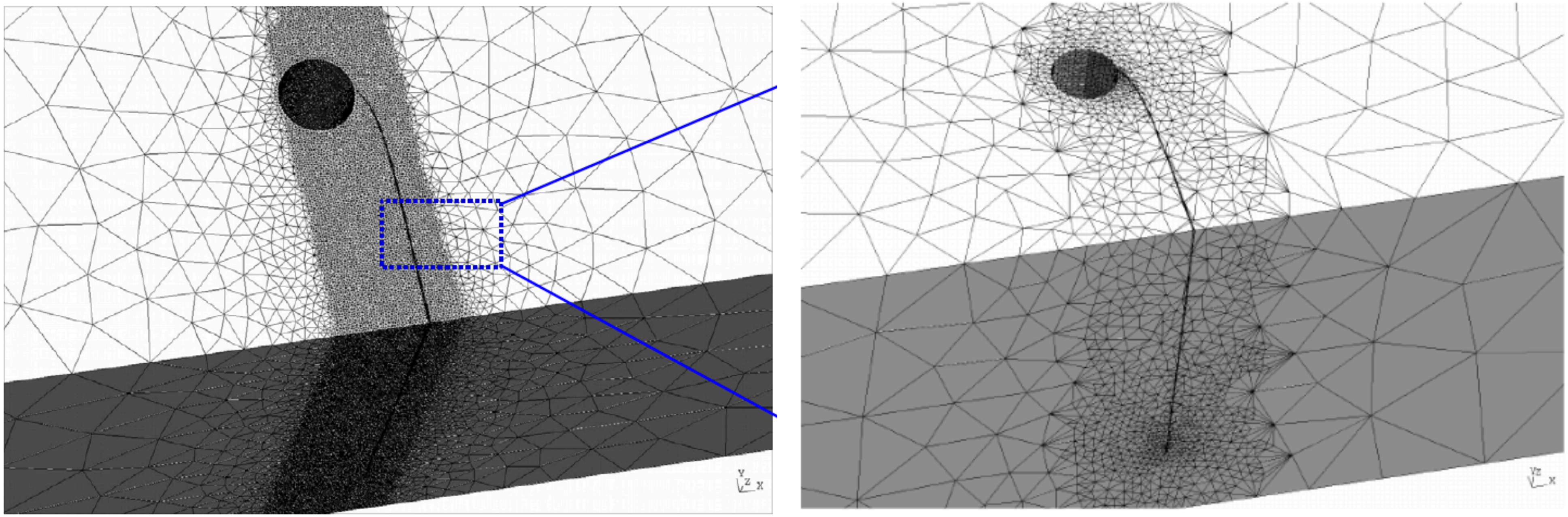
Much better… adapt the discretisation locally



Orders of magnitude fewer elements

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.

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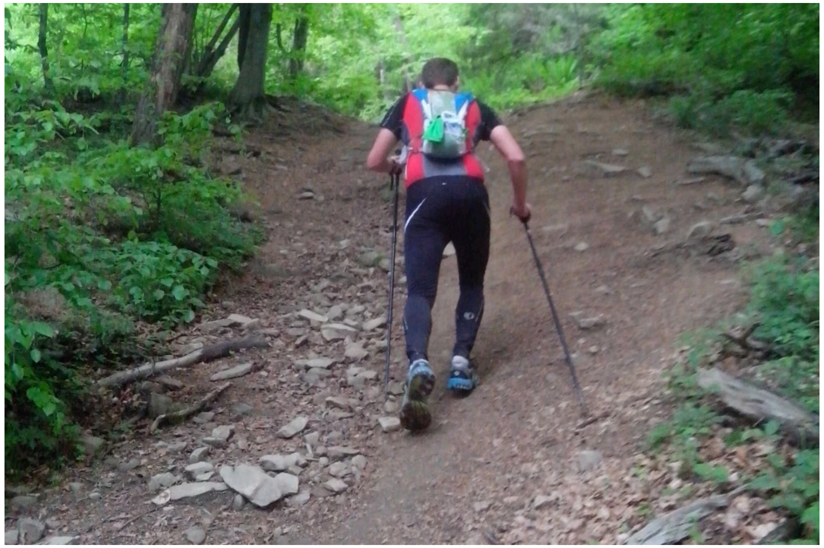
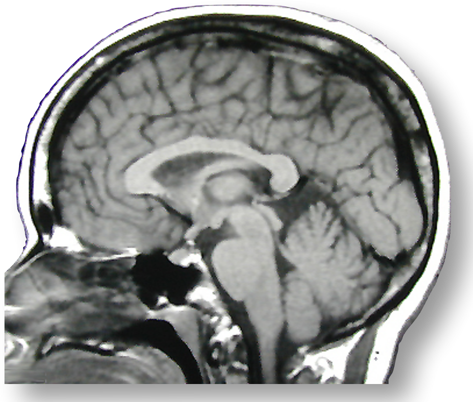
From your first love to the ERC

hiking - 20km D+500m



ultra-marathon 52km D+2500m

aerospace



biomechanics

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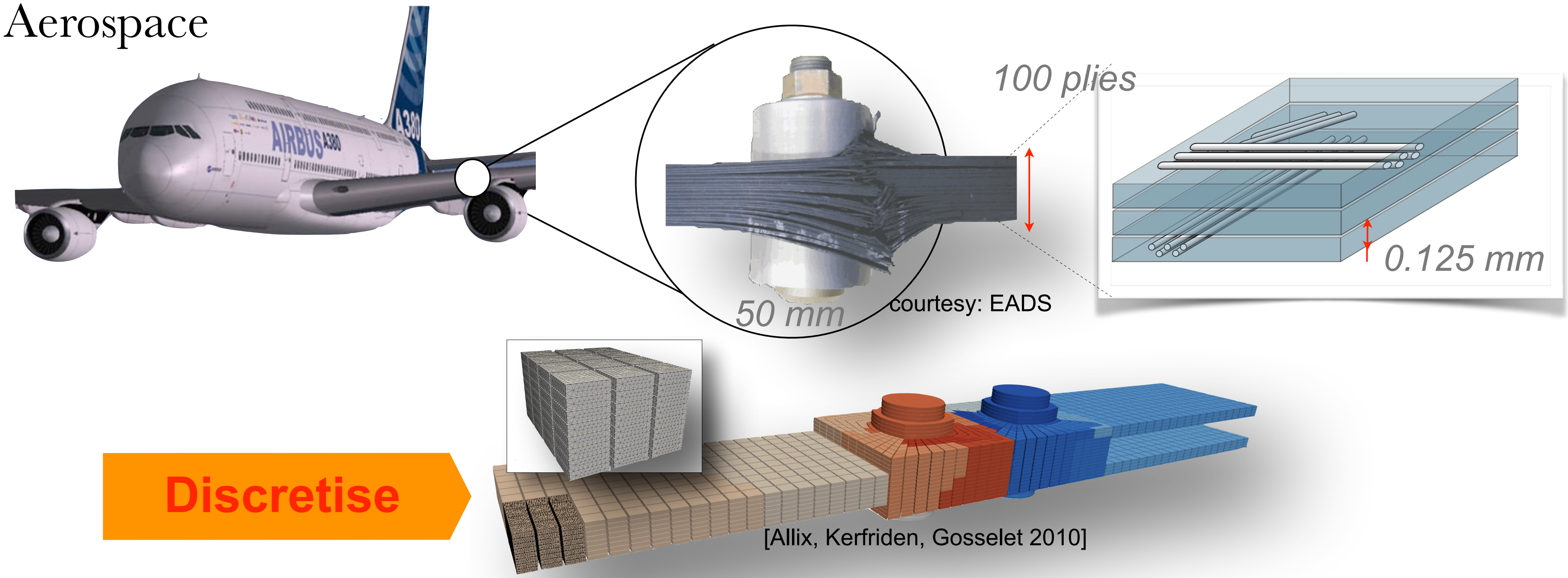
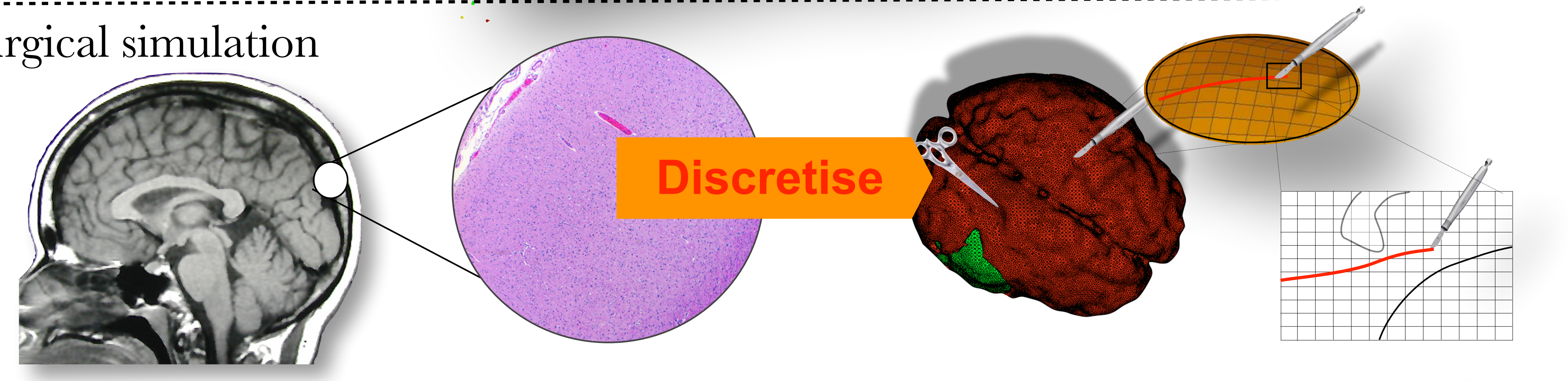
Motivation: multiscale fracture of engineering structures and materials

Aerospace



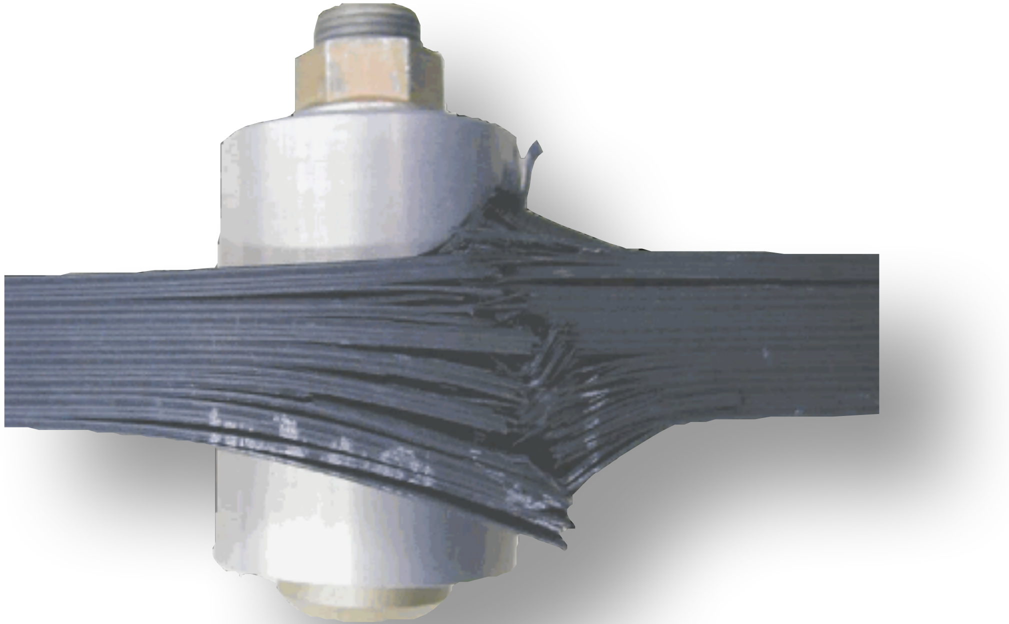
Surgical simulation



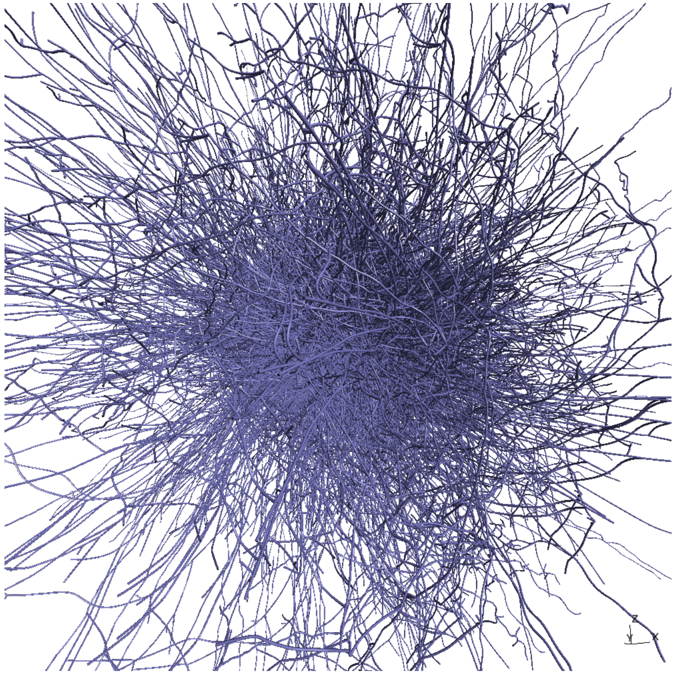
- Reduce the problem size while controlling the quality for problems involving (free) interfaces

Aero

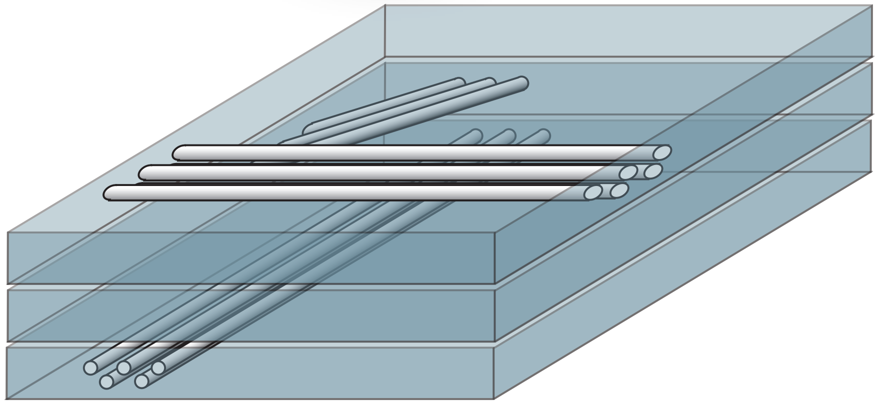
Bio



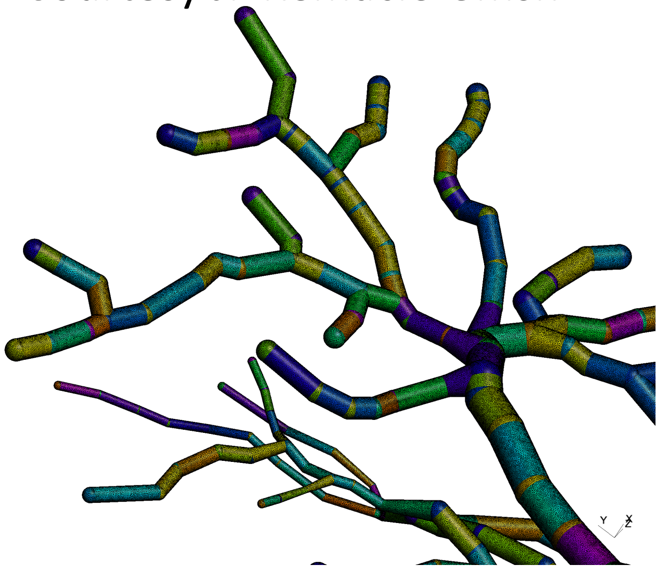
Bolted joint Courtesy EADS



Courtesy JF Remacle Gmsh



Multi-scale fibre lay-up Courtesy EADS



Courtesy JF Remacle Gmsh

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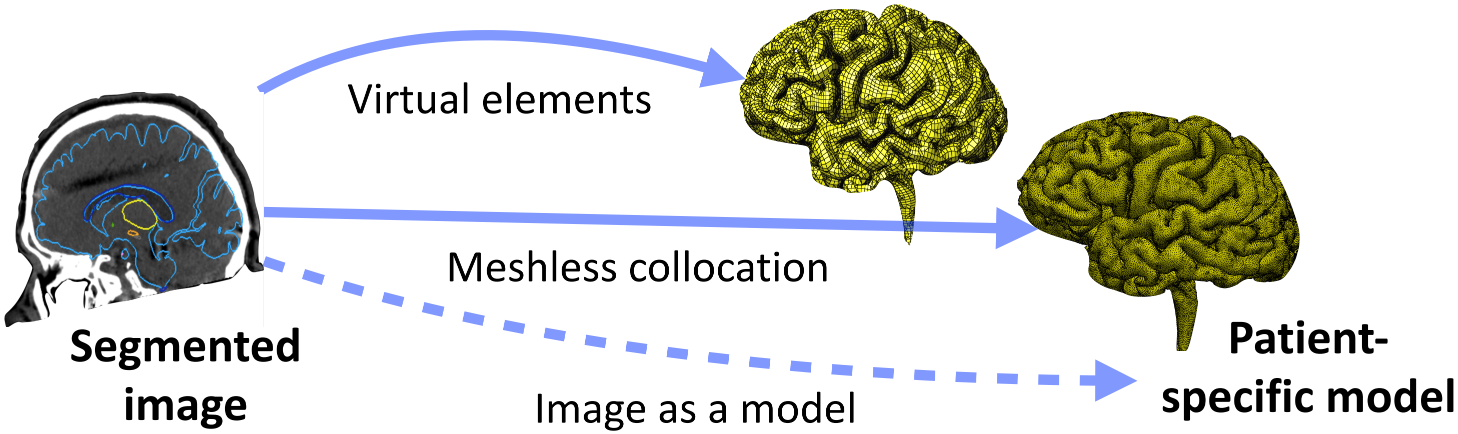
MAIN RESULT: QUALITY-CONTROLLED REAL-TIME SIMULATION

Represent numerically the geometry of a given patient



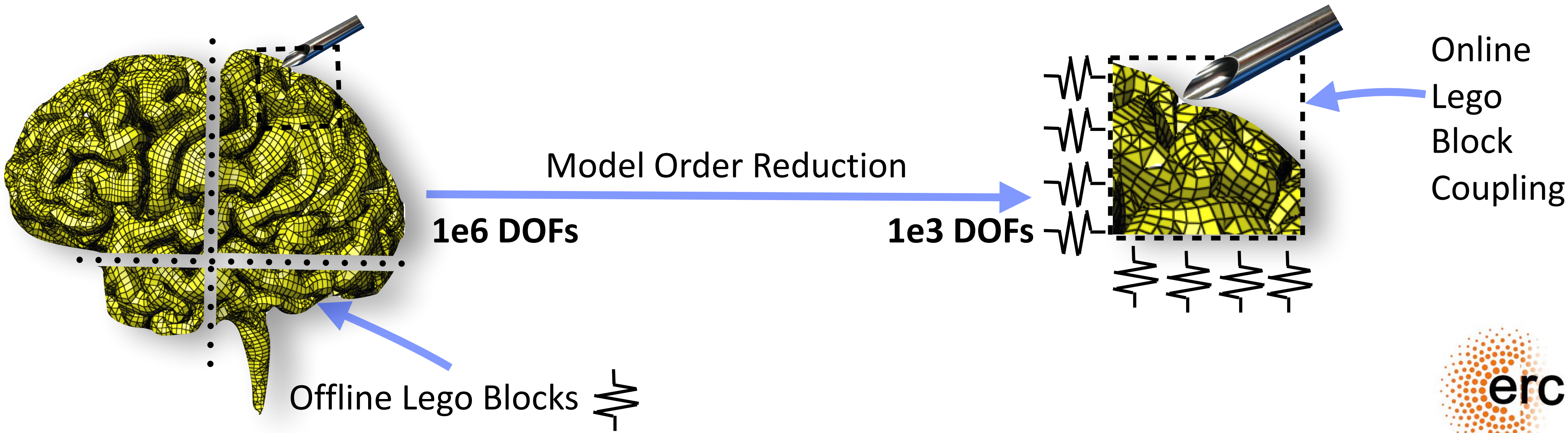
Research questions

- Generation speed?
- Easy adaptivity?
- Incompressibility?
- Mesh distortion?

Solve the problem fast enough and with quality control

Precompute OFFLINE

Real-time ONLINE



RealTCut

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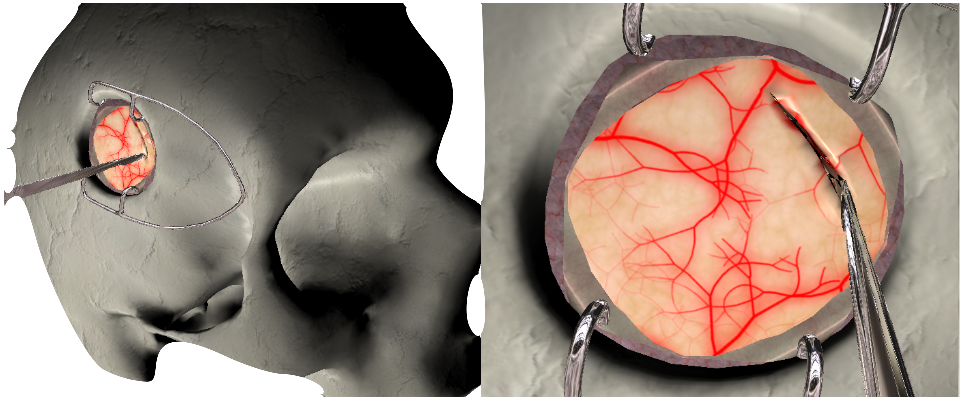
NEXT CHALLENGES

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).

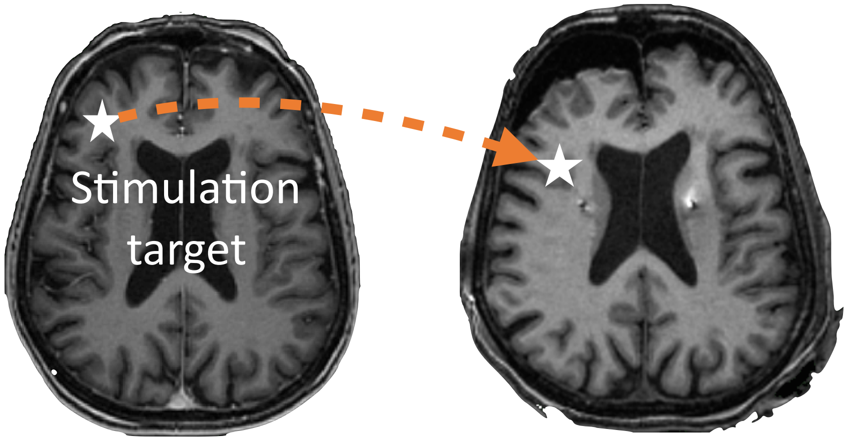


Courtecuisse, 2014, Implicit method for cutting in real-time. MEDIA

A generic organ is sufficient.

Future
Surgical assistance and planning

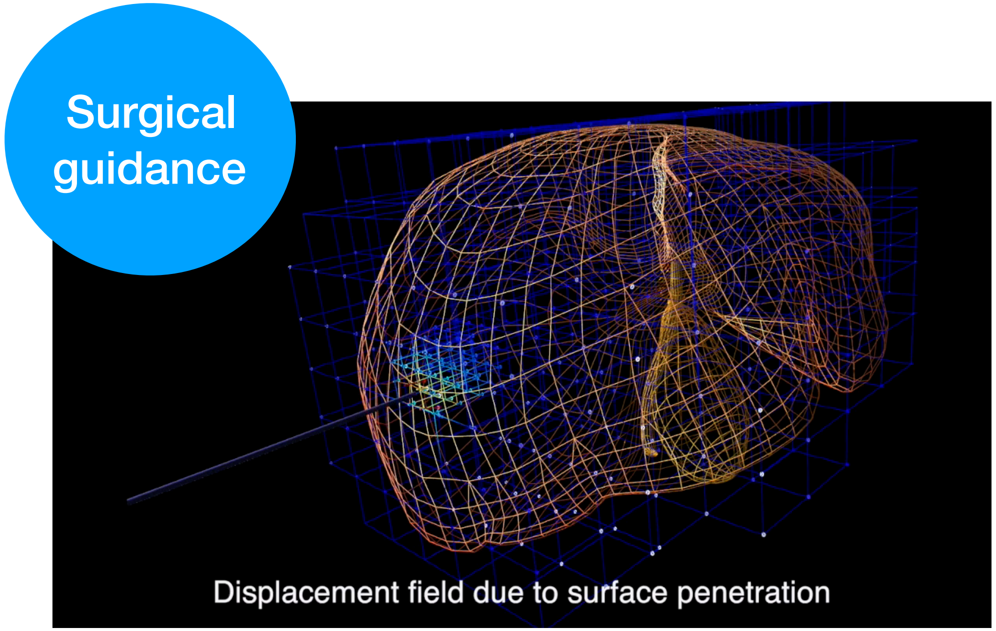
- Data-driven material models (real-time).
- Error control in quantities of interest for strong non-linearities, multi-field…
- Clinical time scales (solution in minutes).



Predict shift of brain target.

Patient specificity is essential.

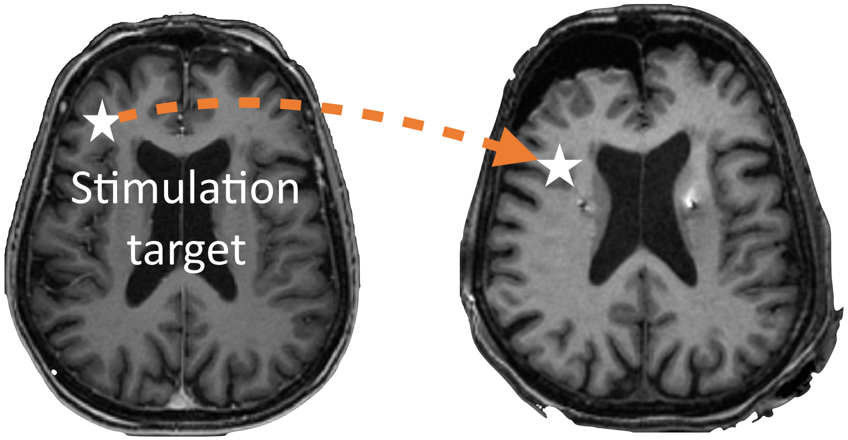
From surgical training to surgical planning and assistance



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).



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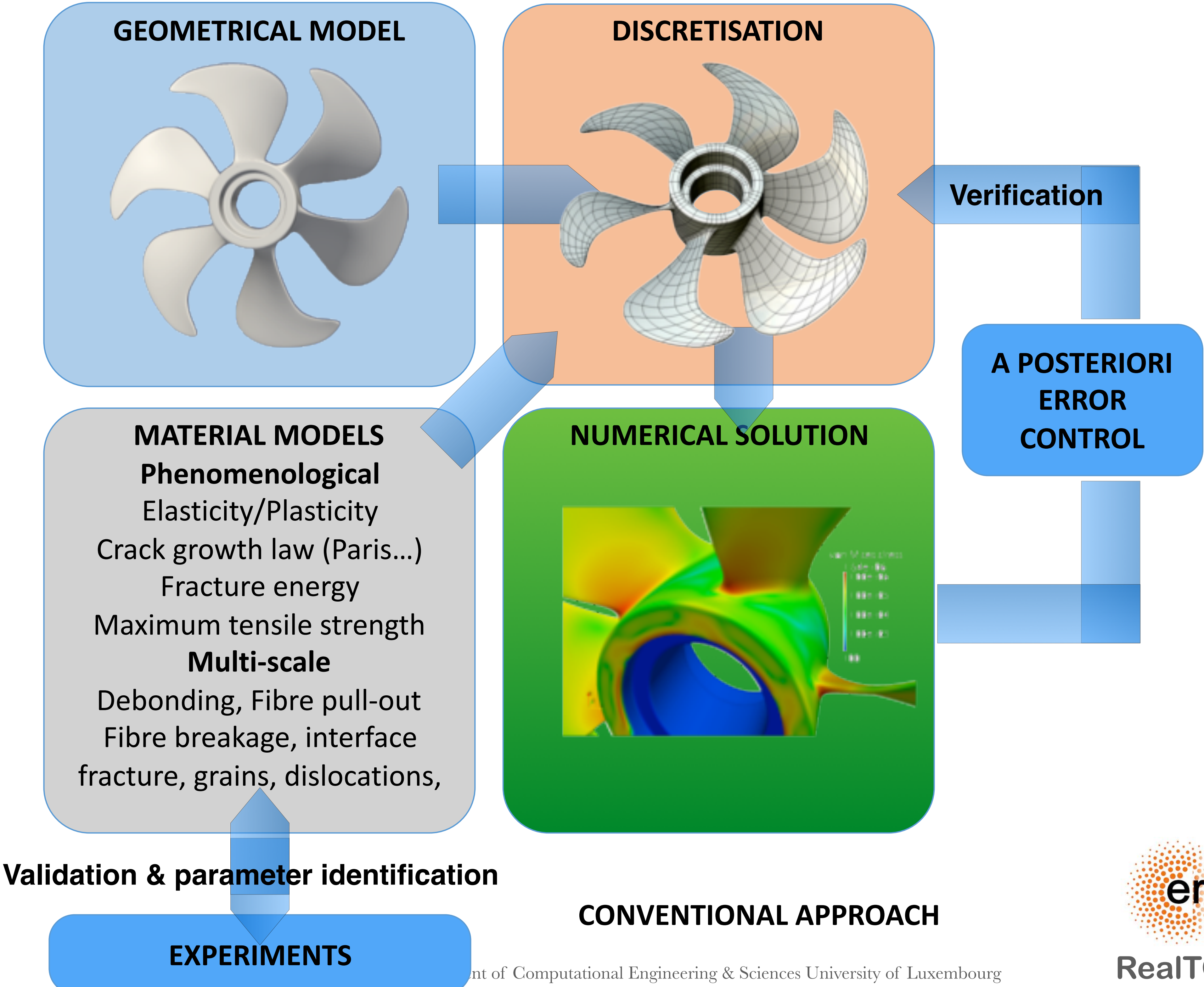
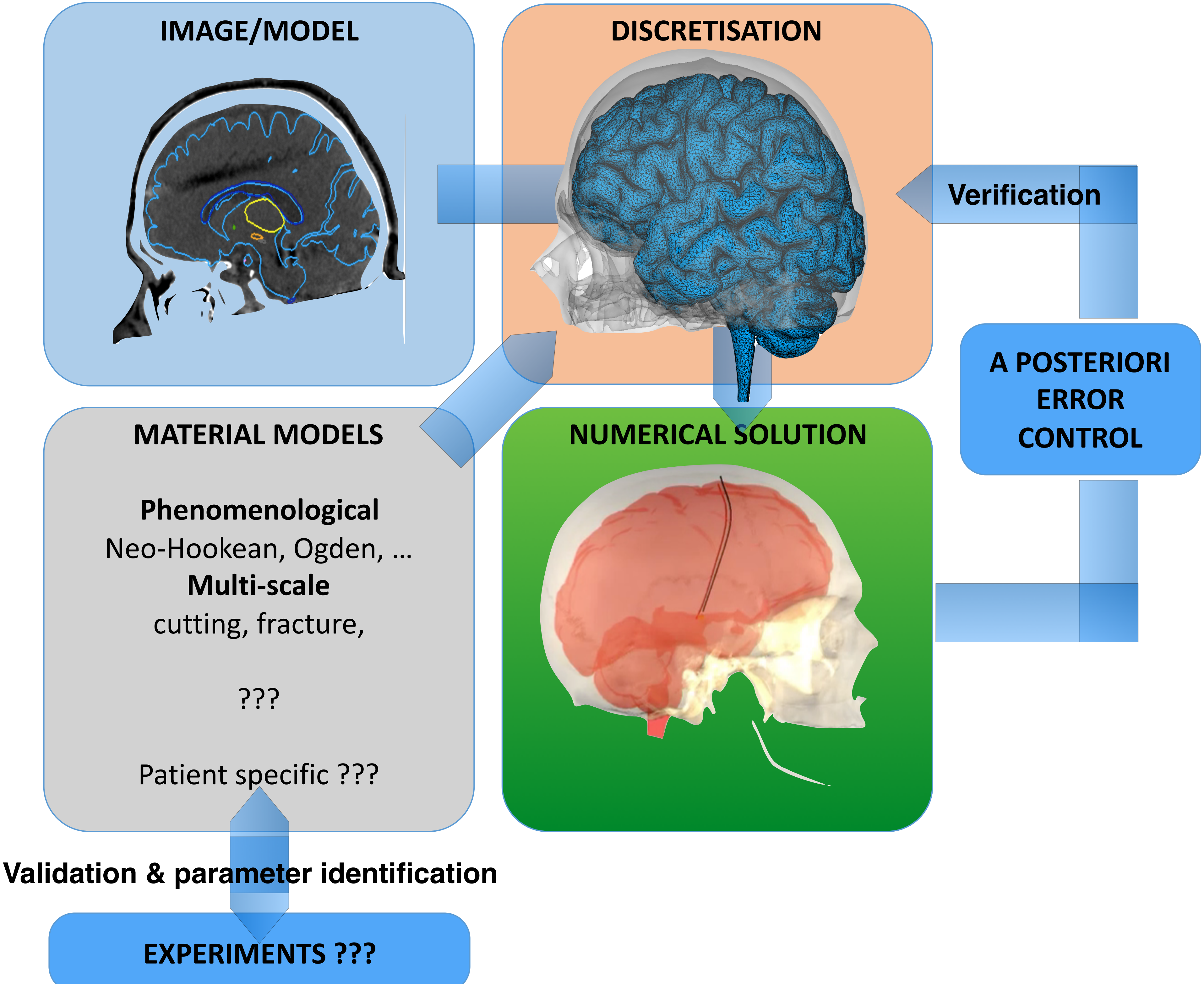
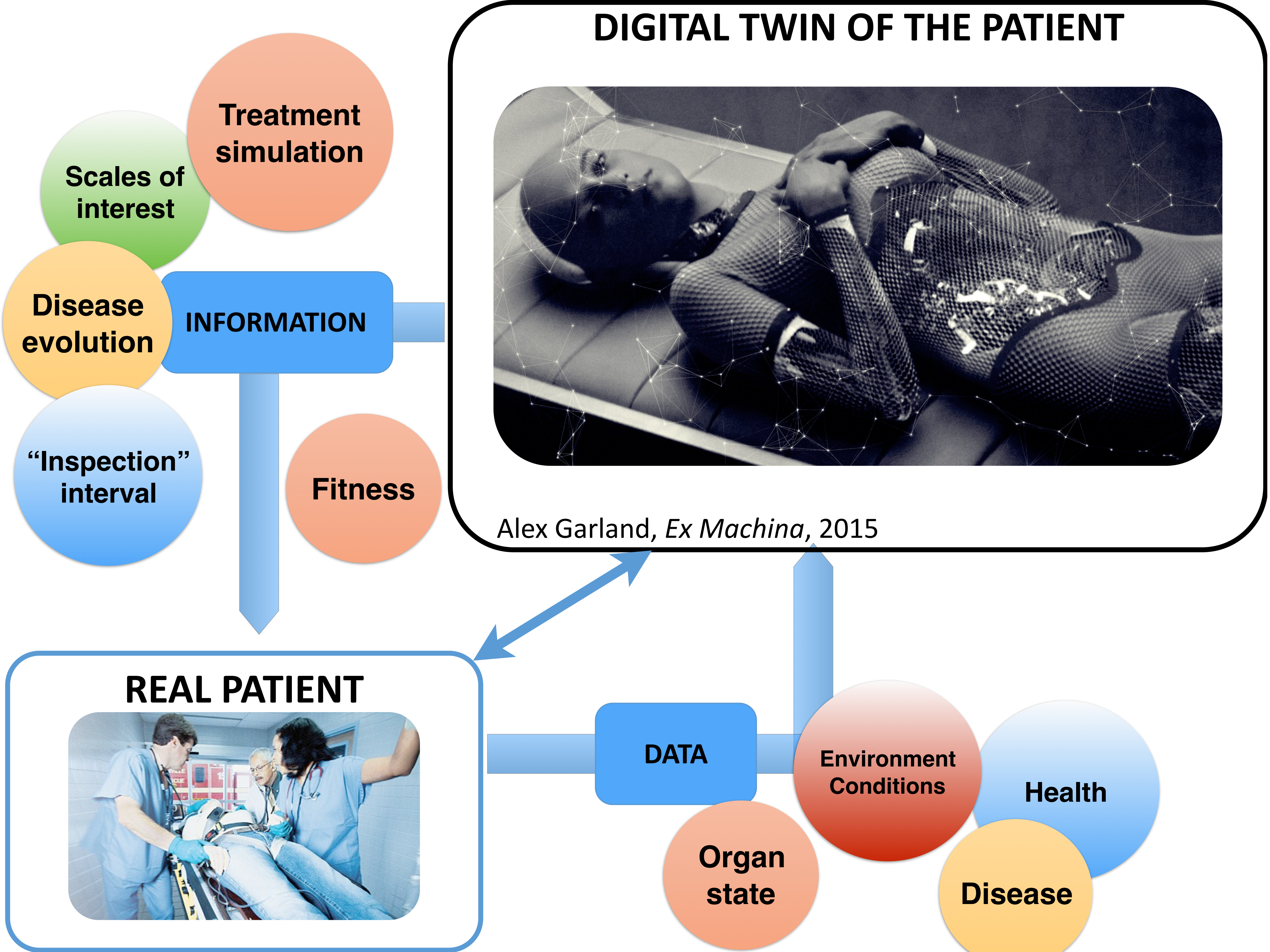

GEOMETRICAL MODEL
DISCRETISATION
Verification
A POSTERIORI ERROR CONTROL
MATERIAL MODELS
Phenomenological
Elasticity/Plasticity
Crack growth law (Paris…)
Fracture energy
Maximum tensile strength
Multi-scale
Debonding, Fibre pull-out
Fibre breakage, interface
fracture, grains, dislocations,
NUMERICAL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

RealTCut


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



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

Prior Knowledge

Prior Knowledge

Hypothesis

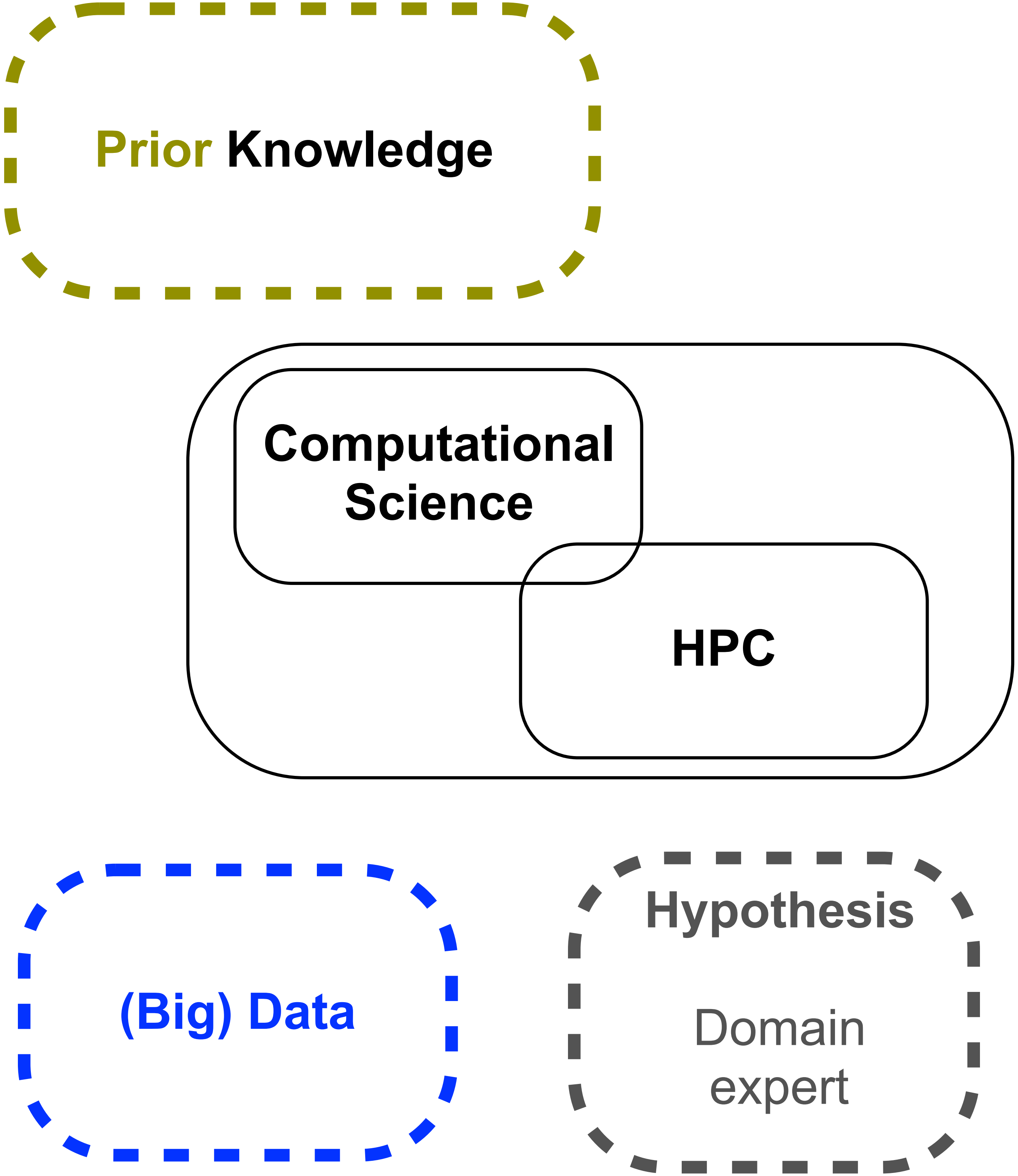
Domain expert

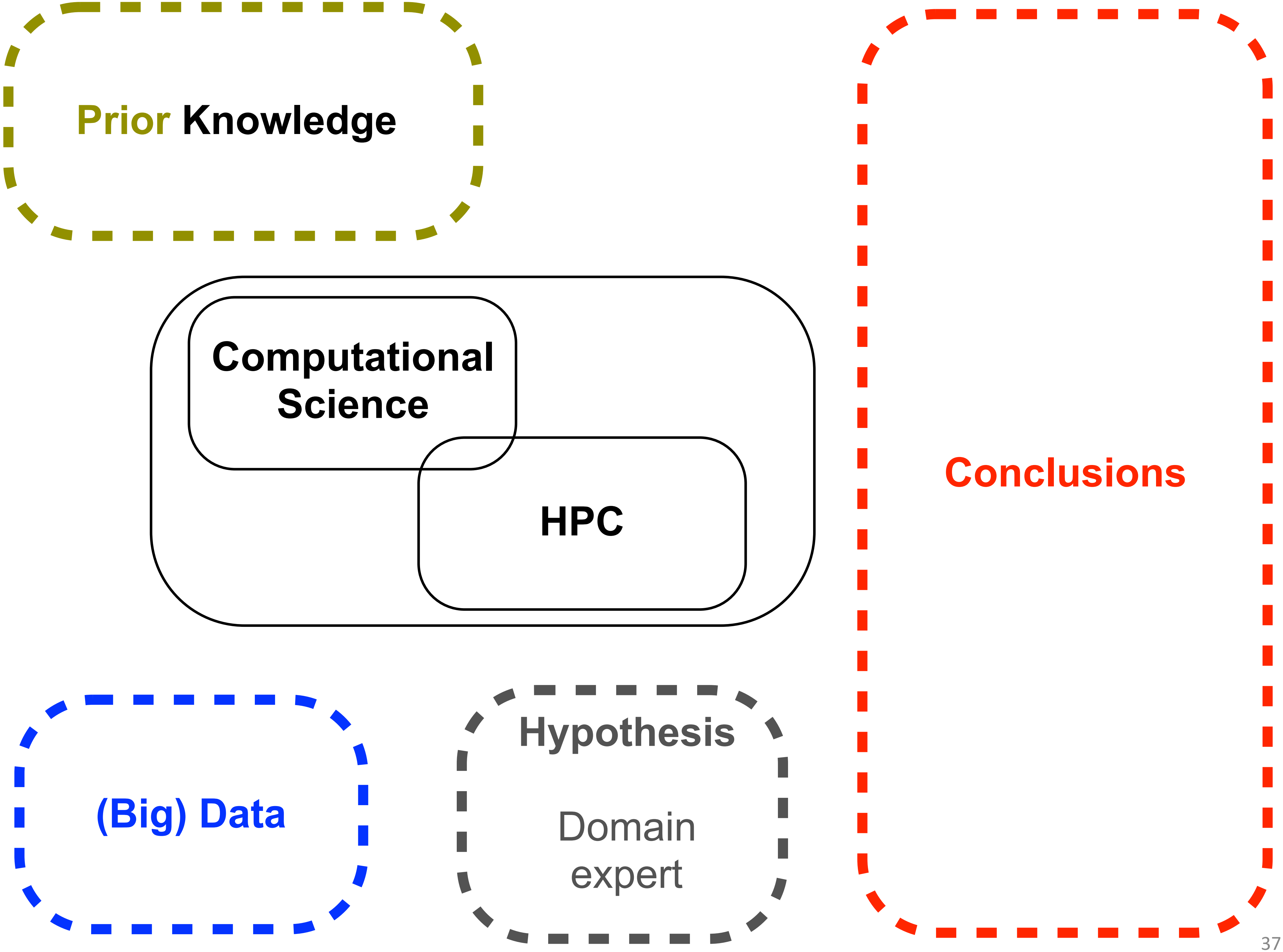
Prior Knowledge

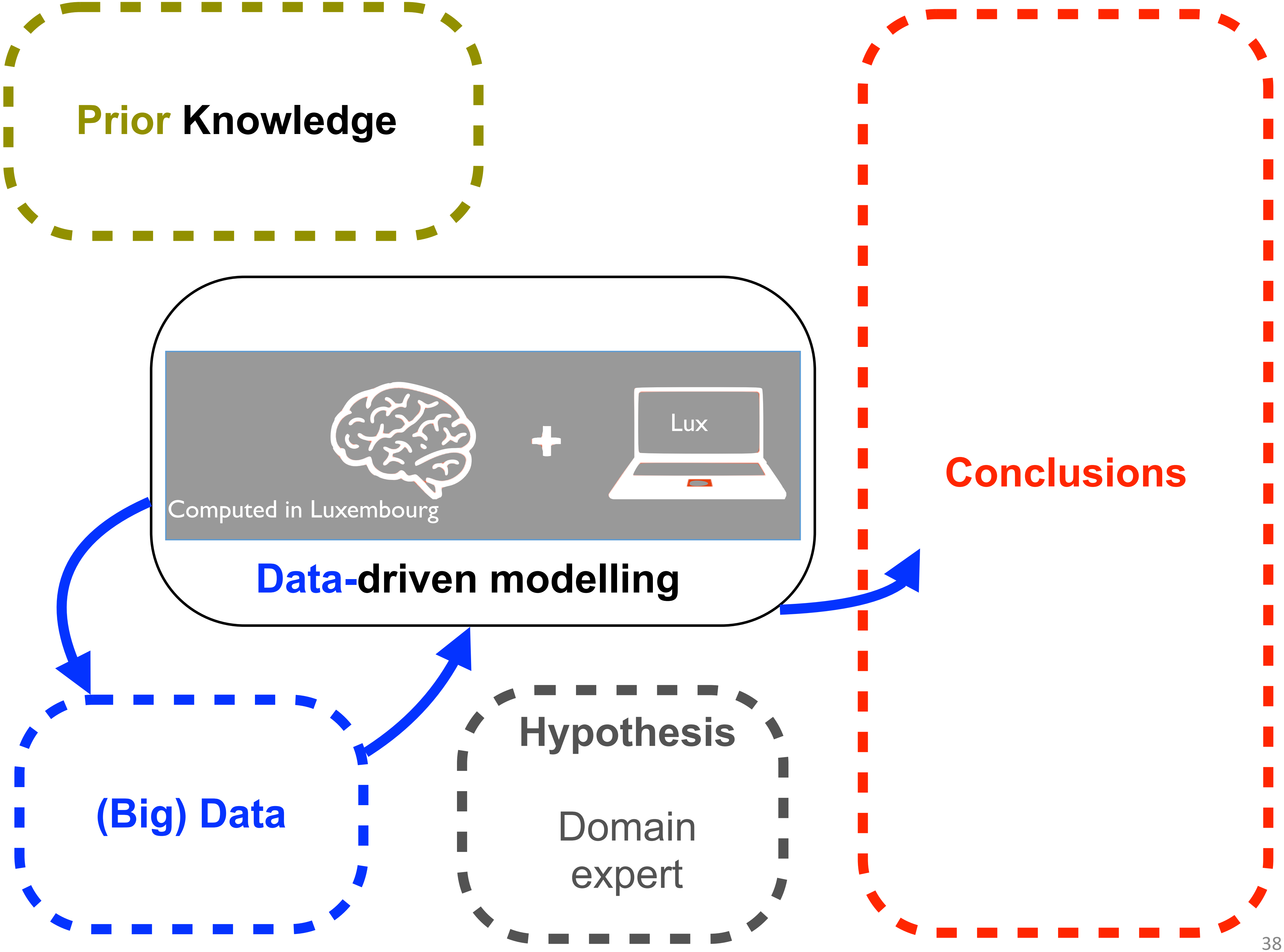
(Big) Data

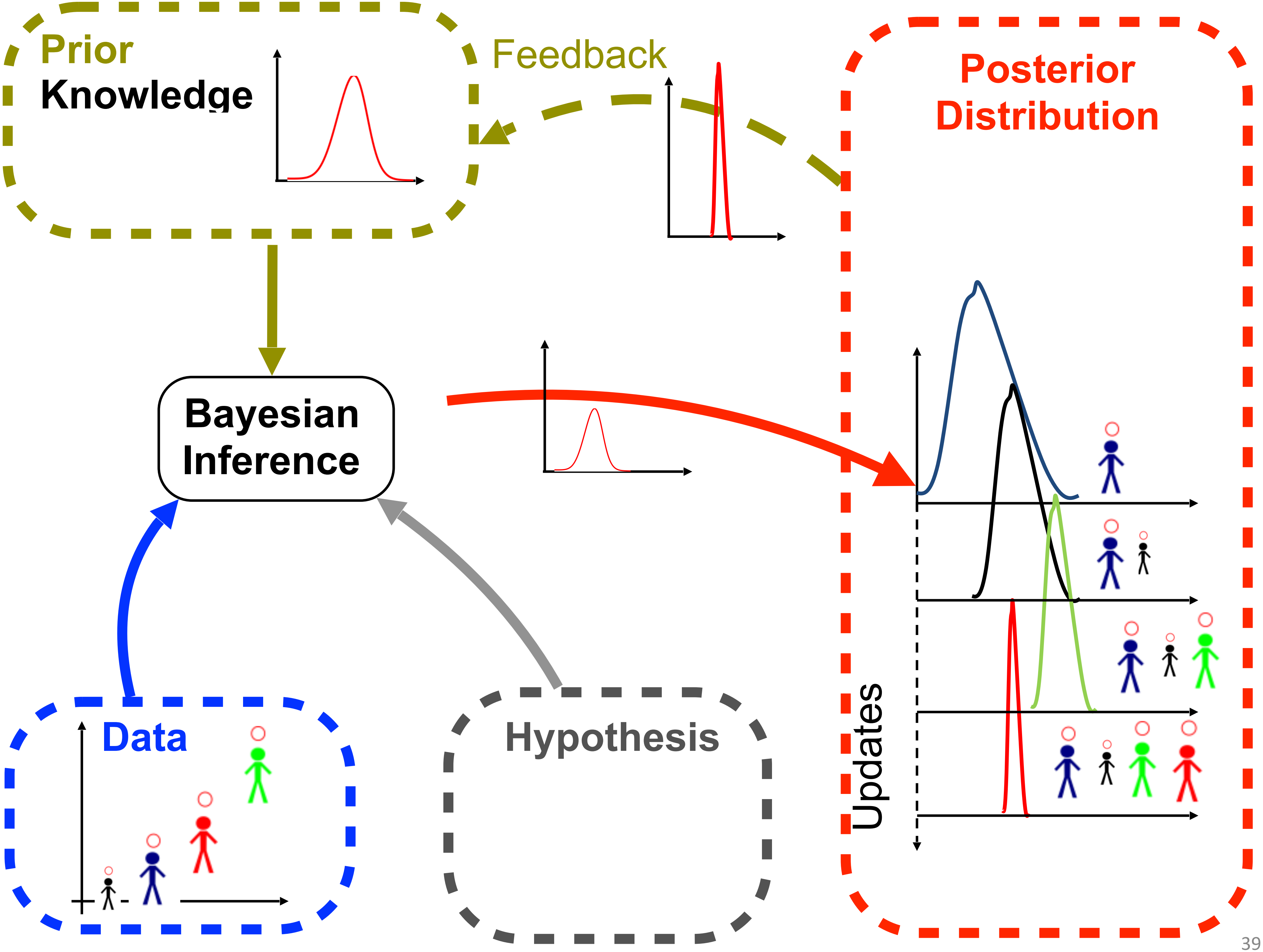
Hypothesis

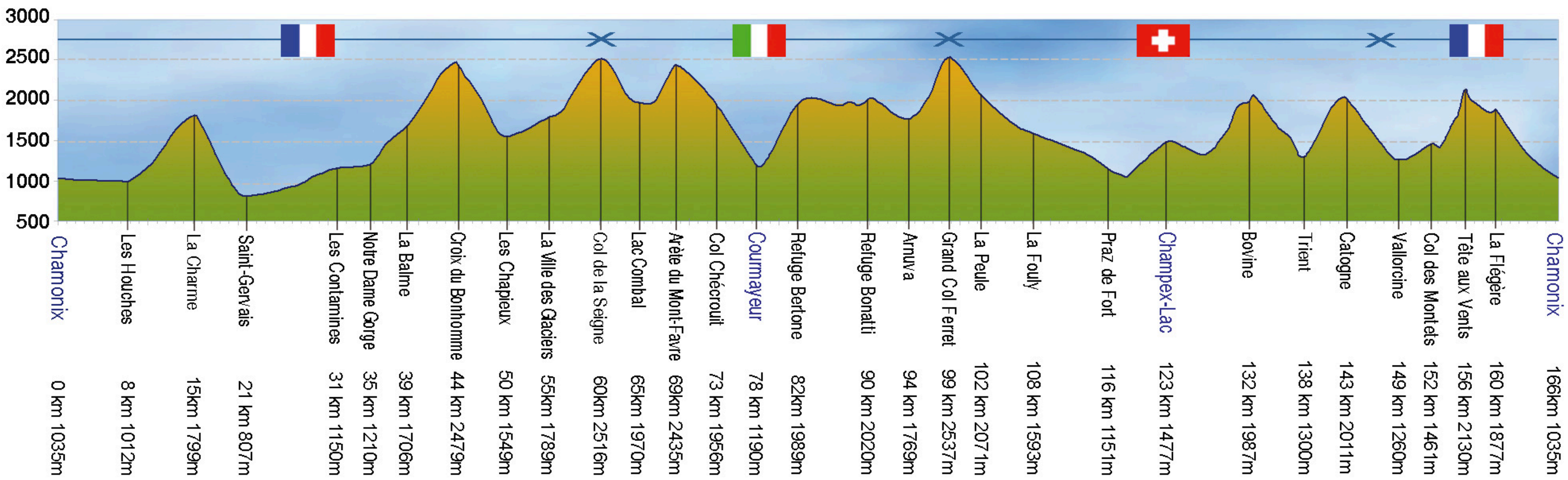
Domain
expert


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


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


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

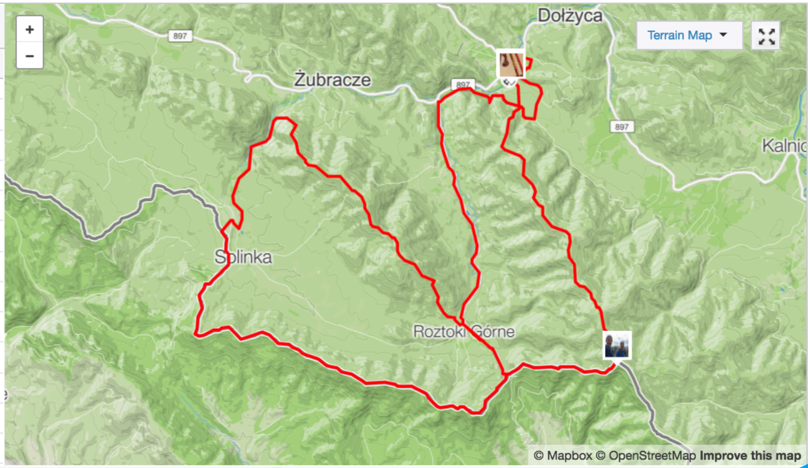

Prior
Knowledge
Feedback
Posterior
Distribution
Bayesian
Inference
Updates
Data
Hypothesis



UTMB 177km running D+ 10,300m

Splits

KM	Pace	GAP	Elev
40	12:40 /km	6:59 /km	126 m
41	10:57 /km	7:00 /km	78 m
42	8:02 /km	6:29 /km	10 m
43	21:32 /km	11:59 /km	112 m
44	9:50 /km	7:12 /km	55 m
45	9:09 /km	7:54 /km	-56 m
46	9:44 /km	8:11 /km	-4 m
47	9:07 /km	8:17 /km	-36 m
48	8:30 /km	7:32 /km	-71 m
49	7:06 /km	6:26 /km	-94 m
50	7:45 /km	6:15 /km	-68 m
51	8:58 /km	7:11 /km	-211 m
0.6	9:17 /km	8:06 /km	-42 m

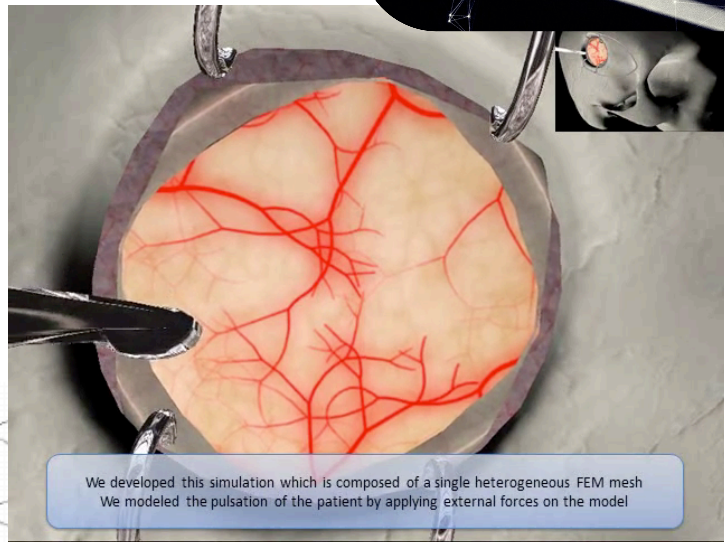


52km running D+ 2500m

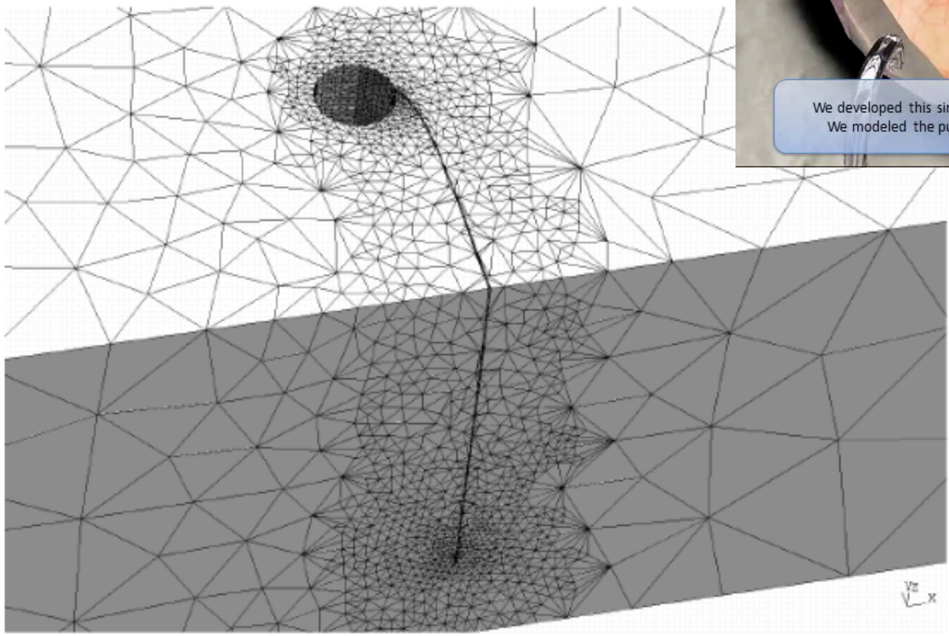
20km walking D+500m

Alex Garland, *Ex Machina*, 2015

Personalised surgery medicine



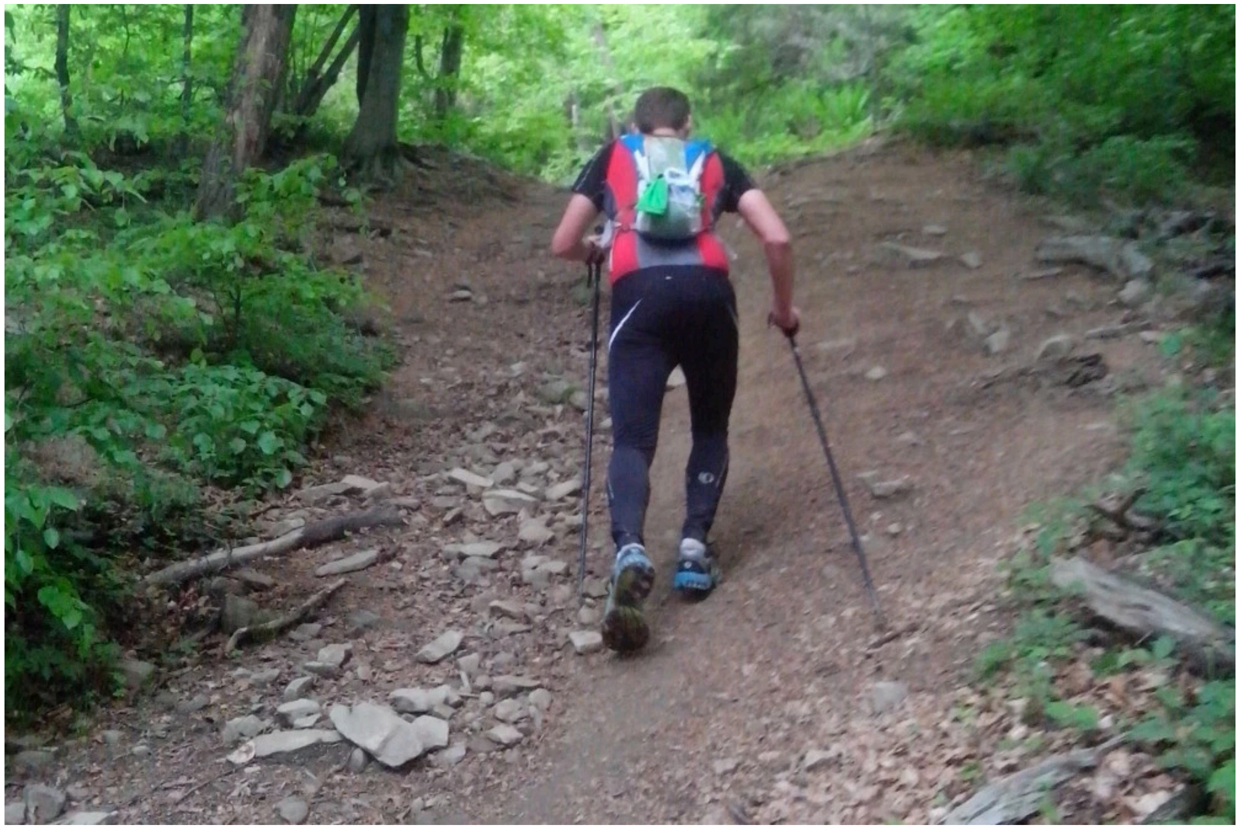
Error-controlled surgical training



Error-controlled fracture mechanics

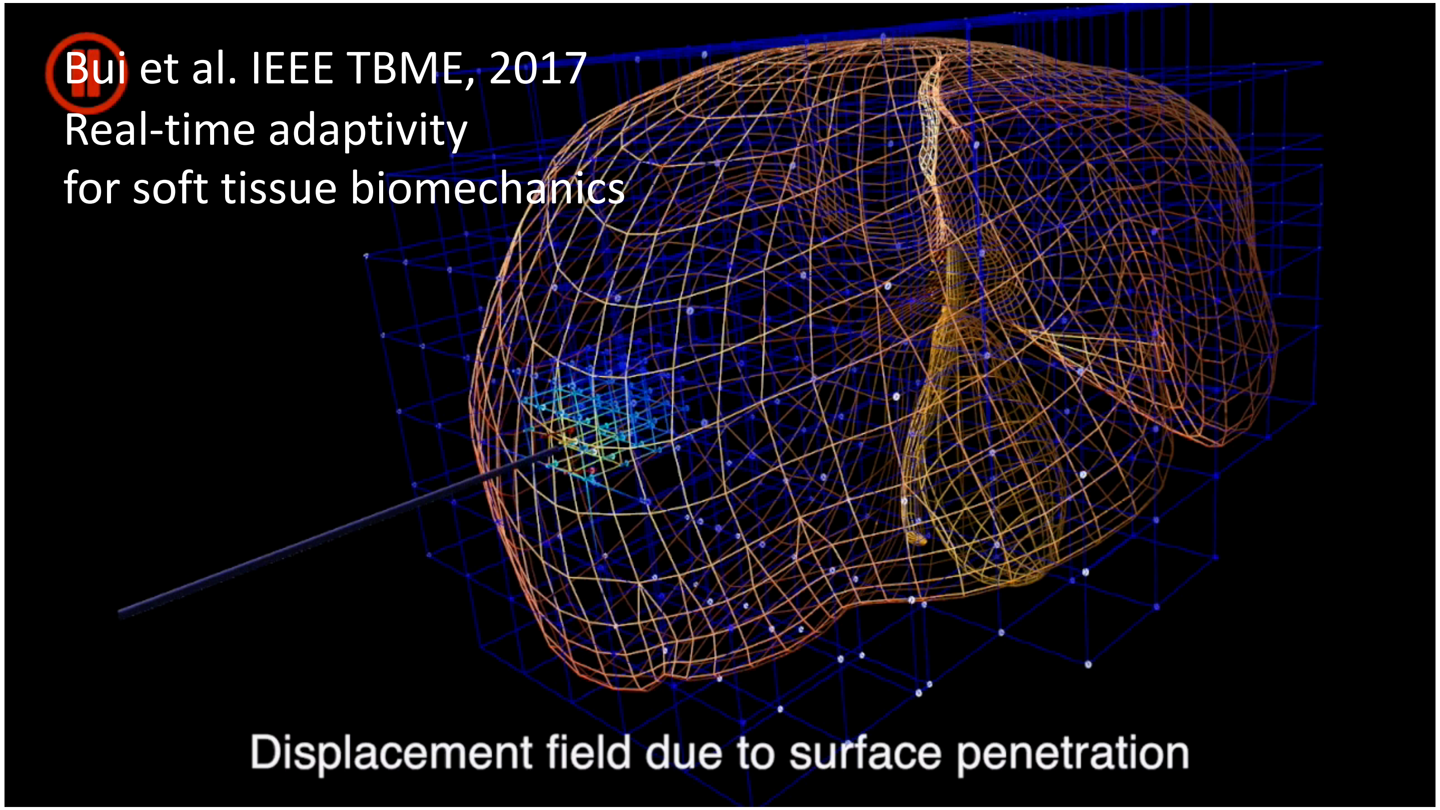
A bit of suffering…

$$\overbrace{\pi(\text{param.}|\text{obs.})}^{\text{Posterior}} = \frac{\overbrace{\pi(\text{param.})}^{\text{Prior}} \times \overbrace{\pi(\text{obs.}|\text{param.})}^{\text{Likelihood}}}{\underbrace{\pi(\text{obs.})}_{\text{Evidence}}}$$



But much more fun!

$$\overbrace{\pi(\text{param.}|\text{obs.})}^{\text{Posterior}} = \frac{\overbrace{\pi(\text{param.})}^{\text{Prior}} \times \overbrace{\pi(\text{obs.}|\text{param.})}^{\text{Likelihood}}}{\underbrace{\pi(\text{obs.})}_{\text{Evidence}}}$$

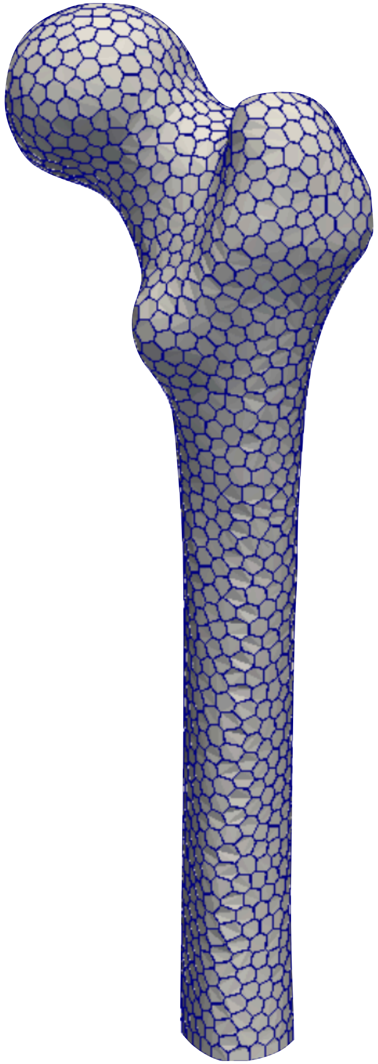


Thank you for your attention!

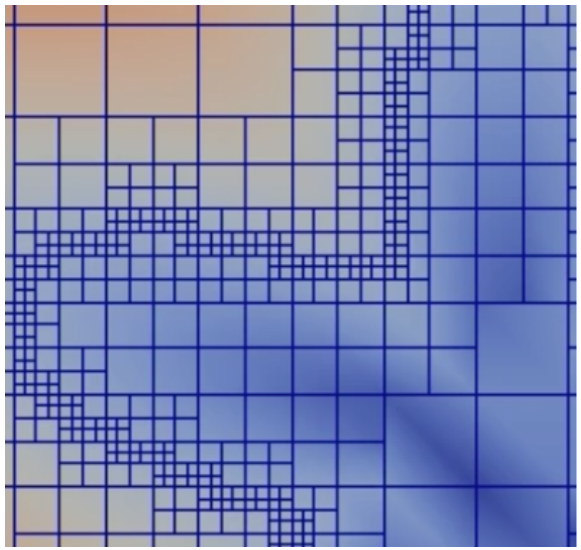
http://legato-team.eu

Data
Abstraction
Method
Discover
Statistical Inversion
POD
Prioritise
Manifold learning
Discrete Systems
Optimize
GRACE data
RD2 Gravity
Maps
Quantify uncertainty
Reduced bases
RD8 Energy harvesting
Experiment snapshots
RD5 3D printing
Best model
RD1 Water Cycle
GNSS data
Accelerate
RD6 PDE selection
RD3 Hydro-Ecology
Bayesian statistics
MapReduce
Principal Component Analysis
in Silico data
Predict
RD16 Neuro-feedback
Select
Continuous Systems
RD4 Materials
RD9 Interfaces
Detect
Gene regulatory network
Information theory
Optimise
Control
Understand
Stochastic PDEs
Propagate uncertainty
Clinical data
RD12 Biomarkers
RD13 Cell re-program
Machine learning
Economic data
Medical image
RD10/11 Cells
Deep learning
Graphs
Design
RD7 Molecular crystals
RD14 Economy
RD15 Psycho-pathology
RD18 Mobility
Social data
Diagnose
RD17 Social Media
Infer
Simulation database
RD19 Well-being
SHARE Data
Instagram
Mobility data
Forecast
Profiling
Network Analytics
Classify

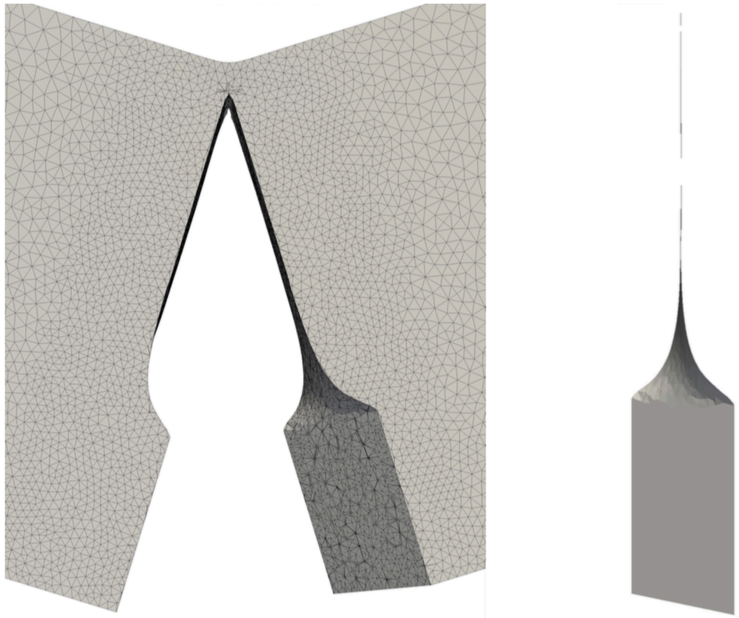
Finite Elements



polyhedral elements



unfitted FEM



extended FEM

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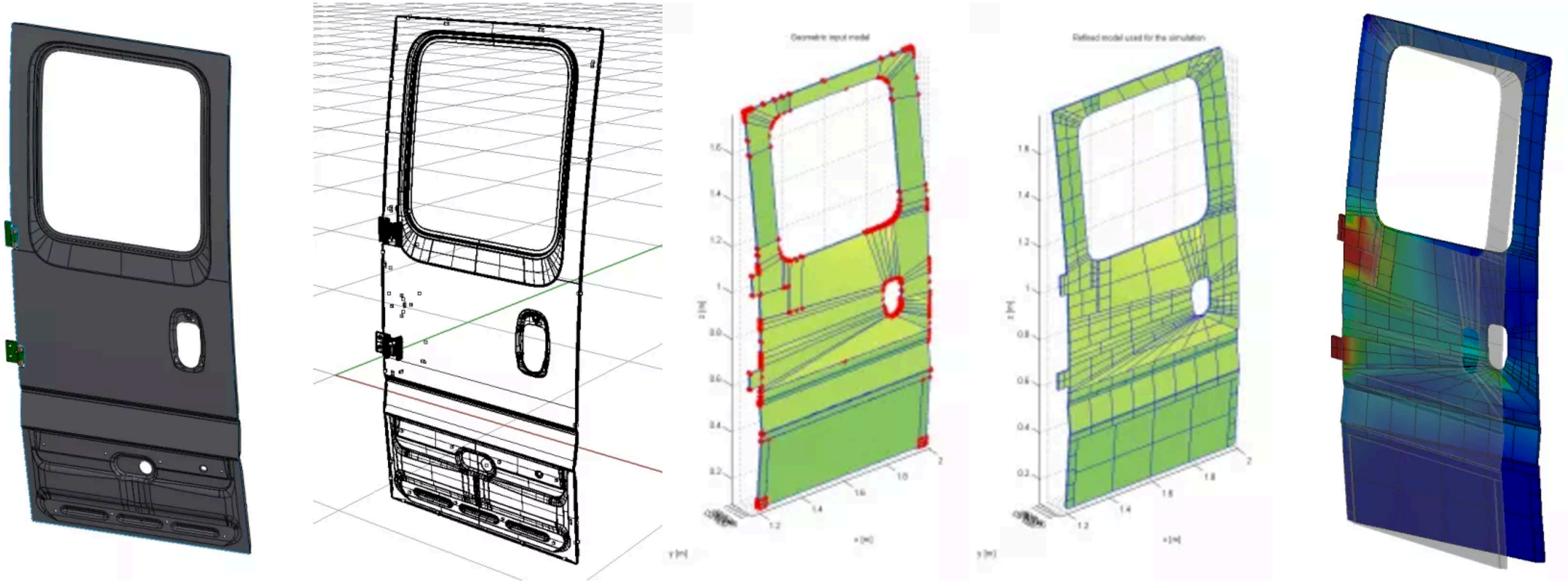
CAD-CAE integration



Geometry-Independent Field approximaTion - Isogeometric Analysis -Point collocation methods

http://legato-team.eu/project/cad-cae-integration/

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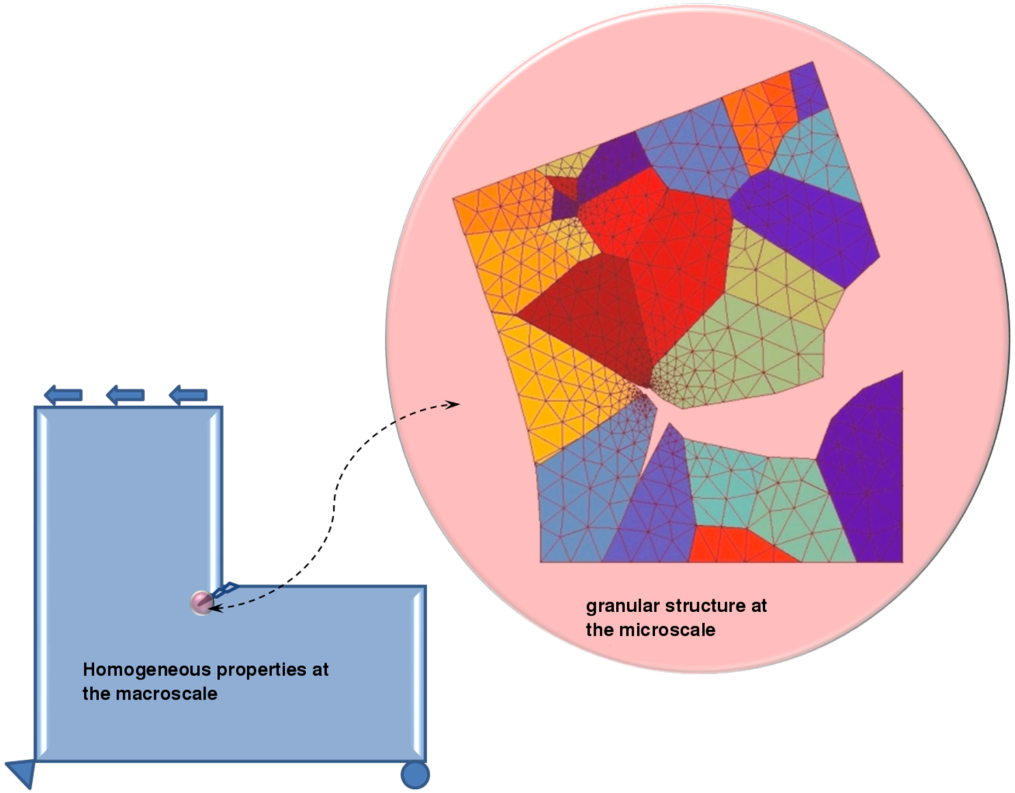
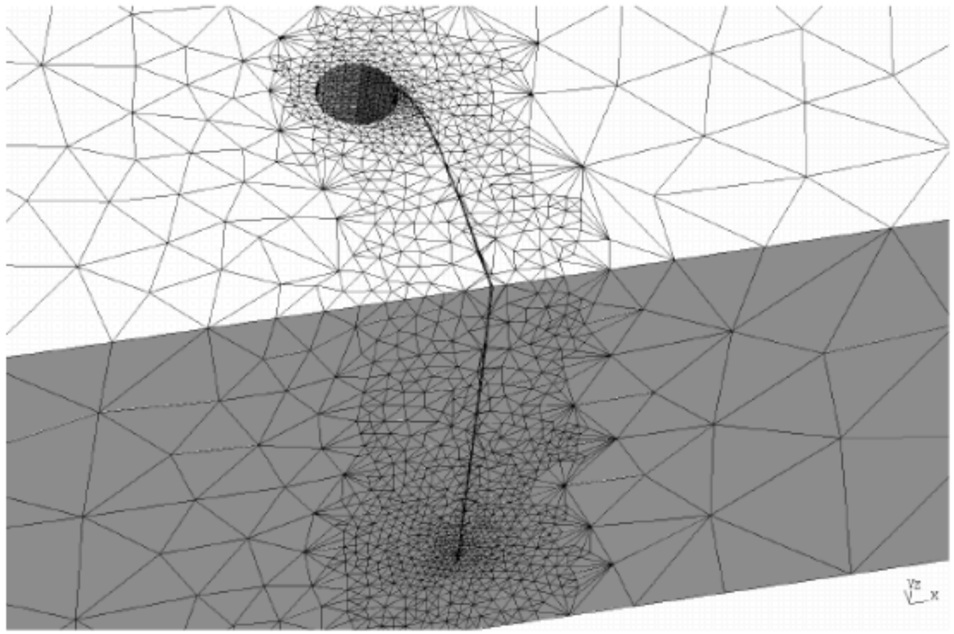
Error estimation





Most economical mesh

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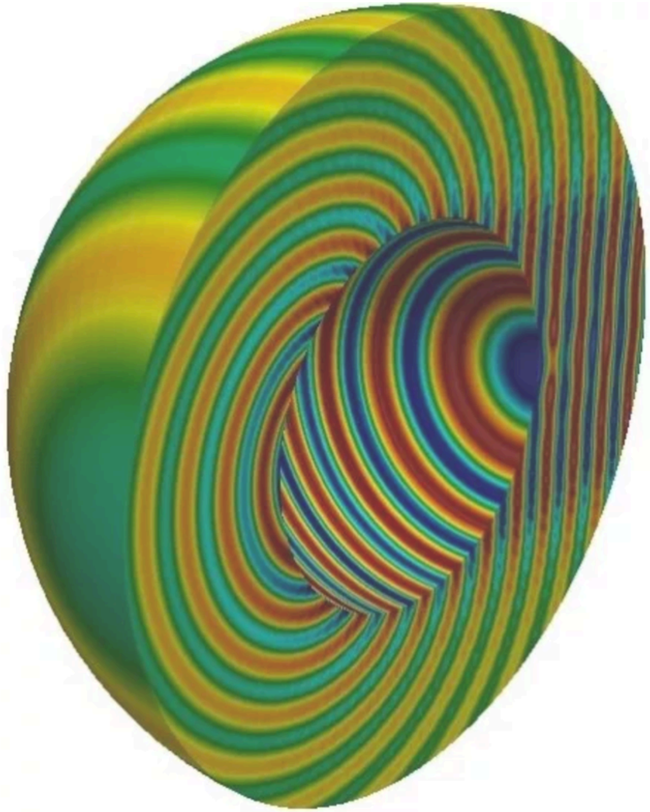
Coupled problems

Electromagnetics



Exterior acoustics

with Tahsin Khajaj U.T. Tyler

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