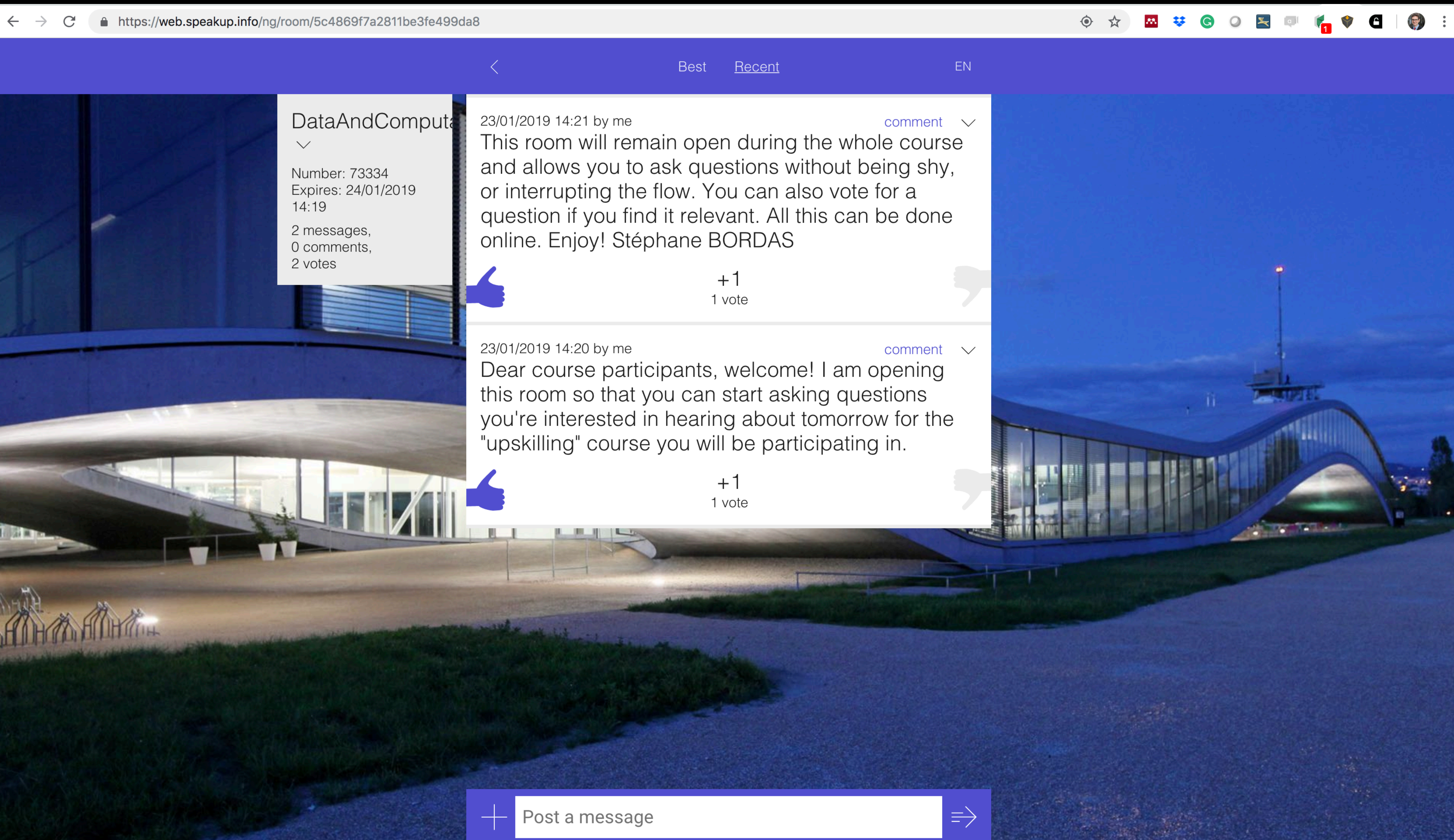
Modelling and Simulating Complex Systems

Stéphane P.A. Bordas
University of Luxembourg
stephane.bordas@alum.northwestern.edu
legato-team.eu

Speak up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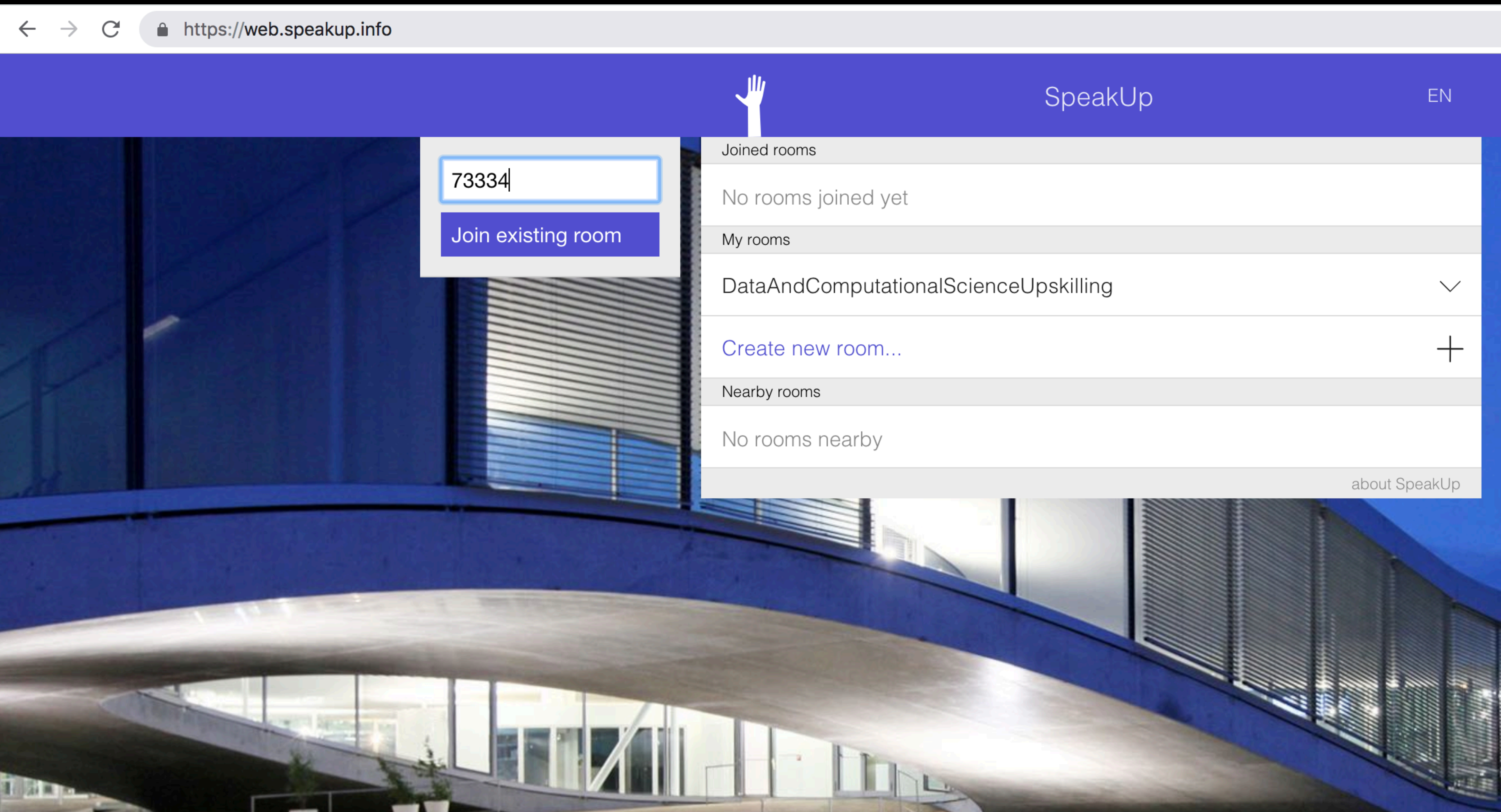
Recent
EN
DataAndComputa
Number: 73334
Expires: 24/01/2019 14:19
2 messages,
0 comments,
2 votes
23/01/2019 14:21 by me
comment
This room will remain open during the whole course and allows you to ask questions without being shy, or interrupting the flow. You can also vote for a question if you find it relevant. All this can be done online. Enjoy! Stéphane BORDAS
+1
1 vote
23/01/2019 14:20 by me
comment
Dear course participants, welcome! I am opening this room so that you can start asking questions you're interested in hearing about tomorrow for the "upskilling" course you will be participating in.
+1
1 vote
Post a message

Speak up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Join existing room
Joined rooms
No rooms joined yet
My rooms
DataAndComputationalScienceUpskilling
Create new room...
Nearby rooms
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Acknowledgements

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The University of Luxembourg

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Department of Computer Science

Pierre Kerfriden, PhD
Mines Paris-Tech, Paris, France

The legato-team
legato-team.eu

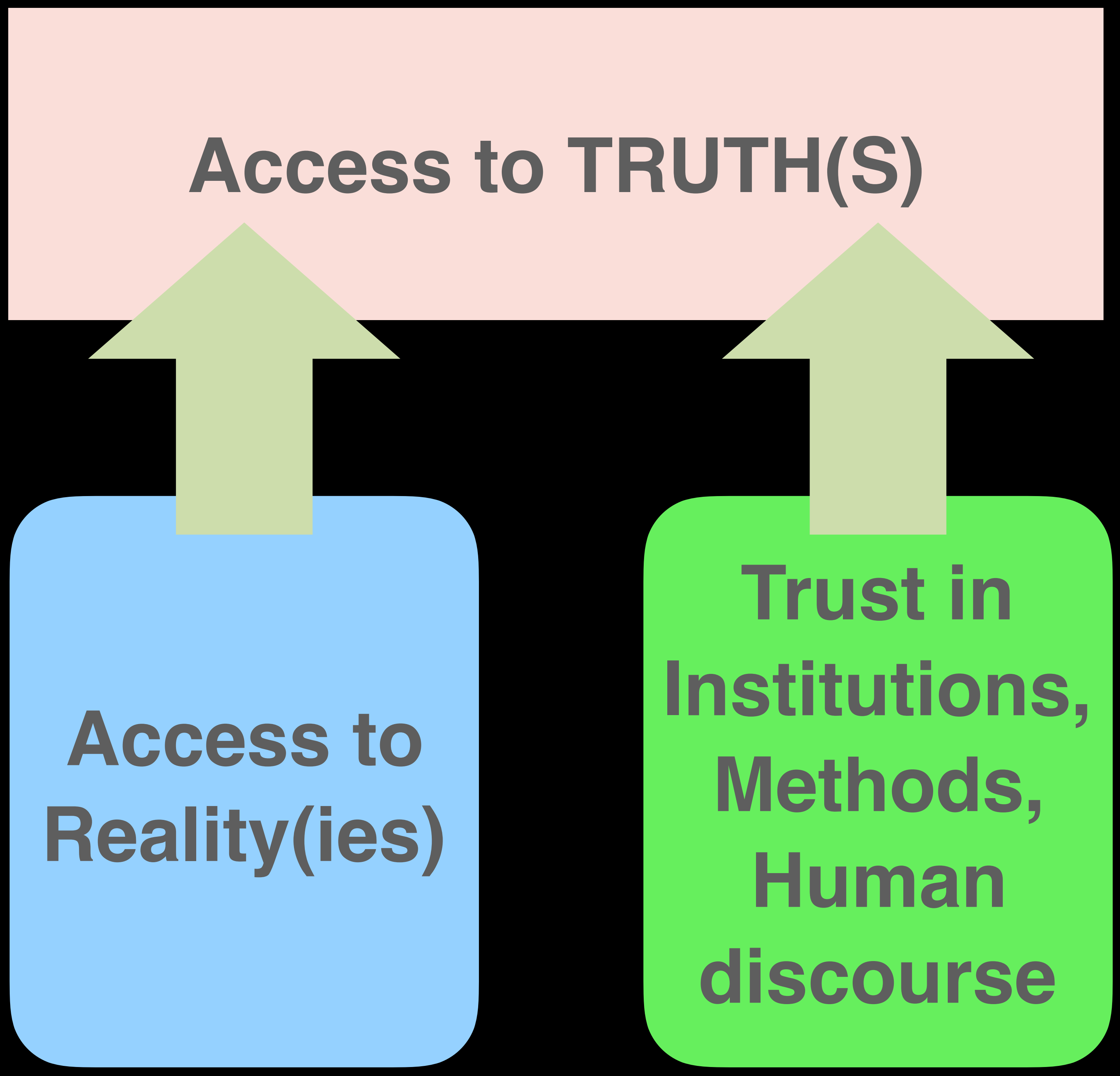
COMPLEXITY EXPLORER
SANTA FE INSTITUTE

What is Truth?

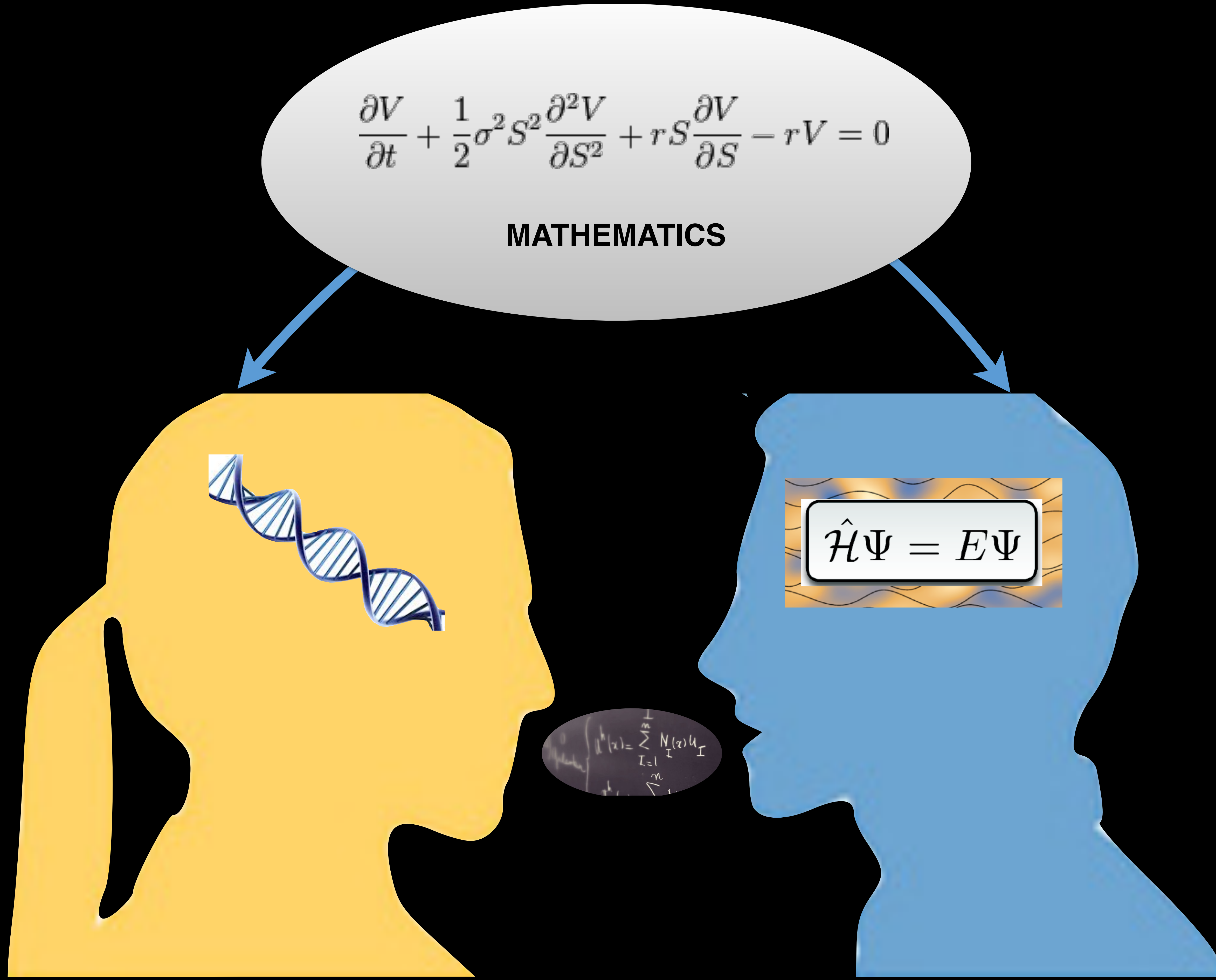
- Sciences are plural, they have validity domains, hence truth has multiple faces;
- Knowledge is never complete and Research never finished;
- Knowledge itself is less important than the method used to acquire it;
- What we discover through research is the BEST we can discover at a given instant in time;
- Investing in Research indicates trust in the scientific method.

Data

- 90% of the data available today was generated in the last two years;
- Developing new scientific methodologies to optimise the acquisition of new understanding from data;
- Develop methodological core based on the language of mathematics and common to various application areas;
- These new methodologies will fuel science and technology by creating multi-disciplinary interactions in two fields: personalised medicine and advanced materials.



Access to TRUTH(S)
Access to Reality(ies)
Trust in Institutions, Methods, Human discourse


$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS\frac{\partial V}{\partial S} - rV = 0$
MATHEMATICS
$\hat{\mathcal{H}}\Psi = E\Psi$

Outline

- Scientific method, experiments, analytical methods and models
- What is a complex system?
- What models are available to understand and predict?
- What are agent-based models?
- Equation-based (mathematical) models
- How to choose the “best” model?

The scientific method and the 3 pillars of science

(or should we say 4?)

How do we think about the world?

Aristotle

384-322 BC

Geocentrism

Copernicus

1473-1543

Heliocentrism

Galileo Galilei

1564-1642

innovative combination of experiments and mathematics

Isaac Newton

1643-1727

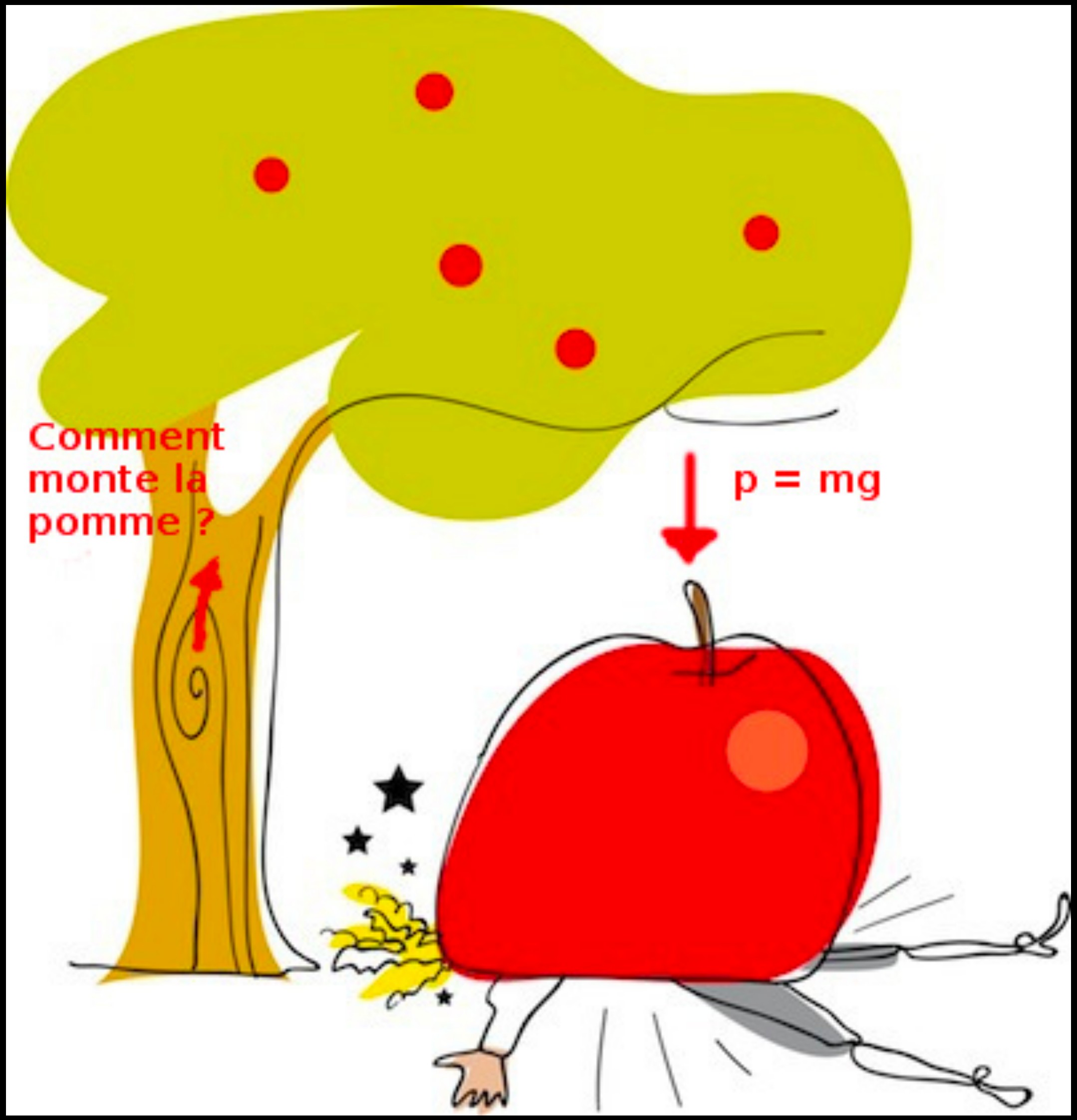
Universality of gravitation…

Pierre Simon Laplace

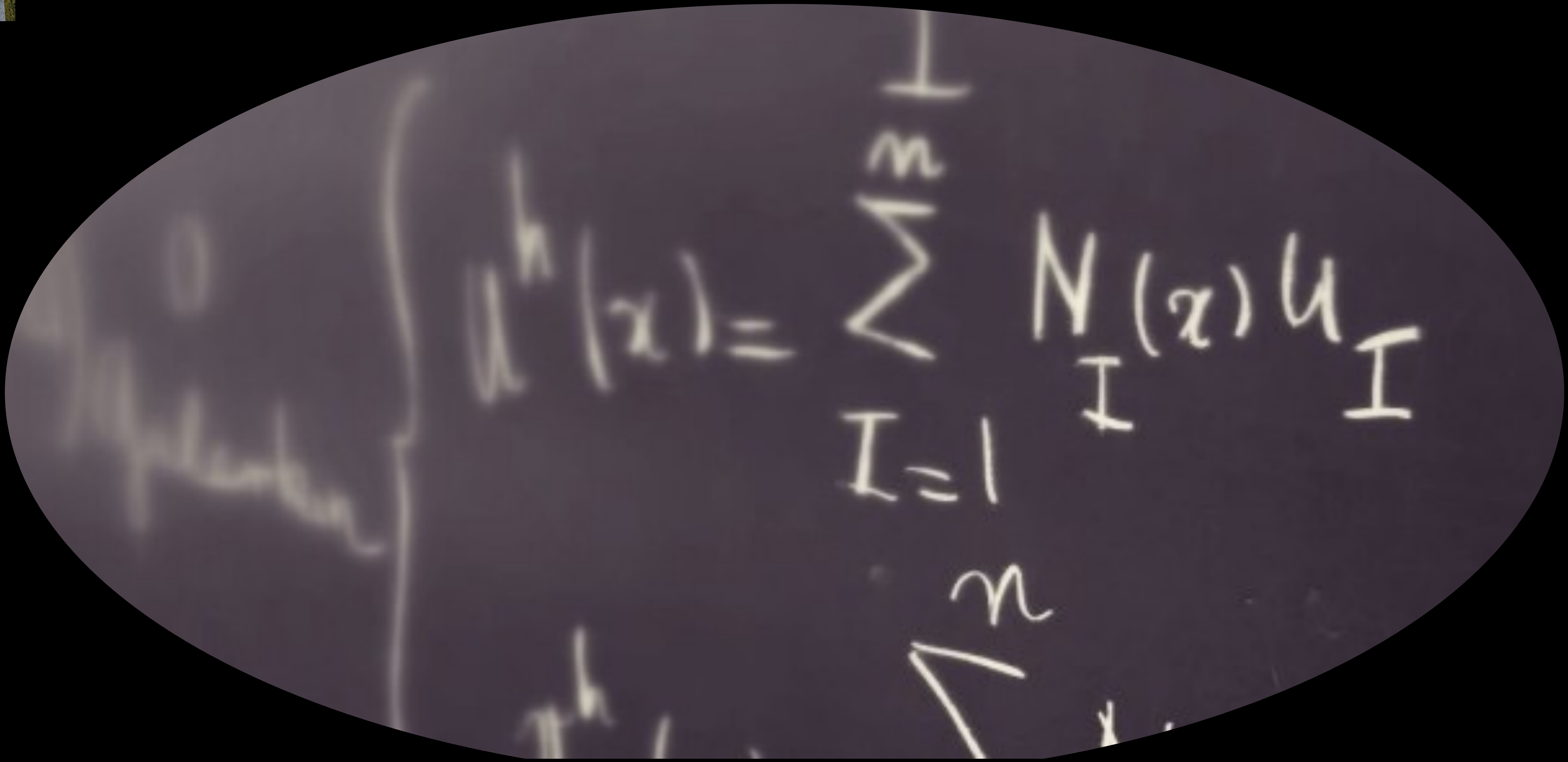
1749-1827

Our lack of knowledge is uncertainty

How do we think about the world?



Inductive thinking
Observations -> conclusions on governing laws



Write mathematical models from observations

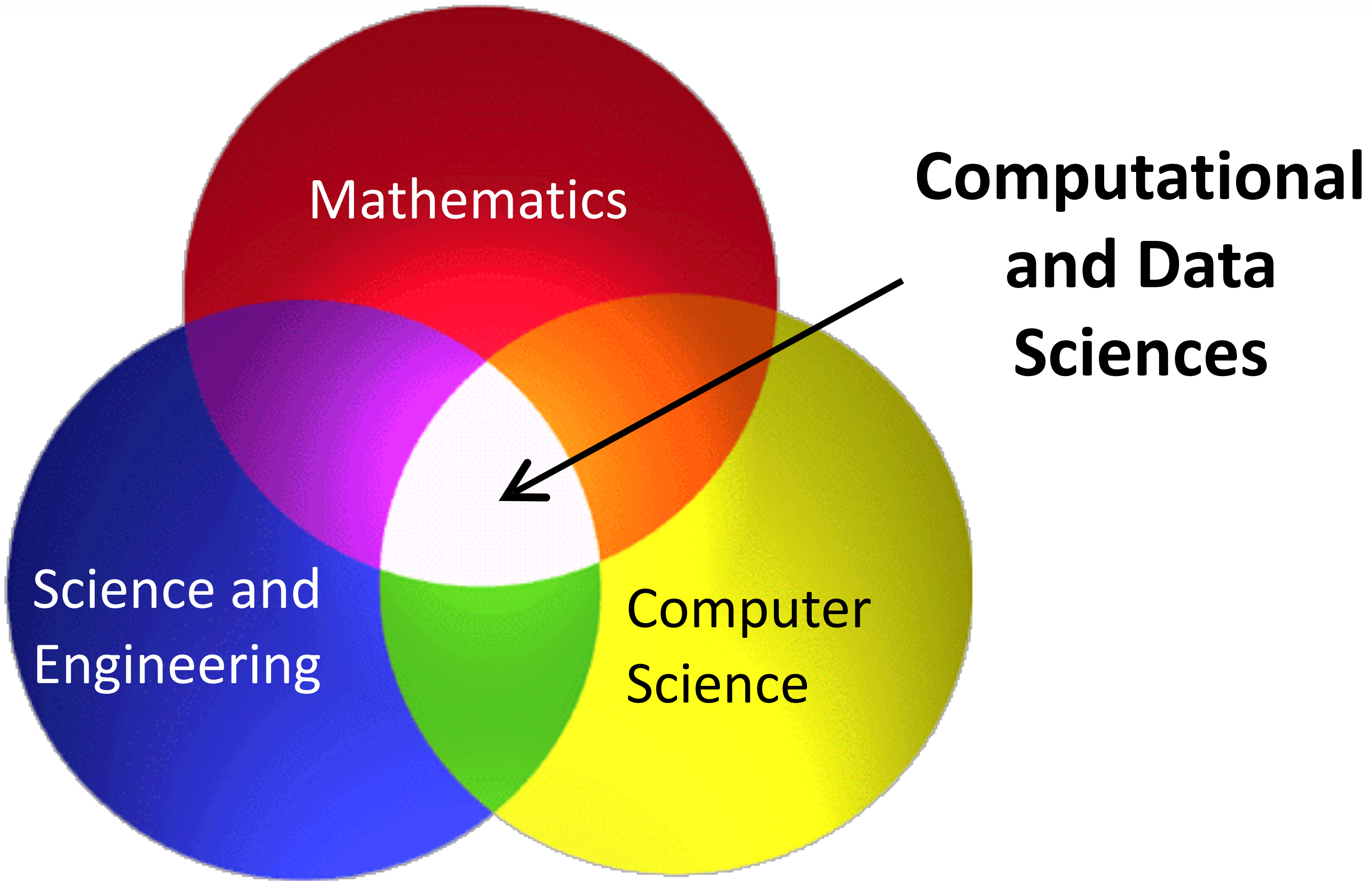
Experiments to

- Formulate hypotheses and laws about the world
- Identify parameters of mathematical models

Conduct numerical experiments to
- Formulate hypotheses and laws about the world
- Identify parameters of mathematical models

Conduct numerical experiments to
- Formulate hypotheses and laws about the world
- Identify parameters of mathematical models

The third pillar of scientific discovery

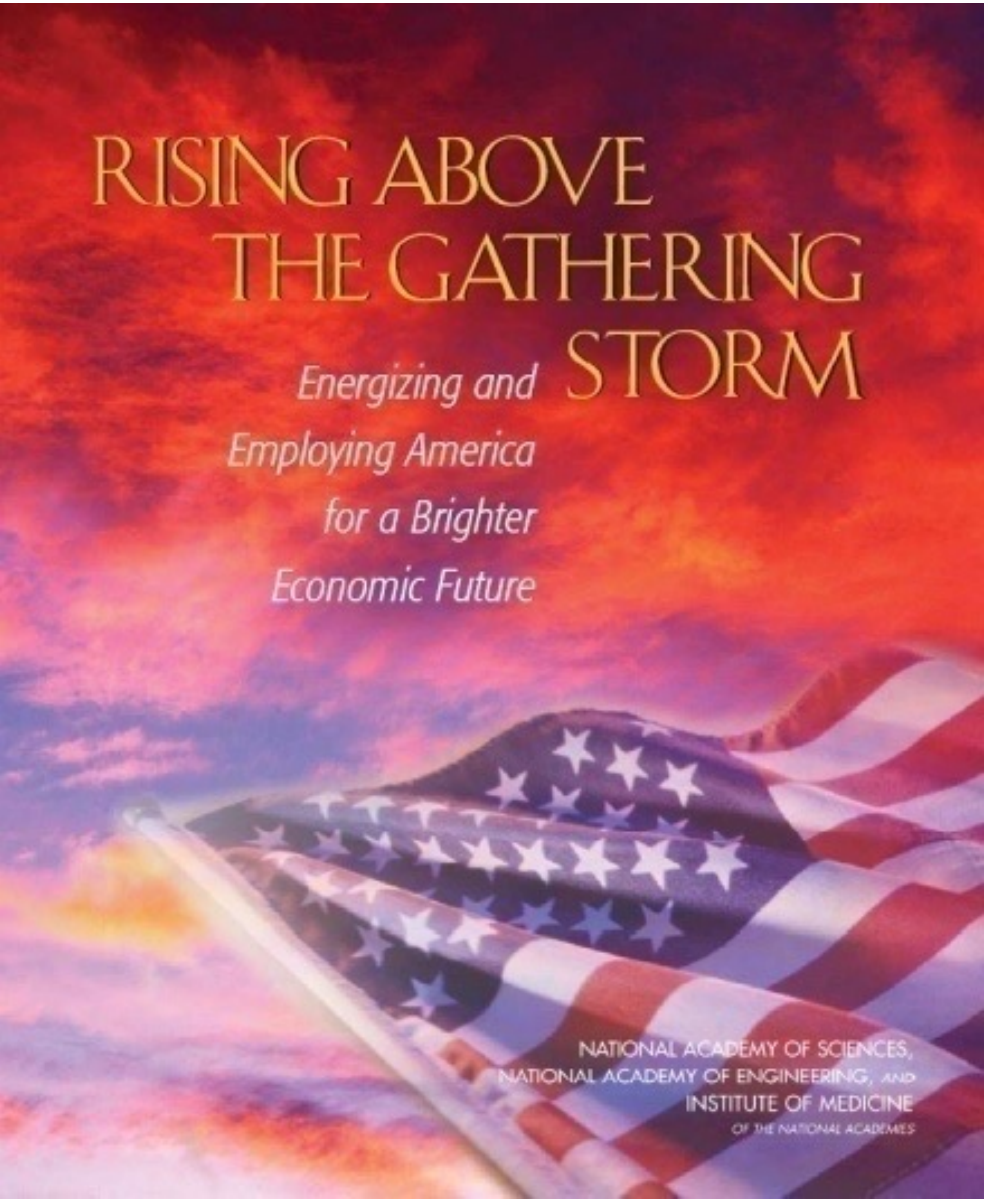


Computational Sciences: the discipline concerned with the use of computational methods and devices to enable scientific discovery and engineering applications of science.

Simulation based science

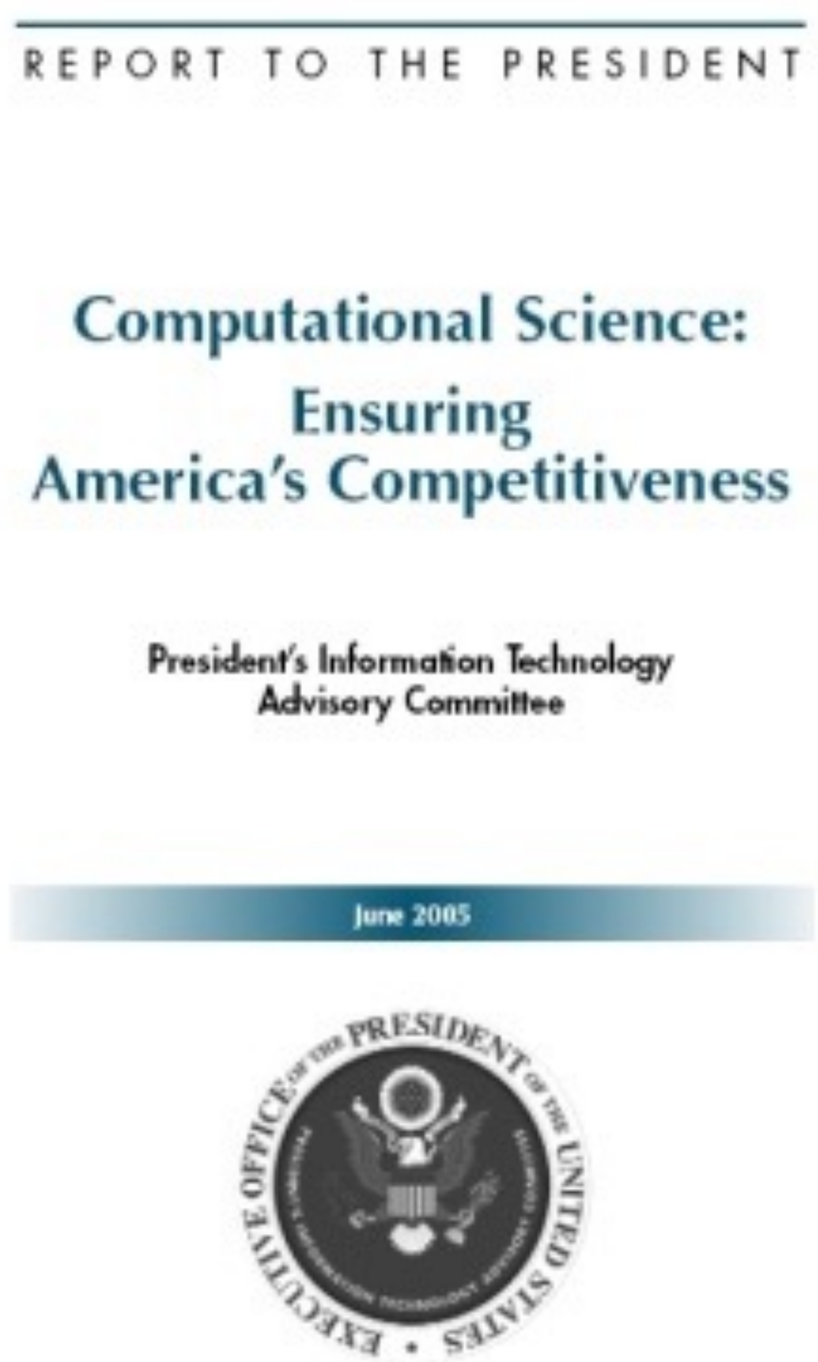
• • •

Simulation based science



National Academy of Sciences
National Academy of Engineering
Institute of Medicine

Simulation based science


REPORT TO THE PRESIDENT

Computational Science:
Ensuring
America's Competitiveness

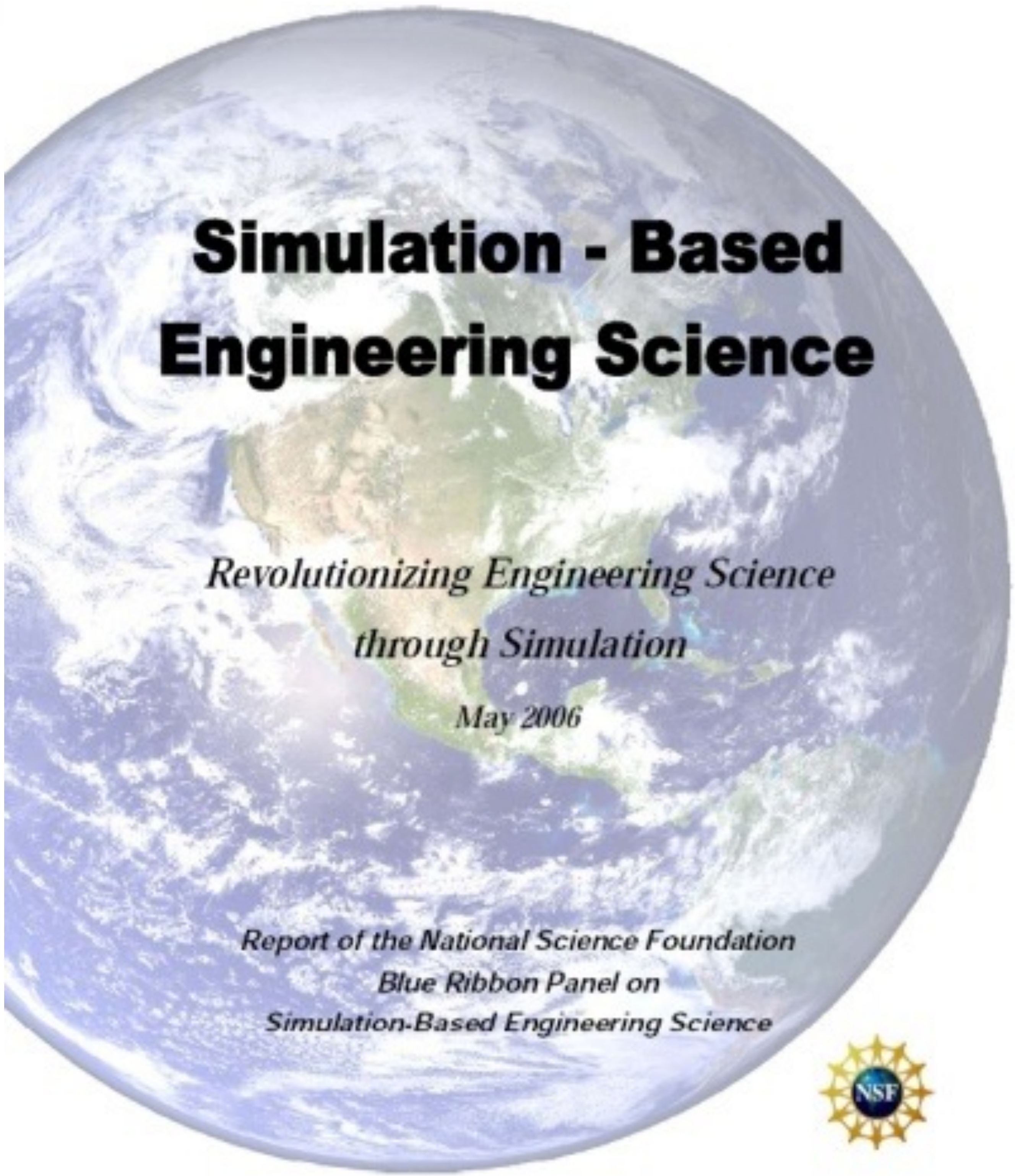
President's Information Technology
Advisory Committee

June 2005

President's Information Technology Advisory Committee

2005

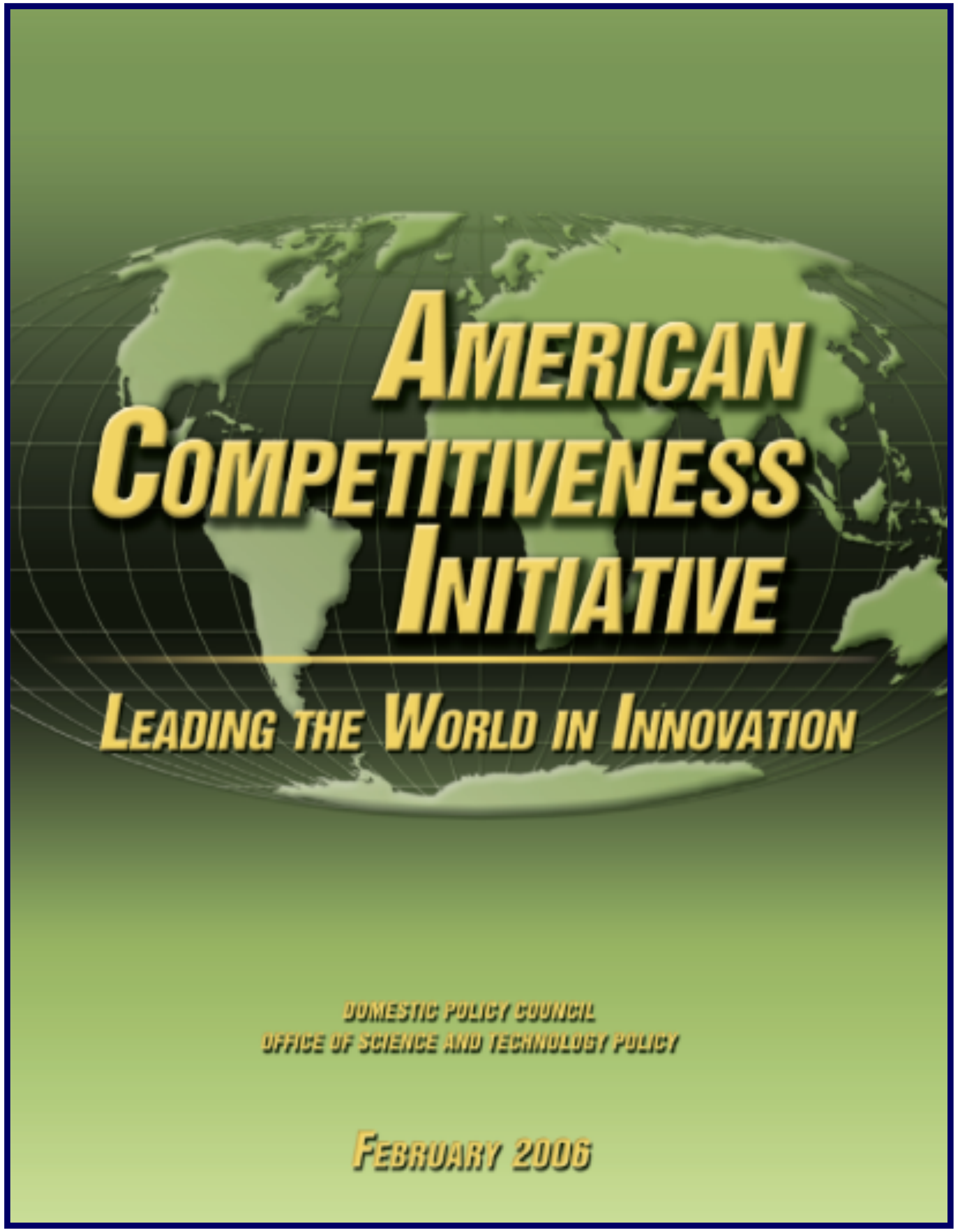
Simulation based science



US National Science Foundation (NSF)

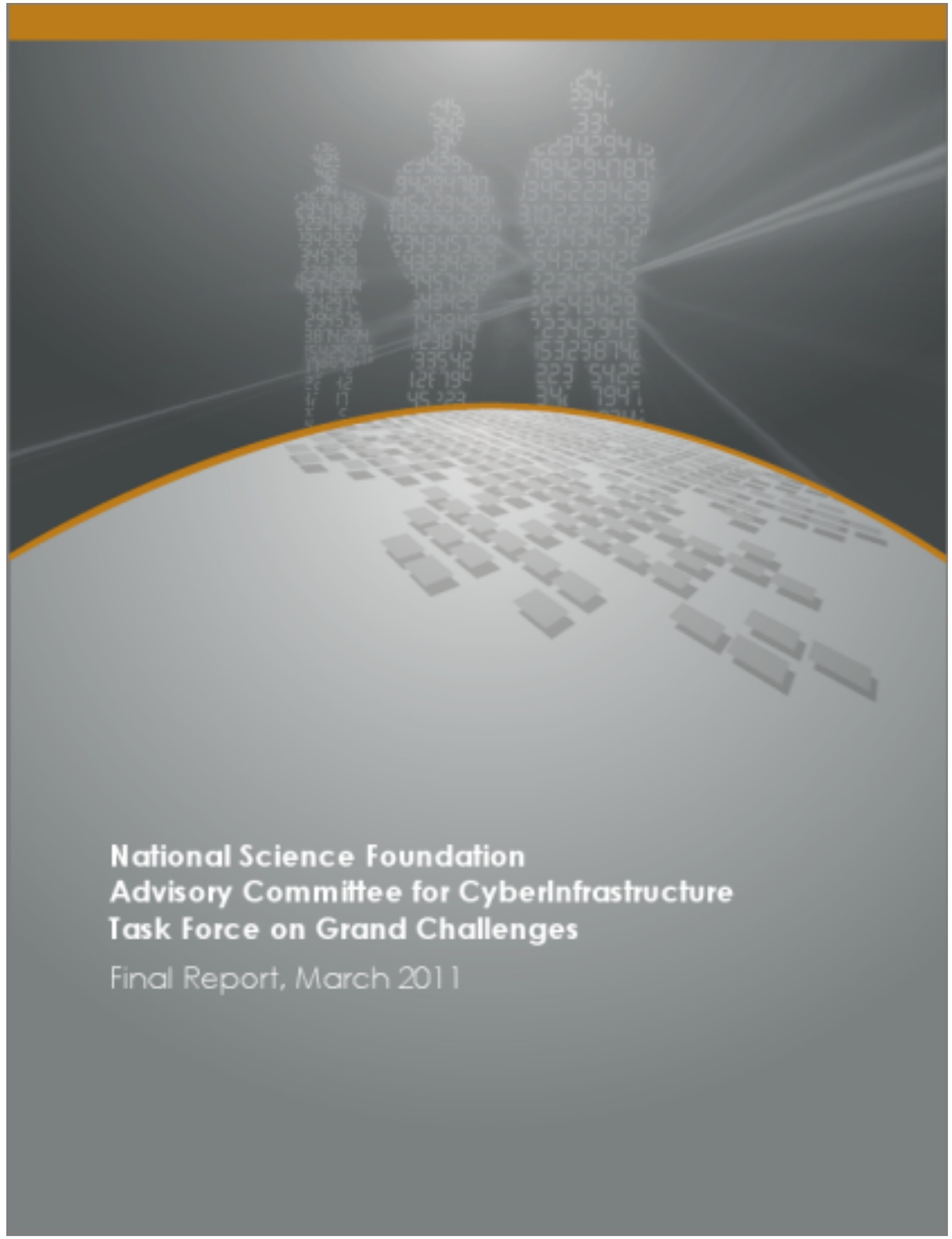
2006

Simulation based science



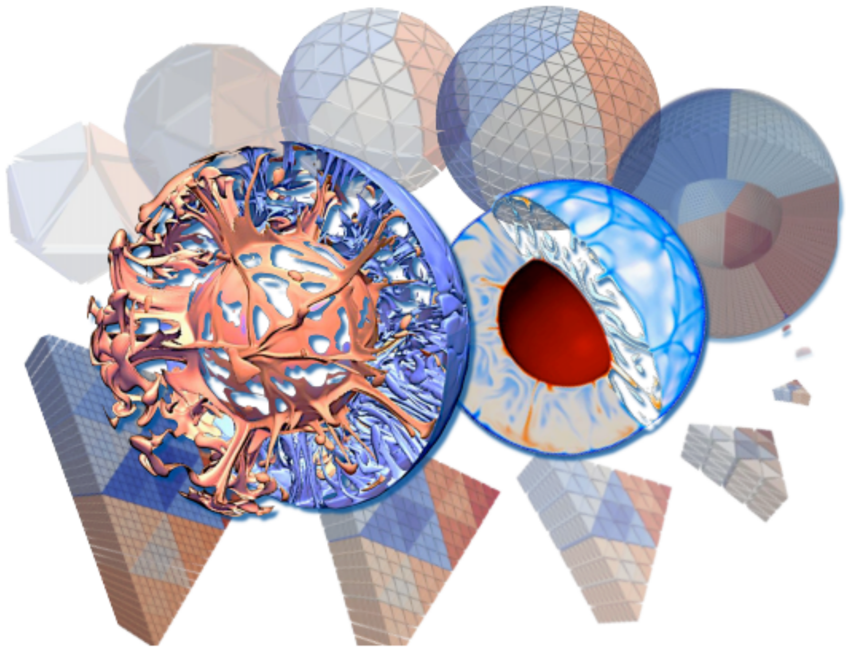
Office of Science and Technology Policy 2006

Simulation based science



Research and Education in Computational Science and Engineering

September 2016



Report from a workshop sponsored by the Society for Industrial and Applied Mathematics (SIAM) and the European Exascale Software Initiative (EESI-2), August 4-6, 2014, Breckenridge, Colorado

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Karen Willcox, Massachusetts Institute of Technology, Vice Chair
Lois Curfman McInnes, Argonne National Laboratory, Program Director
Hans De Sterck, Monash University, Secretary

Additional Contributors:

George Biros, University of Texas at Austin
Hans Bungartz, Technische Universität München
James Corones, Krell Institute
Evin Cramer, Boeing
James Crowley, SIAM
Omar Ghattas, University of Texas at Austin
Max Gunzburger, Florida State University
Michael Hanke, KTH Stockholm
Robert Harrison, Brookhaven National Laboratory and Stonybrook University
Michael Heroux, Sandia National Laboratories
Jan Hesthaven, École Polytechnique Fédérale de Lausanne
Peter Jimack, University of Leeds
Chris Johnson, University of Utah
Kirk E. Jordan, IBM
David E. Keyes, KAUST

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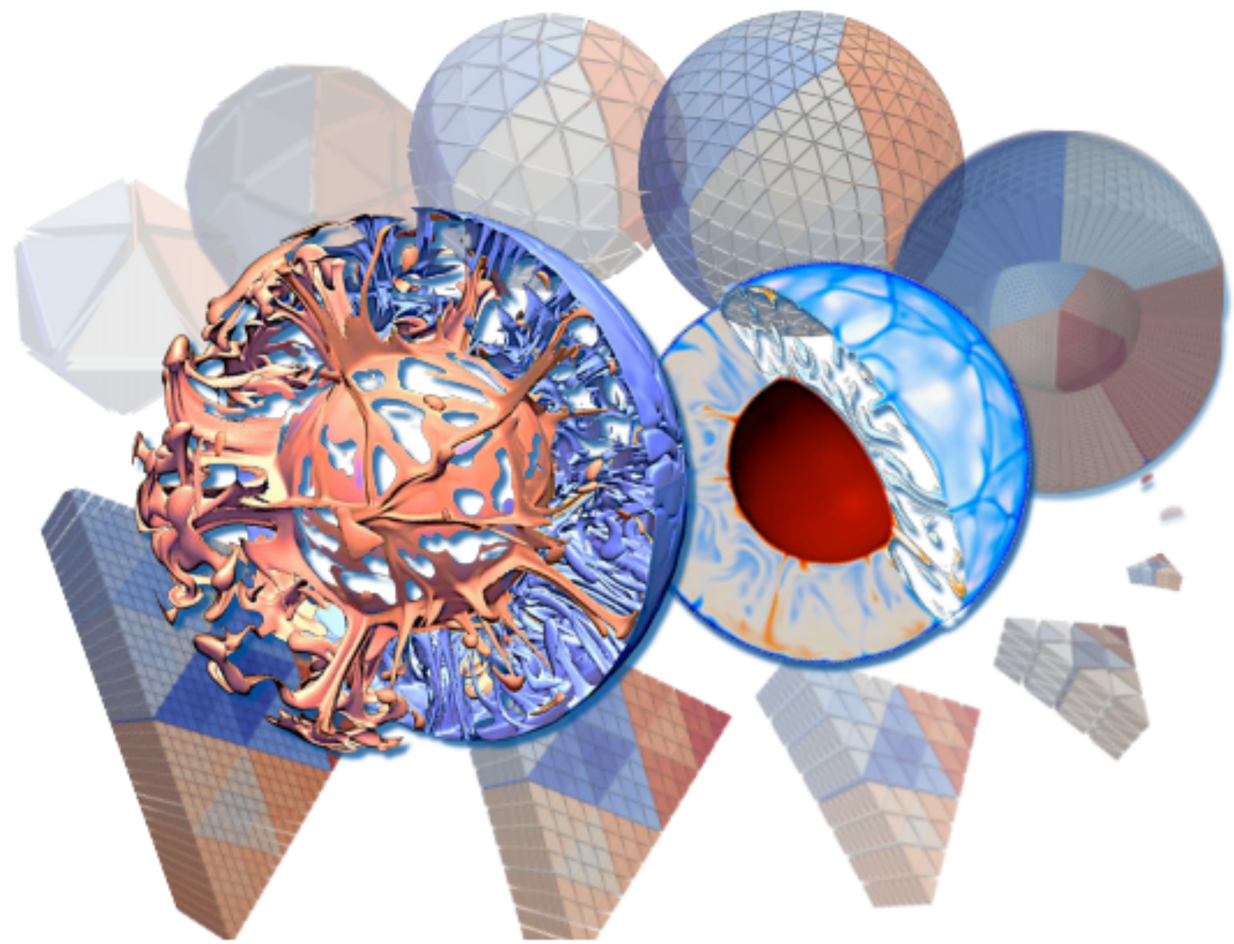
https://arxiv.org/pdf/1610.02608.pdf

Research and Education in Computational Science and Engineering

September 2016



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Additional Contributors:

What computational & data sciences enable that traditional science doesn't

LOOK INTO THE PAST

- Earthquakes, climate, oil discovery, archeology, seismology, law, economics, finance

PROBE THE FUTURE

- Explore the effects of thousands of scenarios
- Drug design, space exploration, climate change, natural disasters, …

CHOOSE MODELS

- Explore consequences of breakdown of models and theory…

OPTIMISE

- Optimize procedures, designs, products, systems, etc.

Why is multi-disciplinary research important?

- Most Grand Challenge problems today involve complex phenomena and systems that lie on **disciplinary boundaries**.
- **Interdisciplinary research** moves beyond simple collaboration and teaming to integrate **data**, methodologies, perspectives, and concepts from multiple disciplines in order to advance fundamental understanding and to solve **real world problems**.
- Interdisciplinary research holds the promise of pushing fields forward and accelerating scientific **discovery**.
- Interdisciplinary study and training **prepares** a **workforce** that undertakes scientific challenges in news and innovative ways.

Mission for Computational and Data Sciences in Luxembourg

UNIVERSITÉ DU LUXEMBOURG

Mission

To provide the infrastructure and intellectual leadership for developing outstanding interdisciplinary research programs in computational and data sciences.

To enable world-leading education in computational and data sciences in Luxembourg.

To promote and facilitate digital literacy and provide the fundamental building blocks necessary to the development of Industry 4.0 in Luxembourg.

Outline

- Scientific method, experiments, analytical methods and models
- What is a complex system?
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- Equation-based (mathematical) models
- How to choose the “best” model?

Complex systems

- Large number of interacting components
- Evolving over time
- Decentralised decisions vs. Centralised control
- **Local** interactions **->** **emergence** of **global** patterns

Examples

- Biological systems (brain, cancer, bacteria…)
- Policy and government
- Environment (weather, ice sheet, pollution…)
- Economy, stock market
- Ecosystems (bats, fish…)
- Functional/sensing materials (graphene…)

Emergence

- Micro (local) level leads to patterns at the macro level
  - Ant/bee colonies
  - Housing patterns, traffic jams
  - Populations in ecosystems
  - Pressure of gases
  - Pricing
  - Effect of individual behaviours in societies

Two questions about emergence

- You know the micro, you want to understand the macro
- You observe the macro, you want to deduce the micro rules

THIS IS HARD

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What is a model?

When we were kids ;-) or grownup kids…

What is a model?

Biologists

What is a model?

If you are in fashion…

What is a model?

- An abstract description of a process, object, system, event which exaggerates certain aspects compared to others
- “Essentially, all models are wrong, but some are useful” George Box, 1987
- The choice of the model depends on the quantities of interest (QoI)

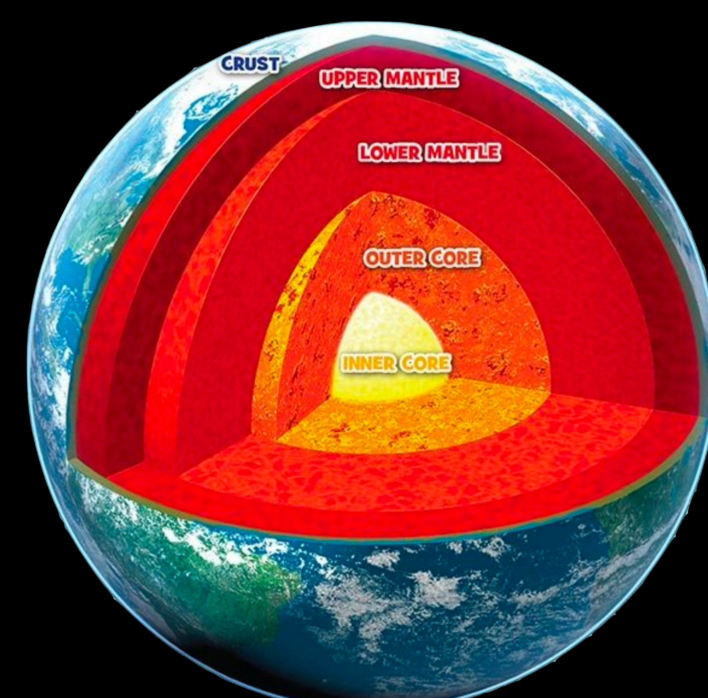
What is a model?

Real World

Projection

Model 1

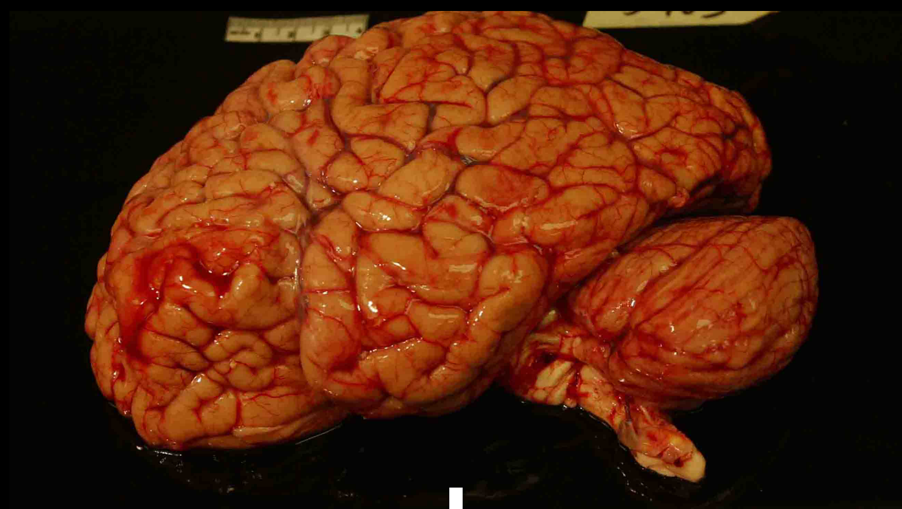
Geophysical layers



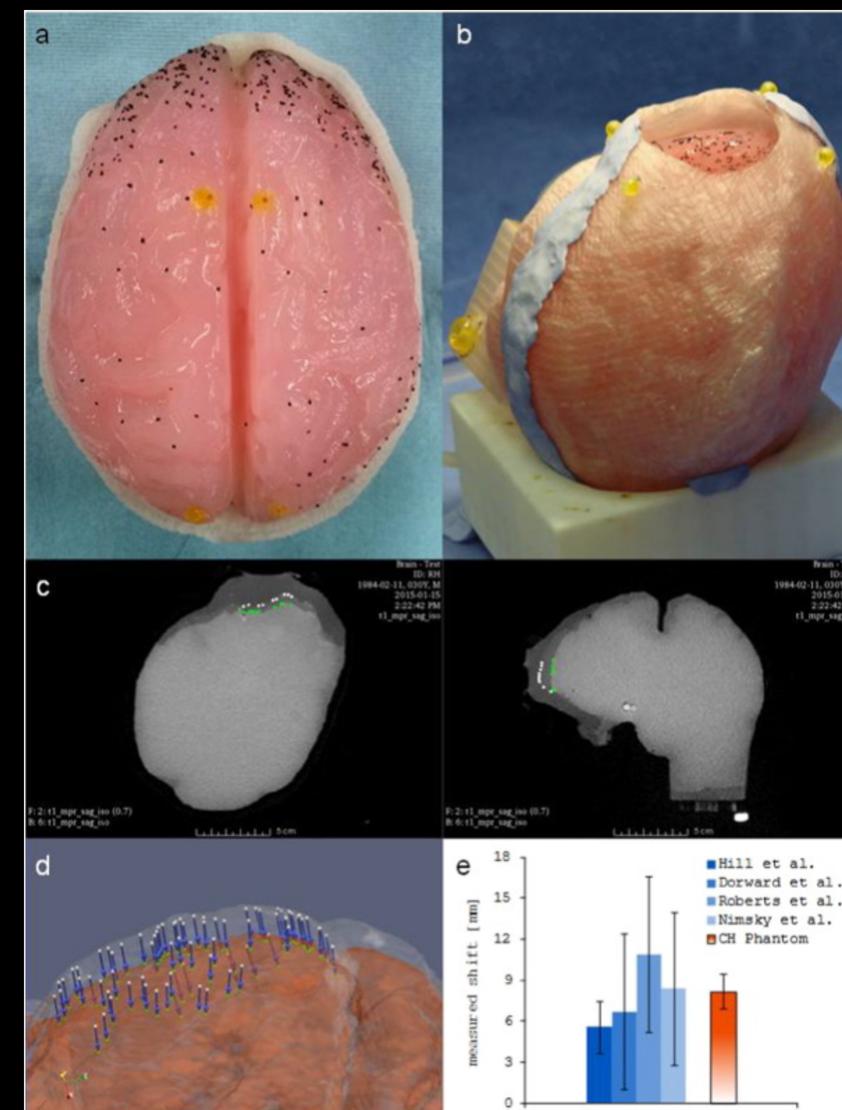
Model 2

If you are into geography or geophysics

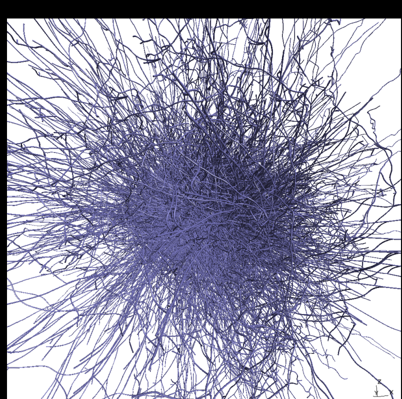
What is a model?

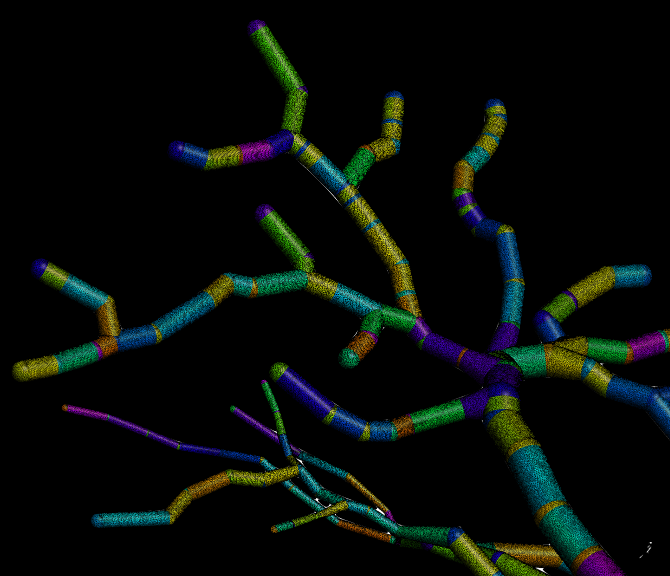


Physical model



Mathematical model

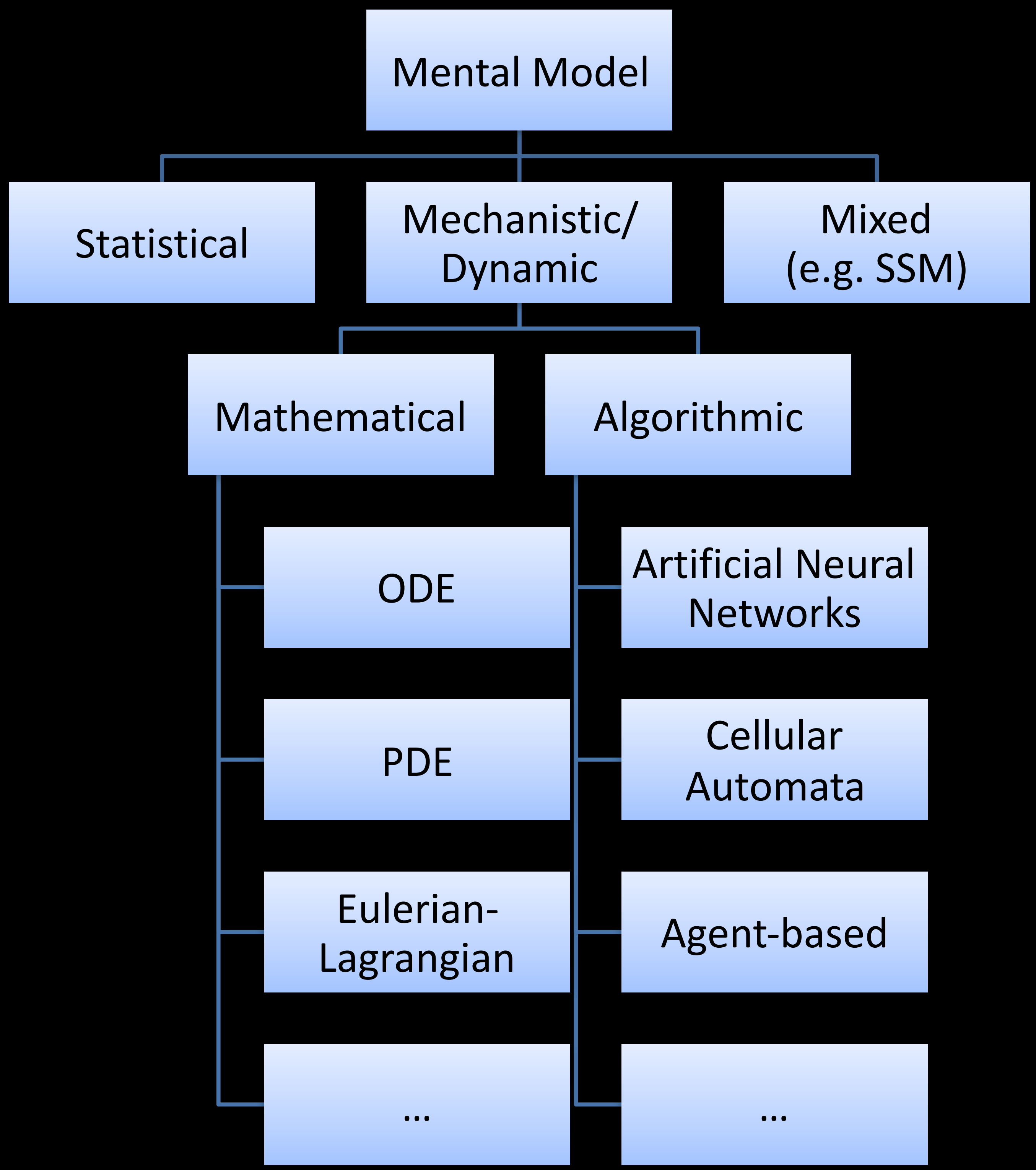




J.F. Remacle
Quantity of Interest: neuro-transmission

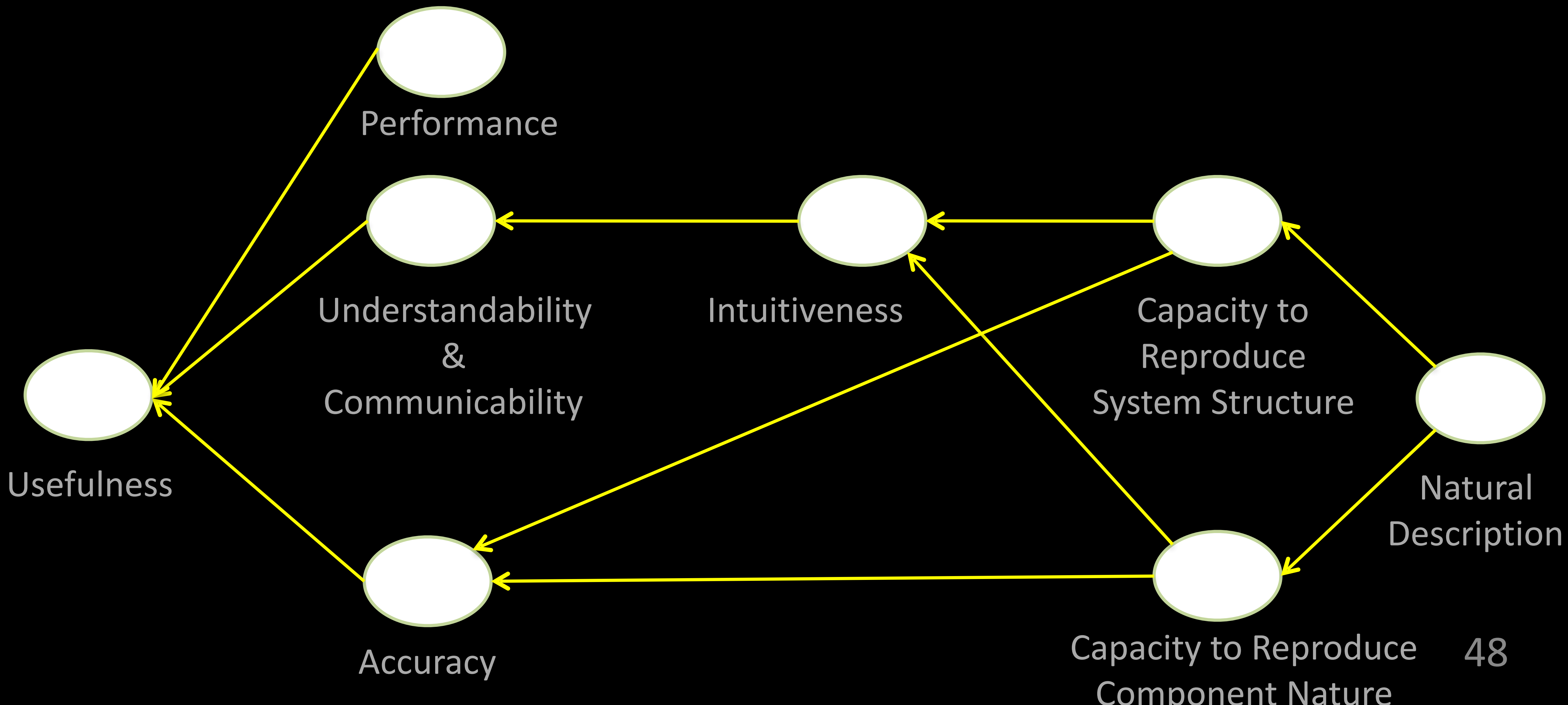
Tissue phantoms/mimics
(Dini, Imperial College London)
Quantity of Interest: stiffness

Types of models

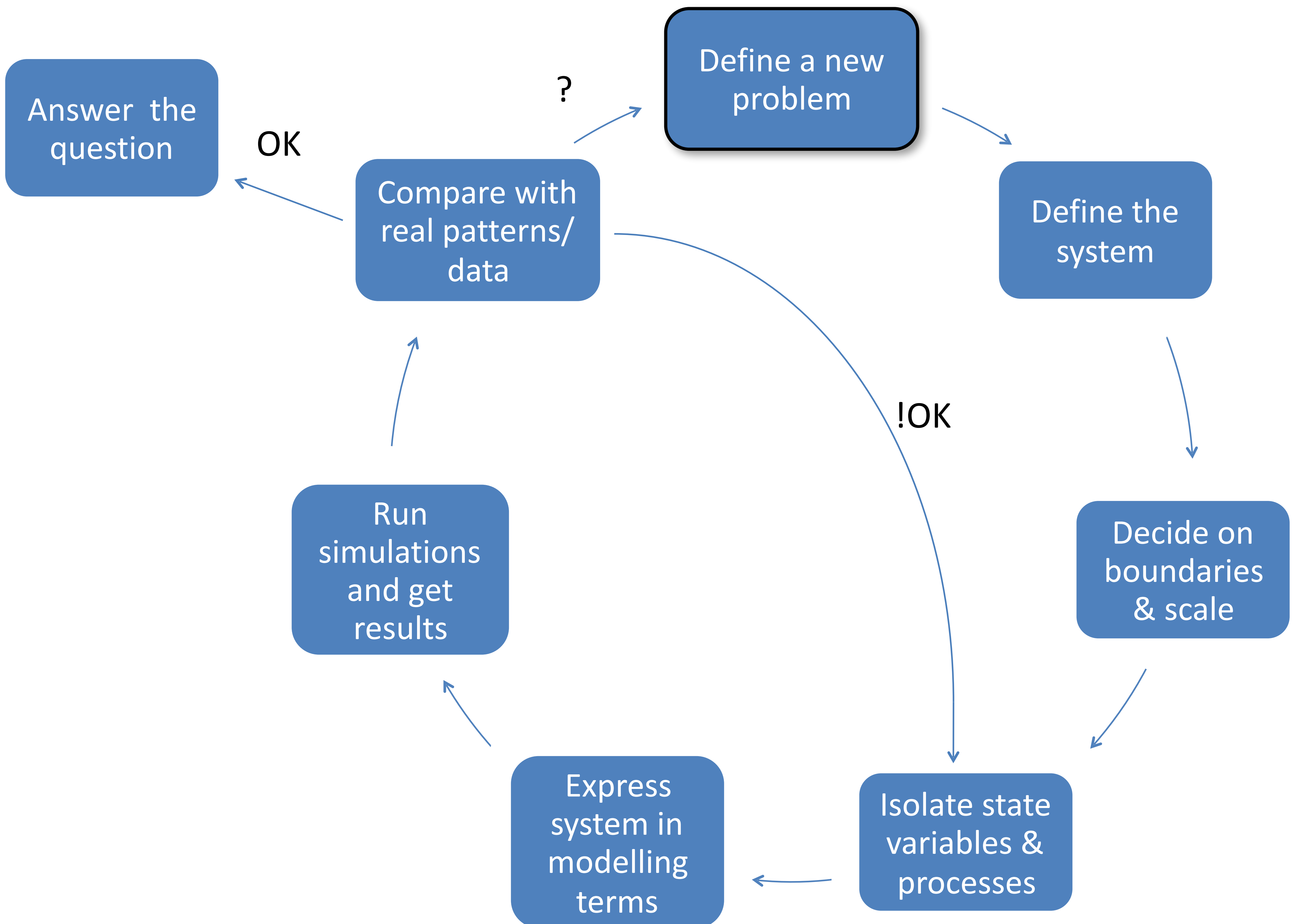


What is a "good" dynamic model?

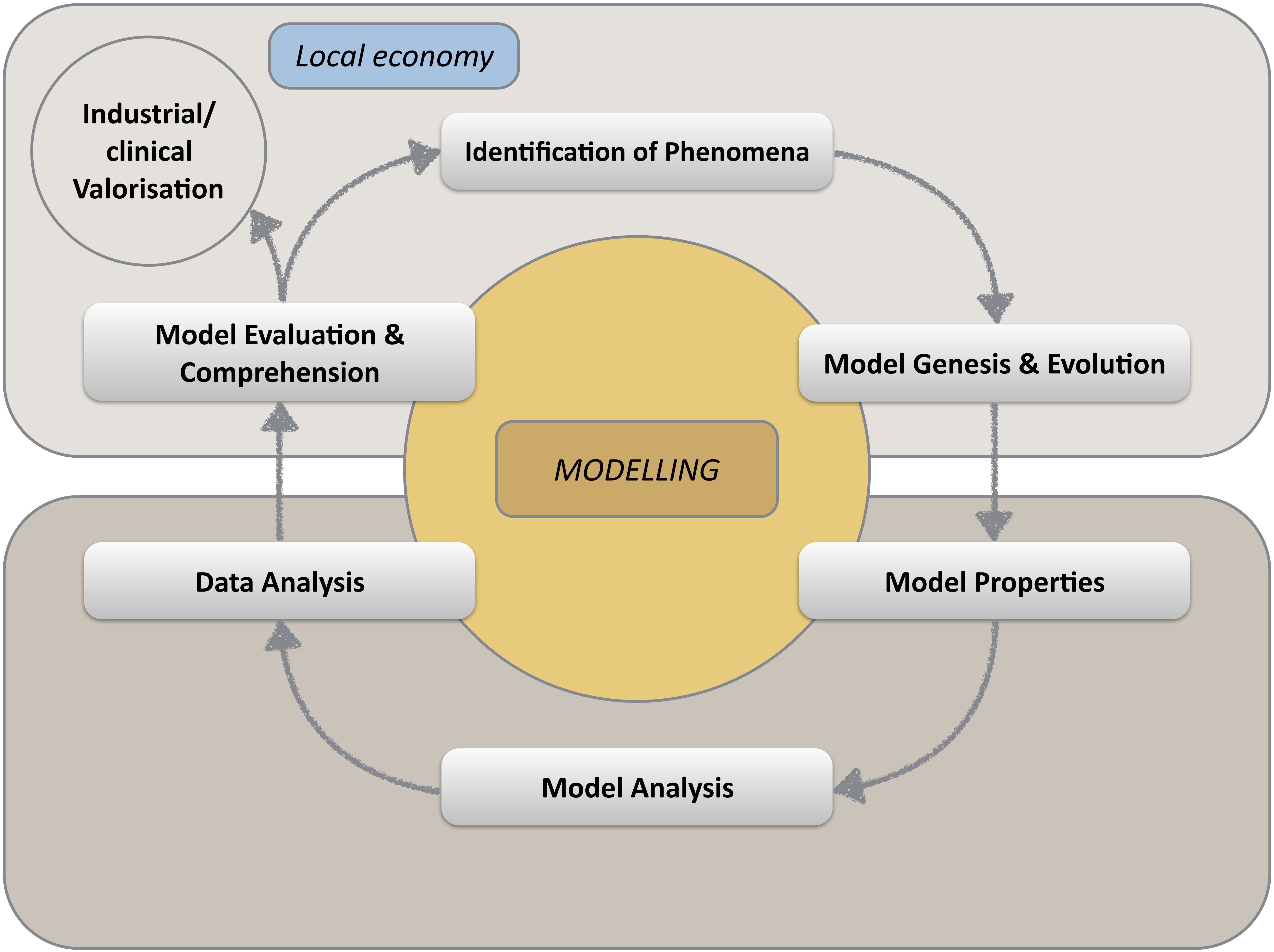
- "All models are wrong. Some of them are **useful.**" -- George E.P. Box (1979)



How to build dynamic models?
The modelling process



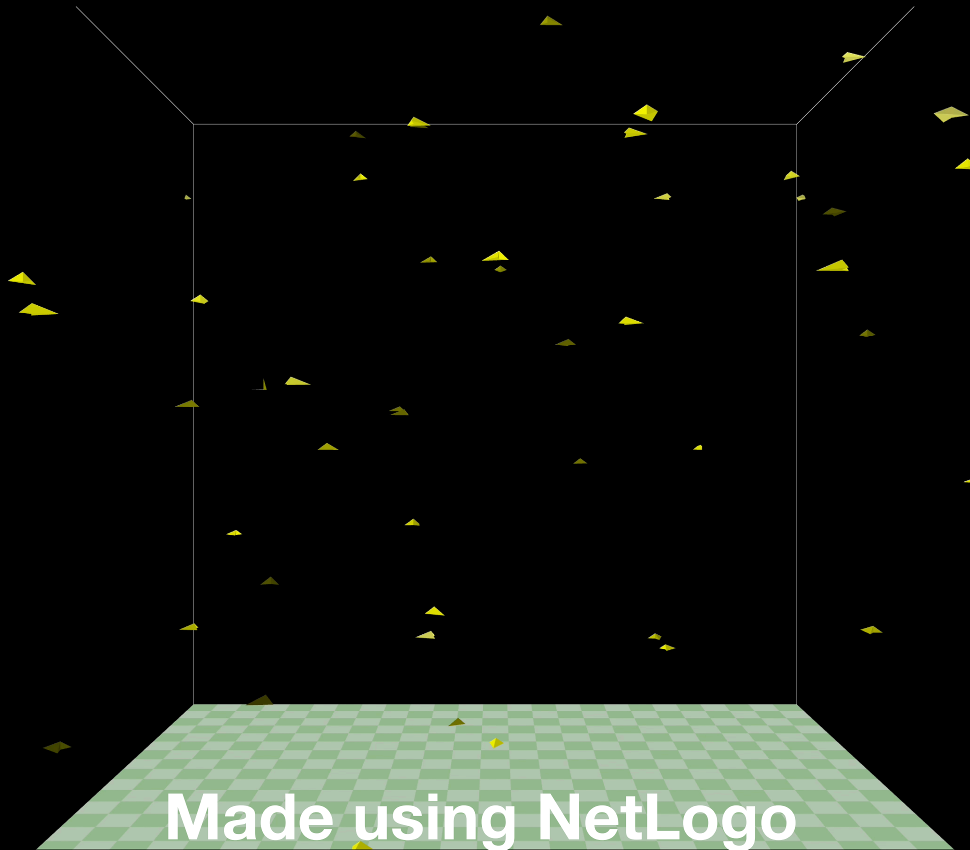
COMPUTATIONAL & DATA SCIENCES



Stirling murmuration (Rome)

Flocking of Stirlings

- Is there a leader?
- Are the global patterns attributable to local rules? Can we derive global equations governing their behaviour? Is the process deterministic?
- What is their acceleration, maximum velocity, reaction time, minimum distance with other birds, line of sight, manoeuvrability?



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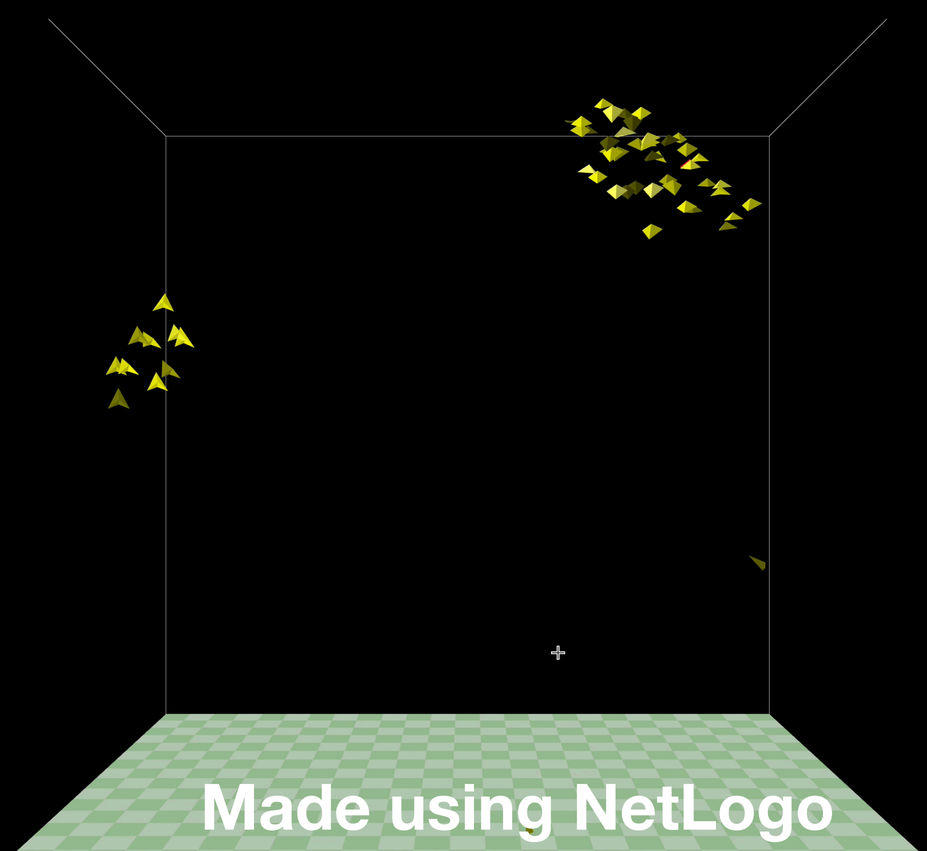
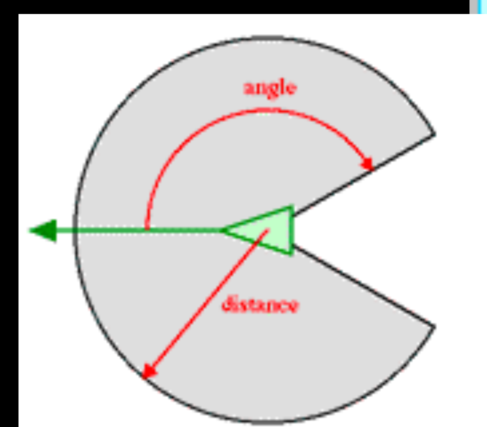
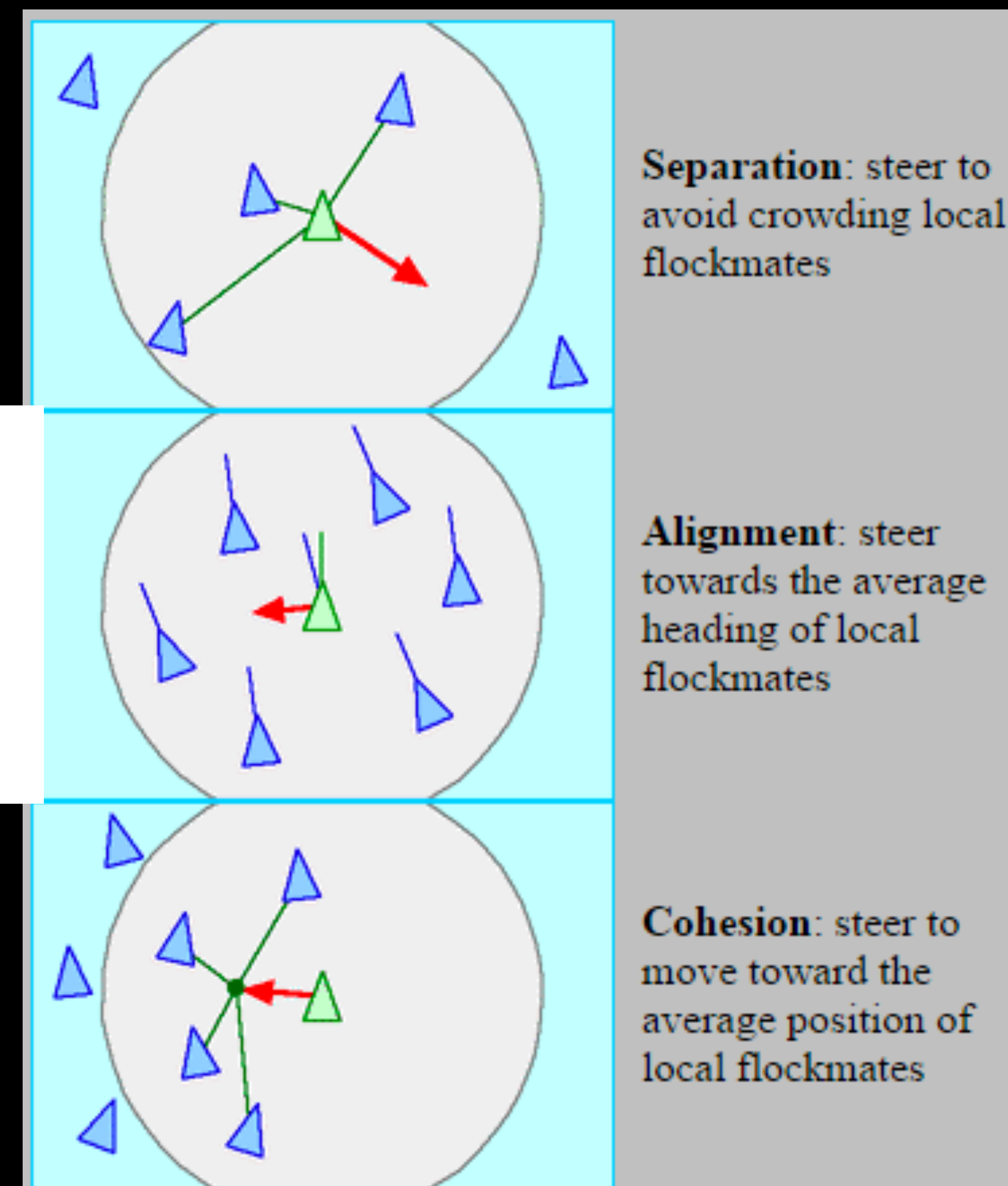
Boids flocking local rules for global behaviour



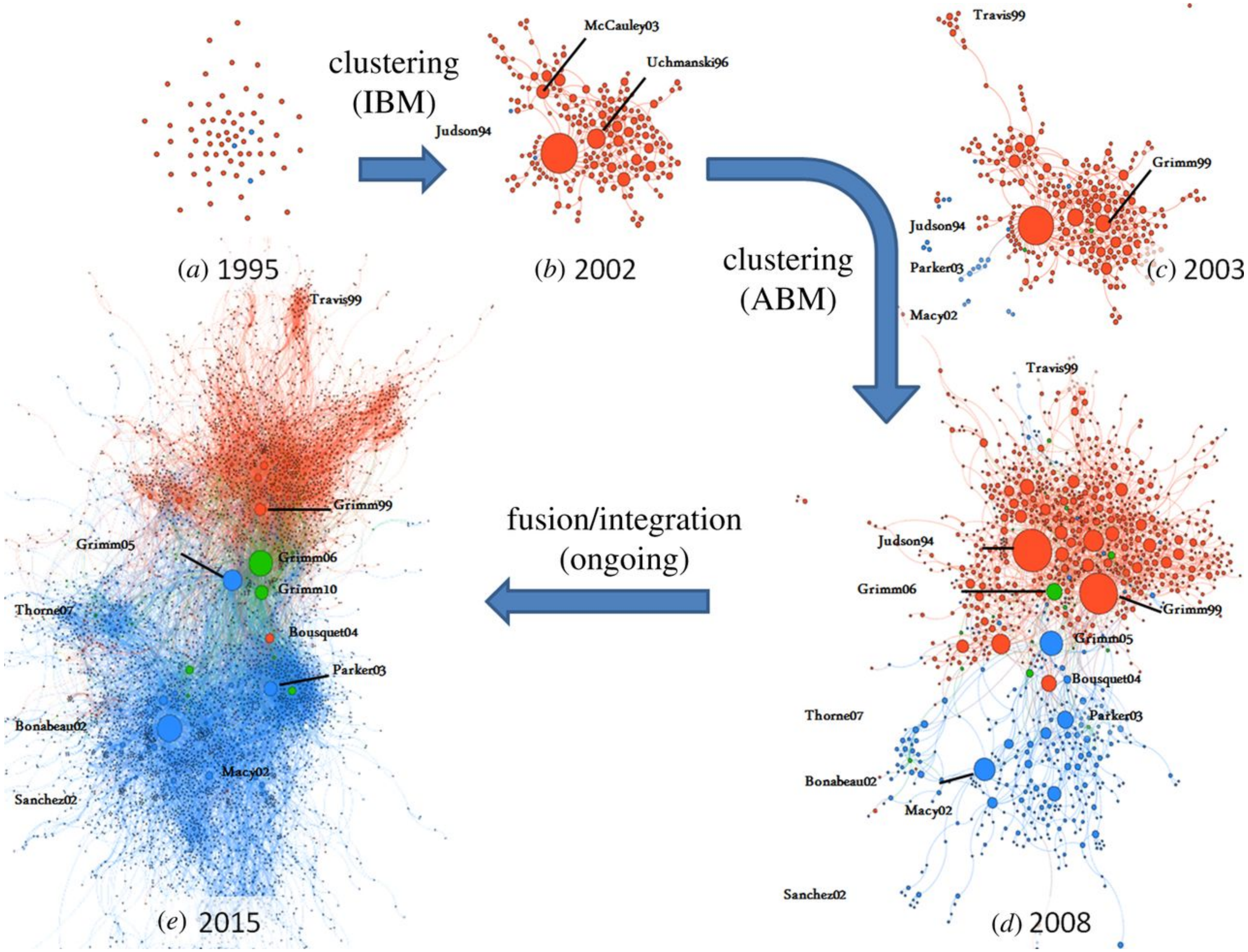




C.W. Reynolds SIGGRAPH, 1987

Applications of ABM/IBM

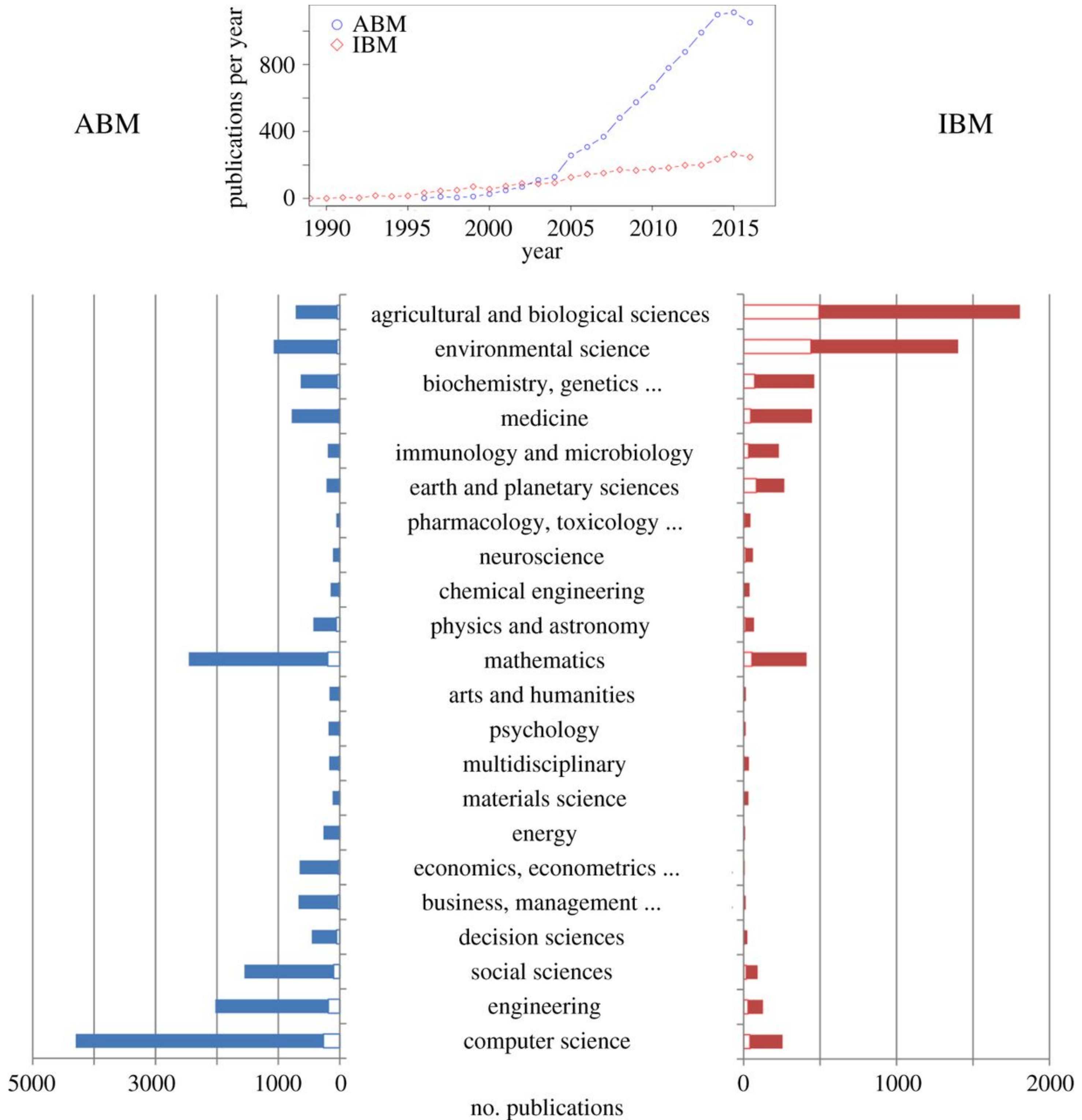
- A growing, unified community



(Vincenot, 2018)

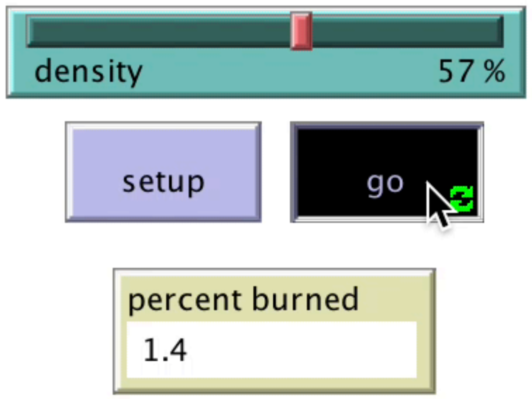
Applications of ABM/IBM

- Over 12,000 publications
- Everywhere in science!



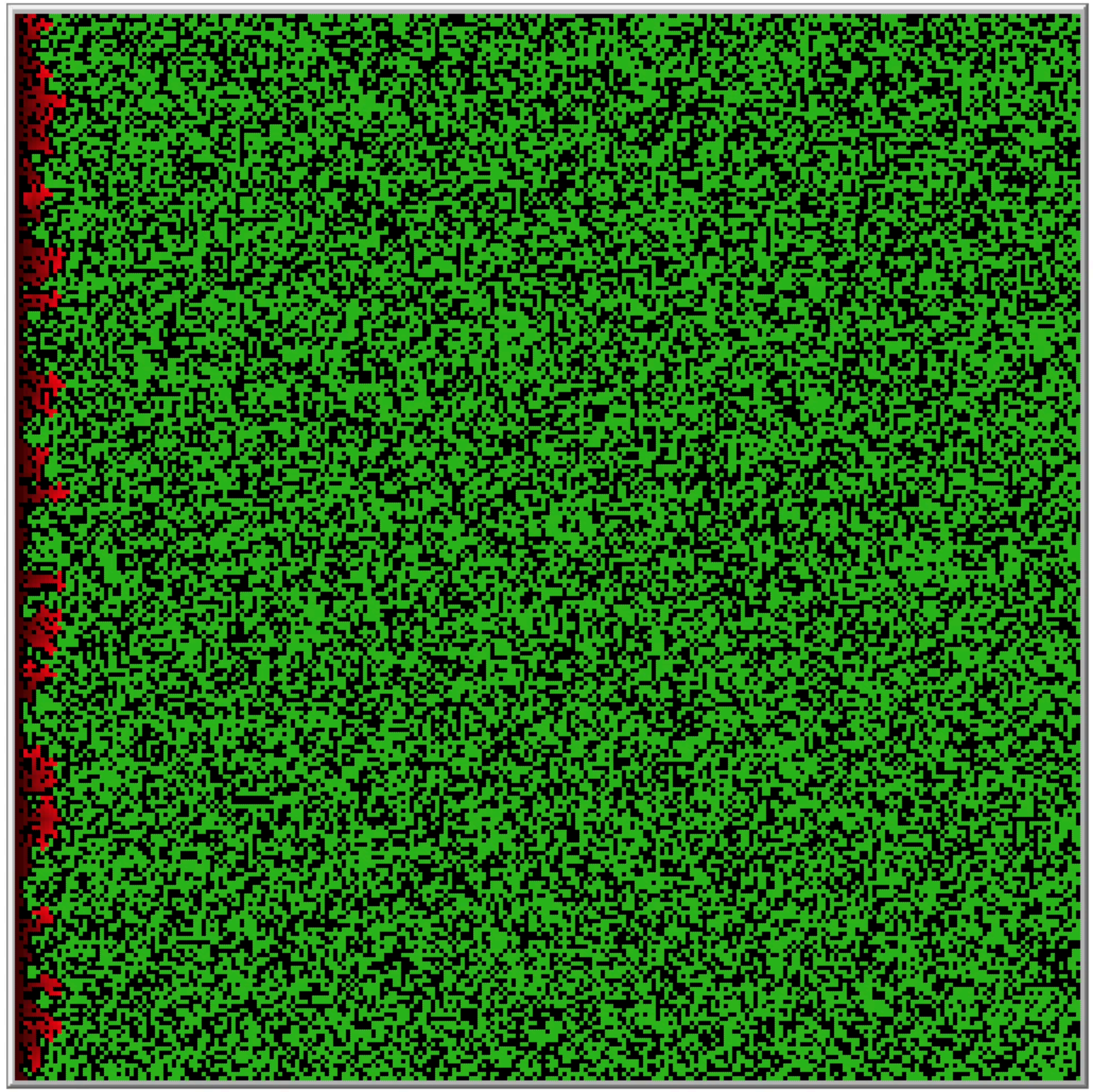
(Vincenot, 2018)

Mathematical models



59% is a threshold (50/50 probability)

Self-Organised Criticality



Fire spreading through a forest for various tree densities by NetLogo

Self-Organised Criticality

The Forest-Fire model belongs to the class of Self-Organized-Critical (SOC) systems, which are governed by a **slow driving energy input and burst (avalanches) of dissipative outputs** resulting often in **fractal** structures. These systems were introduced by P. Bak et al. [2] in 1987 using the example of a **sandpile** model. These SOC models can be applied to many different fields, famous applications are for instance: **earthquakes, solar flares, co-evolution, forest fires, hydraulic fracture and more. In addition they show scaling laws** and are related to critical phenomena.

http://guava.physics.uiuc.edu/~nigel/courses/563/Essays_2010/PDF/Funke.pdf

https://pdfs.semanticscholar.org/ec58/3f6f99f1d15a1d1ae2de1d243b648efd2ba8.pdf

http://www.uvm.edu/pdodds/files/papers/others/1993/grassberger1993.pdf

https://www.sciencedirect.com/science/article/pii/B9780128001301000047

Algorithmic Languages

- ABMs are always coded as algorithms
- Most often, simple deductive behavior:

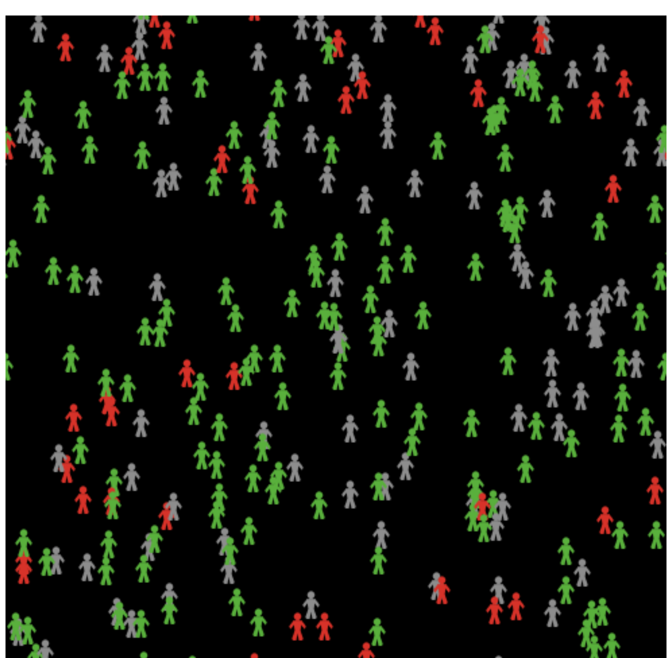
  e.g. "if hungry, search food"

  condition *action*

- Implementations require coding skills, but simplified languages exist

Netlogo

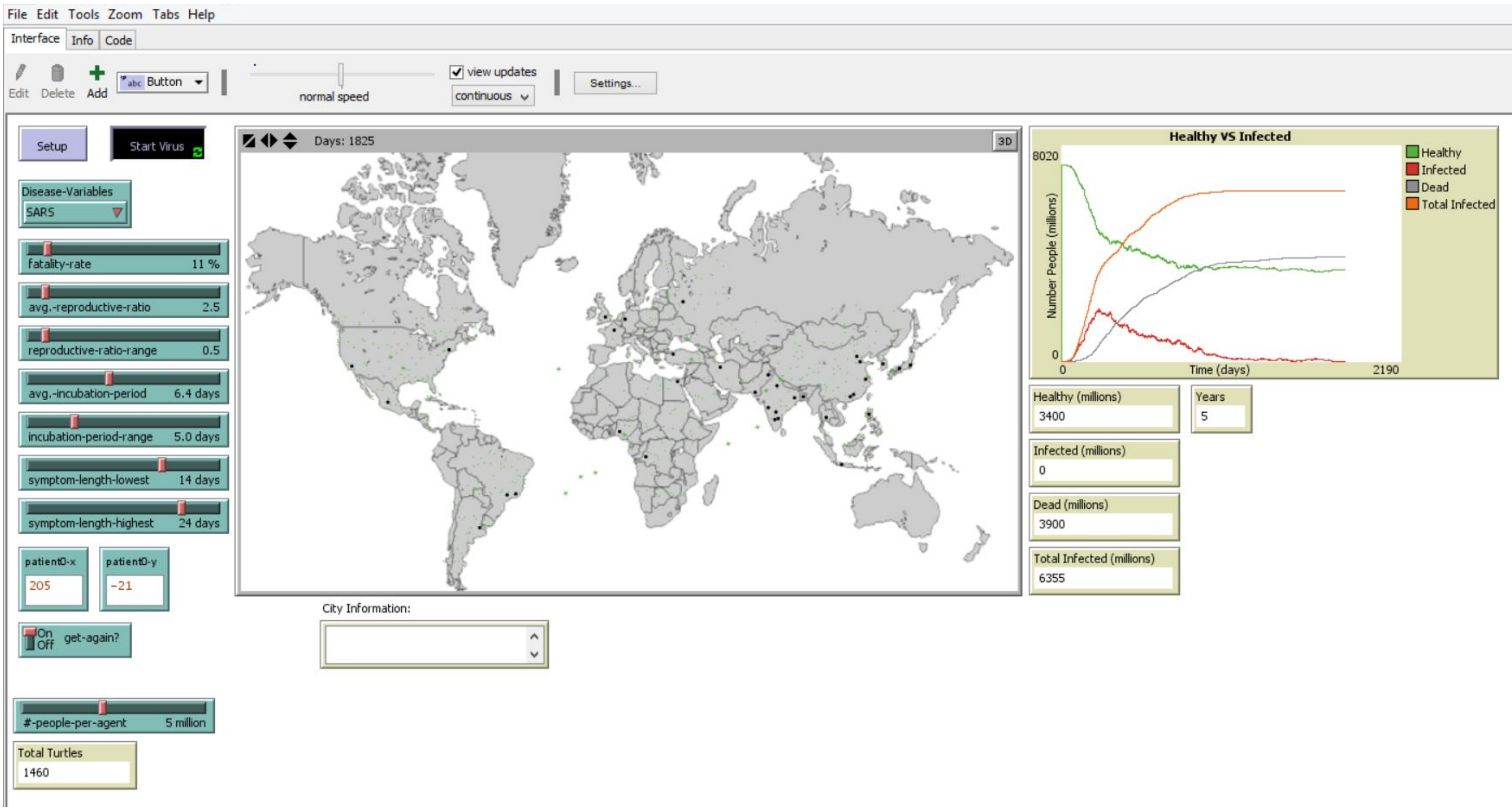
- Most used by ecologists
- Simplified language
- Slow, but good for relatively simple models
- Simple random movement model →



```
to setup
        clear-all
        create-turtles 10
        reset-ticks
end

to go
        ask turtles [
                fd 1 ;; forward 1 step
                rt random 10 ;; turn right
                lt random 10 ;; turn left
        ]
        tick
end
```

Netlogo


File Edit Tools Zoom Tabs Help
Interface Info Code
Edit Delete Add
Button
normal speed
view updates
continuous
Settings...
Setup
Start Virus
Disease-Variables
SARS
fatality-rate 11 %
avg.-reproductive-ratio 2.5
reproductive-ratio-range 0.5
avg.-incubation-period 6.4 days
incubation-period-range 5.0 days
symptom-length-lowest 14 days
symptom-length-highest 24 days
patient0-x
205
patient0-y
-21
On
Off
get-again?
#-people-per-agent 5 million
Total Turtles
1460
Days: 1825
3D
City Information:
Healthy VS Infected
8020
0
Number People (millions)
Time (days)
2190
Healthy
Infected
Dead
Total Infected
Healthy (millions)
3400
Years
5
Infected (millions)
0
Dead (millions)
3900
Total Infected (millions)
6355

Gama

- Computer scientists
- More complex language
- Powerful, but difficult

```
model SI_city

global{
	geometry shape<-envelope(square(500));
	init{
		create people number:1000;
	}
}

species people skills:[moving]{
	float speed <- 5.0 + rnd(5);
	bool is_infected <- flip(0.01);
	reflex move{
		do wander;
	}
	reflex infect when: is_infected{
		ask people at_distance 10 {
			if flip(0.01) {
				is_infected <- true;
			}
		}
	}
	aspect circle{
		draw circle(5) color:is_infected ? rgb("red") : rgb("green");
	}
}

experiment main_experiment type:gui{
	output {
		display map {
			species people aspect:circle;
		}
	}
}
```

Definition of the world geometry

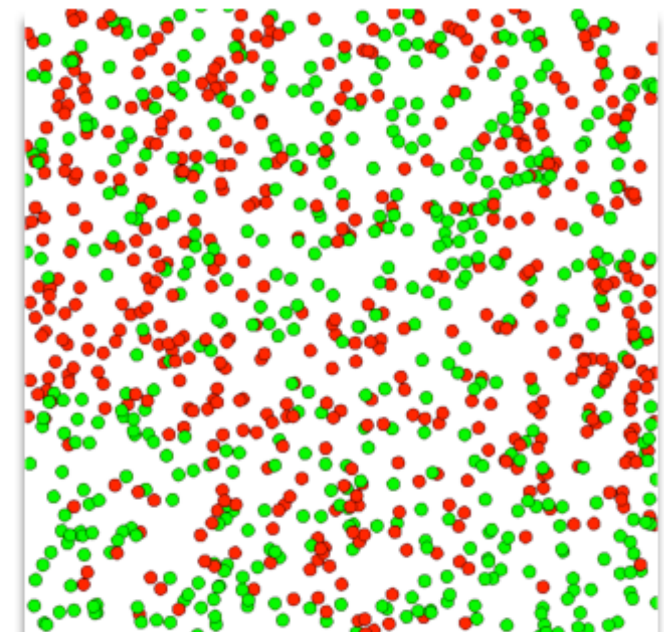
People agent creation

variables of the people agents

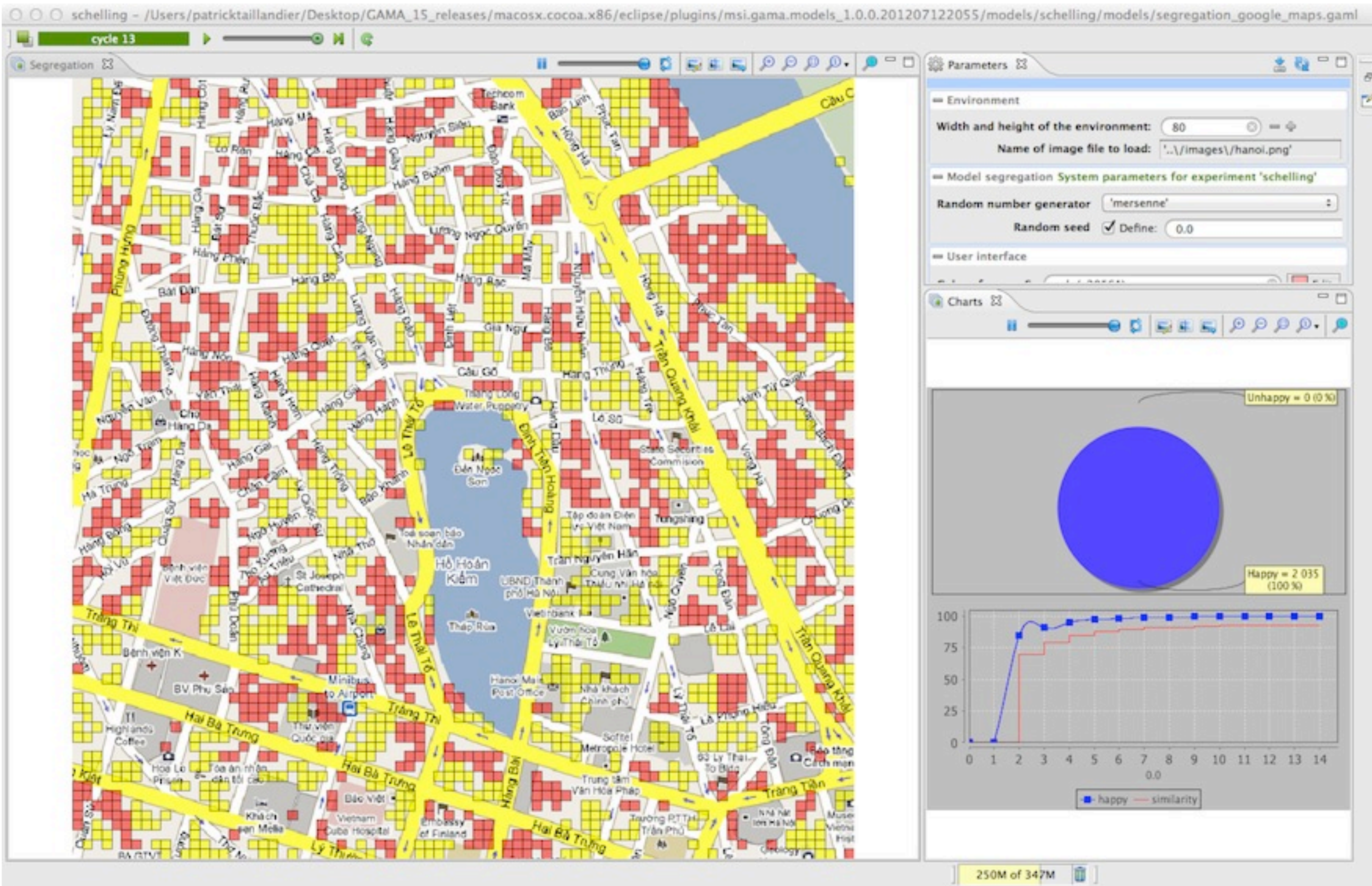
reflexes of the people agents

Aspect of the people agents

Definition of an agent display



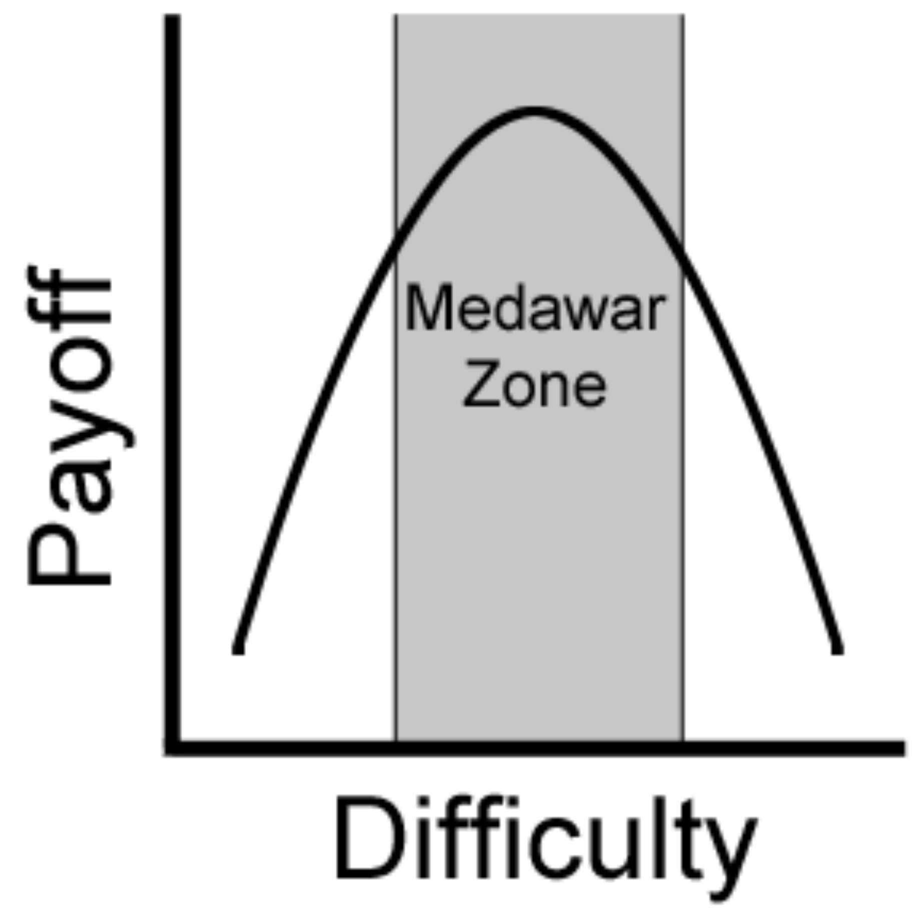
Gama



schelling – /Users/patricktaillandier/Desktop/GAMA_15_releases/macosx.cocoa.x86/eclipse/plugins/msi.gama.models_1.0.0.201207122055/models/schelling/models/segregation_google_maps.gaml
cycle 13
Segregation
Parameters
Environment
Width and height of the environment: 80
Name of image file to load: '..\/images\/hanoi.png'
Model segregation System parameters for experiment 'schelling'
Random number generator 'mersenne'
Random seed Define: 0.0
User interface
Charts
Unhappy = 0 (0 %)
Happy = 2 035 (100 %)
happy
similarity
250M of 347M

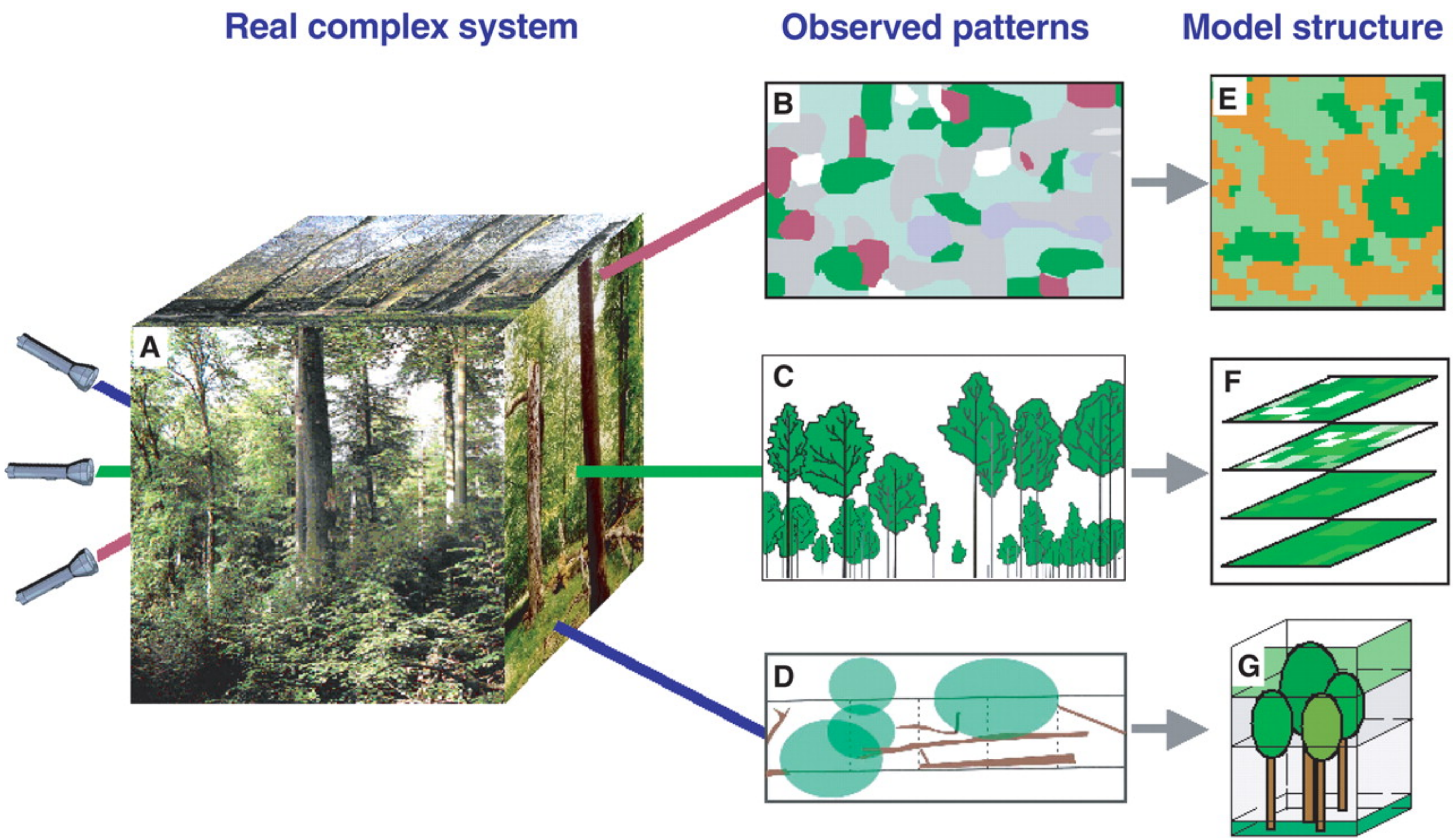
KISS

- "Keep it Simple, Stupid" (KISS) principle
- Try to make models as simple as possible
- Many processes/parameters <u>does NOT mean</u> better accuracy!!

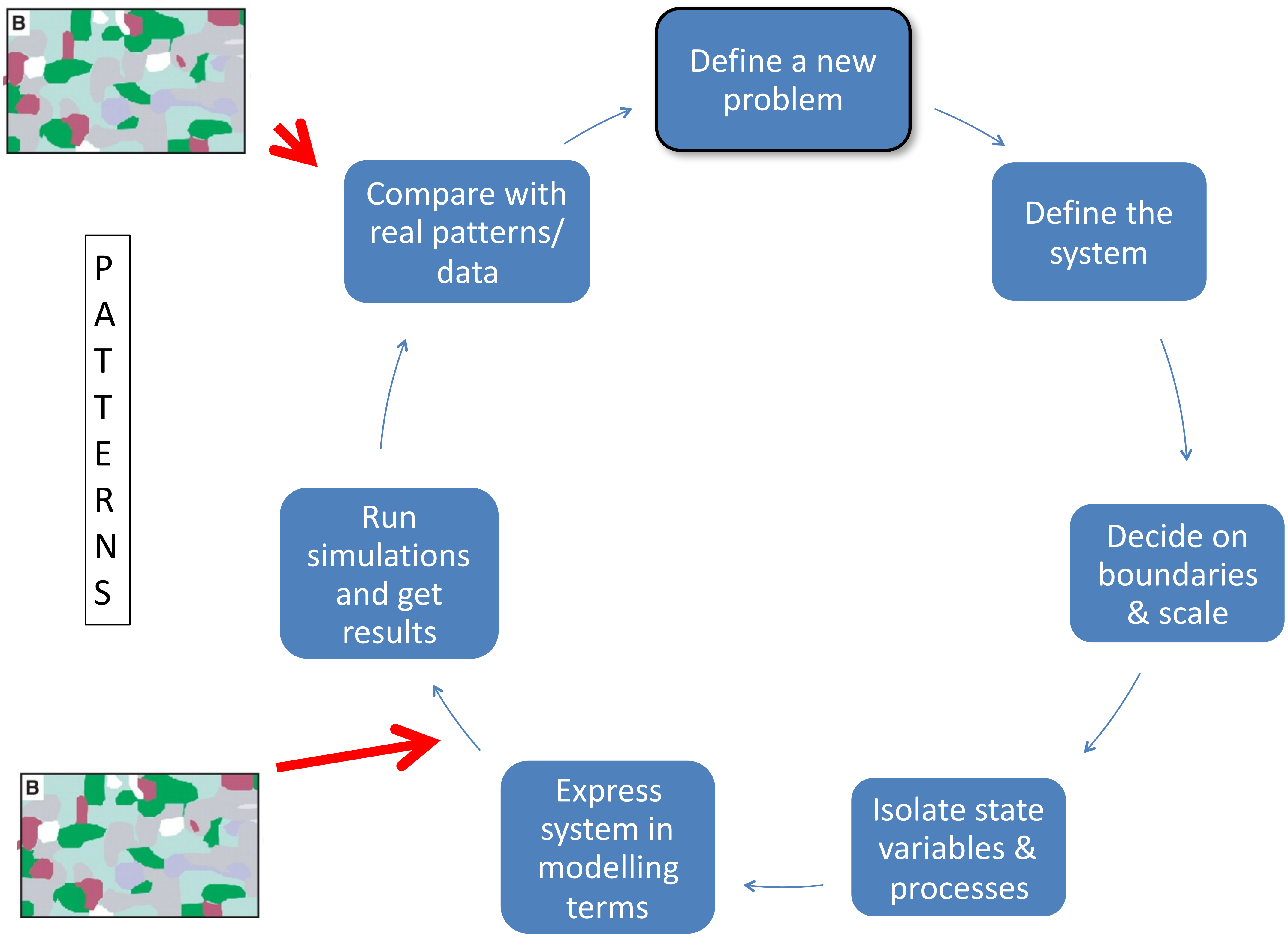


Pattern-oriented Modelling

- Use patterns instead of numerical fitting to validate model (Grimm et al. 2005)



Pattern-oriented Modelling



ODD: Describing ABM Models

- The ODD Protocol
  - Overview, Design concepts, and Details (ODD)
  - A strict set of guidelines to describe and publish ABMs
  - Guarantees the replicability of models and studies
  - More than 2000 citations
  - 2nd version already; 3rd version in preparation
  - See Grimm et al. (2006 and 2010)
- Please <u>always</u> use when developing ABMs!

Useful Reads

Agent-based Modelling

- Grimm V. and Railsback S.F. 2011. *Individual-based Modeling and Ecology*. **Princeton University Press**.
- Janssen M. 2017. *Introduction to Agent-based Modeling.* [Online book] https://cbie.gitbook.io/introduction-to-agent-based-modeling/

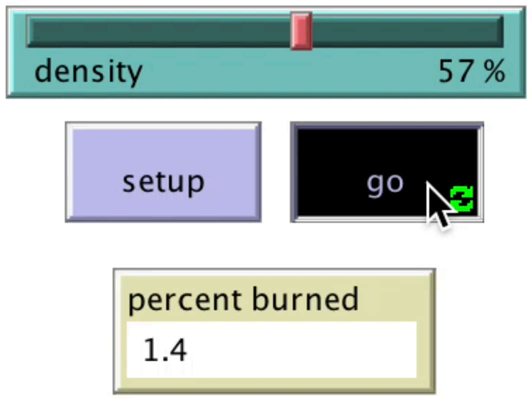
Vegetation model

- Vincenot C.E., Carteni F., Bonanomi G., Mazzoleni S., Giannino F. 2017. *Plant-soil negative feedback explains vegetation dynamics and patterns at multiple scales*. **Oikos**, 126:1319-1328.
- Vincenot C.E., Carteni F., Mazzoleni S., Rietkerk M., Giannino F. 2016. *Spatial Self-Organization of Vegetation Subject to Climatic Stress—Insights from a System Dynamics—Individual-Based Hybrid Model*. **Frontiers in Plant Science** fpls.2016.00636.

Outline

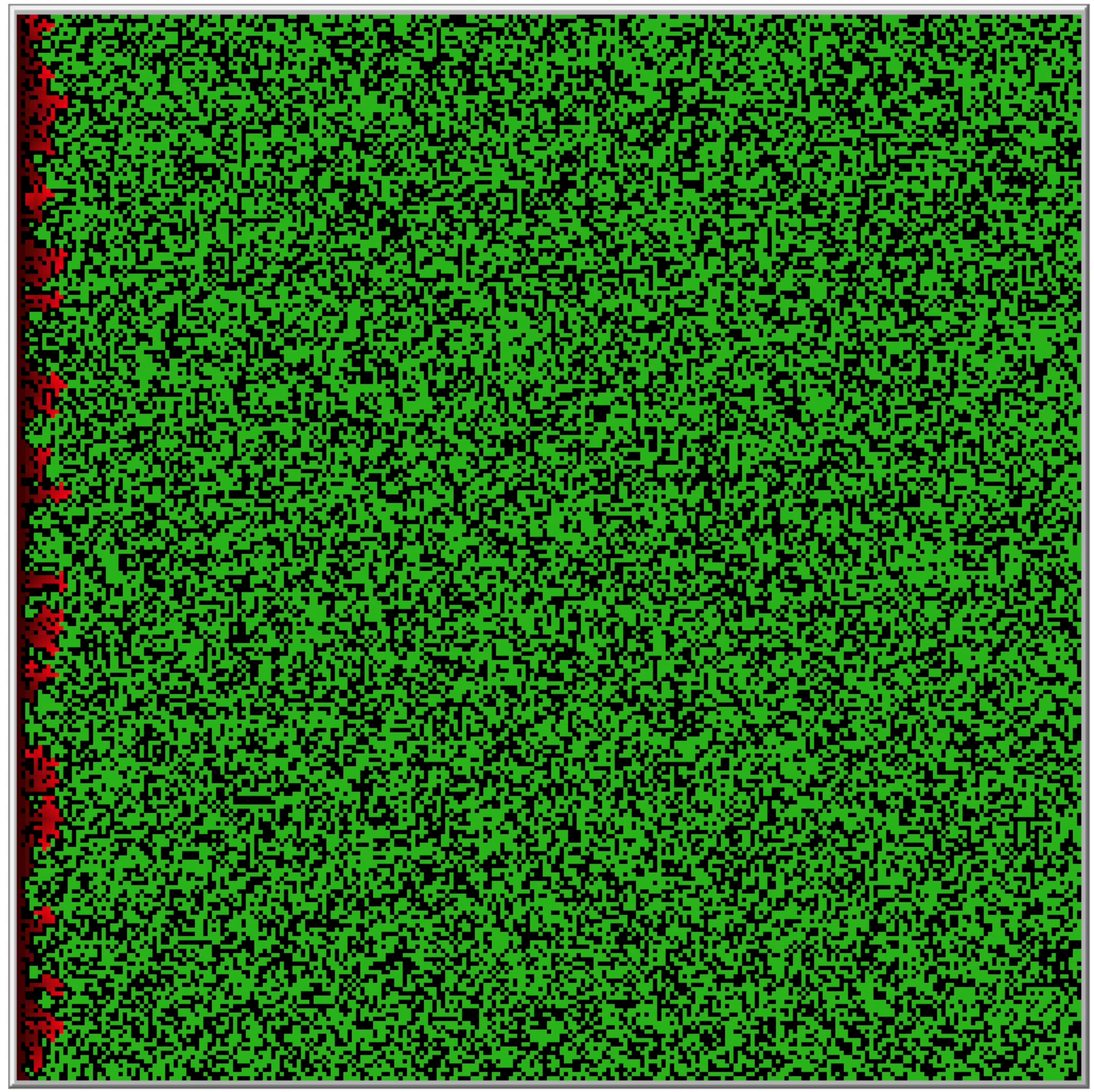
- Scientific method, experiments, analytical methods and models
- What is a complex system?
- What models are available to understand and predict?
- What are agent-based models?
- Equation-based (mathematical) models
- How to choose the “best” model?

Mathematical models



59% is a threshold (50/50 probability)

Self-Organised Criticality



Fire spreading through a forest for various tree densities by NetLogo

Physics-based or mathematical models

Physics-based model

T (K) is the temperature of the fire layer,
$S \in [0,1]$ is the fuel supply mass fraction (the relative amount of fuel remaining),
k $(m^2 s^{-1})$ is the thermal diffusivity,
A $(K s^{-1})$ is the temperature rise per second at the maximum burning rate with full initial fuel load and no cooling present,
B (K) is the proportionality coefficient in the modified Arrhenius law,
C (K^{-1}) is the scaled coefficient of the heat transfer to the environment,
C_S (s^{-1}) is the fuel relative disappearance rate,
T_a (K) is the ambient temperature, and
$\overrightarrow{v}$ (ms^{-1}) is the wind speed given by atmospheric data or model.

The model is derived from the conservation of energy, balance of fuel supply, and the fuel reaction rate:

$$\frac{dT}{dt} = \nabla \cdot (k \nabla T) - \overrightarrow{v} \cdot \nabla T + A \left(S e^{-B/(T-T_a)} - C(T - T_a) \right), \qquad (1)$$

$$\frac{dS}{dt} = -C_S S e^{-B/(T-T_a)}, \quad T > T_a, \qquad (2)$$

https://arxiv.org/pdf/0709.0086

$$\frac{dT}{dt} = \nabla \cdot (k \nabla T) - \vec{v} \cdot \nabla T + A \left(S e^{-B/(T-T_a)} - C (T - T_a) \right), \tag{1}$$

Heat diffusion — Advection — Fuel consumption

$$\frac{dS}{dt} = -C_S S e^{-B/(T-T_a)}, \quad T > T_a, \tag{2}$$

with the initial values

$$S(t_{\text{init}}) = 1 \text{ and } T(t_{\text{init}}) = T_{\text{init}}. \tag{3}$$

The diffusion term $\nabla \cdot (k \nabla T)$ models short-range heat transfer by radiation in a semi-permeable medium, $\vec{v} \cdot \nabla T$ models heat advected by the wind, $S e^{-B/(T-T_0)}$ is the rate fuel is consumed due to burning, and $AC(T - T_a)$ models the convective heat lost to the atmosphere. The reaction rate $e^{-B/(T-T_a)}$ is obtained by modifying the reaction rate $e^{-B/T}$ from the Arrhenius law by an offset to force zero reaction at ambient temperature, with the resulting reaction rate smoothly dependent on temperature.

Questions: Identification of parameters?

https://arxiv.org/pdf/0709.0086

Outline

- Scientific method, experiments, analytical methods and models
- What is a complex system?
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- What are agent-based models?
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When use agent-based models

- Not too few, nor too many - medium numbers of entities
- Heterogeneous systems
- Local interactions
- Rich environments

Not too many, not too few

- Casti ,1996
  - Too few agents, the system is too simple: game theory and ethnography are sufficient
  - Too many agents, averages work well, statistical descriptions

Richness of the environments

- Social networks
- Geographical systems
- The environment can itself be an agent

Compare agent-based models (ABM), mathematical models (MM), statistical models (SM)

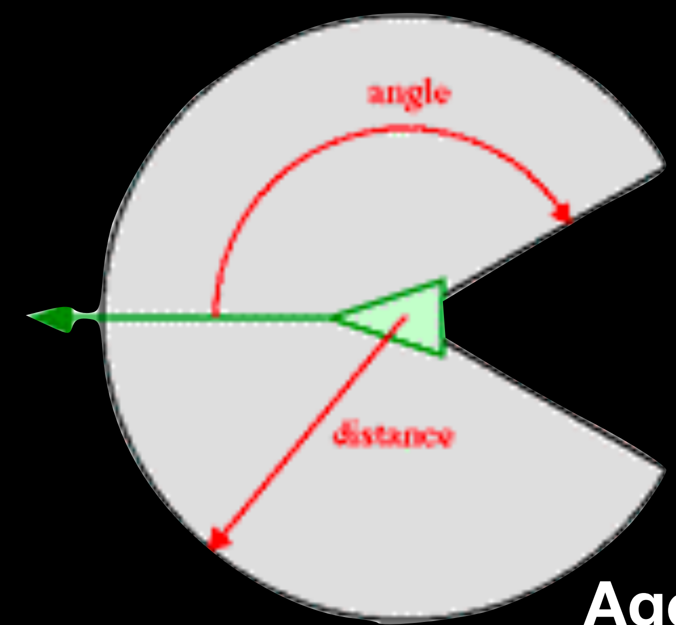
- MM are often continuous: Nano-wolf problem (Wilson 1998), but if you can write equations, do it
- ABM and MM approaches need parameters which are difficult to measure (agents need local parameters and rules)
- SM need large data sets of high quality
- ABM can be coupled to MM
- Both ABM and MM can learn from SM and Machine Learning and become adaptive

Some future prospects

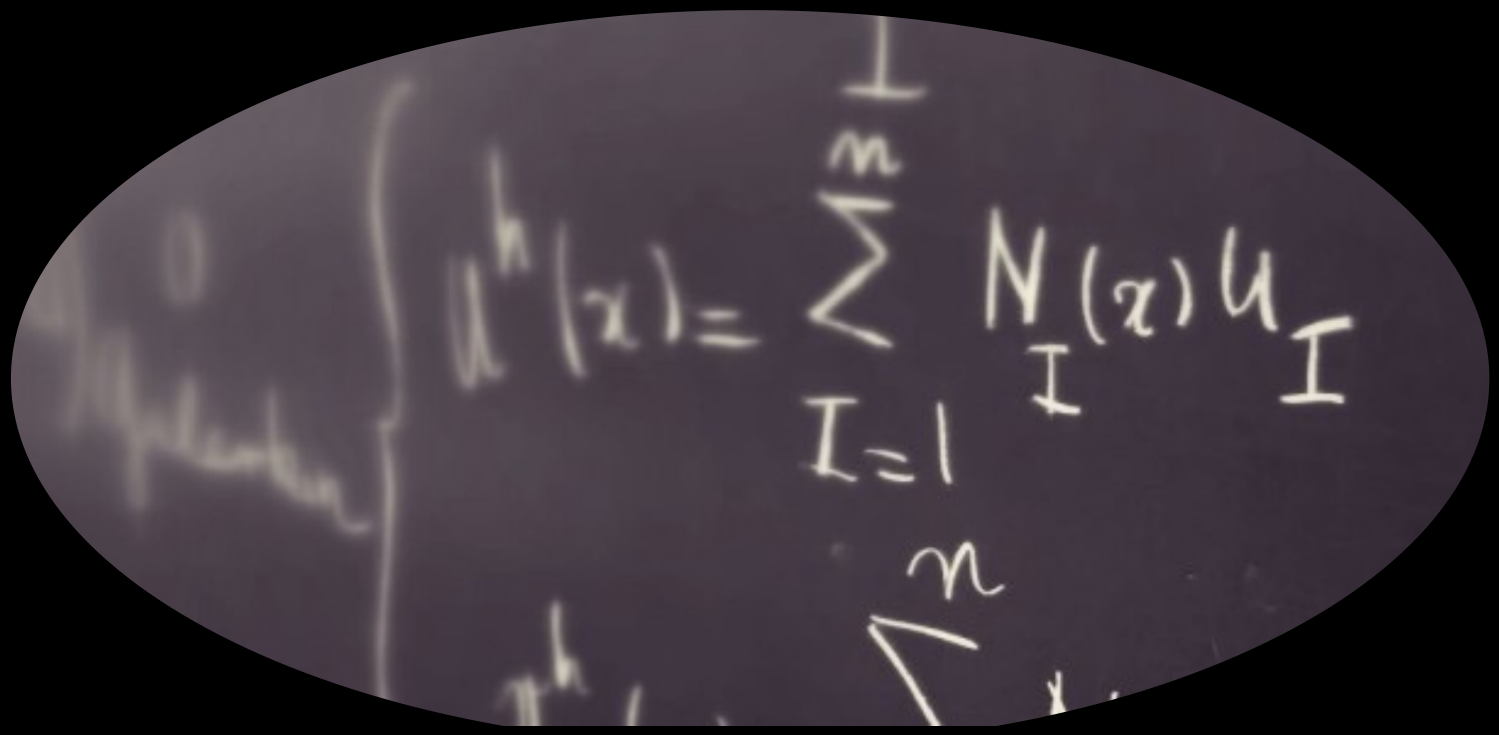
- Lab experiments are costly, they are sometimes impossible, dangeours… they can help generate theories
- ABM or MM can be created from lab experiments
- Models can help scale up from experiments
- Experiments are done within a laboratory setting, far removed from real-life, where the models would be used
- Digital twins can avoid such issues, but are still illusory in practice
- Models can help provide insights into sensitivities and uncertainties

Use of models

- Describe systems
- Explain behaviour
- Experiment and test systems
- Measure sensitivities
- Create analogies
- Educate
- Predict



Agents



Mathematical models

Thank you to

COMPLEXITY
EXPLORER
SANTA FE INSTITUTE

Outline

A focus on equation-based models

- How can we control the quality of simulations, verification and validation?

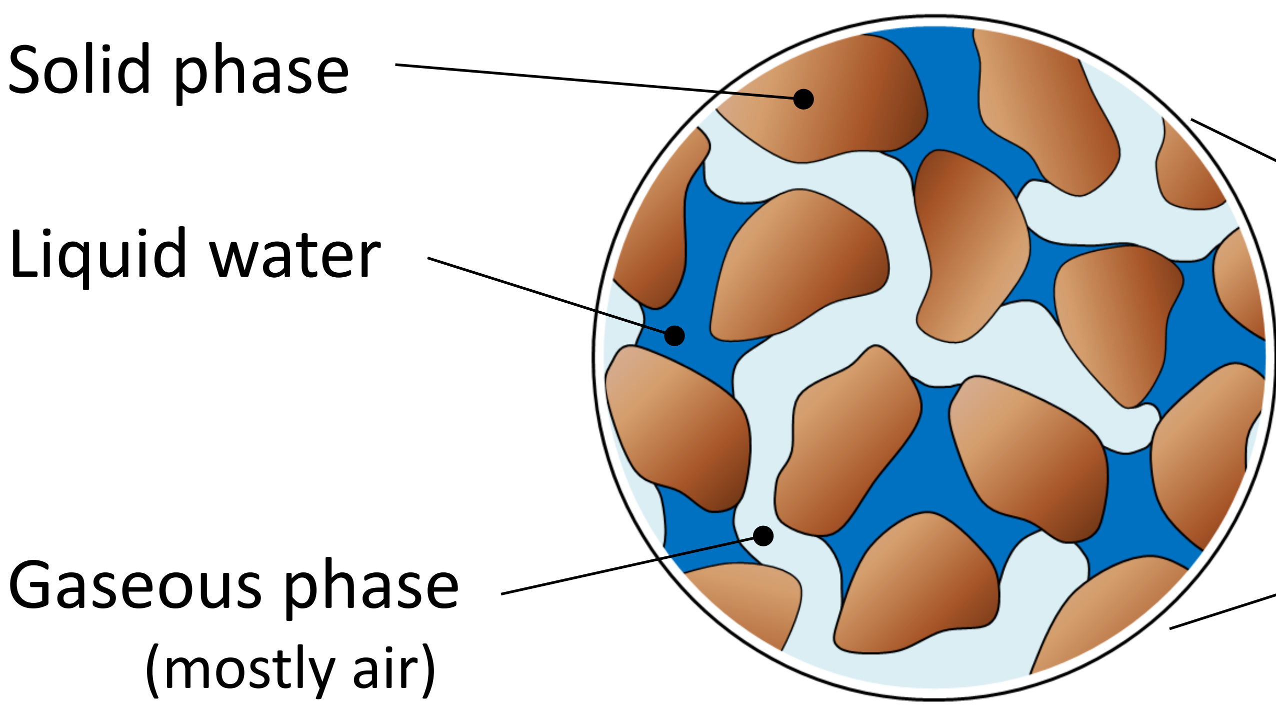
- Why are set-in-stone-models limited?

- How can we leverage statistical models to improve our models?

Porous media models

Microscale (pore scale)

Interfaces identifiable



RVE

Macroscale (Darcy scale)

At each point more phases coexist

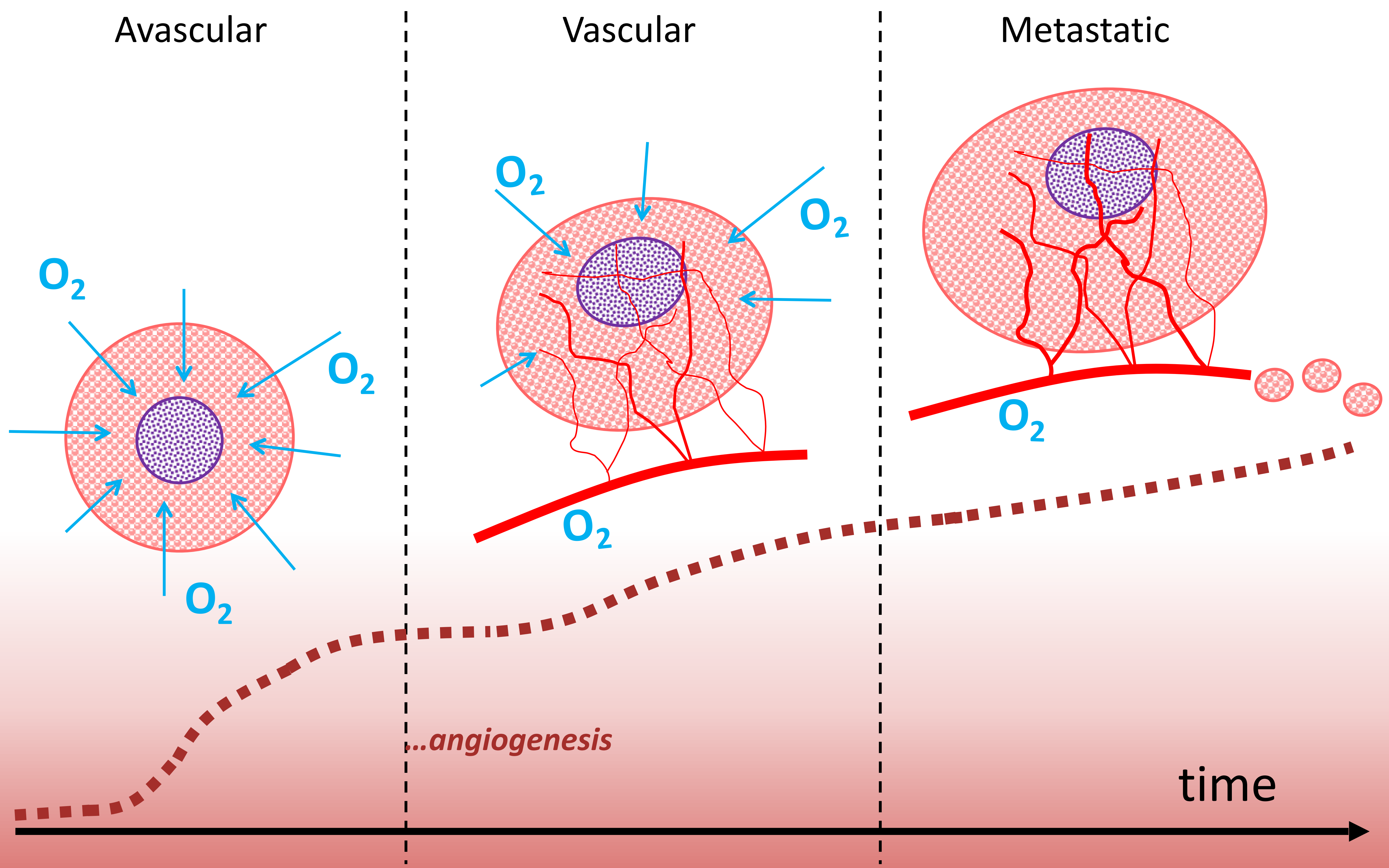
From Ms. Stanton – Science (http://www.oconee.k12.sc.us/)

Microscale
Conservation EQS

TCAT
Thermodynamically Constrained Averaging Theory
(Gray & Miller, 2005)

Macroscale
Conservation EQS

Can also help model tumours



MANY PROBLEMS SHARE THE SAME FORMALISM

Option Pricing

Black, Fischer, and Myron Scholes. "The pricing of options and corporate liabilities." The journal of political economy (1973): 637-654.

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS\frac{\partial V}{\partial S} - rV = 0$$

MANY PROBLEMS HAVE THE SAME FORMALISM

Option Pricing

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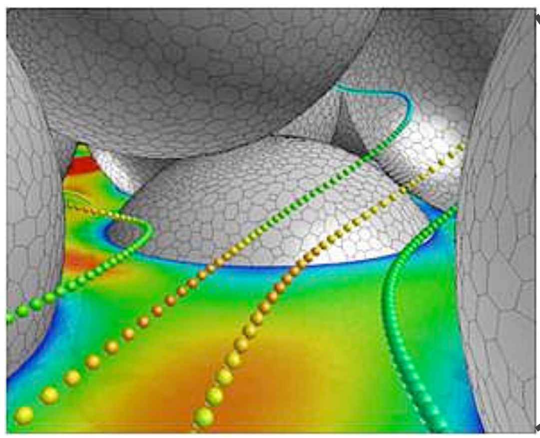
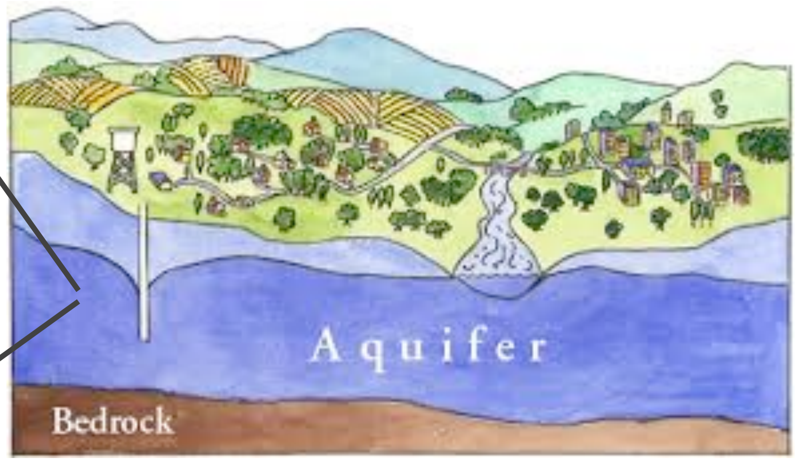
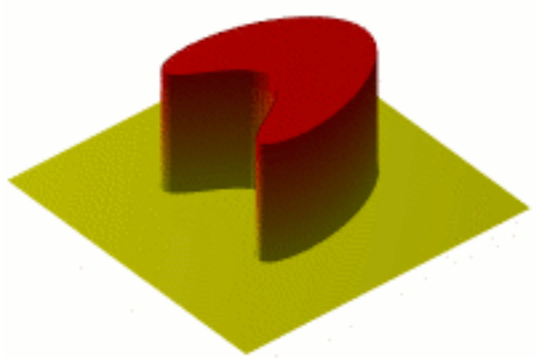
$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS\frac{\partial V}{\partial S} - rV = 0$$

Transport in Porous Media







Barenblatt, Grigory Isaakovich. Scaling, self-similarity, and intermediate asymptotics: dimensional analysis and intermediate asymptotics. Vol. 14. Cambridge University Press, 1978.

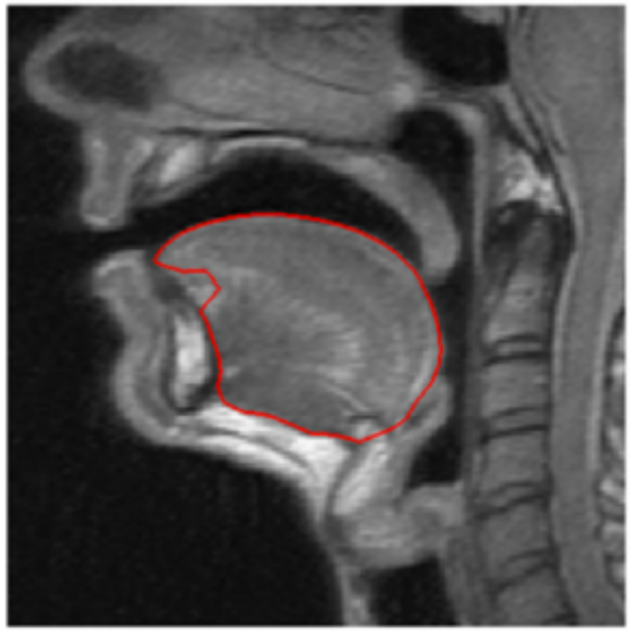

BUY
SELL
STOP

Mathematical Modelling

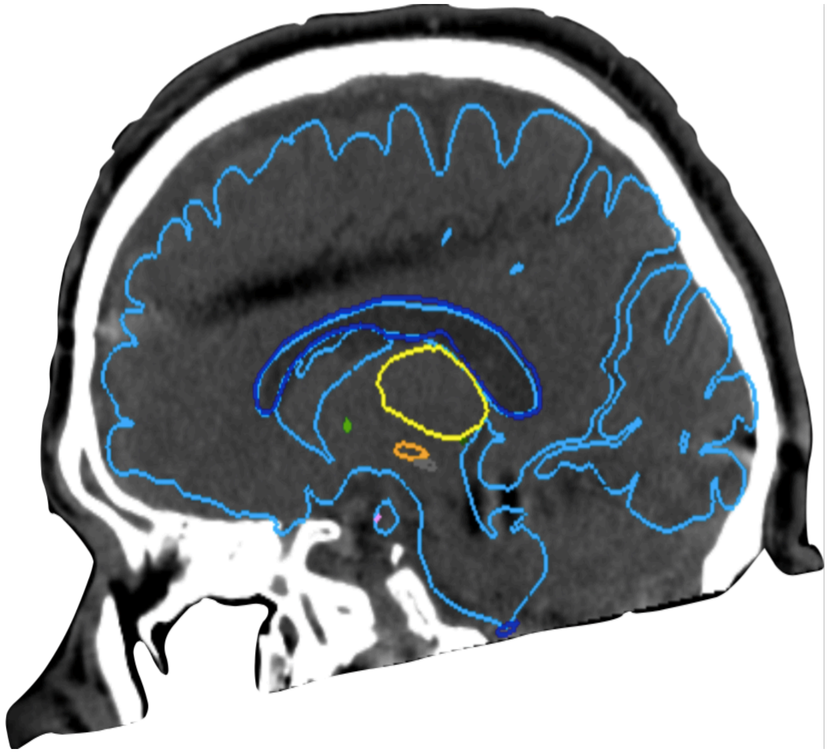
Continuous Problem

Mathematical Modelling

Continuous Problem



Bijar, Rohan, Perrier & Payan 2015



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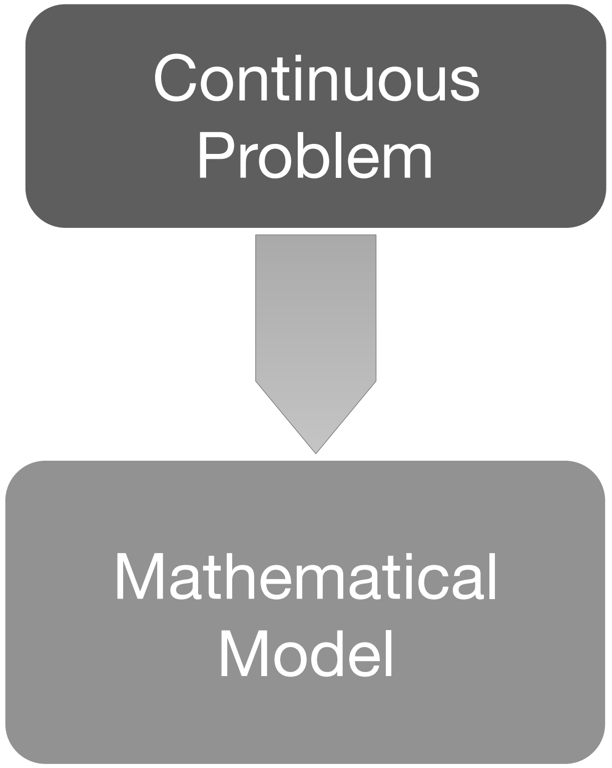
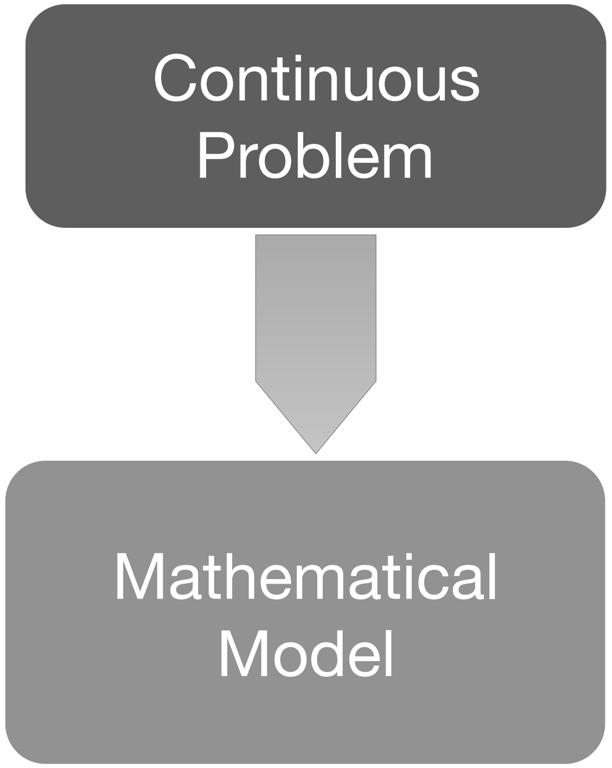
Mathematical Modelling



Mathematical Modelling



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

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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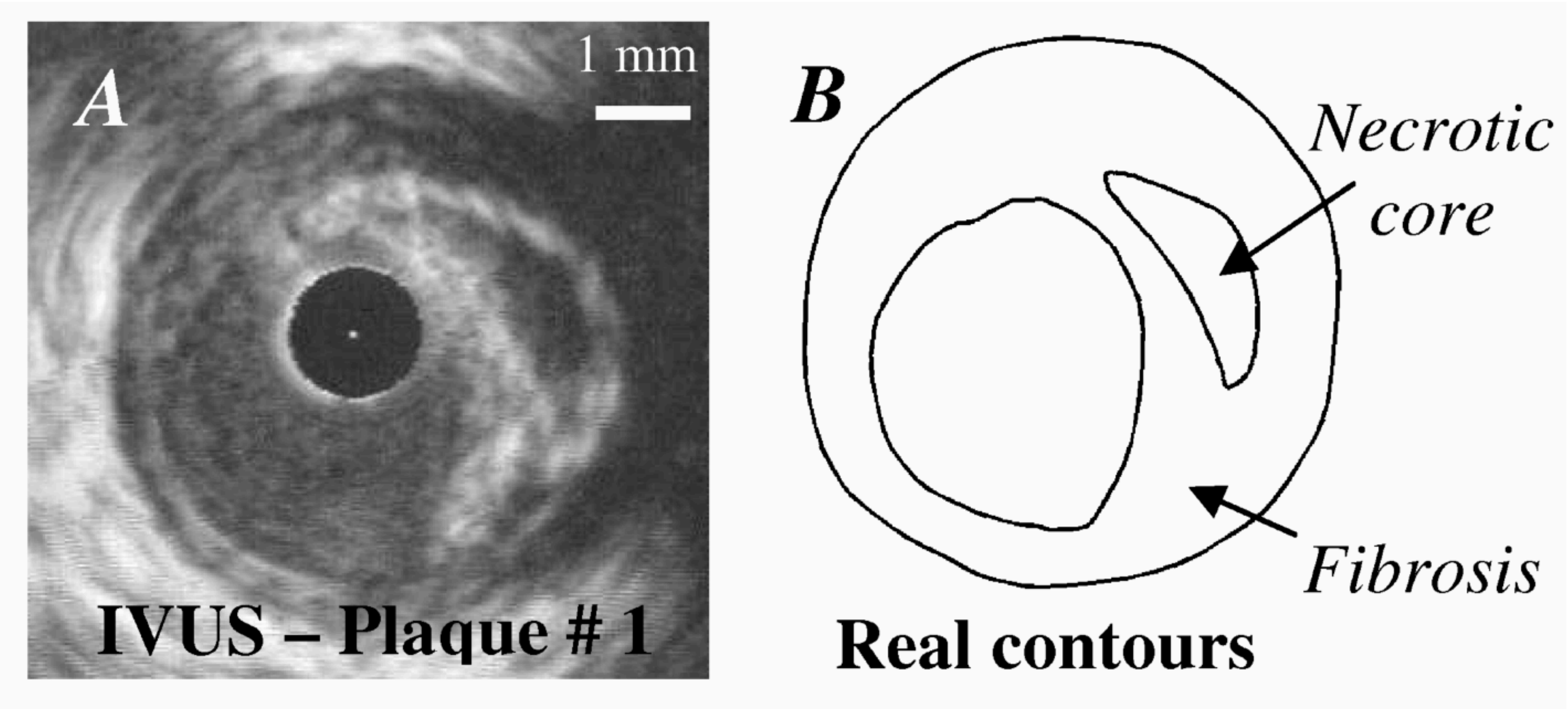
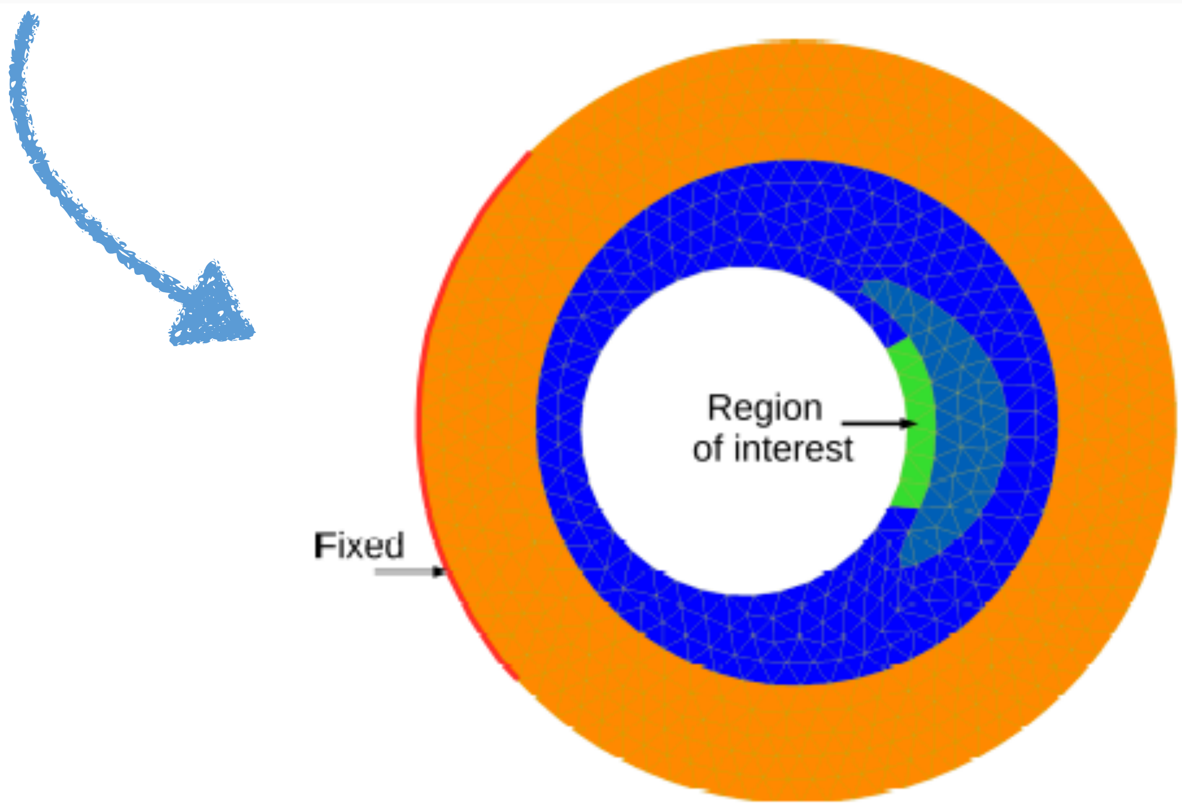
Mathematical Modelling

Continuous Problem

↓

Mathematical Model





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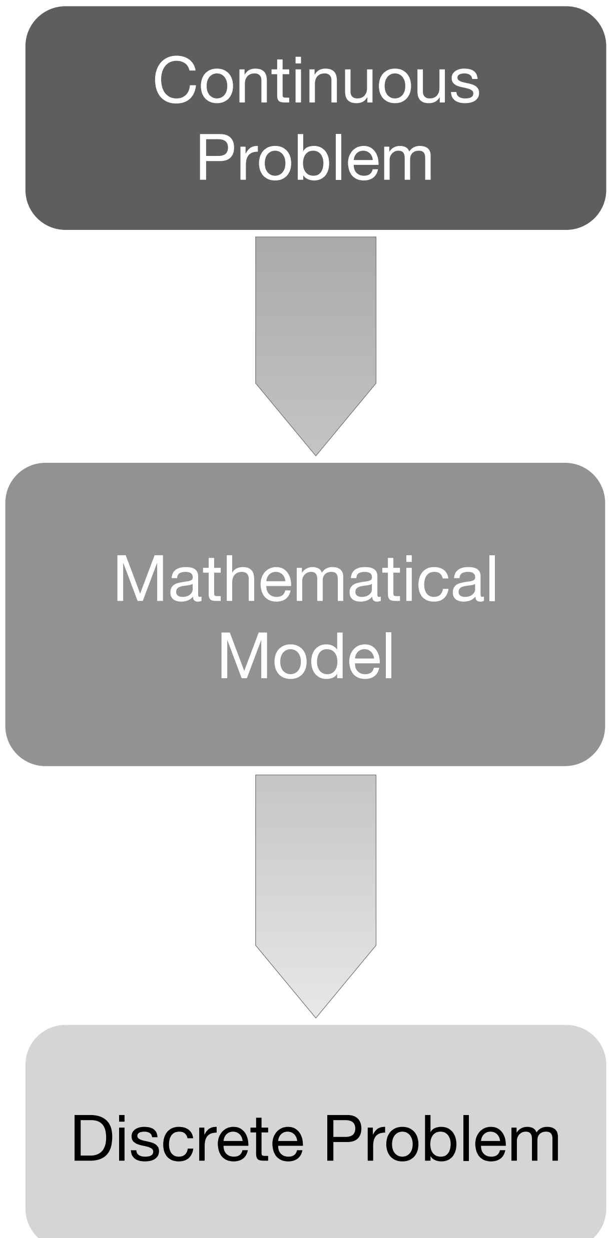
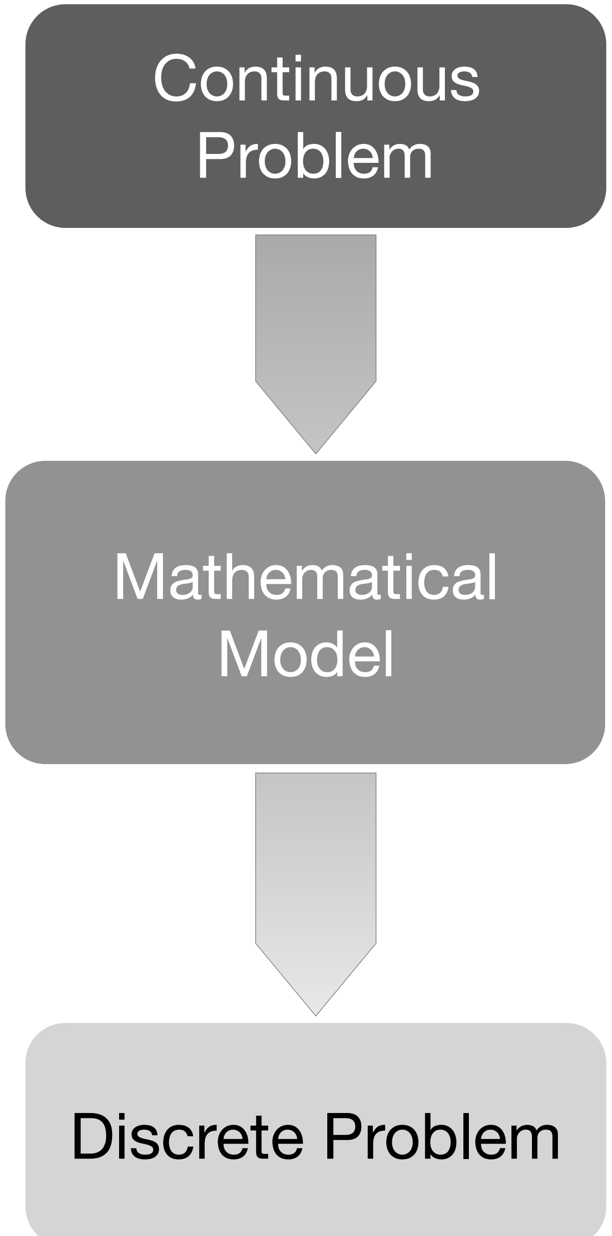
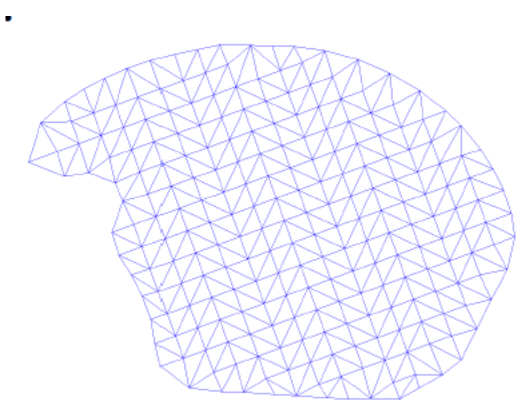
Mathematical Modelling



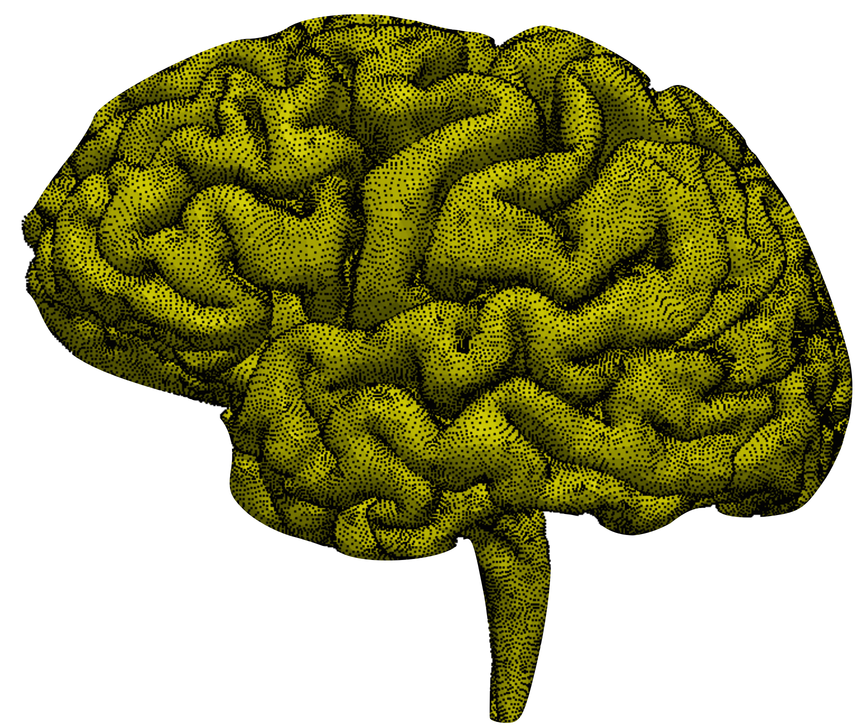
Mathematical Modelling





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

↓

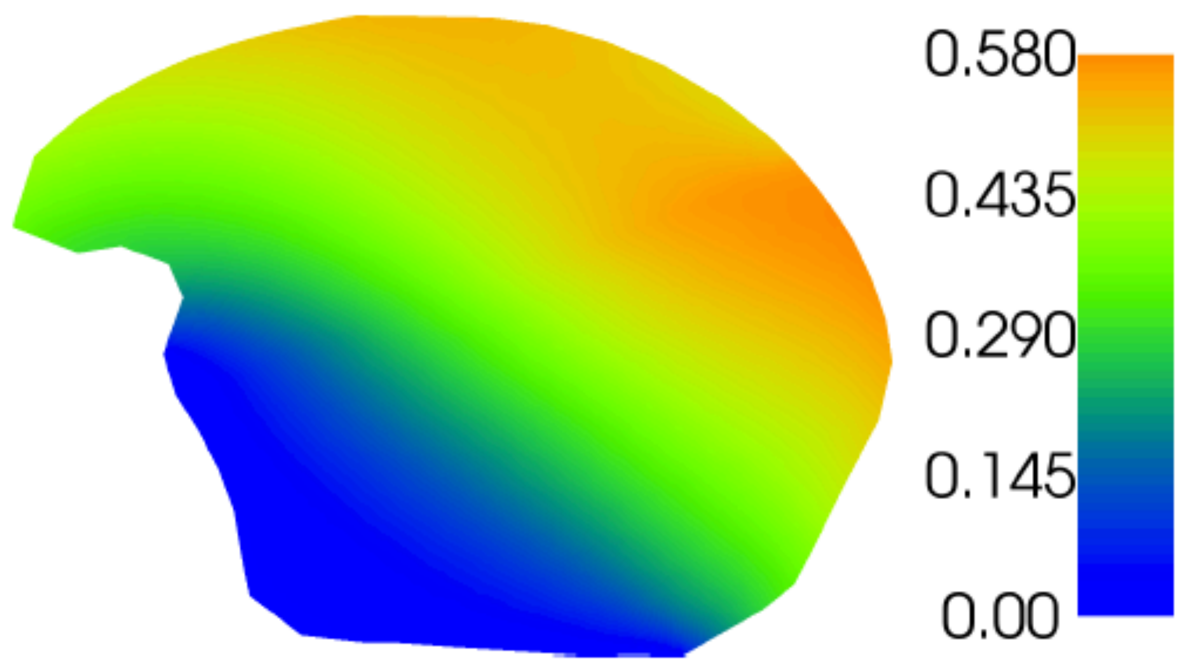
Mathematical Model

↓

Discrete Problem

↓

Numerical Solution



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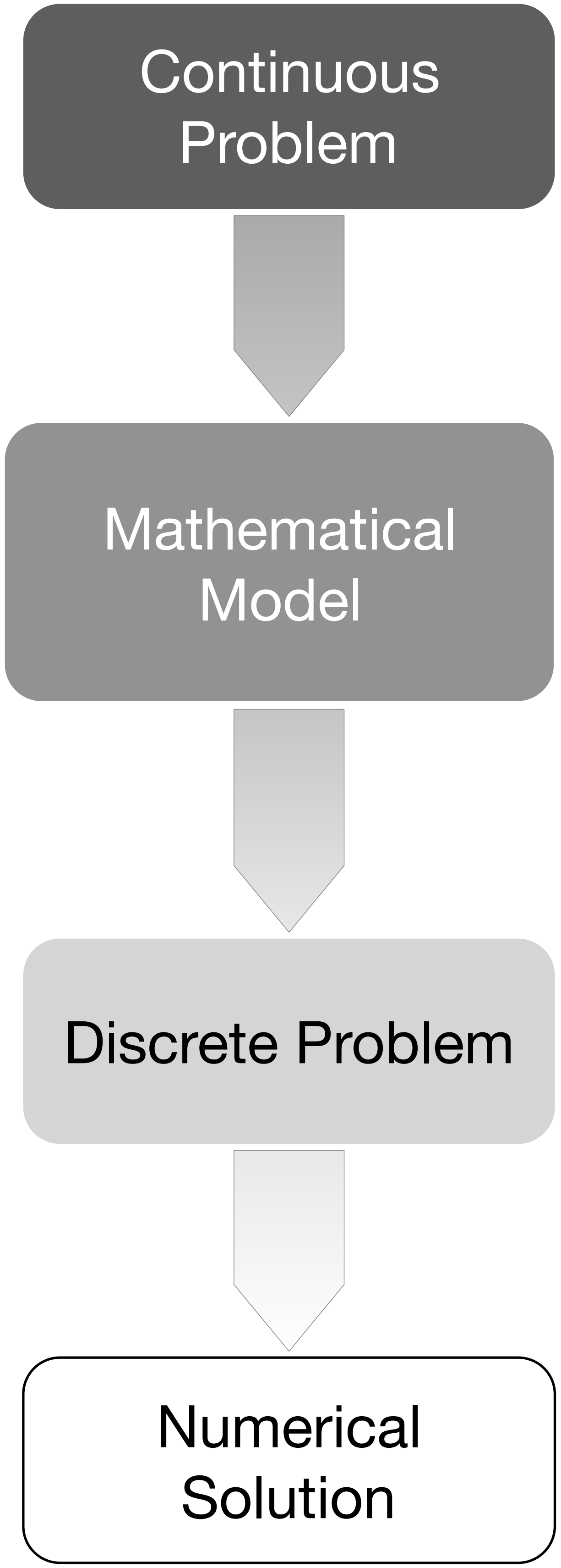
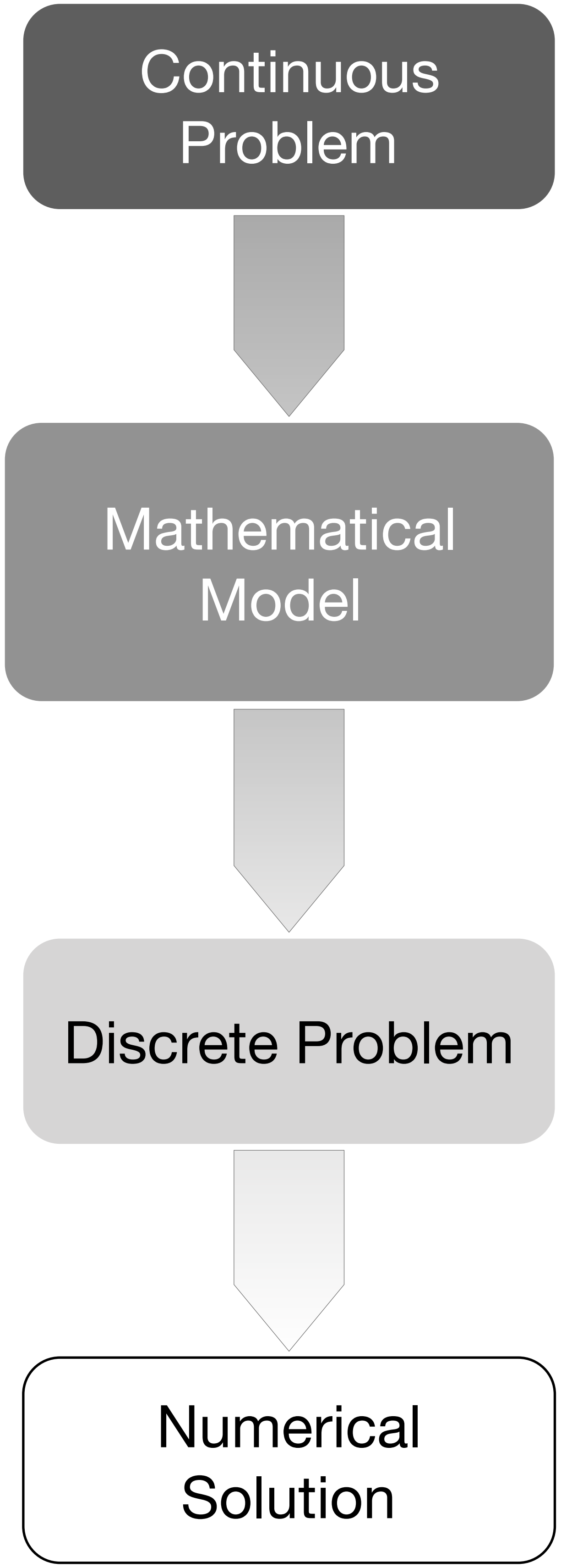
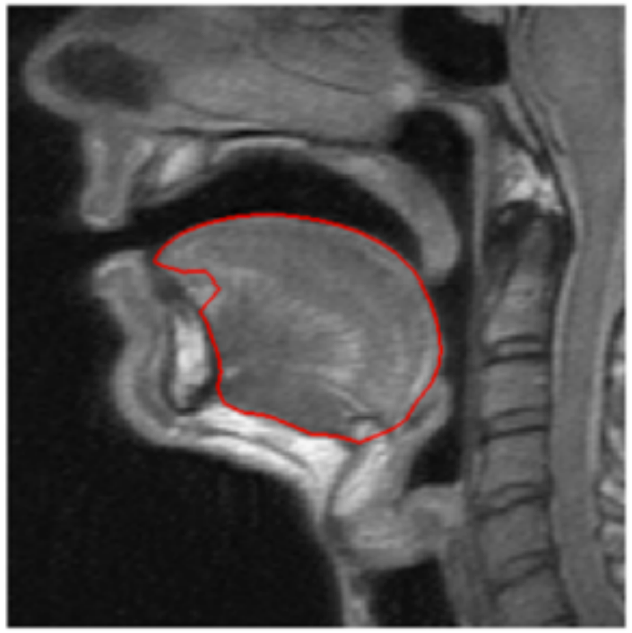
Mathematical Modelling



Mathematical Modelling





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

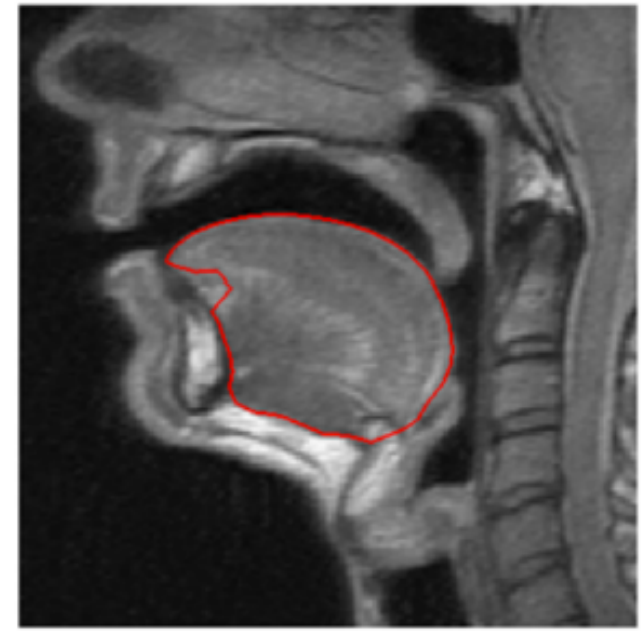
Continuous Problem

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

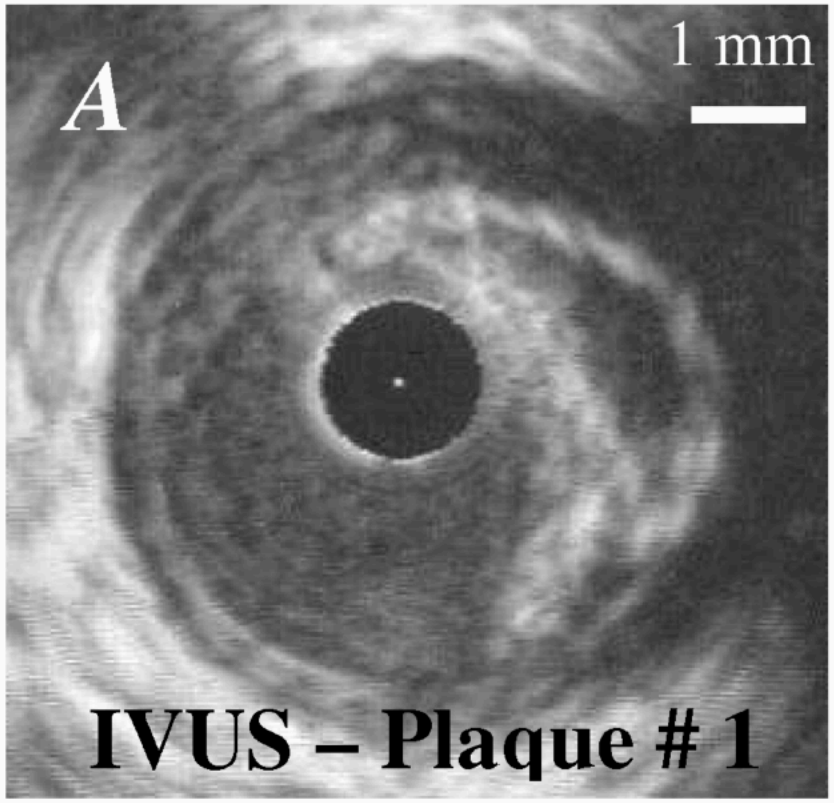
Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error



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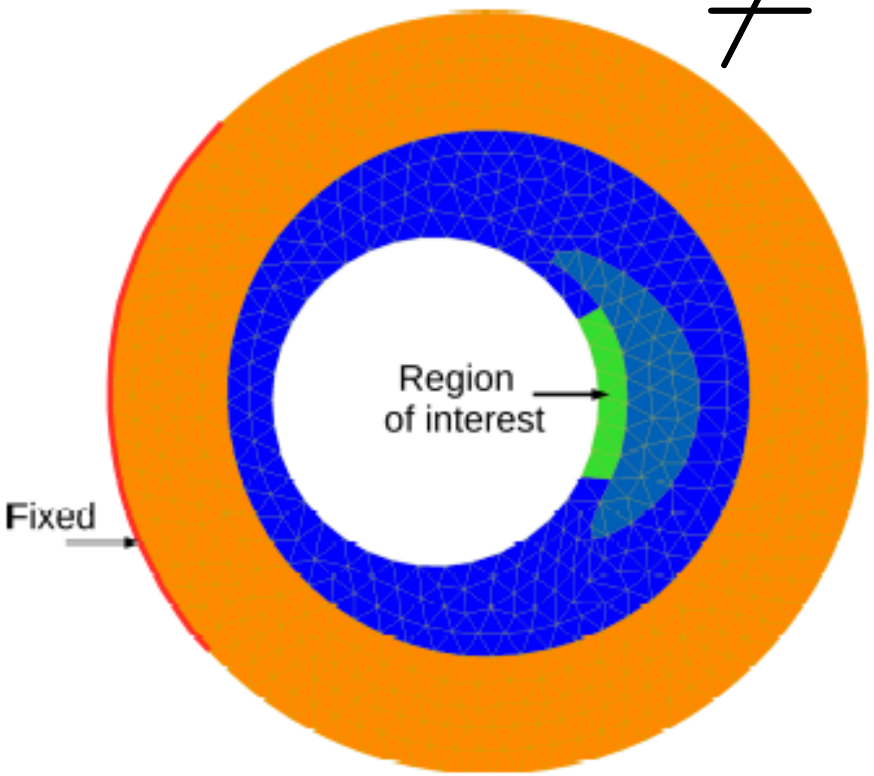

Geometry
Boundary conditions

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Mathematical Modelling

Continuous Problem

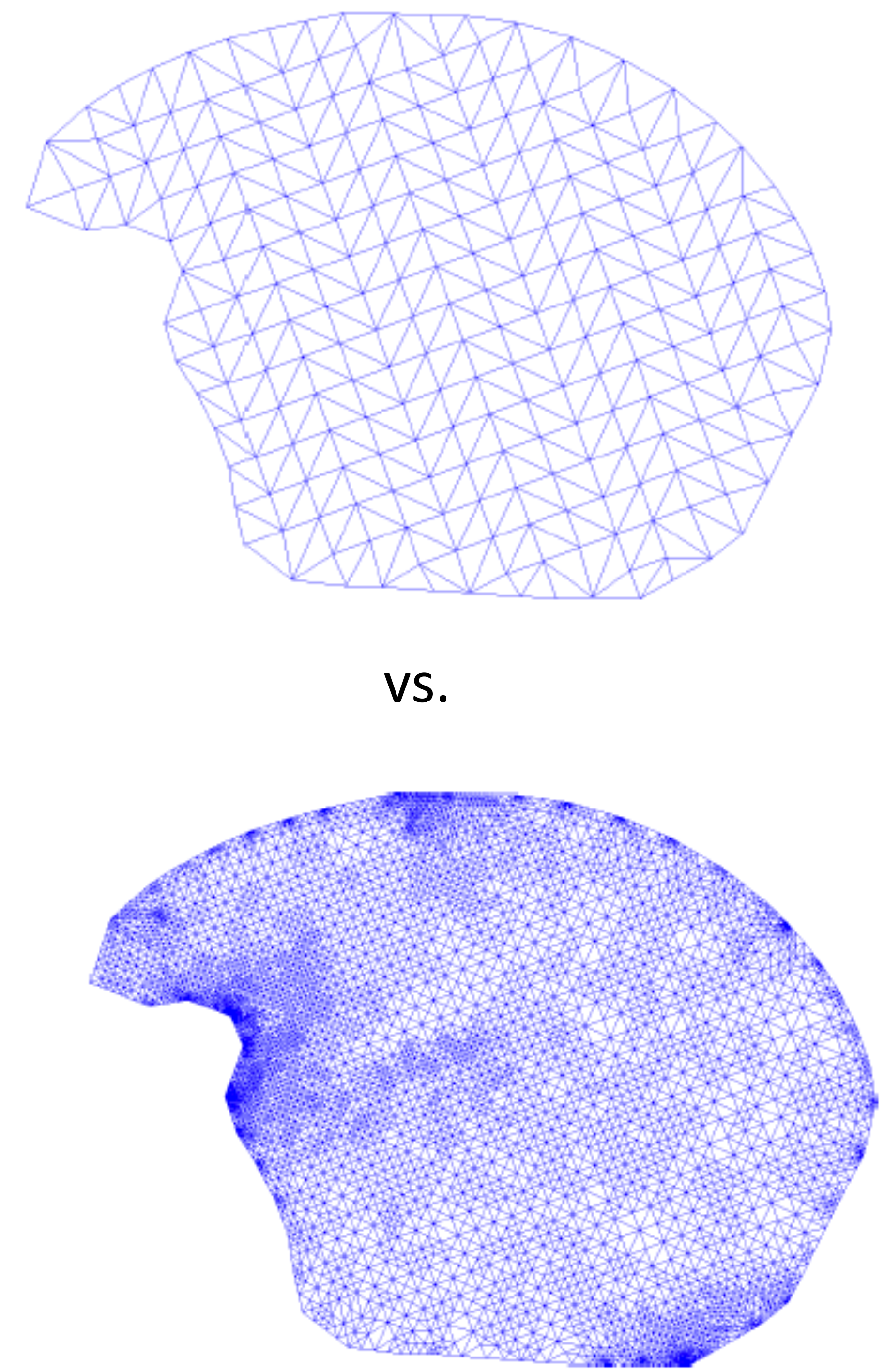
Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Discretization Error



Mathematical Modelling

Continuous Problem

↓

Mathematical Model

↓

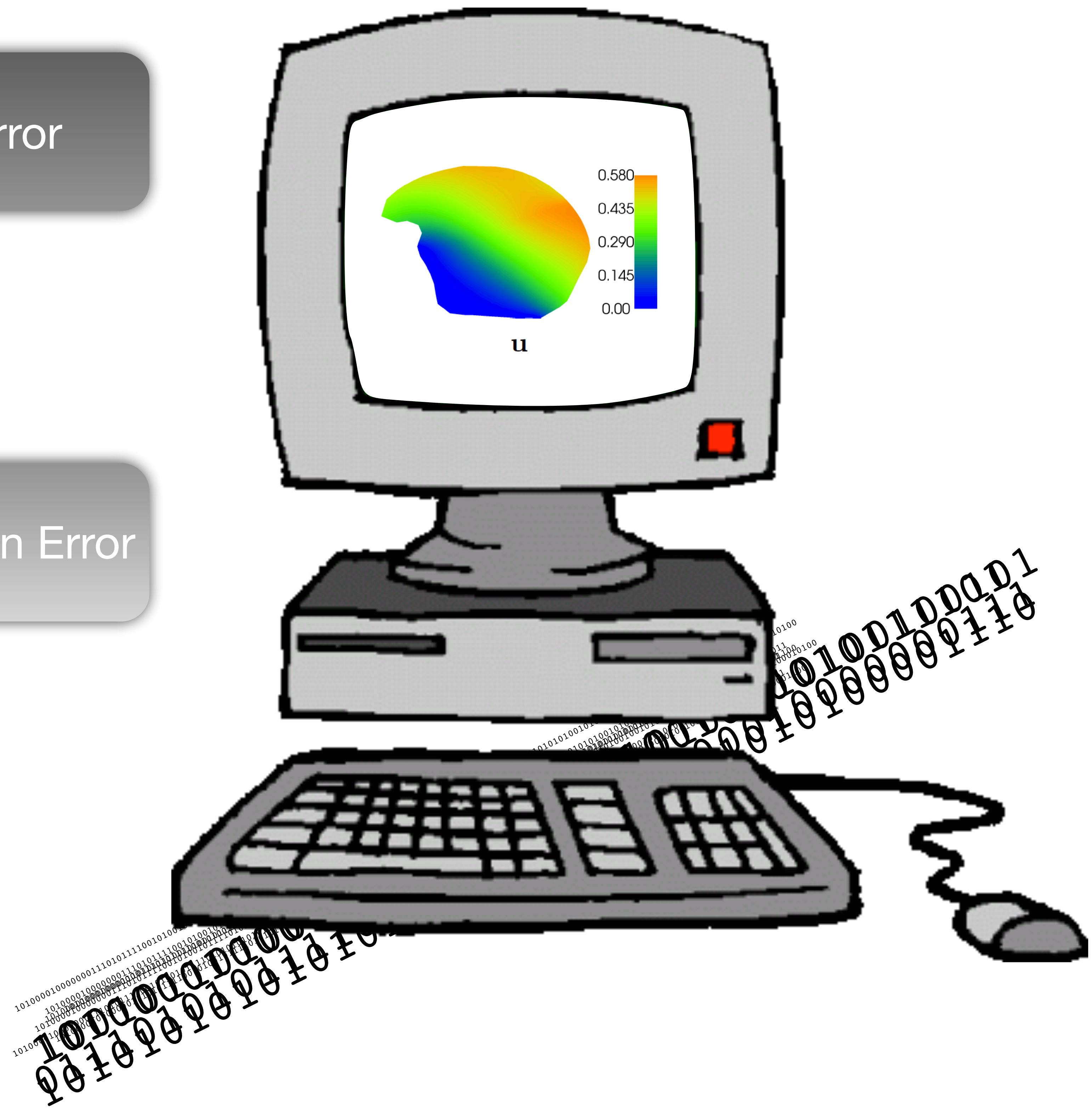
Discrete Problem

↓

Numerical Solution

Model Error

Discretization Error



Mathematical Modelling

Continuous Problem

Mathematical Model

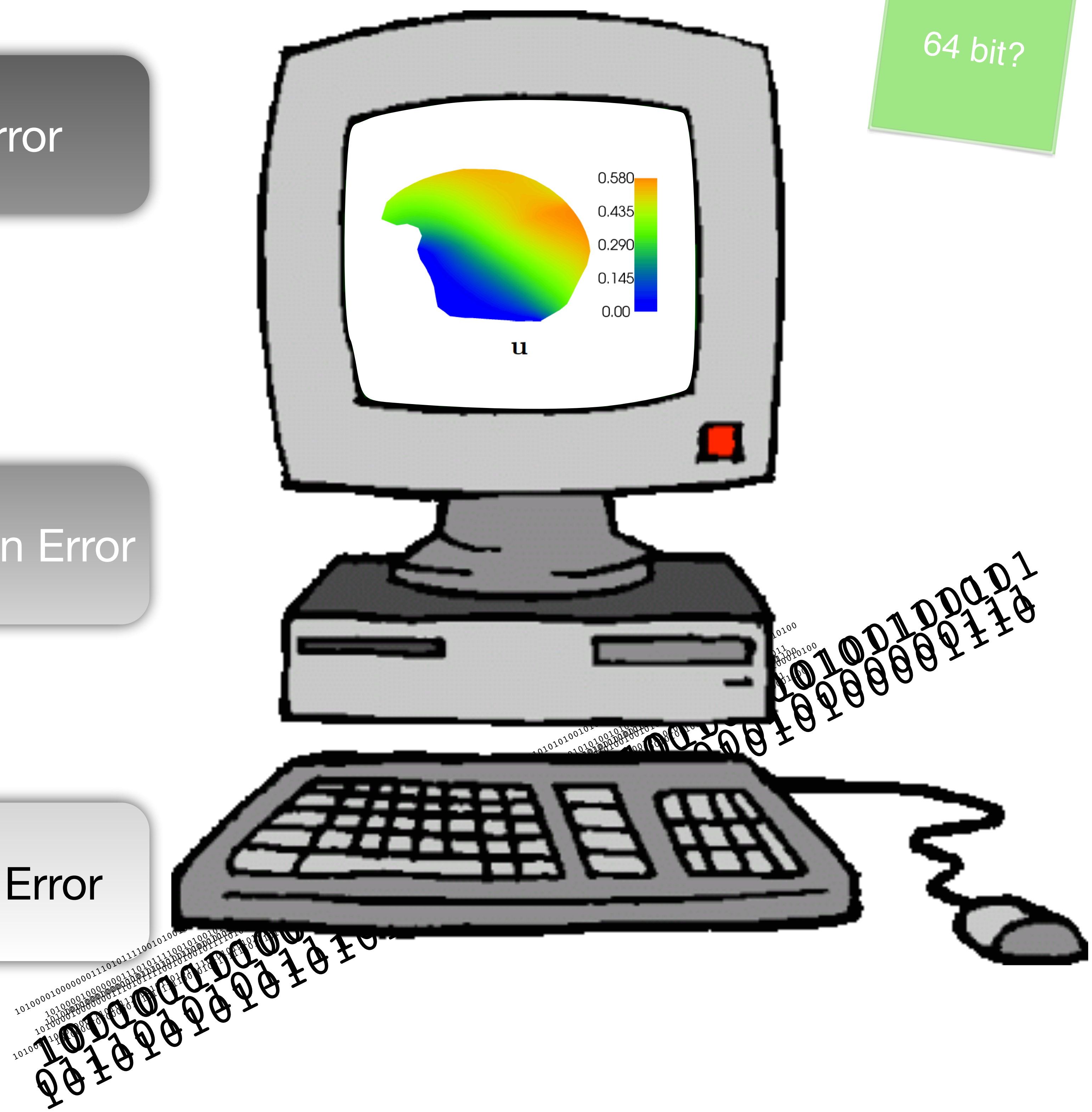
Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error



32 bit?

64 bit?

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Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

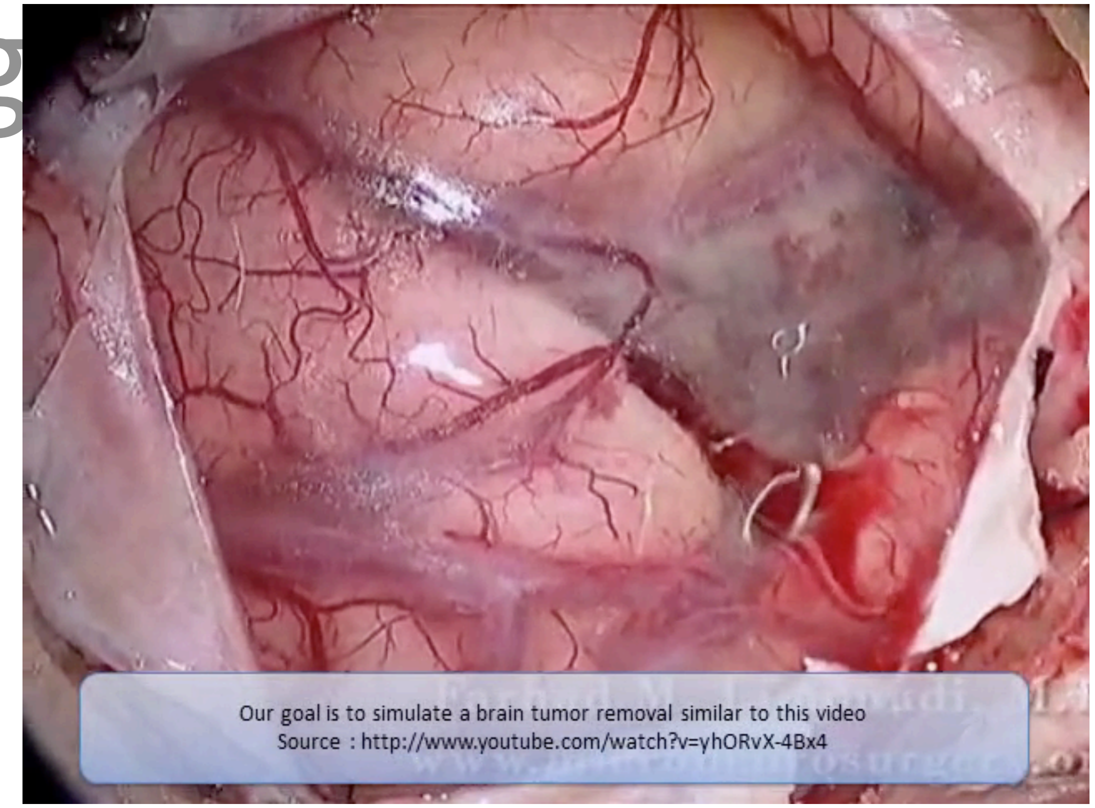
Numerical Solution

Model Error

Discretization Error

Numerical Error

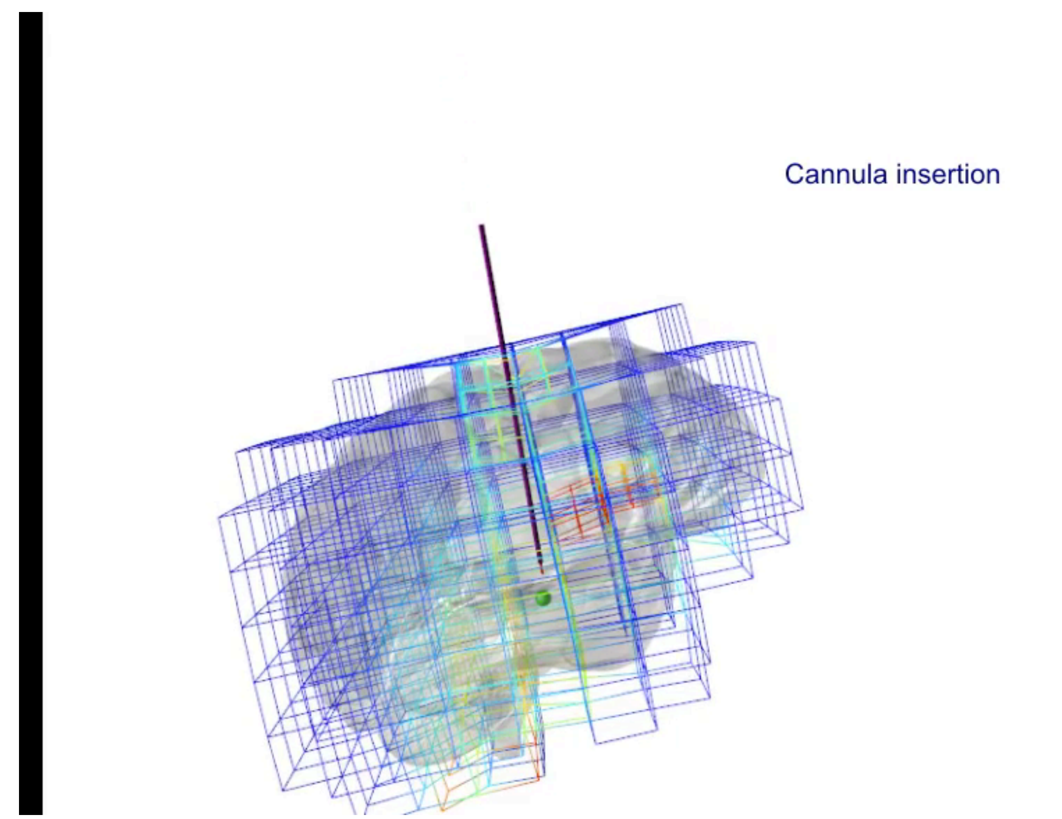
Total Error



Reality

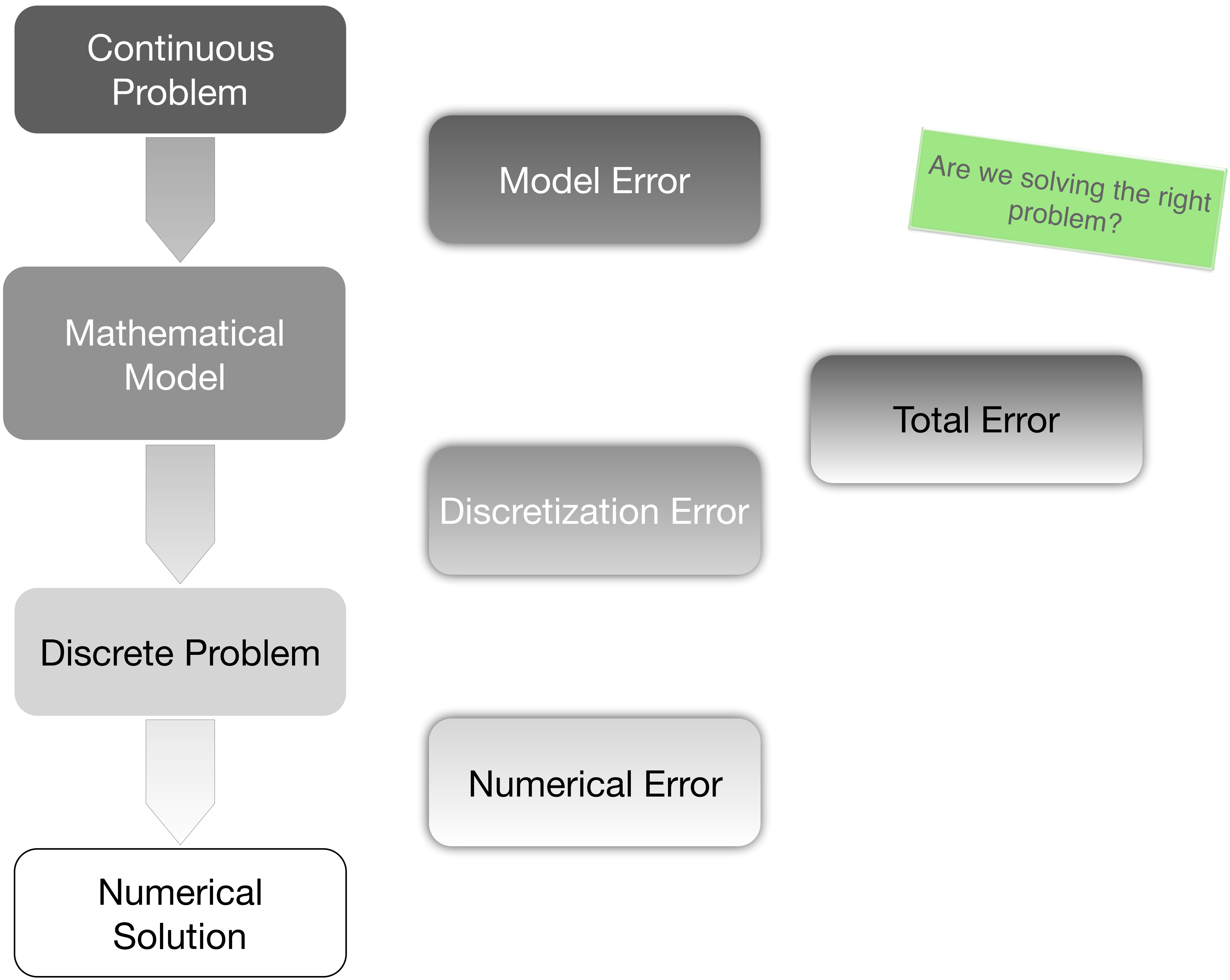
vs.

Simulation

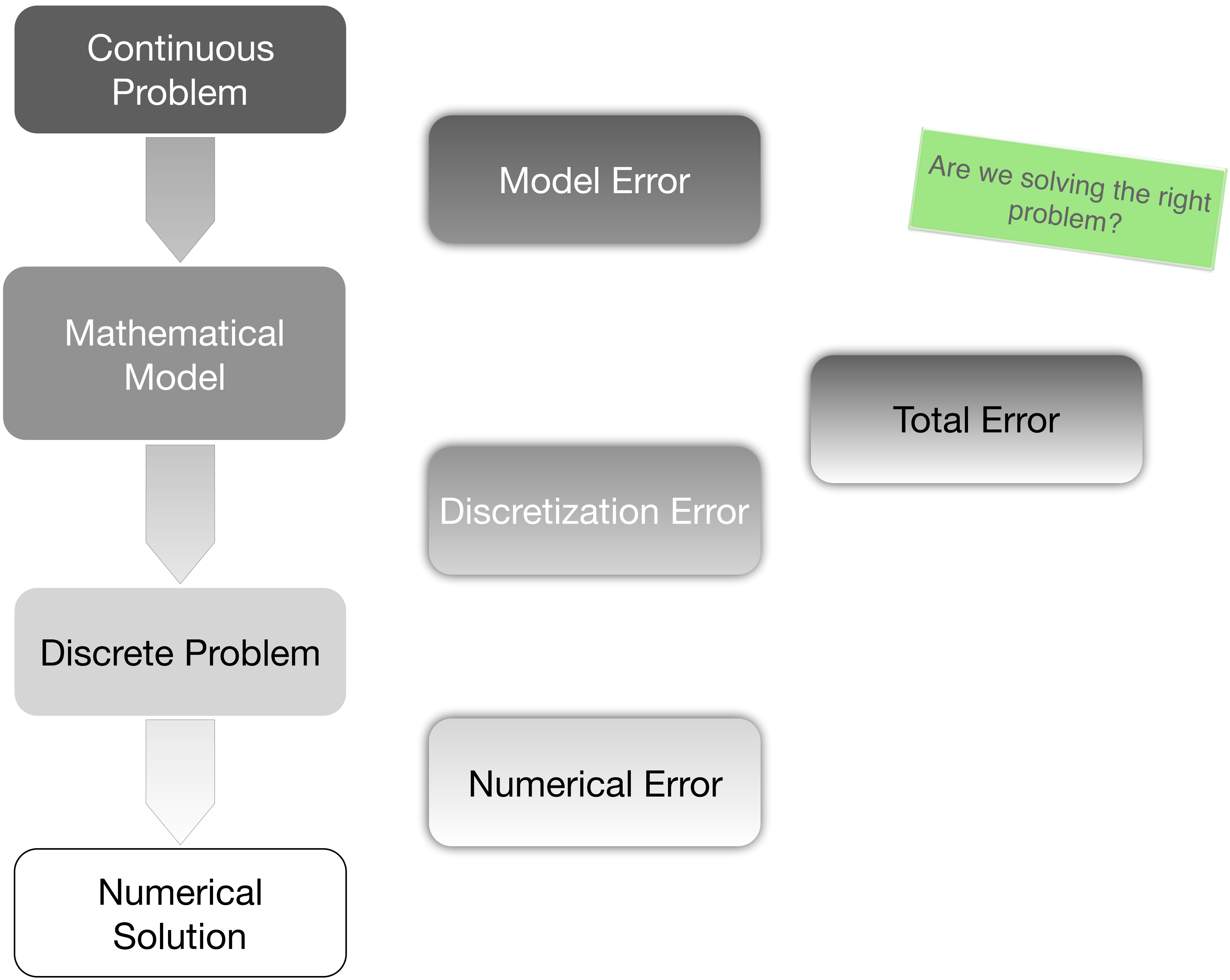


RealTCut

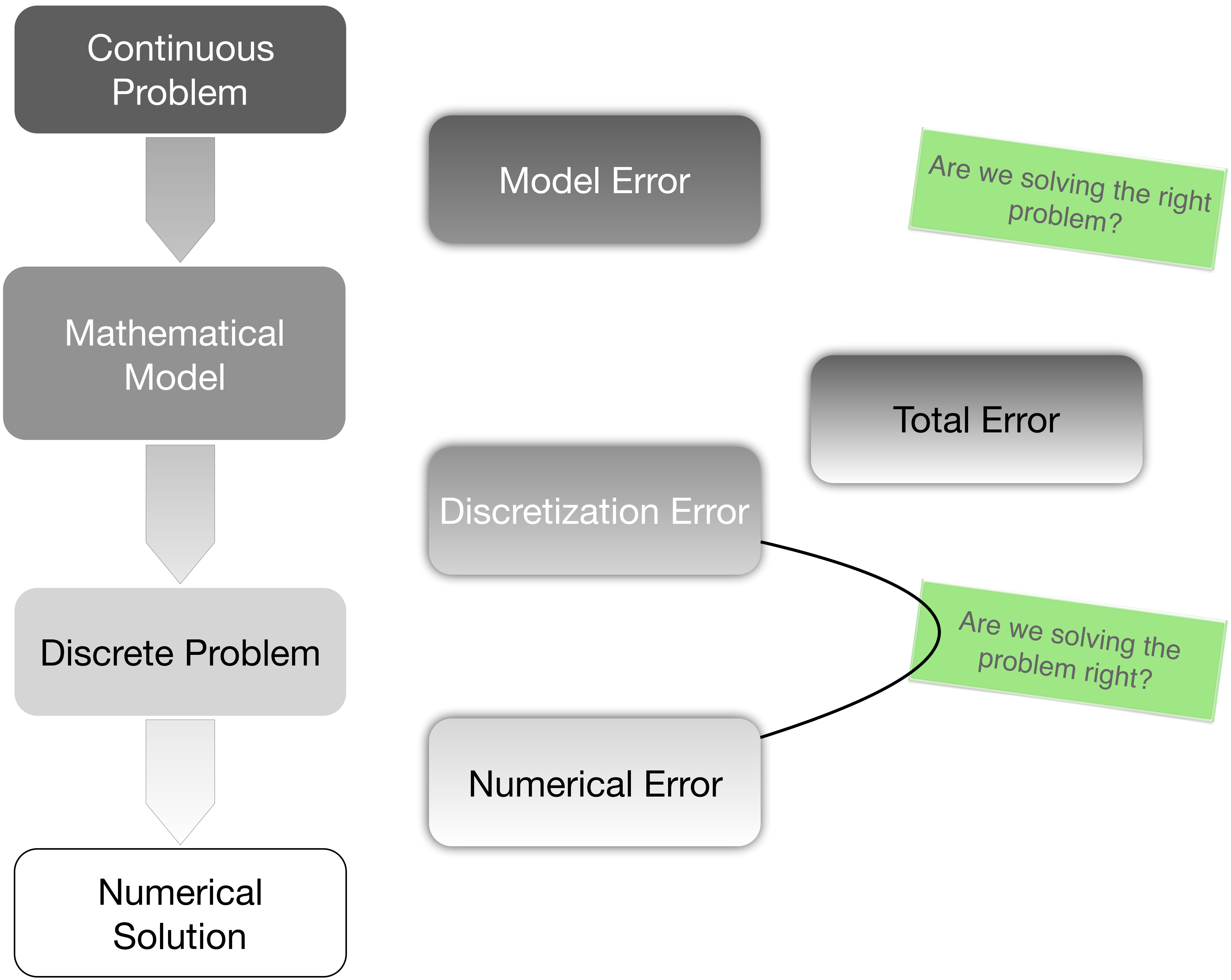
Mathematical Modelling



Mathematical Modelling



Mathematical Modelling



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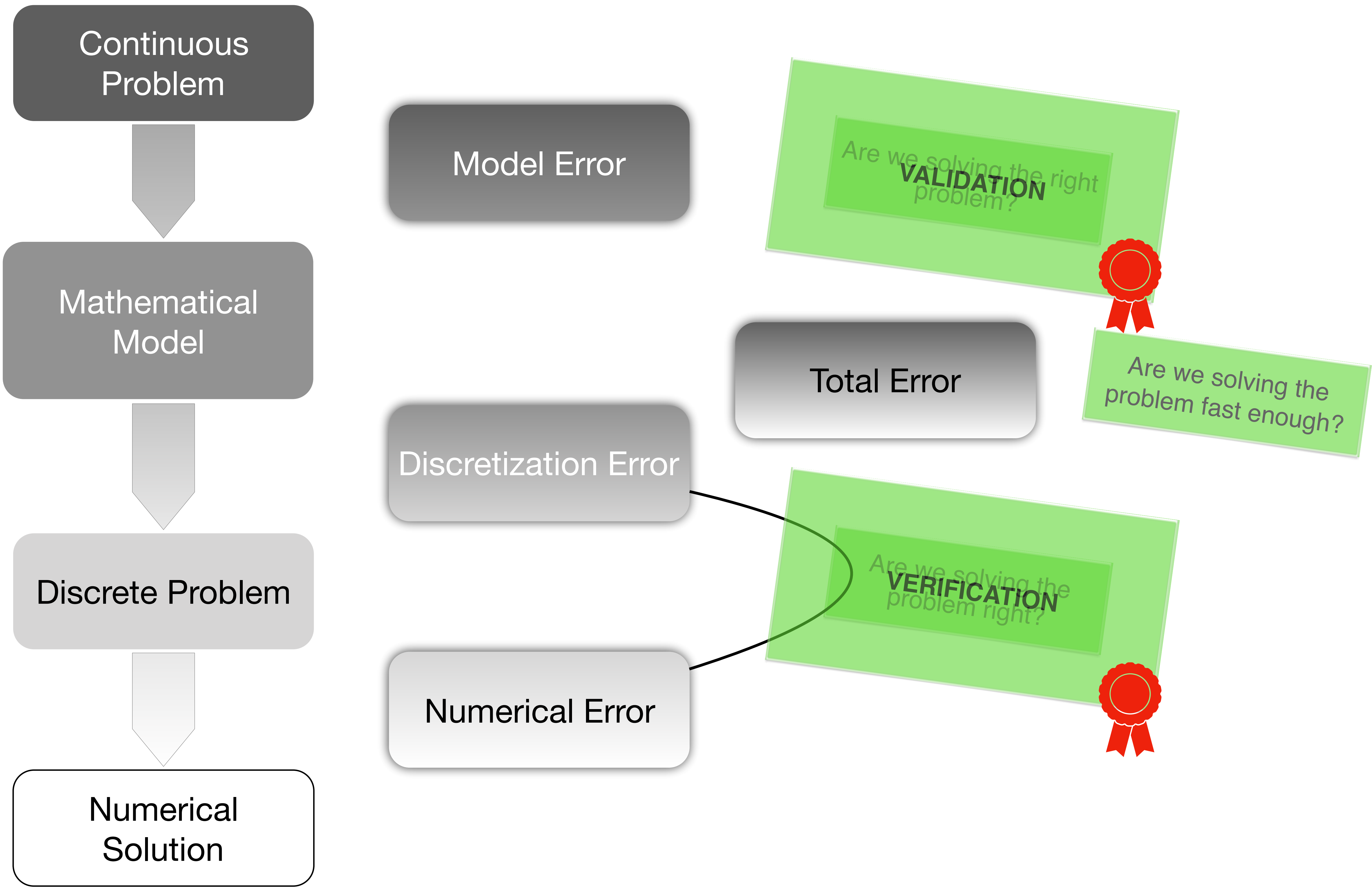
Mathematical Modelling



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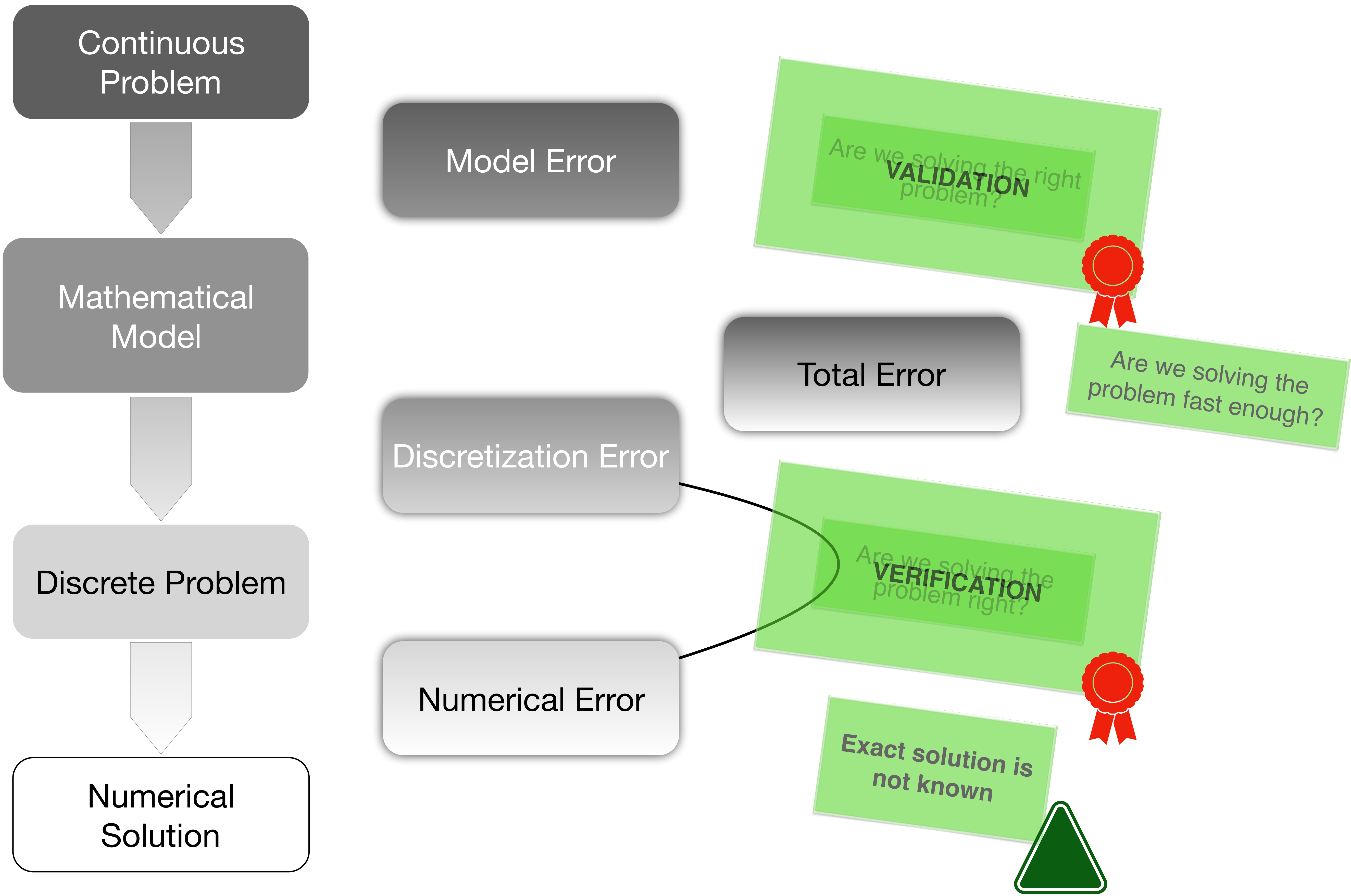
Mathematical Modelling



Outline

A focus on equation-based models

- How can we control the quality of simulations, verification and validation?
- Why are set-in-stone-models limited?
- How can we leverage statistical models to improve our models?

Outline

- **Data-driven modelling: Beyond setting models in stone**
  - Data assimilation
    - How can we learn from observations “on-the-fly”.
    - The power of digital twins.
- **Future challenges**

Introduction to data assimilation

- Bayesian inference
- Kalman filtering

Model and parameter identification through Bayesian inference in solid mechanics

Hussein Rappel

h.rappel@gmail.com

September 07, 2018

UNIVERSITÉ DU LUXEMBOURG

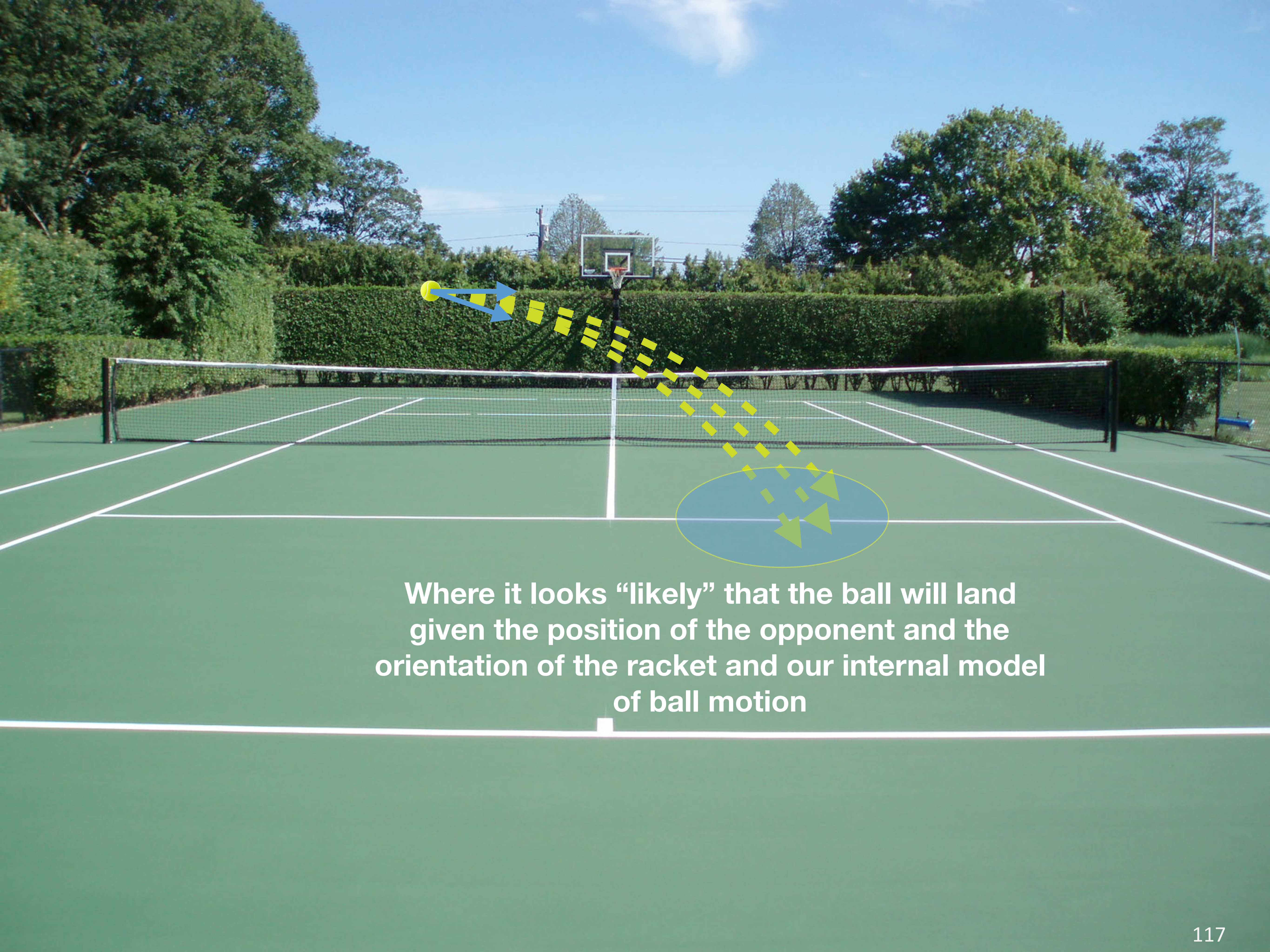
Université de Liège

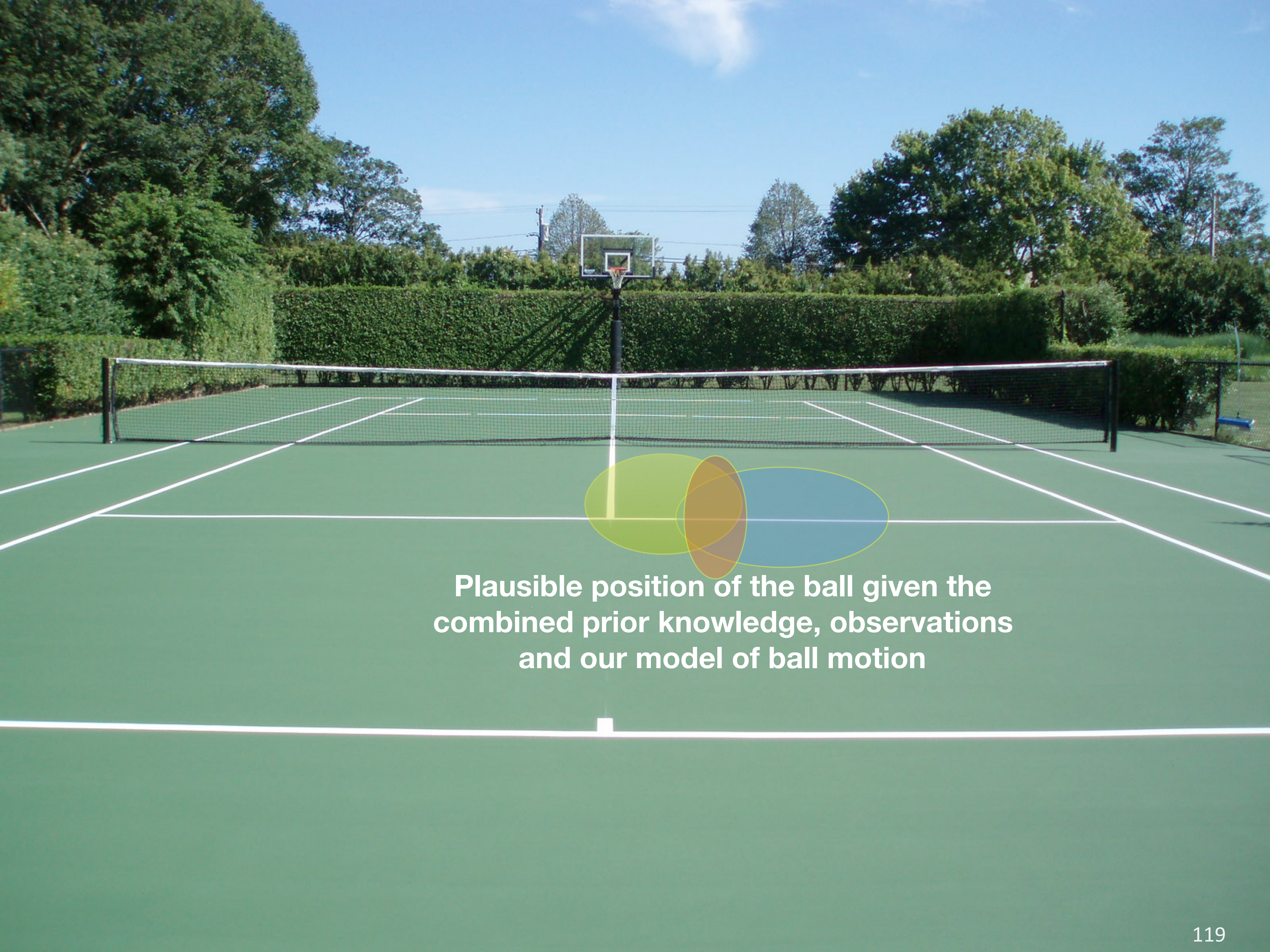
Bayesian inference

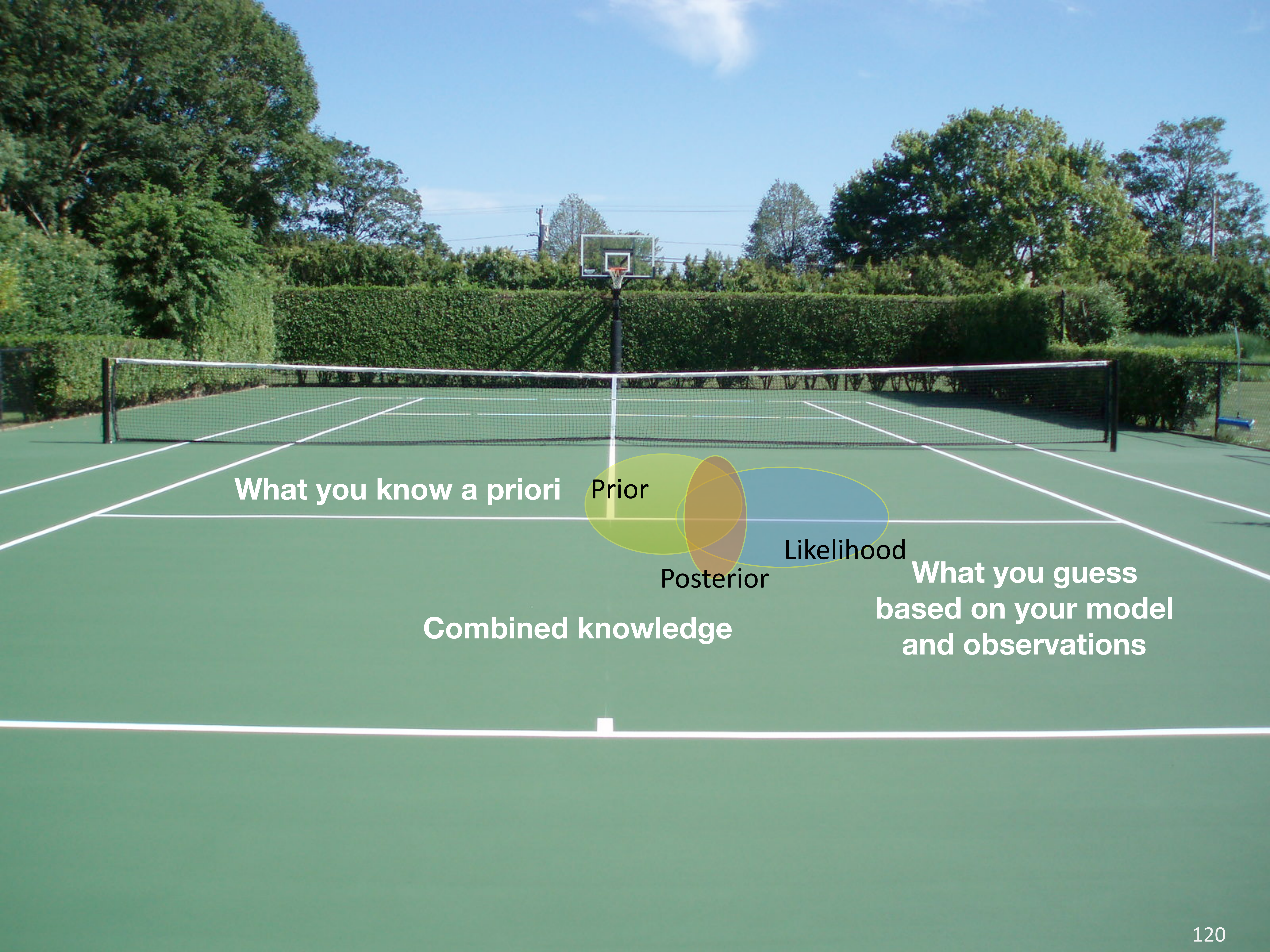
Primer

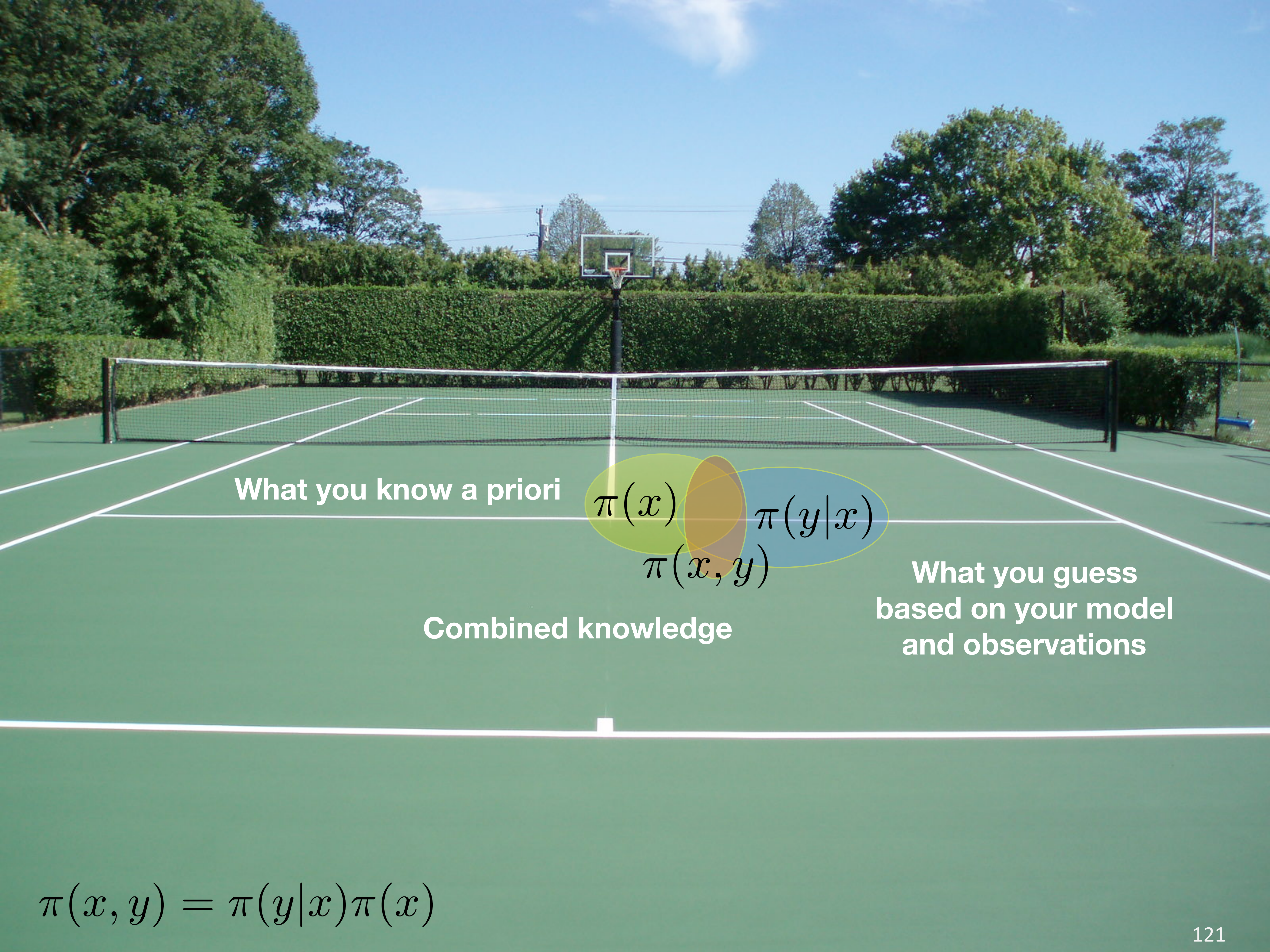

Where the ball “usually” lands
based on experience


Where the ball "usually" lands
based on experience


Where it looks "likely" that the ball will land
given the position of the opponent and the
orientation of the racket and our internal model
of ball motion

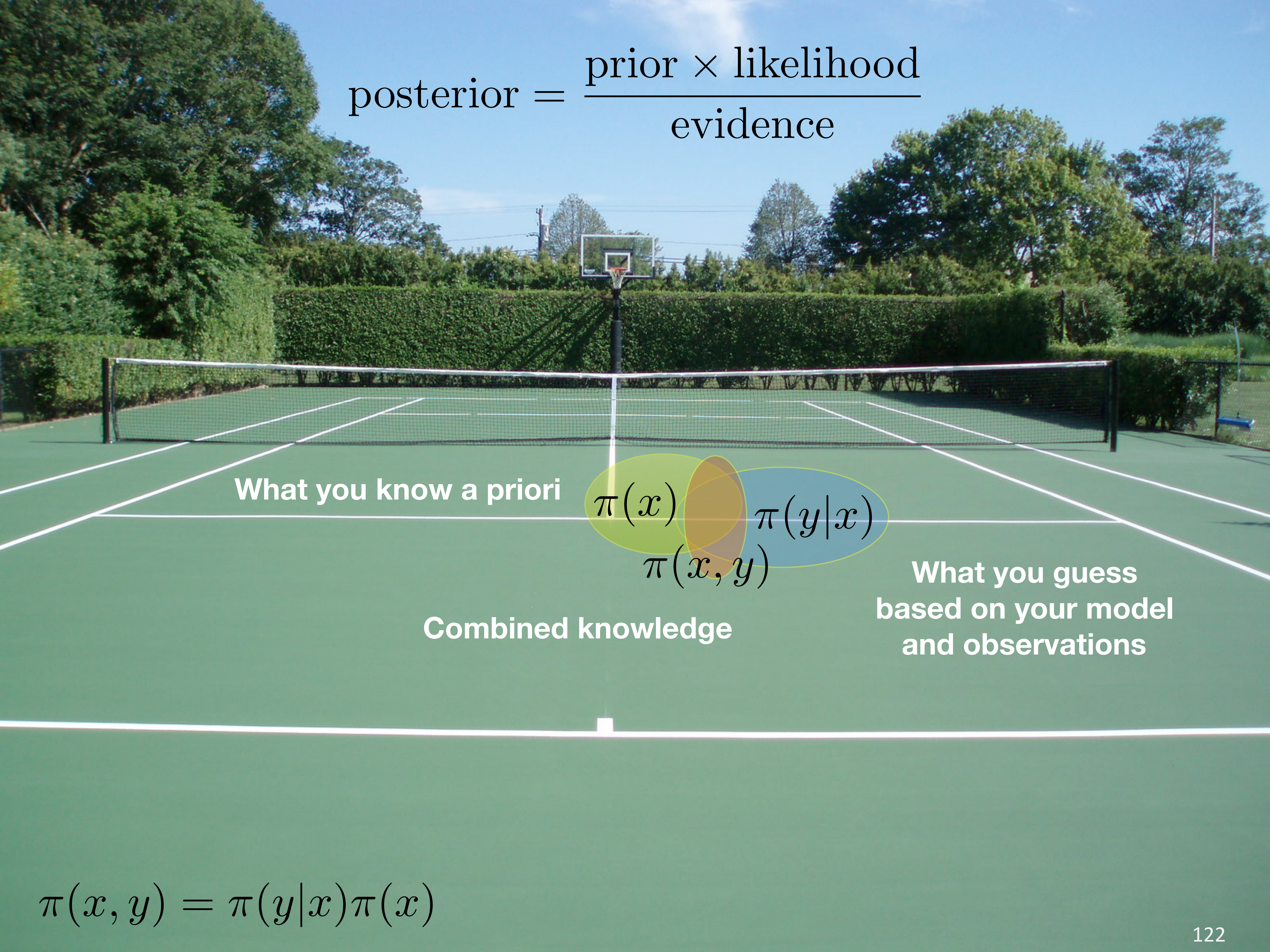

Plausible position of the ball given the
combined prior knowledge, observations
and our model of ball motion


What you know a priori
Prior
Likelihood
Posterior
What you guess based on your model and observations
Combined knowledge



$$\pi(x, y) = \pi(y|x)\pi(x)$$

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

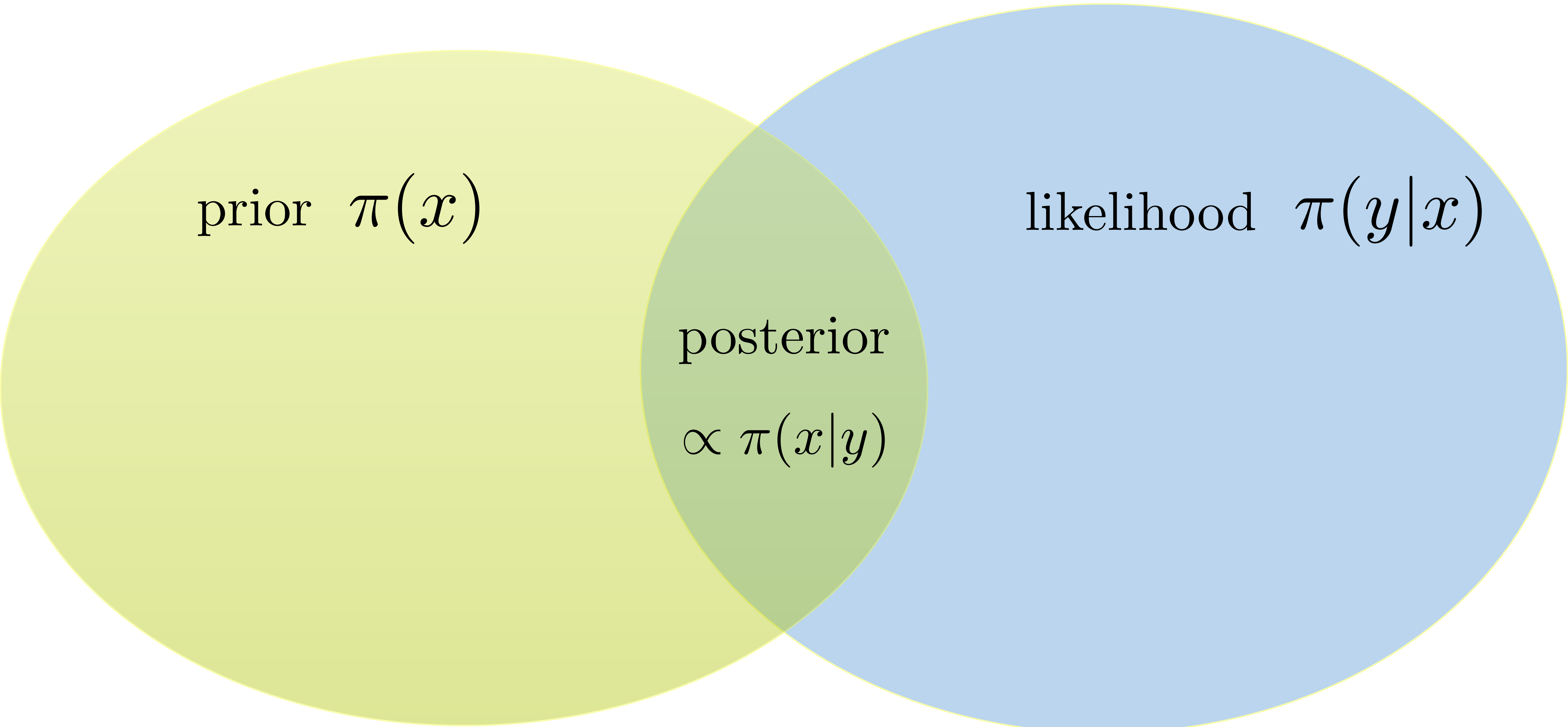


$$\pi(x, y) = \pi(y|x)\pi(x)$$

Bayes' theorem

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$



Parameter identification: Bayesian approach

Bayes' theorem

$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

$\pi(.)$: probability distribution function

$\pi(.|.)$: conditional probability distribution function

x : material parameter

y : observations

Parameter identification: Bayesian approach

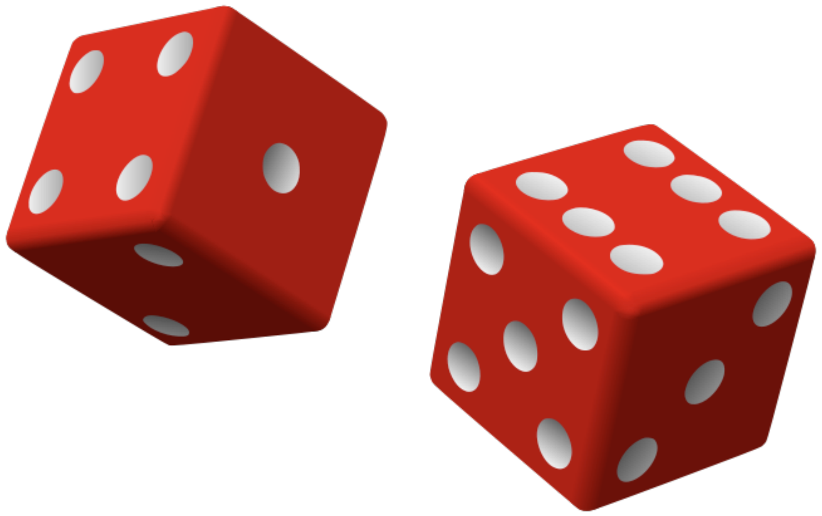
Bayes' theorem

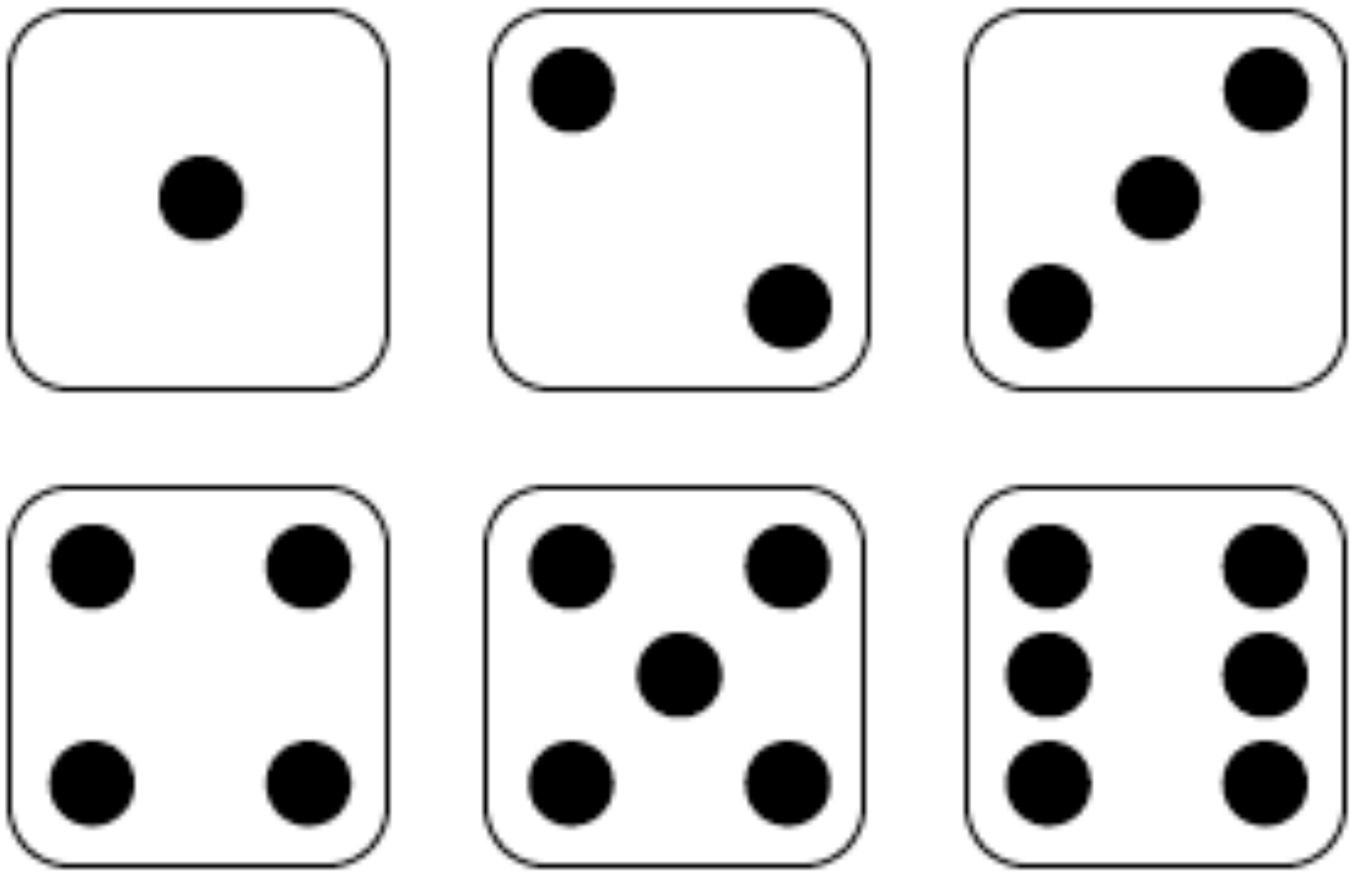
$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

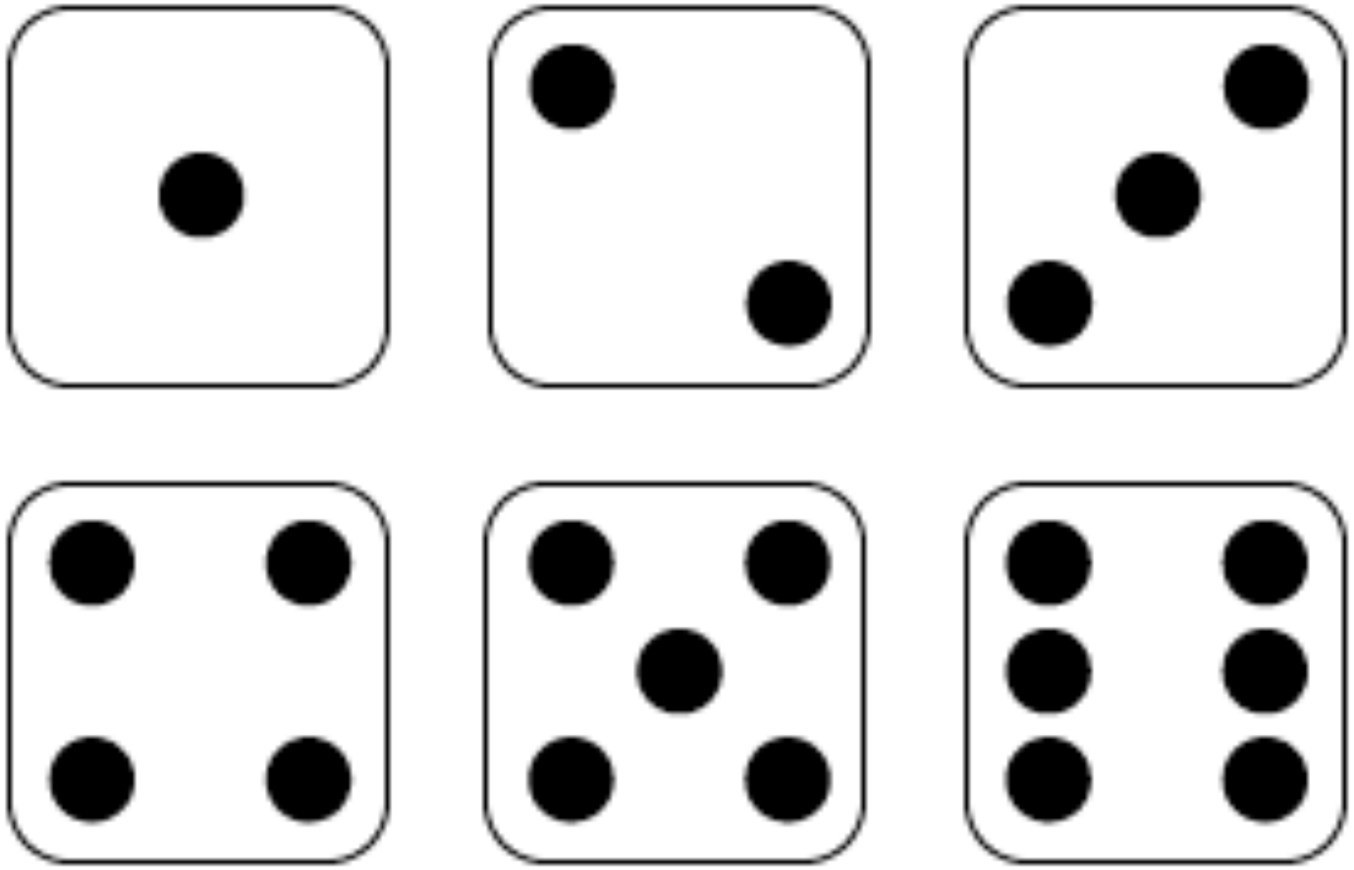
Descriptive formula

$$\text{Posterior} = \frac{\text{Prior} \times \text{Likelihood}}{\text{Evidence}}$$

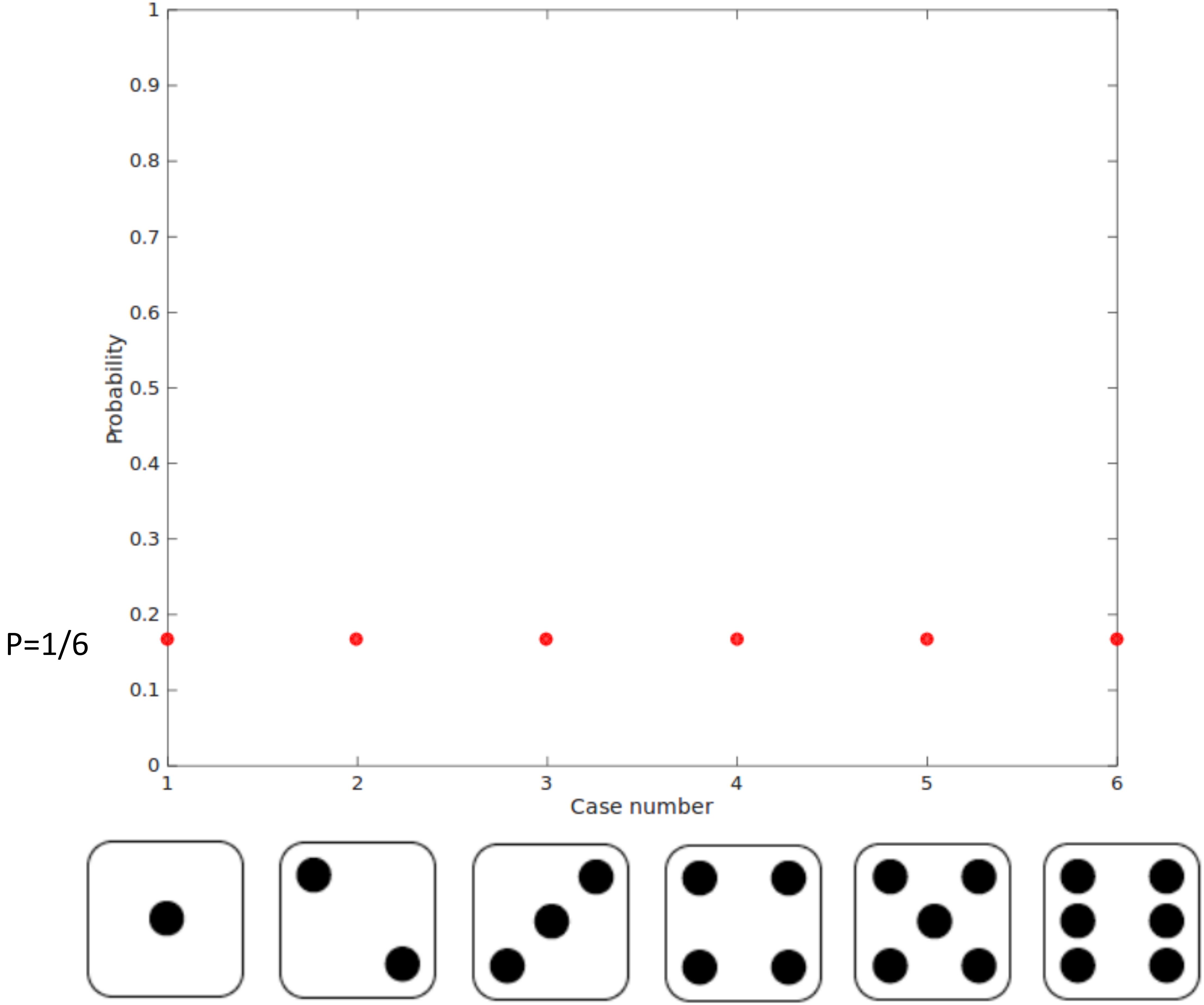
A discrete example of Bayes' theorem







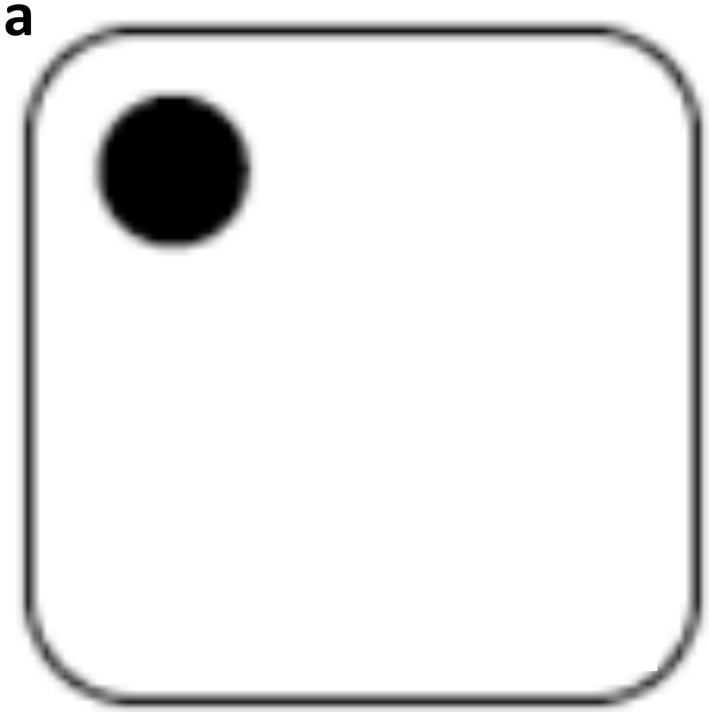
This is our prior information for the probability of each face: 1/6

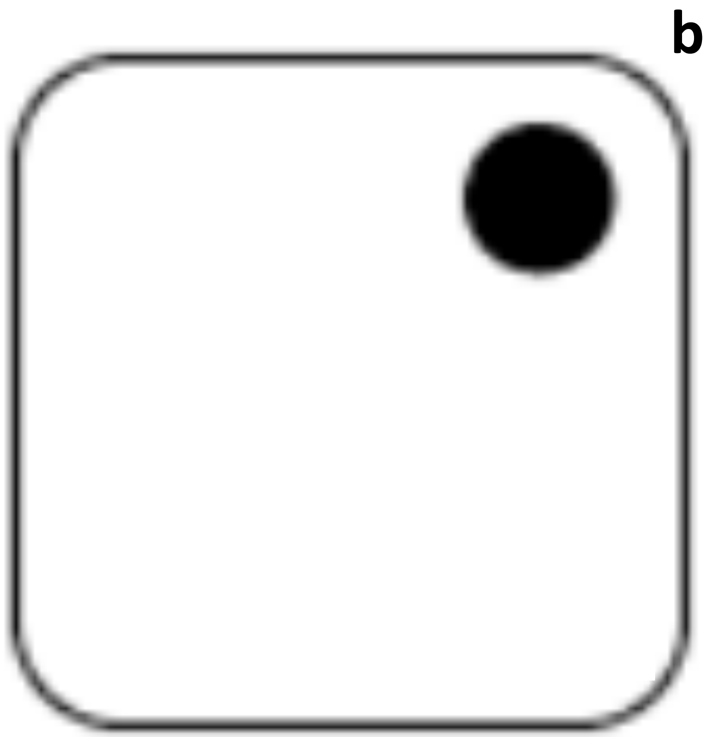

P=1/6
Probability
Case number
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1
2
3
4
5
6

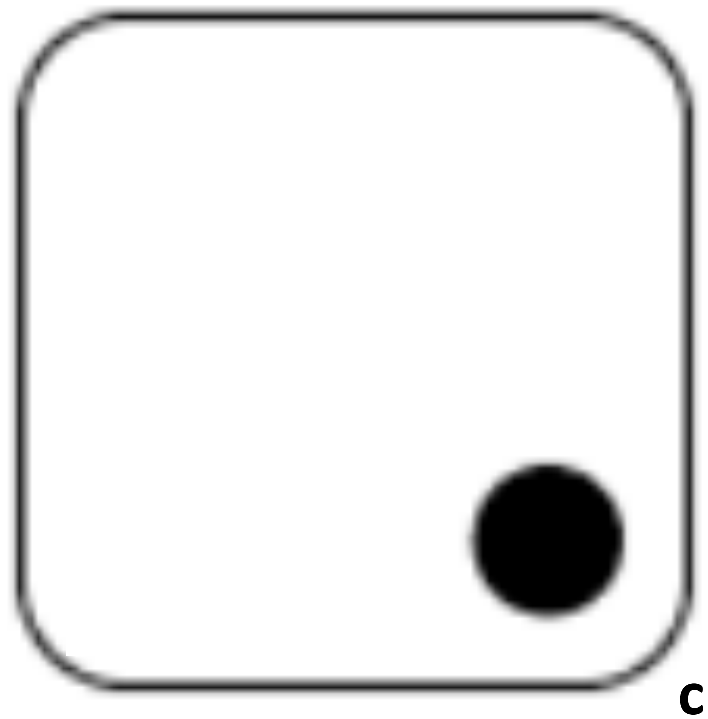
Assume that after throwing the dice, you see the above evidence

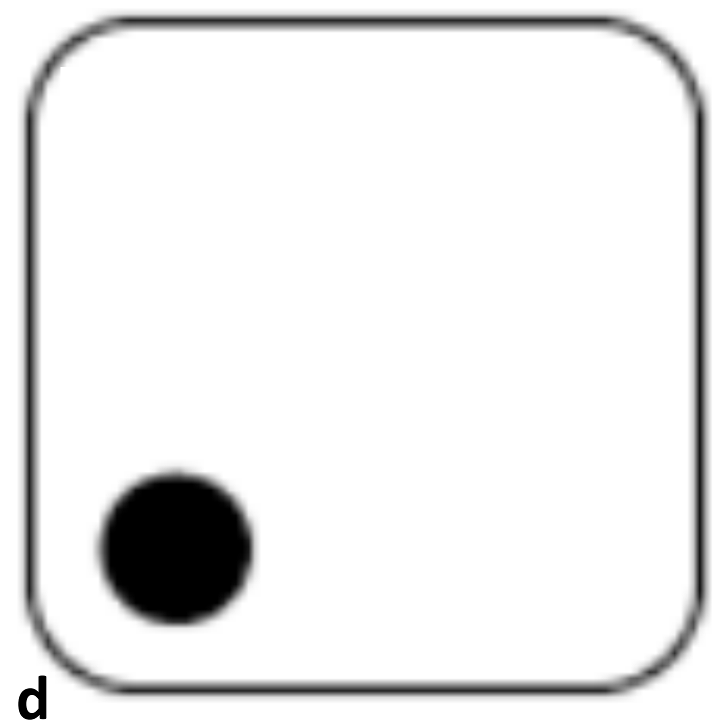
Goal: determine the probability of this evidence for each face of the dice

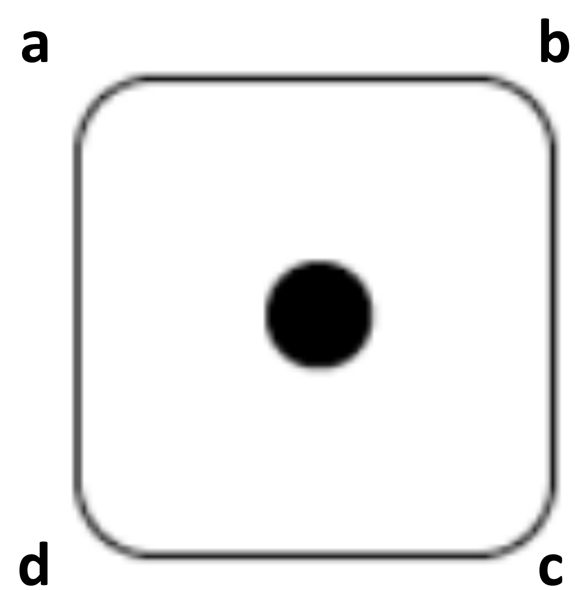
a

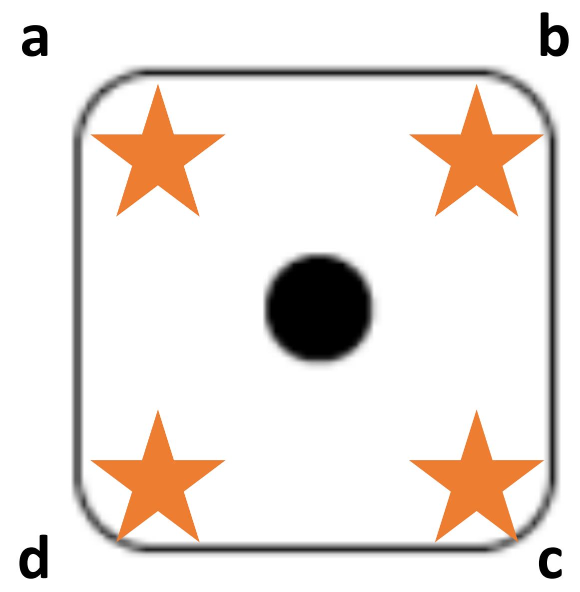


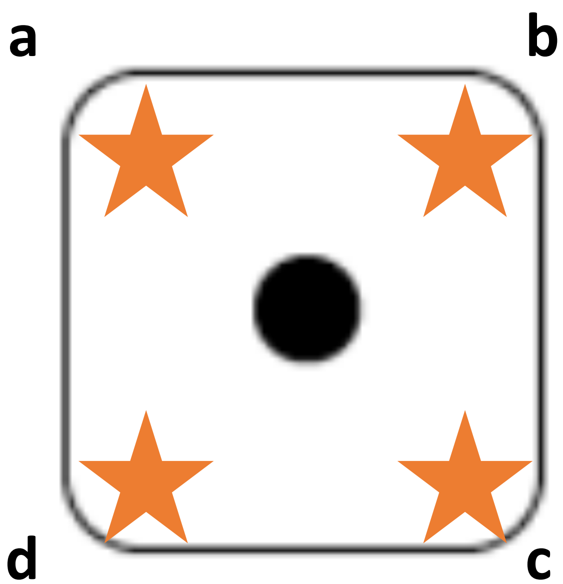

b


c

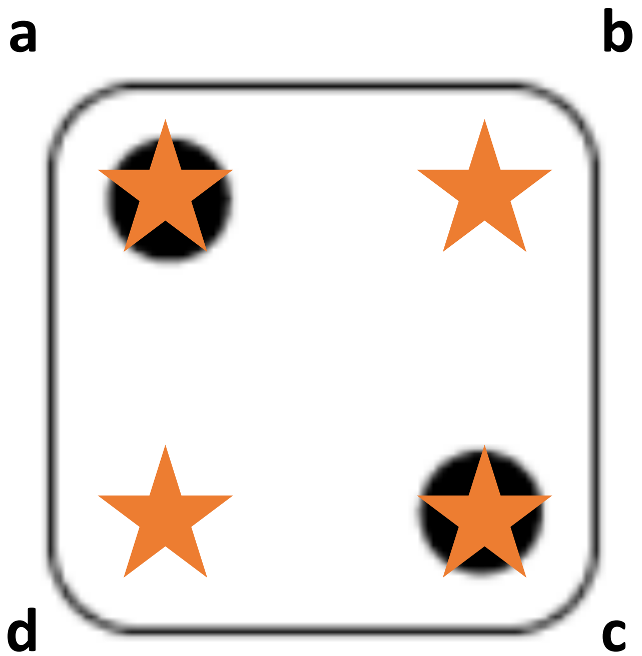

d

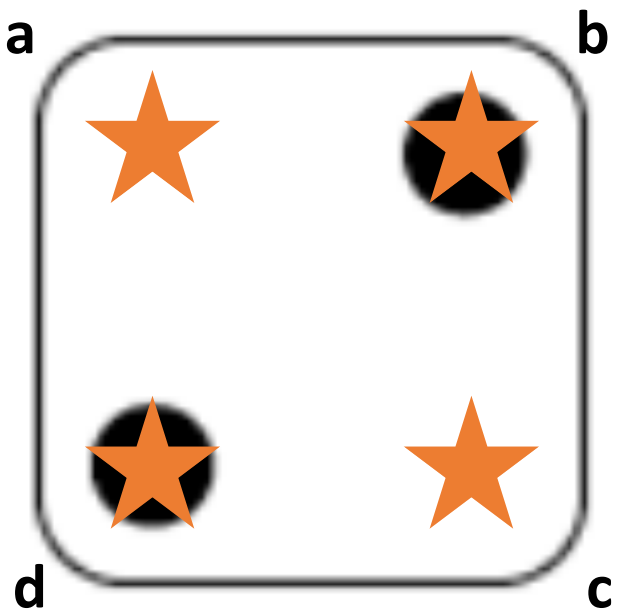

a
b
d
c


a
b
d
c

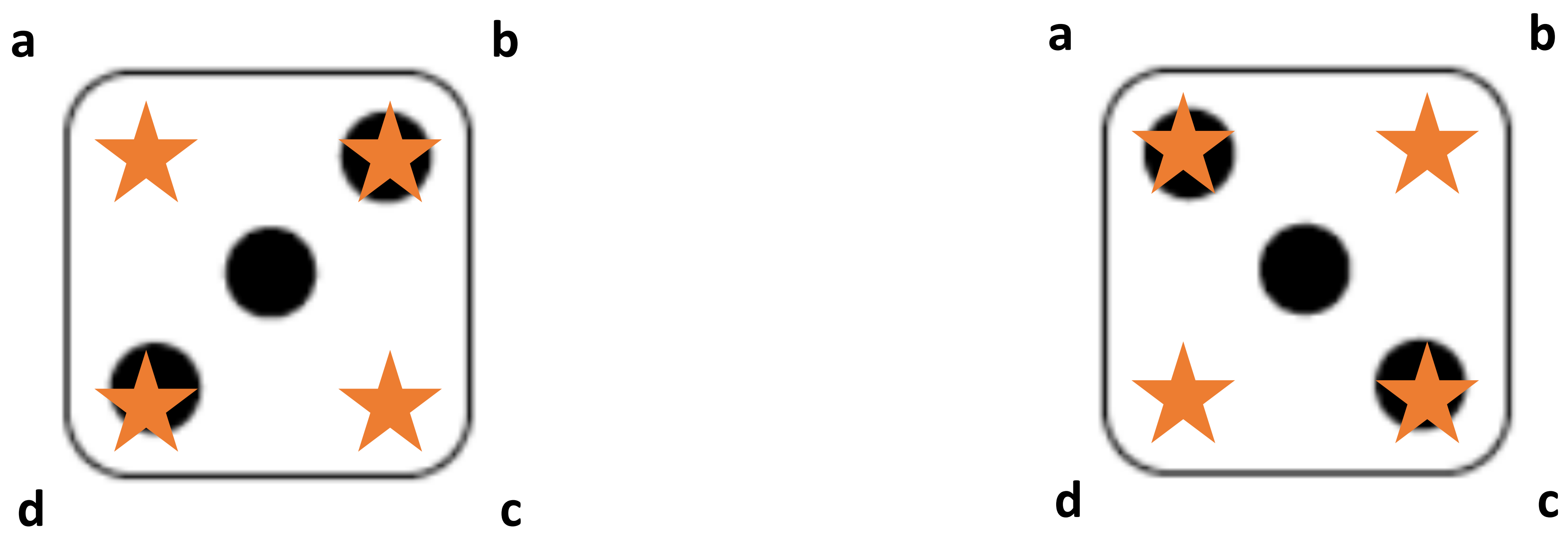


One would never see a dot at the star positions for this face
The probability of the evidence is *zero*

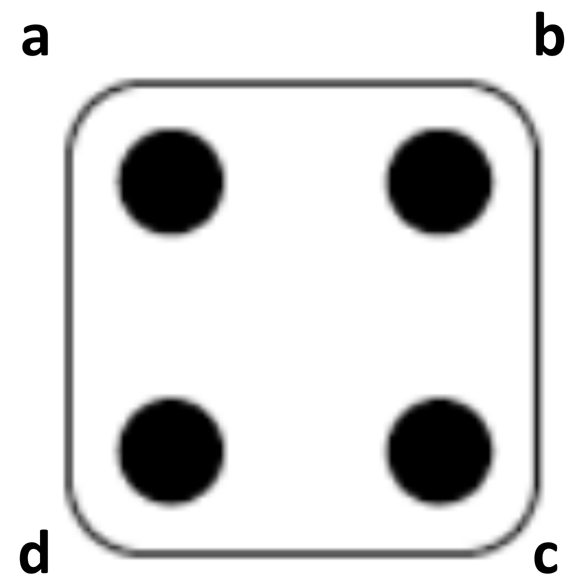


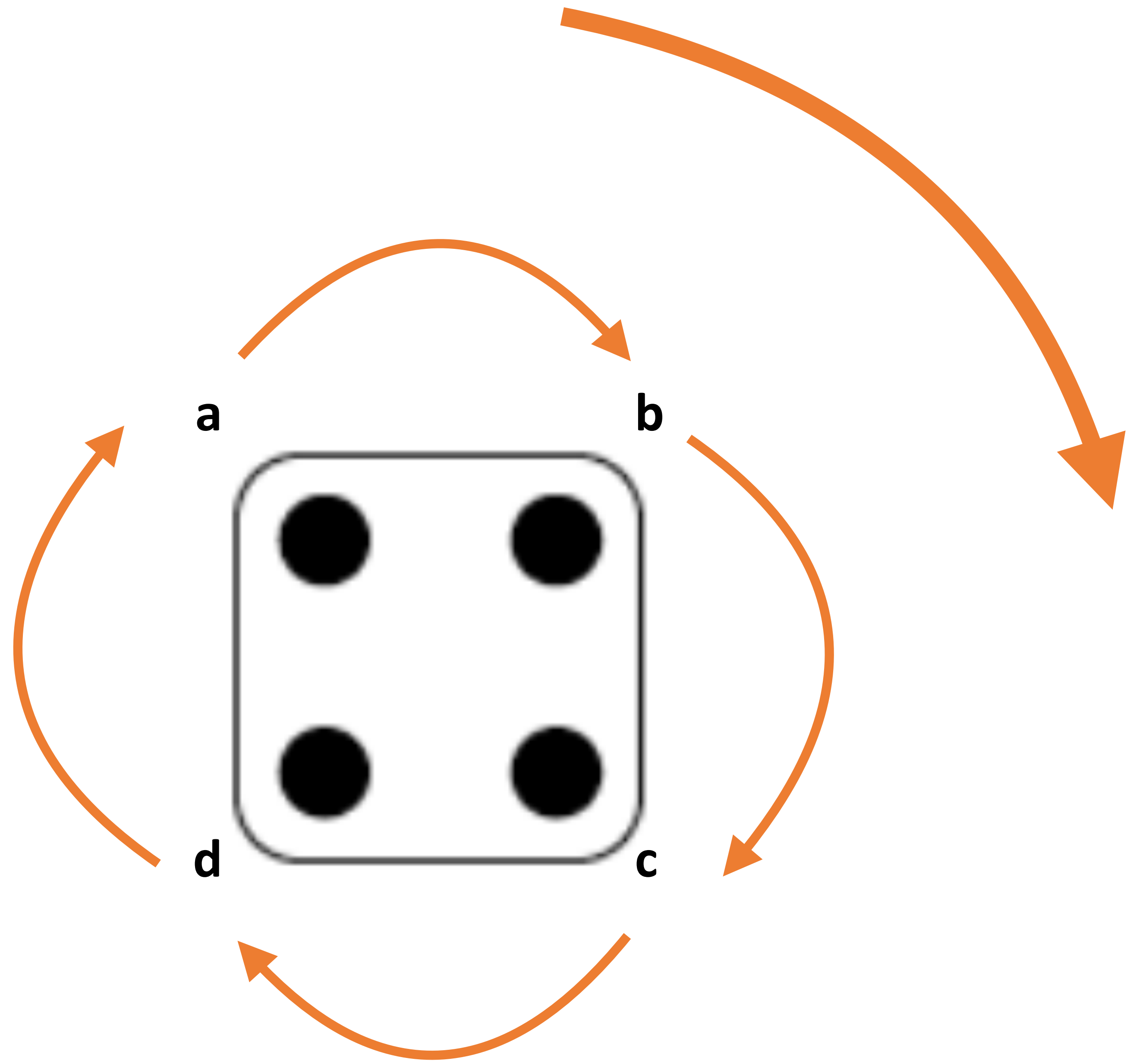


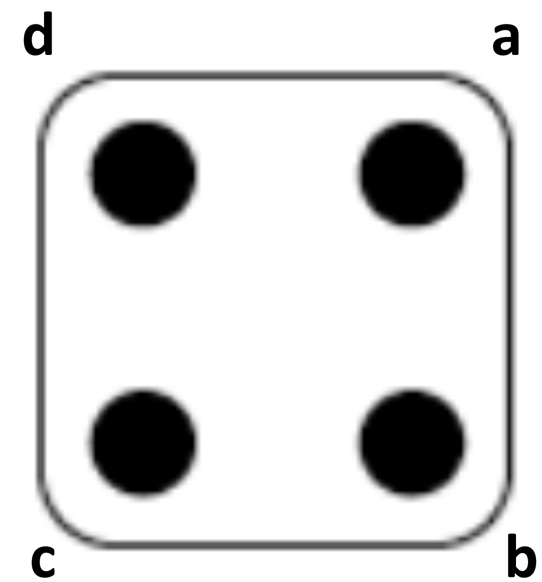
Two possibilities (a,c) and (b,d)

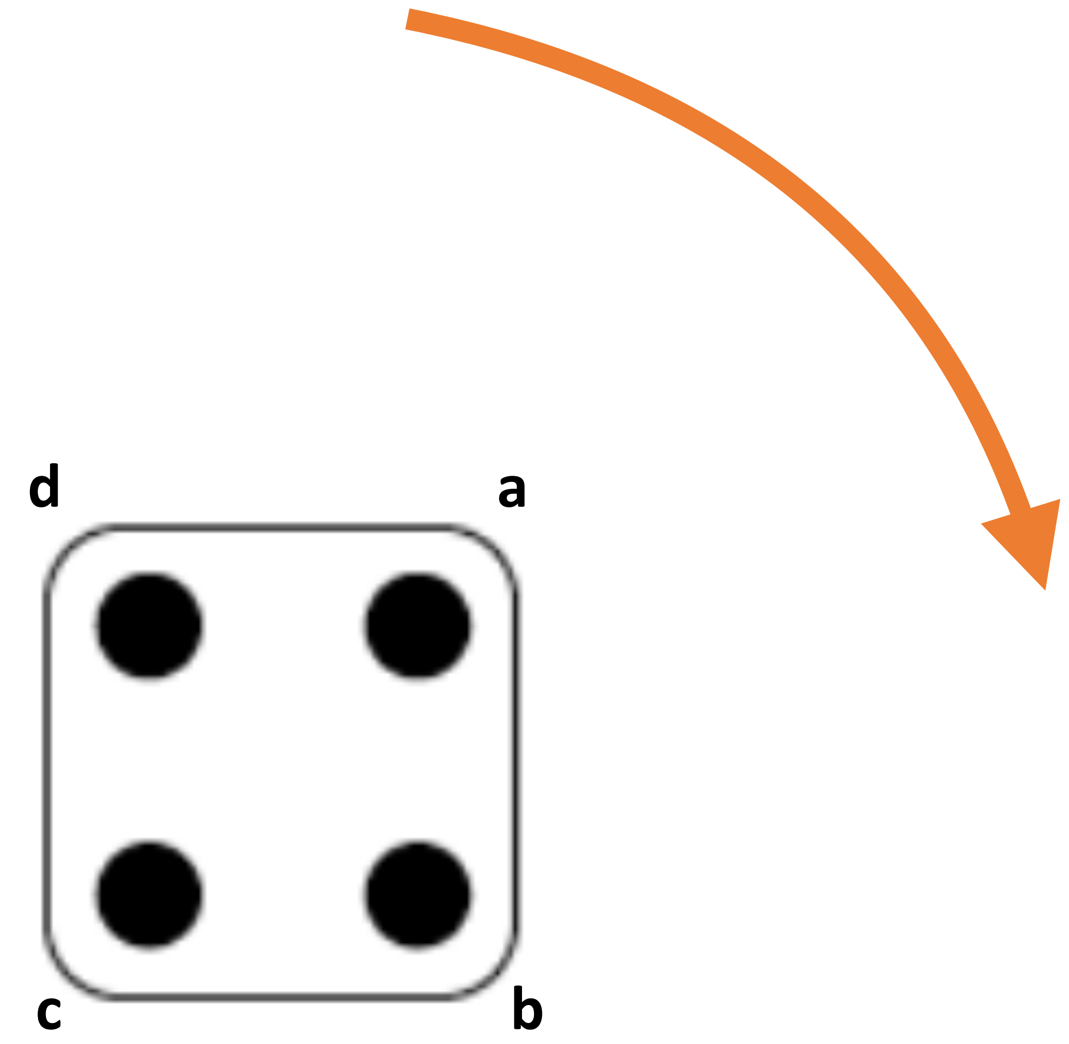


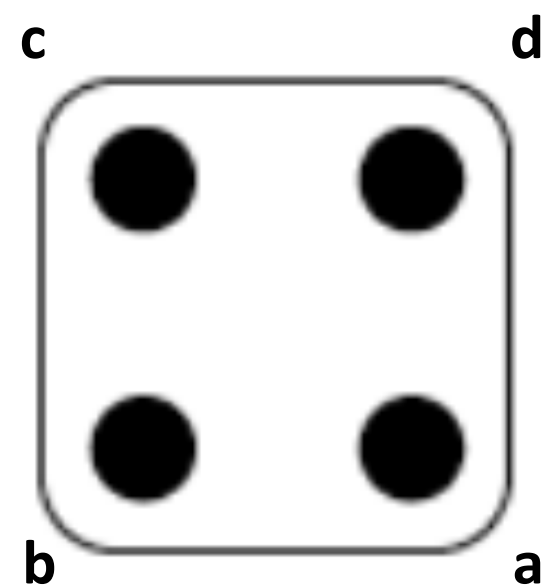
Also two possibilities (a,c) and (b,d)

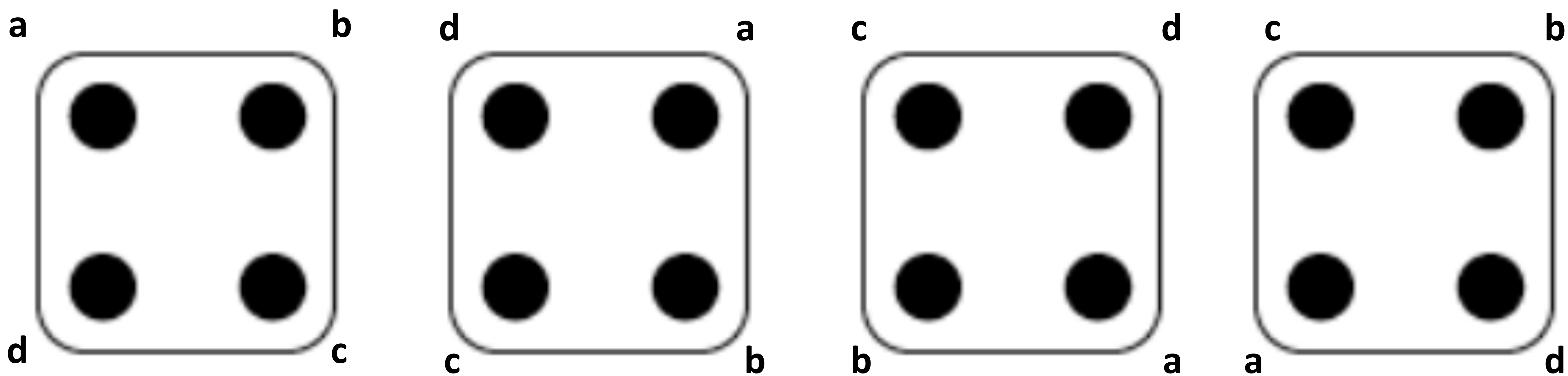

a
b
d
c

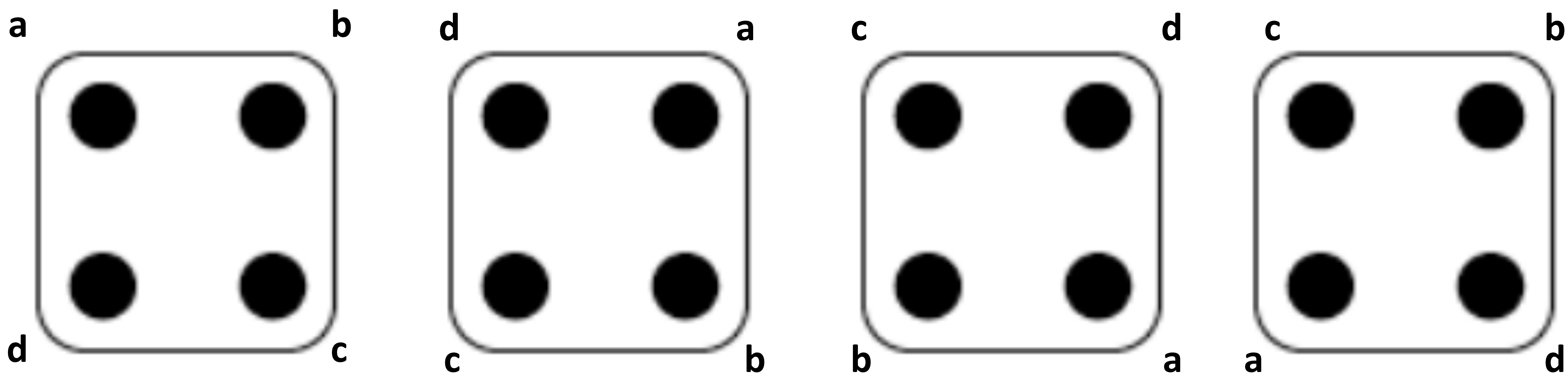

a
b
c
d


d
a
c
b

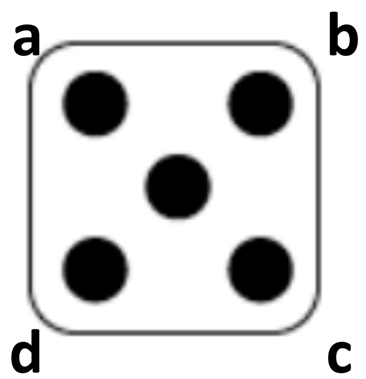

d
a
c
b


c
d
b
a

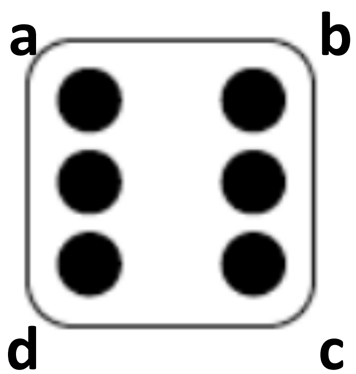

a
b
d
c
d
a
c
b
c
d
b
a
c
b
a
d



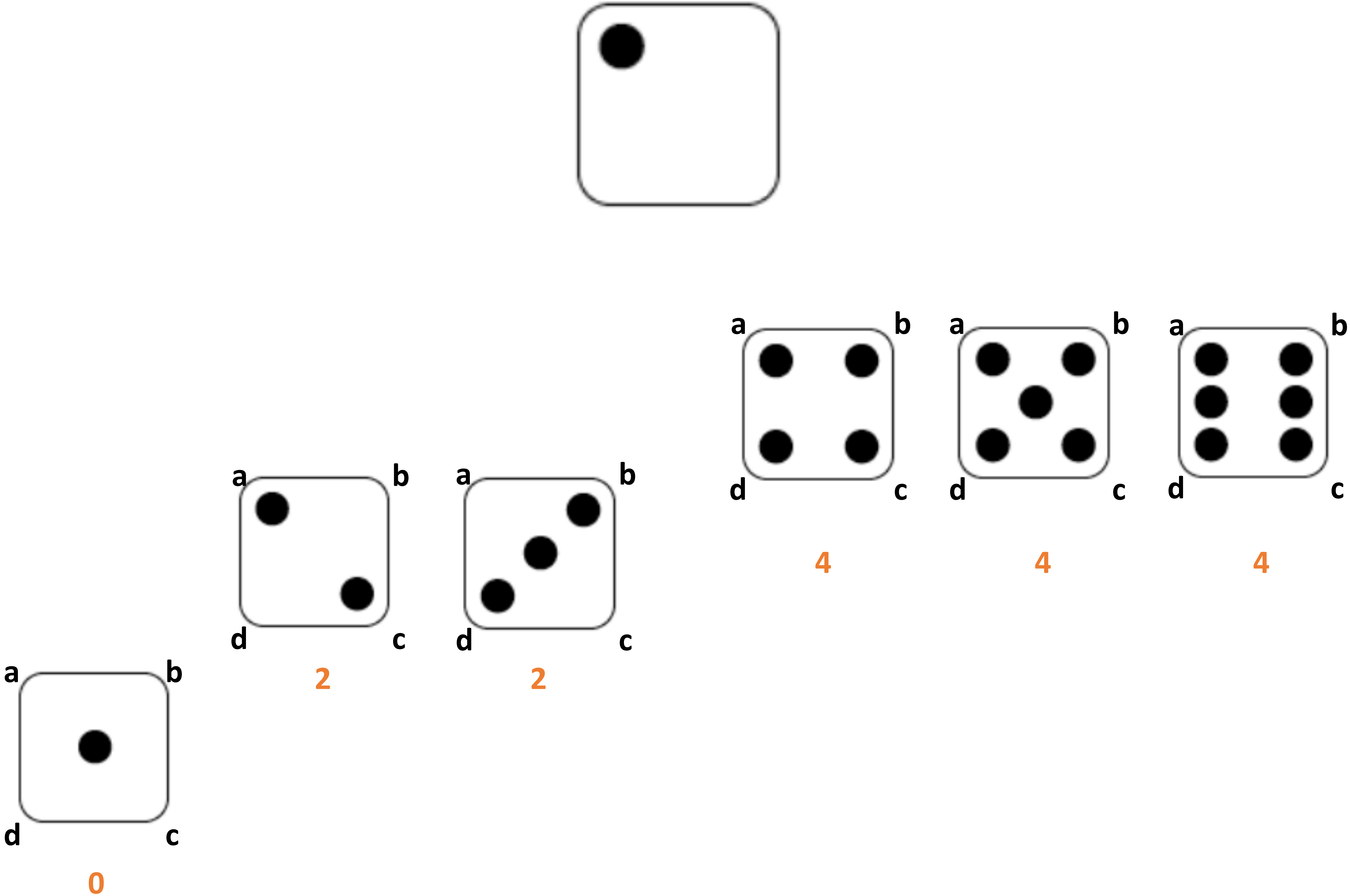
Four possibilities

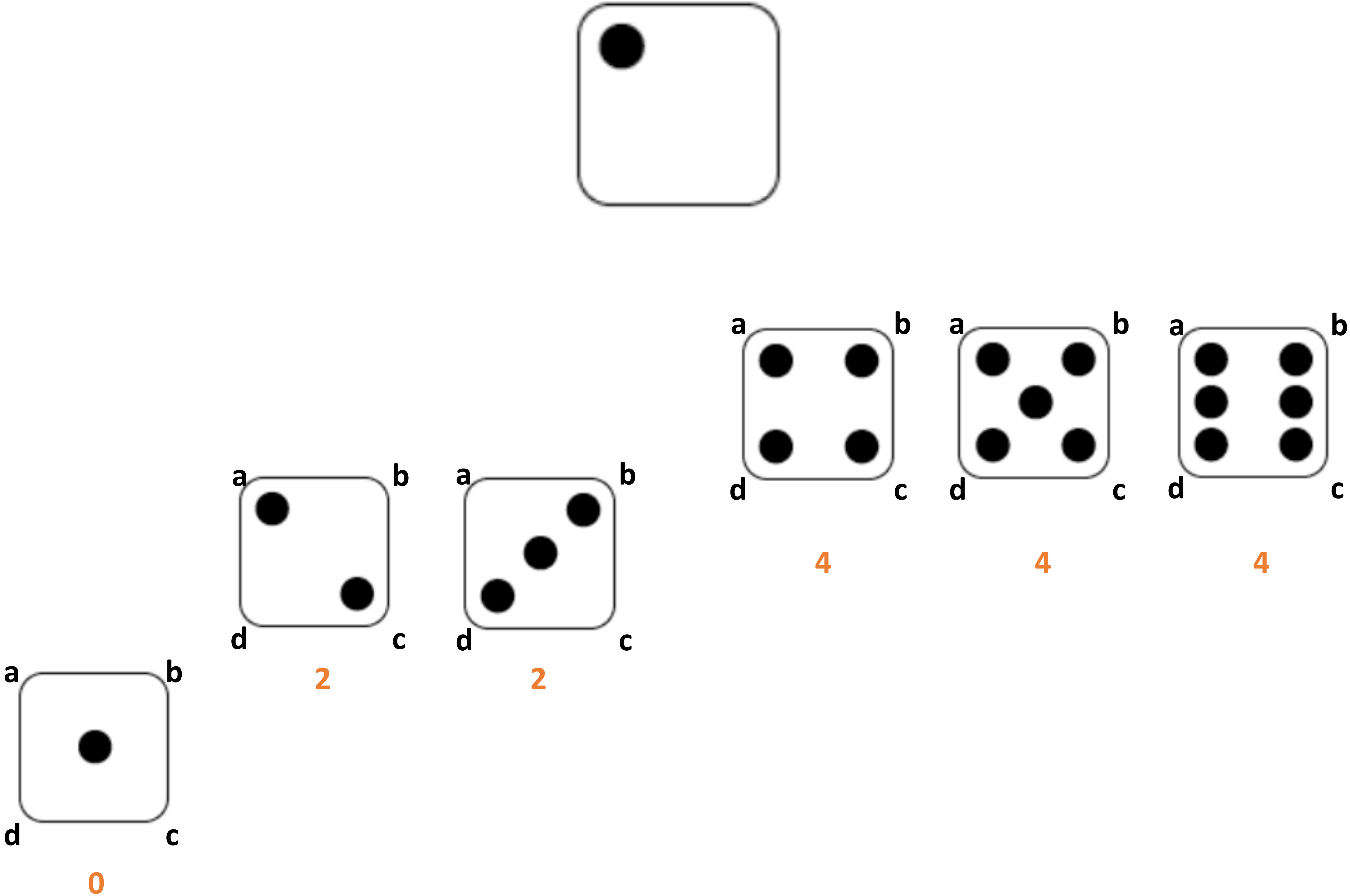


Four possibilities



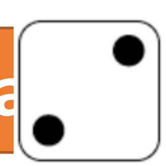
Four possibilities

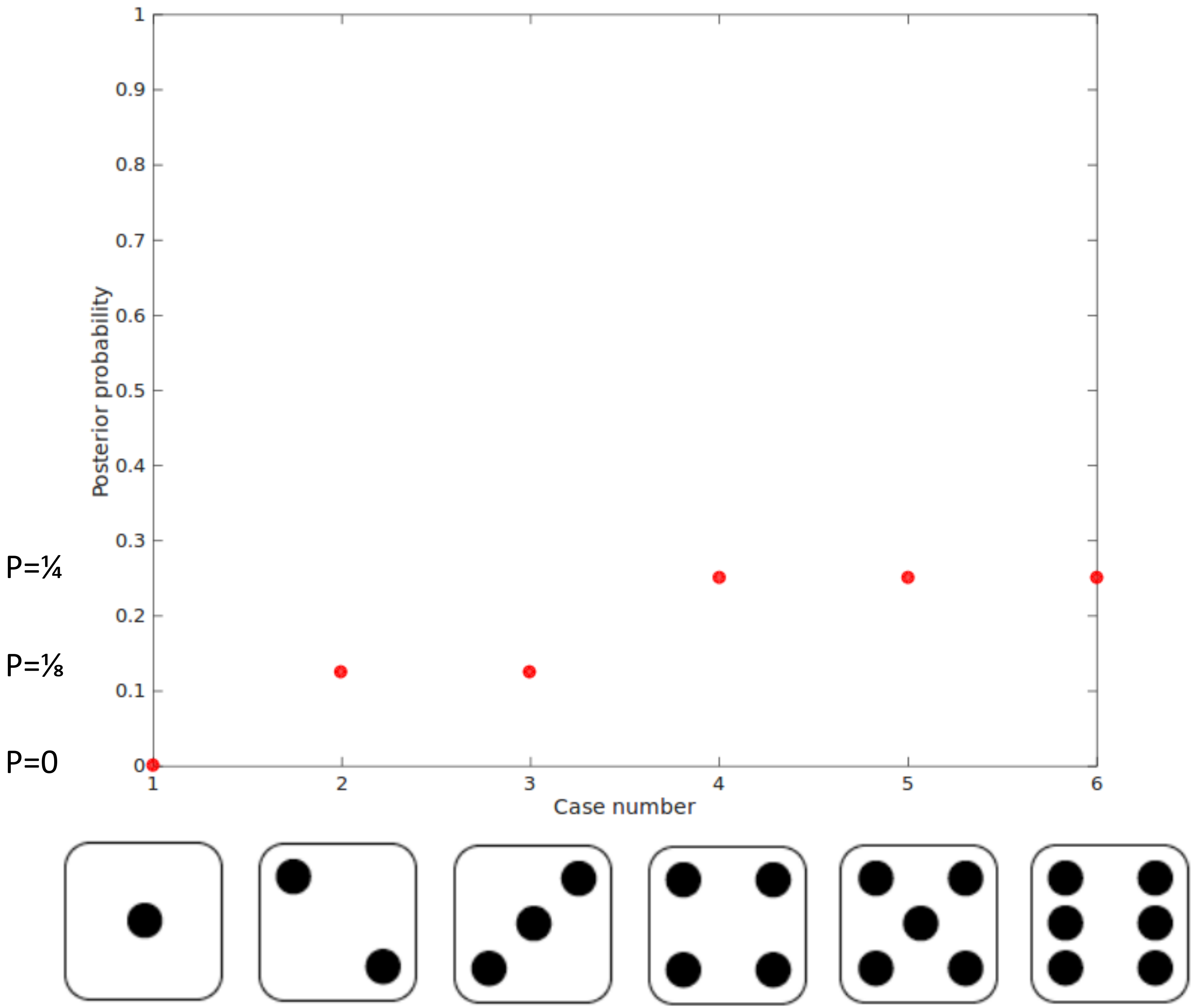

a b c d
0
2
2
4
4
4

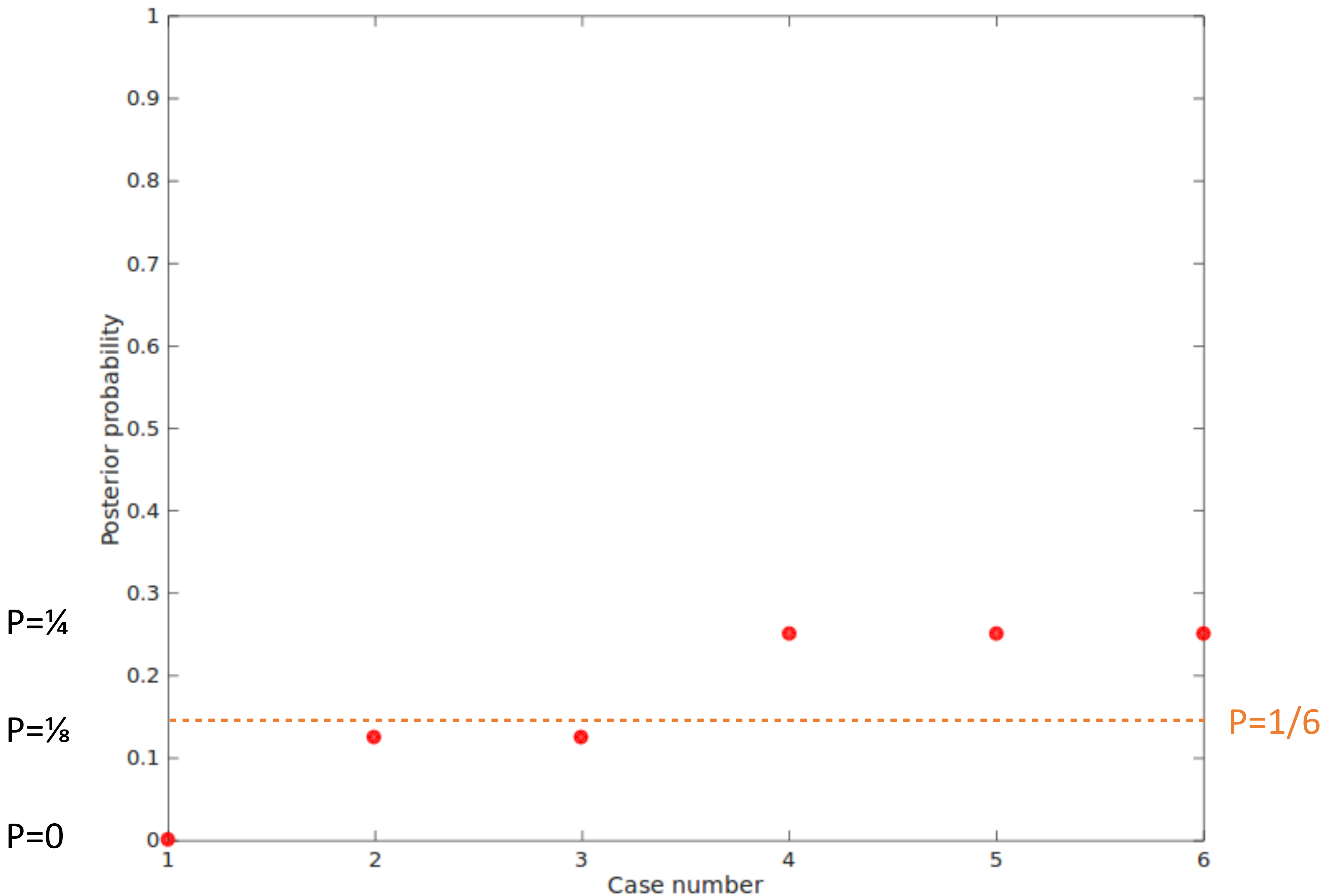


$$\pi(y) = \frac{0+2+2+4+4+4}{6 \times 4} = \frac{16}{24}$$

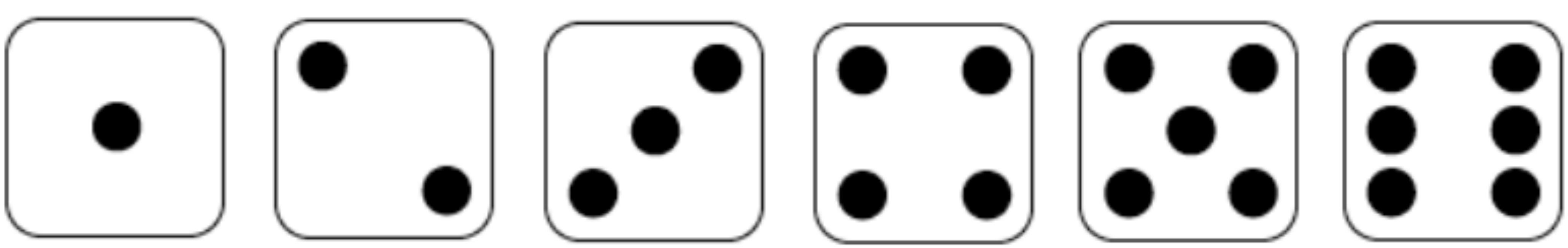
$$\pi(x|y) = \frac{\text{Prior} \times \text{Likelihood}}{\text{Evidence}} = \frac{\frac{1}{6} \times \frac{1}{2}}{\frac{16}{24}} = 0.125$$

Probability tha  **s was the face of the dice knowing**

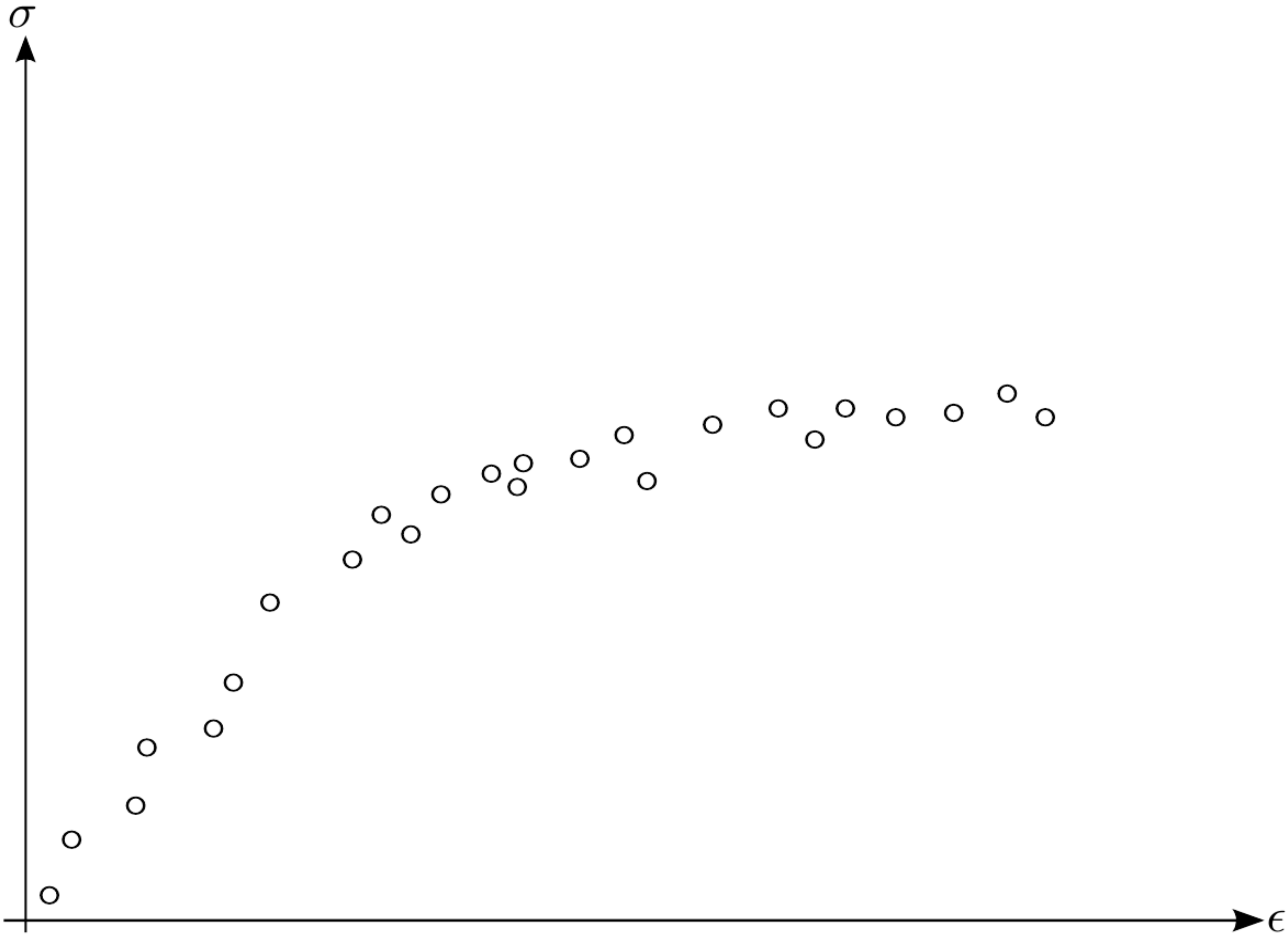

P=¼
P=⅛
P=0
Posterior probability
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1
2
3
4
5
6
Case number



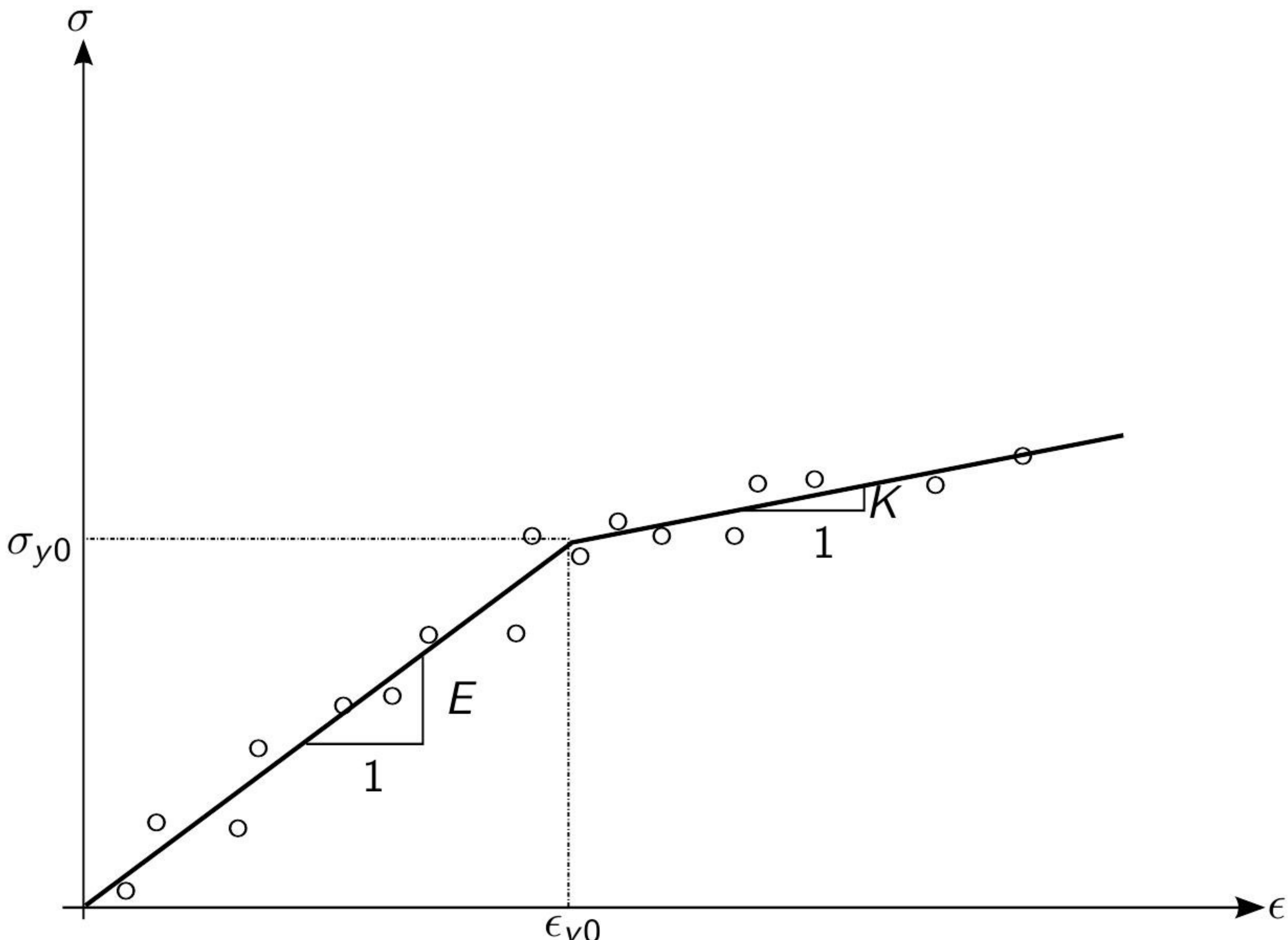
P=¼
P=⅛
P=0
P=1/6
Posterior probability
Case number
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1
2
3
4
5
6



Stress-strain data



Identify the parameters



Construct the likelihood function

Model

$Y = f(X, \Omega)$ observations=f(parameters, error)

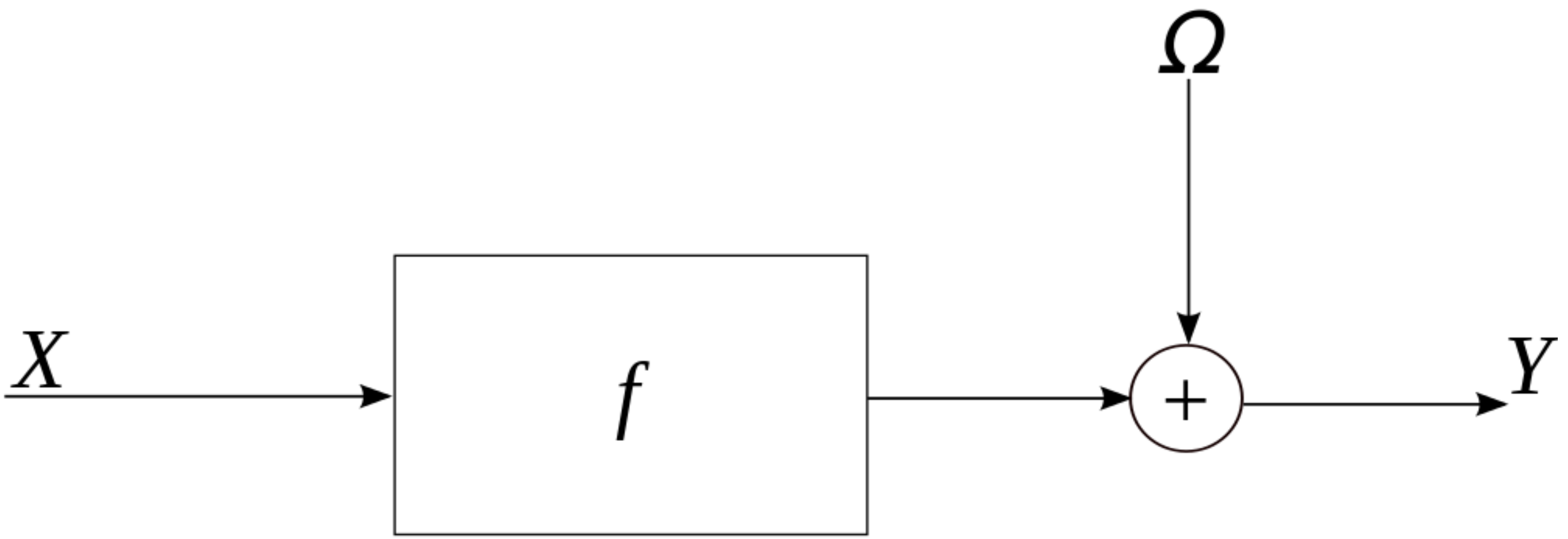
Ω : Error

X : Material parameter

Noise model

Additive noise model

$$Y = f(X) + \Omega$$



Likelihood function

Likelihood function for additive model

$$\pi(y|x) = \pi(\omega) = \pi(y - f(x))$$

$$Y = f(X) + \Omega$$

Constitutive law: linear elasticity

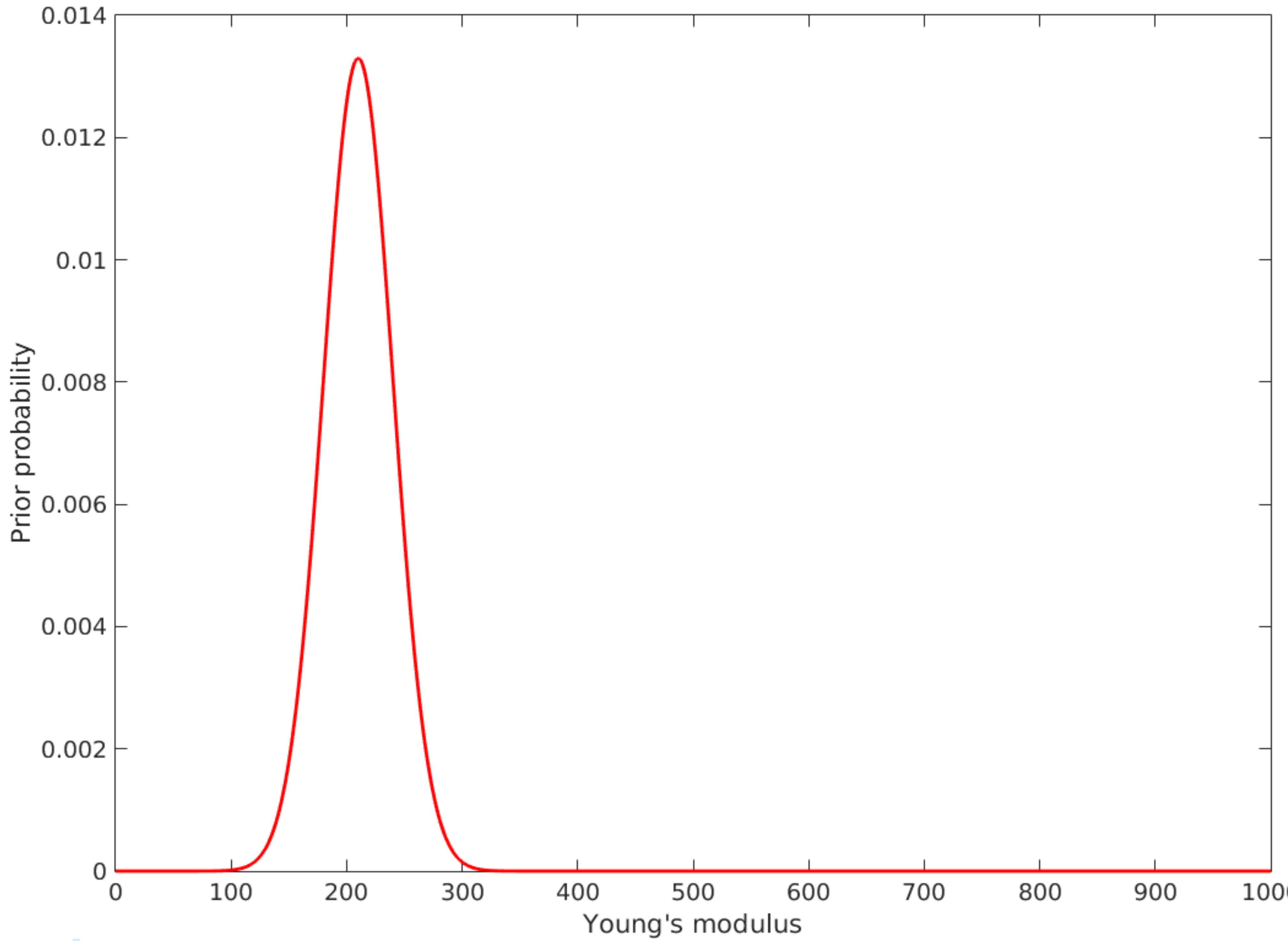
Constitutive model

$$\sigma = E\epsilon \text{ or } \sigma = x\epsilon$$

Observed data

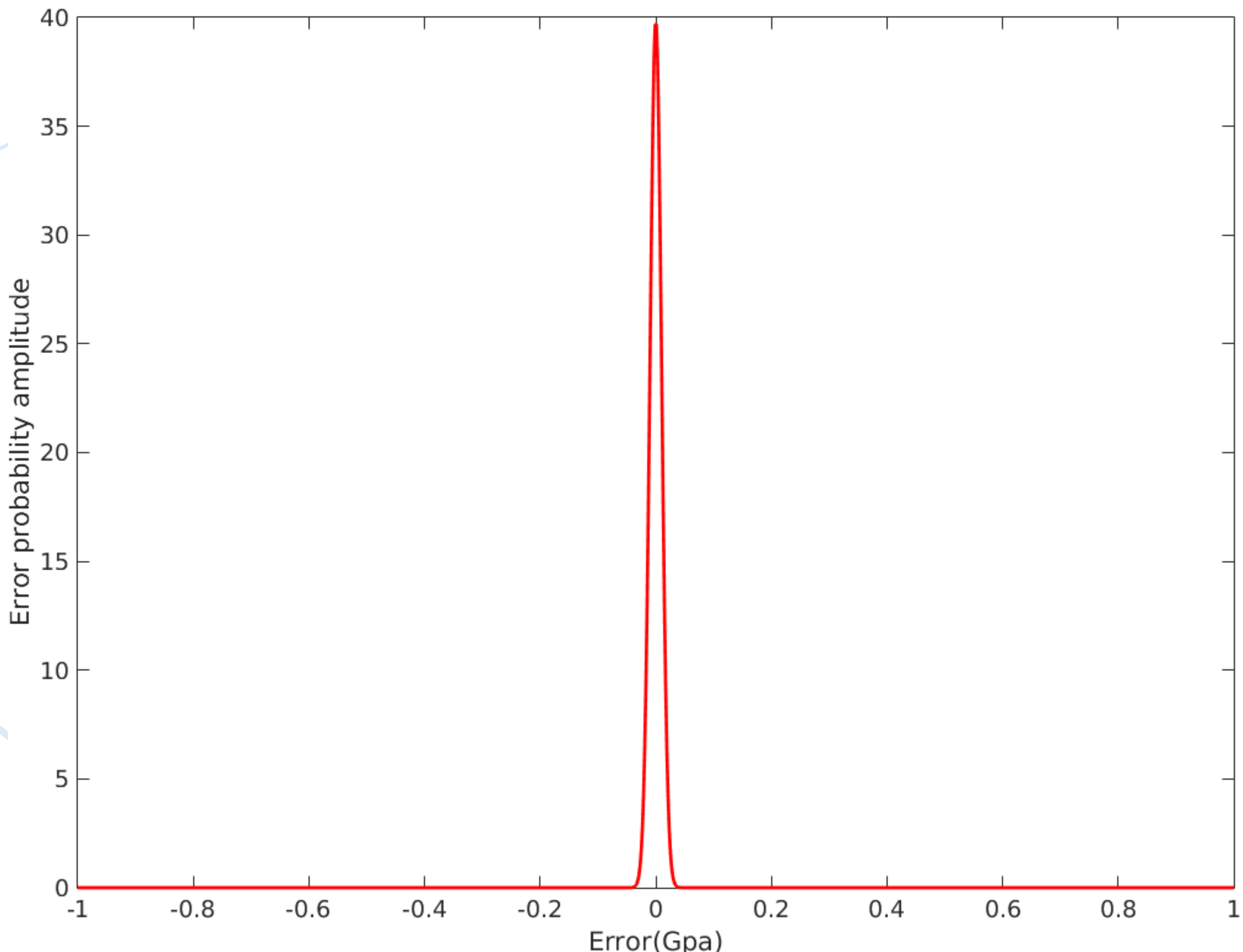
$$Y = X\epsilon + \Omega$$

Prior information on Young's modulus



$$\pi_{prior}(x) = N(210, 900)$$

Error model (noise)



$$\pi(e)_{error} = N(0, 0.0001)$$

Likelihood function

Likelihood function

$$\pi(y|x) = N(y - x\epsilon, 0.0001)$$

$$\pi(y|x) = \pi(\omega) = \pi(y - f(x))$$

Bayes' theorem: calculate the posterior

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

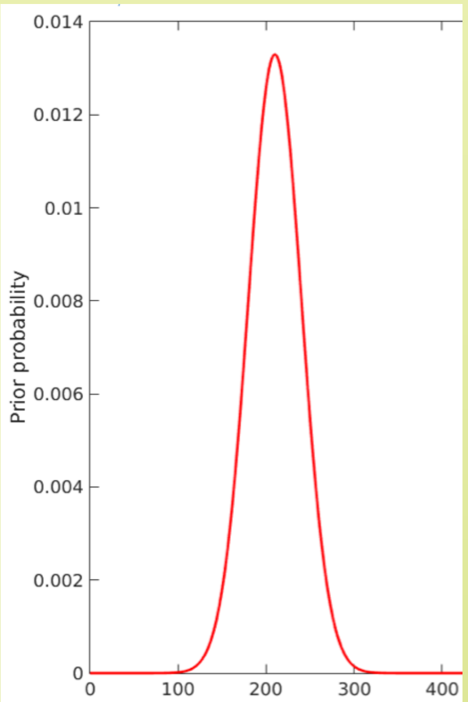
$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

Bayes' theorem: calculate the posterior

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

prior $\pi(x)$



Bayes' theorem: calculate the posterior

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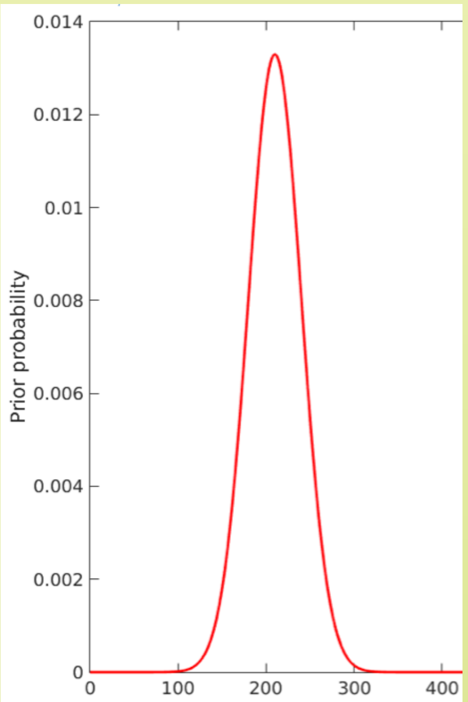
$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

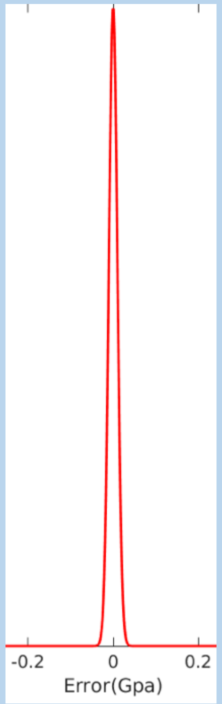
prior $\pi(x)$



likelihood $\pi(y|x)$

$$\pi(y|x) = N(y - x\epsilon, 0.0001)$$

$$\pi(y|x) = \pi(\omega) = \pi(y - f(x))$$

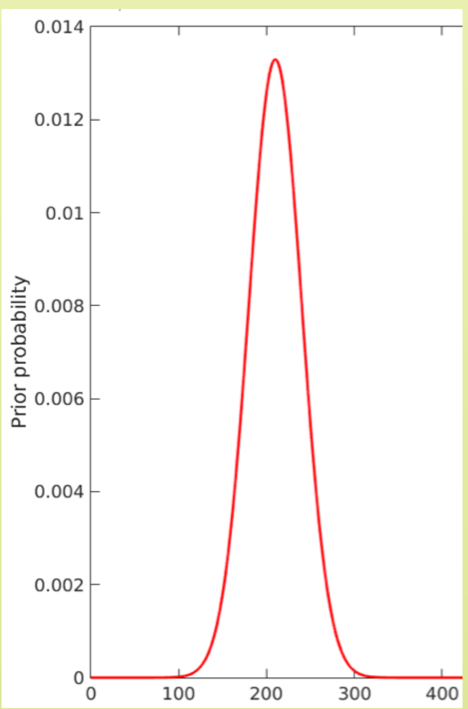


Bayes' theorem: calculate the posterior

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

prior $\pi(x)$

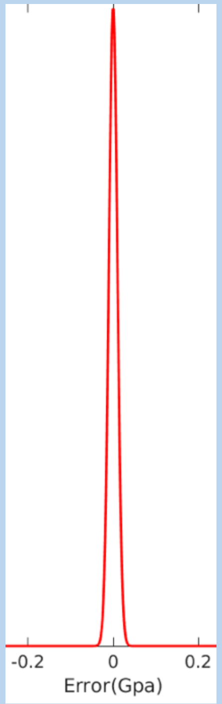


posterior

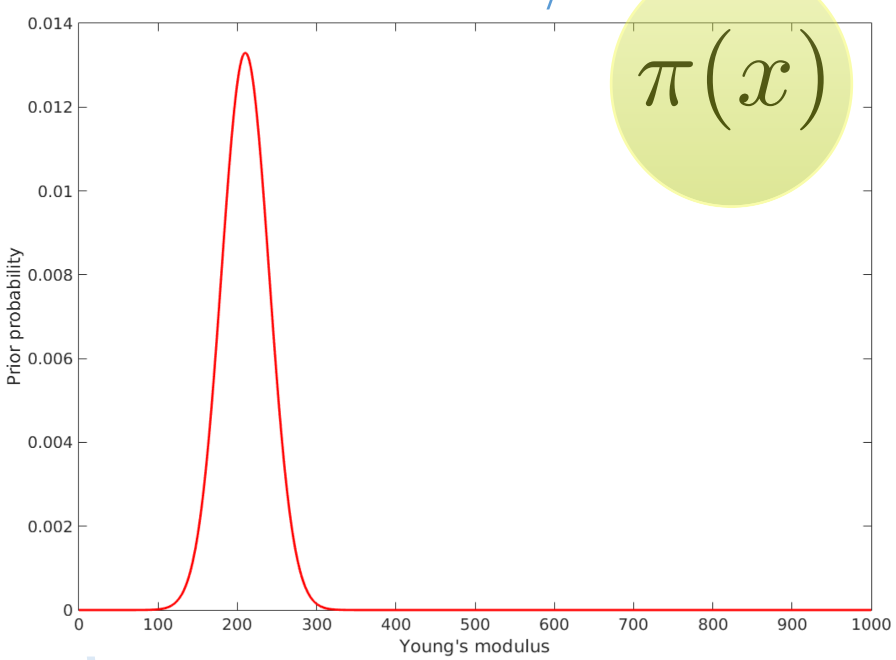
$\propto \pi(x|y)$

likelihood $\pi(y|x)$

$$\pi(y|x) = N(y - x\epsilon, 0.0001)$$
$$\pi(y|x) = \pi(\omega) = \pi(y - f(x))$$

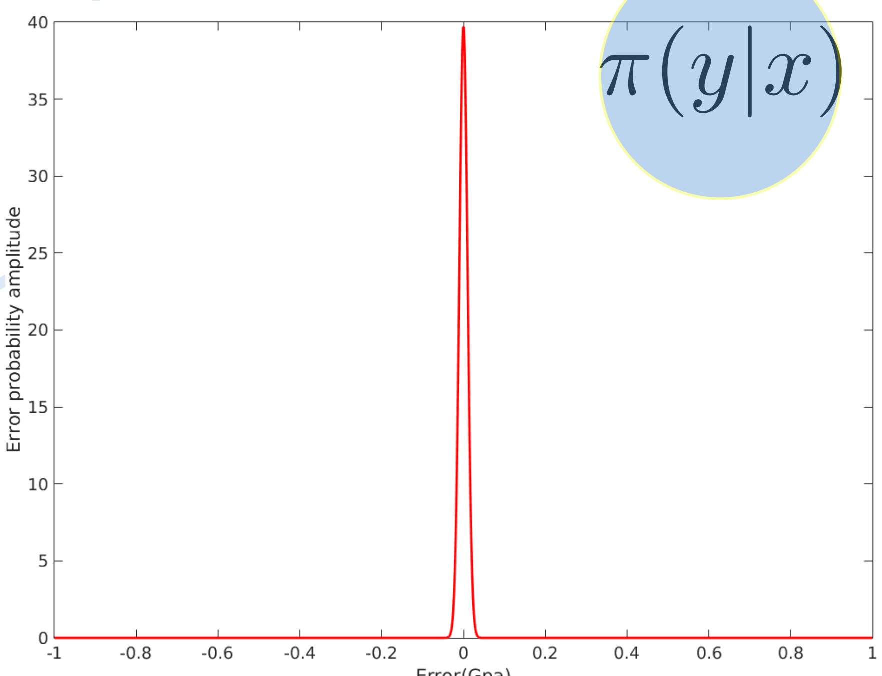


Posterior probability



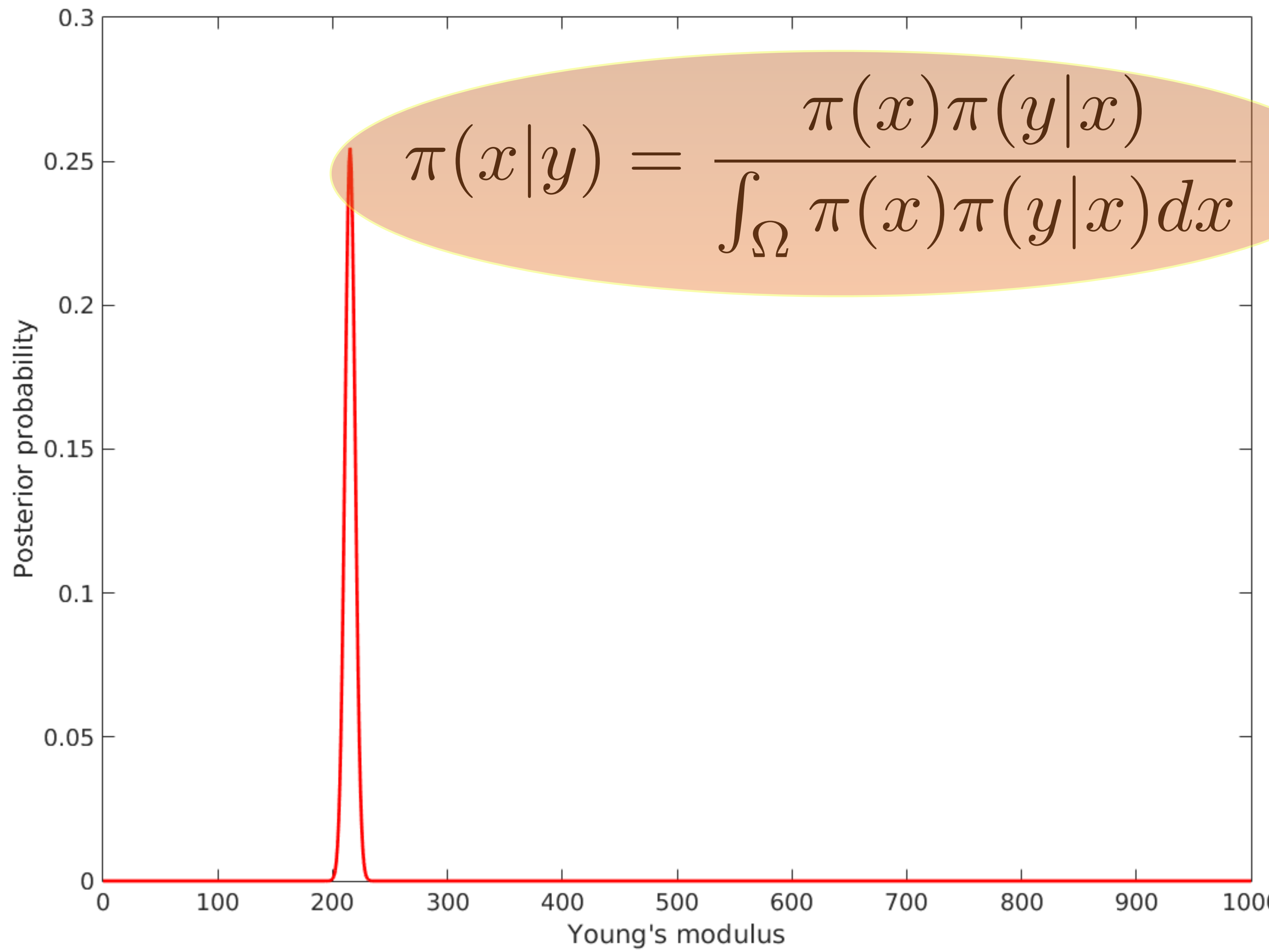
$$\pi(x)$$

$$\pi_{prior}(x) = N(210, 900)$$



$$\pi(y|x)$$

$$\pi(e)_{error} = N(0, 0.0001)$$



$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int_\Omega \pi(x)\pi(y|x)dx}$$

$$\pi_{posterior} = N(215.1533, 19.6168)$$

$$N_{sample} = 10$$

Outline

A focus on equation-based models

- How can we control the quality of simulations, verification and validation?
- Why are set-in-stone-models limited?
- How can we leverage statistical models to improve our models?

Outline

- **Data-driven modelling: Beyond setting models in stone**
  - Data assimilation
    - How can we learn from observations “on-the-fly”.
    - The power of digital twins.
- **Future challenges**

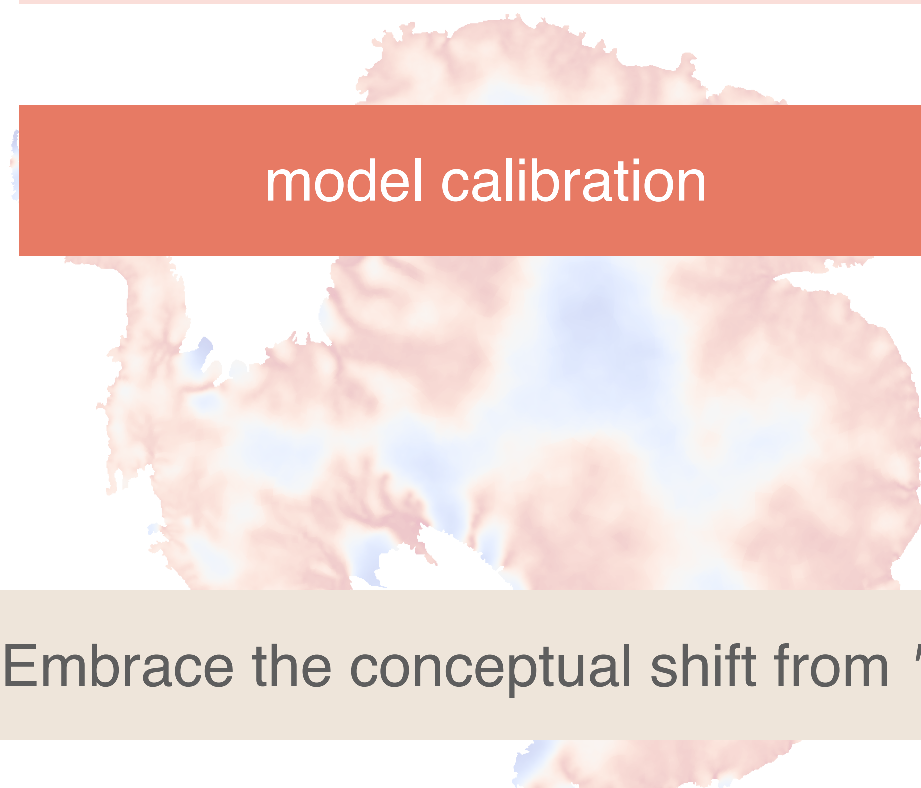
Data-driven Modelling

input → model → output

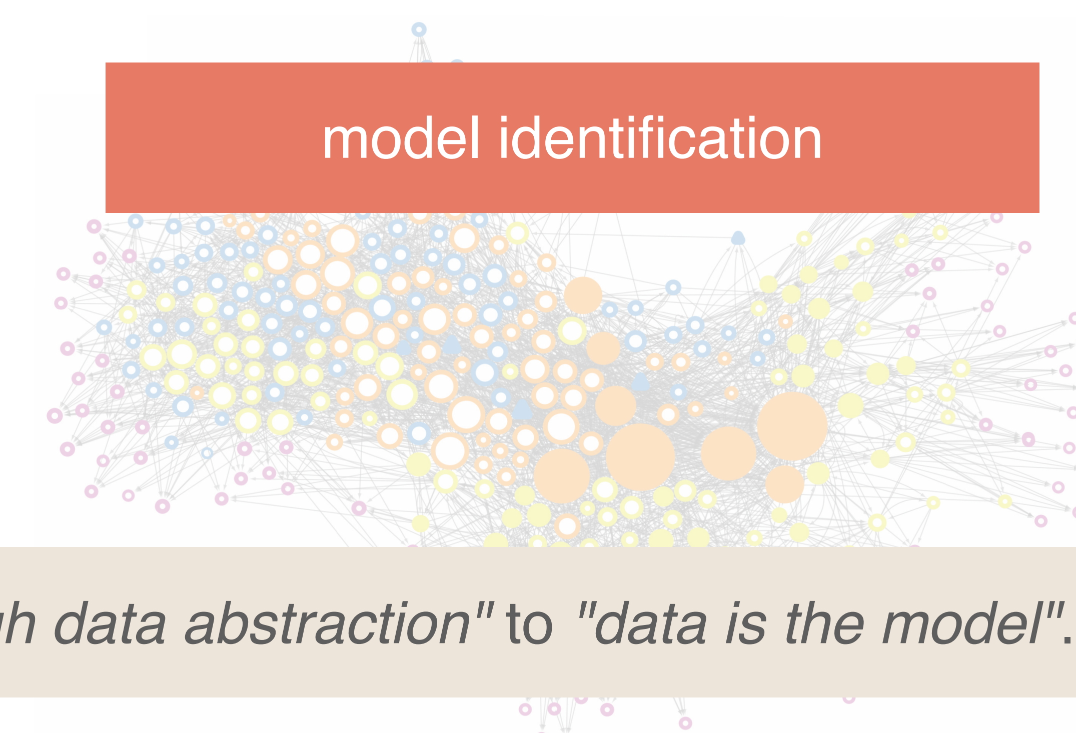
$$f : \mathbf{x} \rightarrow \mathbf{y}$$

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

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



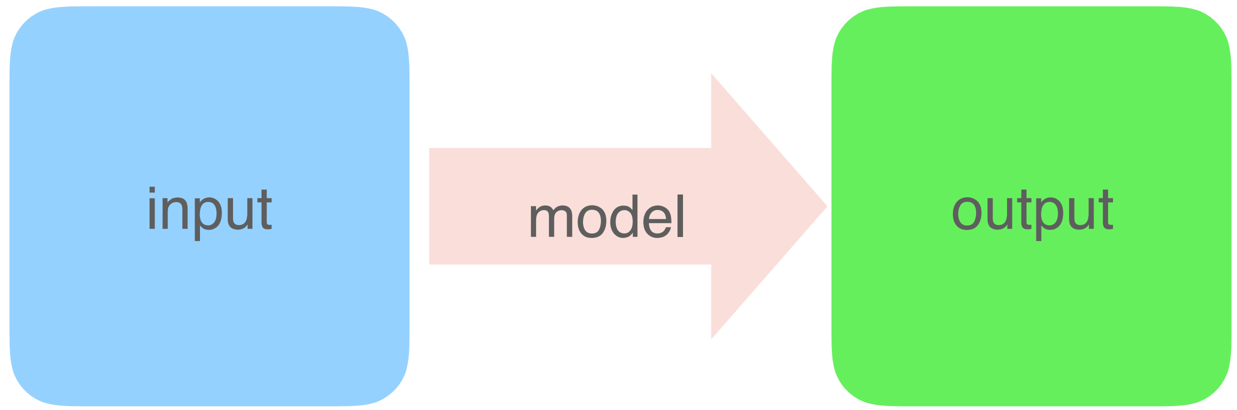
model calibration



model identification

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

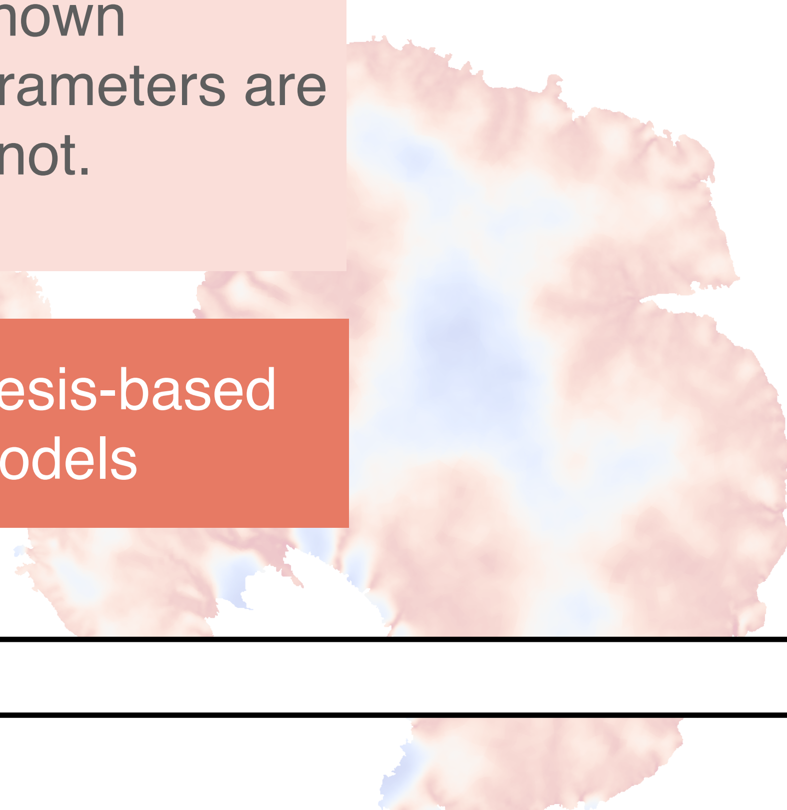
Data-driven Modelling

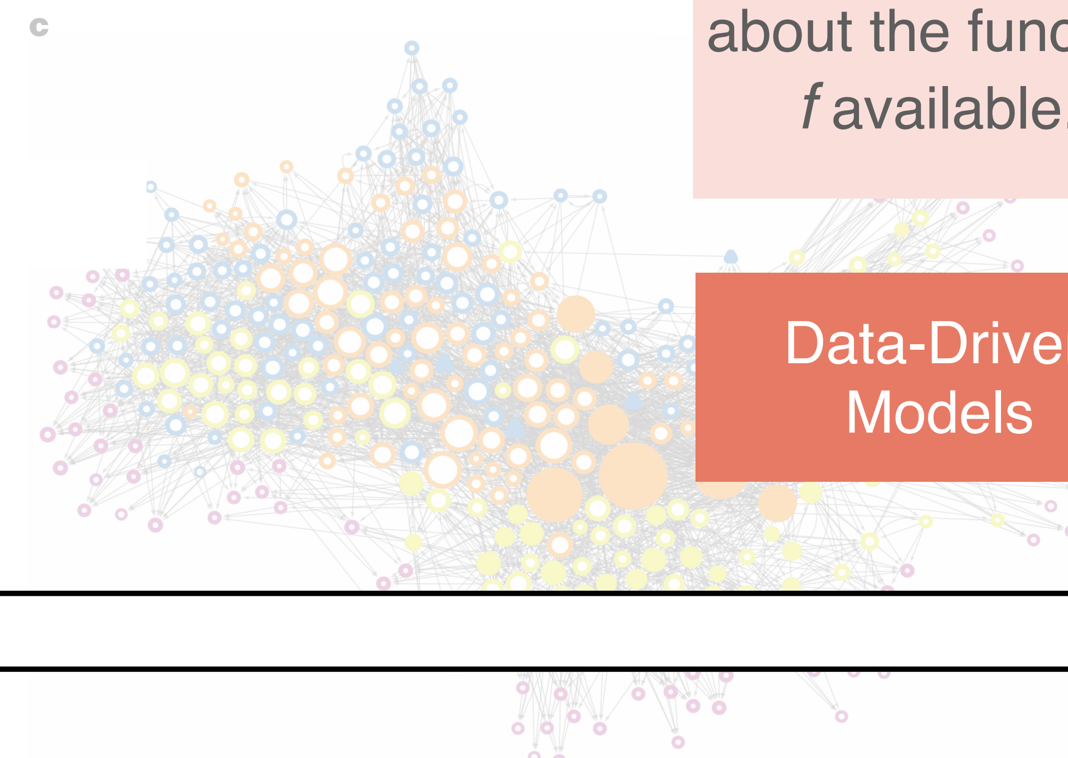


$$f : \mathbf{x} \rightarrow \mathbf{y}$$

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

Hypothesis-based Models

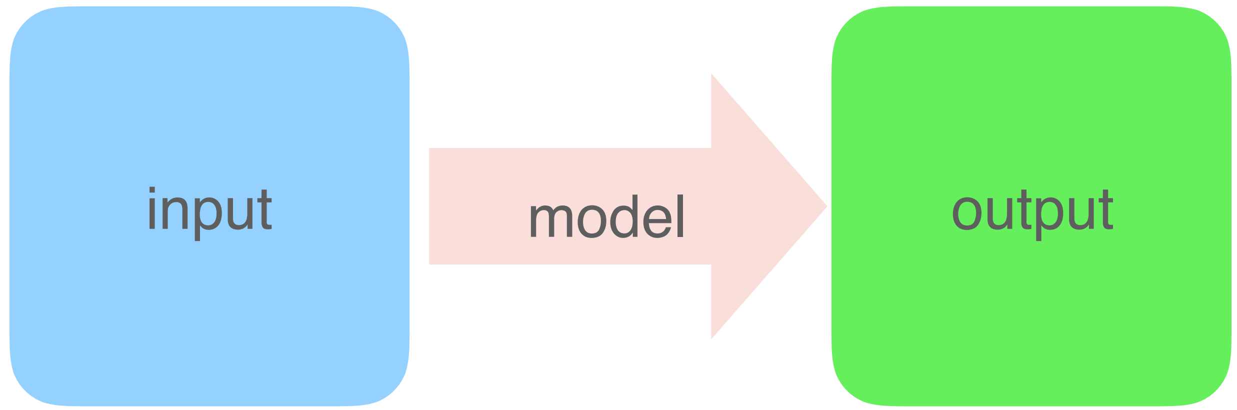




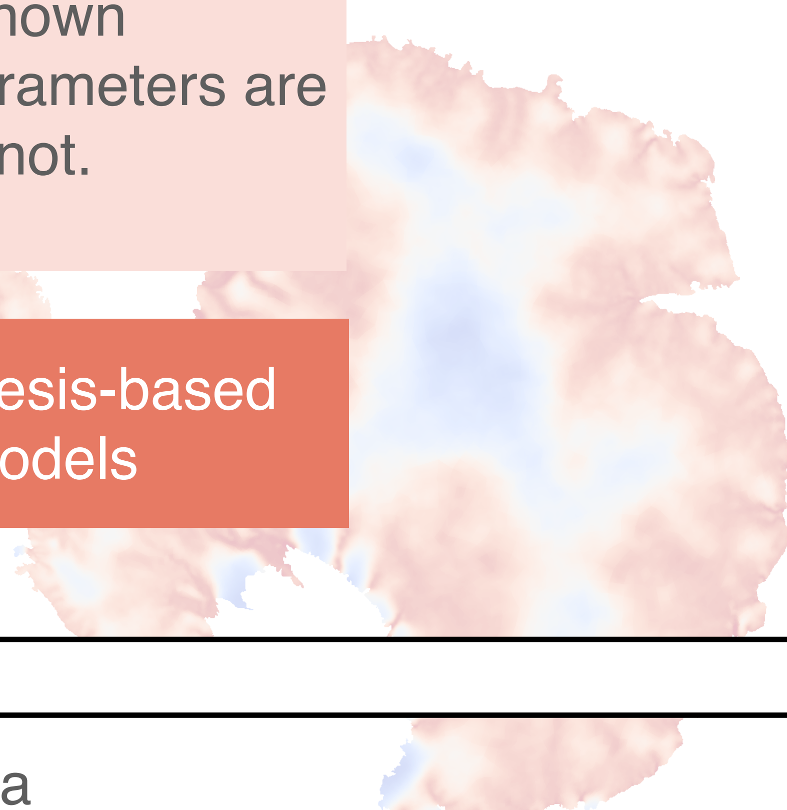
There is no a priori knowledge about the function *f* available.

Data-Driven Models

Data-driven Modelling

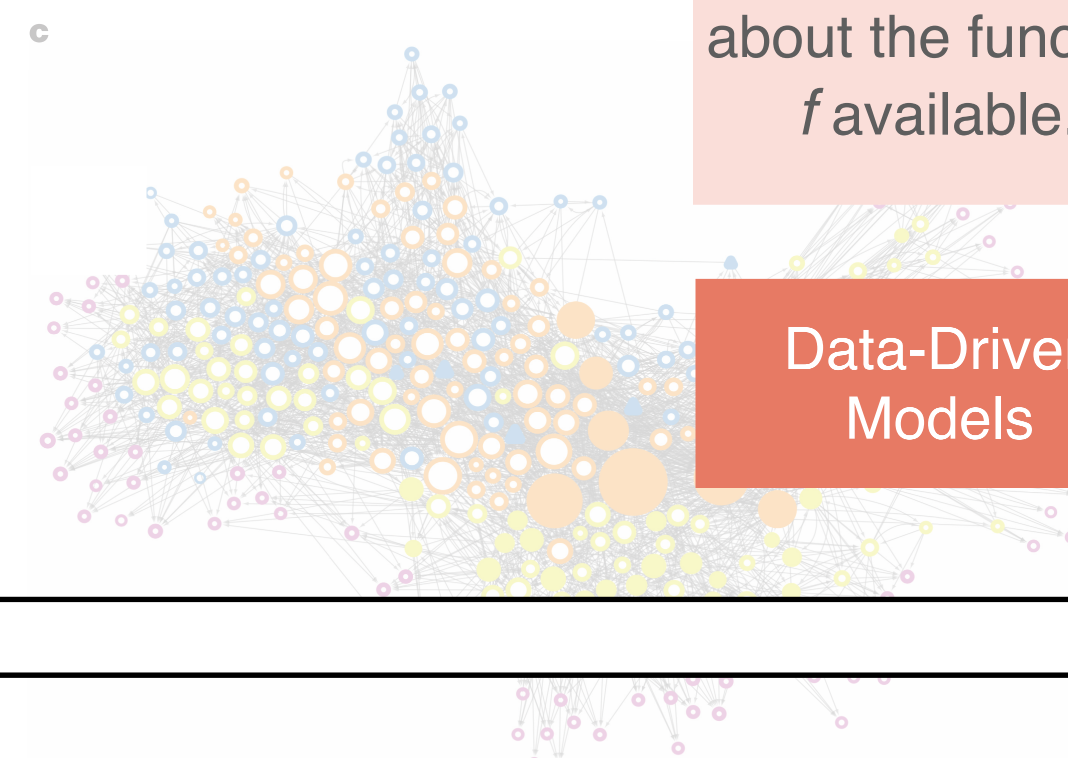


$f : \mathbf{x} \rightarrow \mathbf{y}$



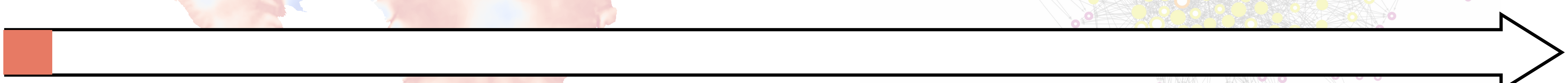
The structure of *f* is known
but its parameters are not.

Hypothesis-based Models



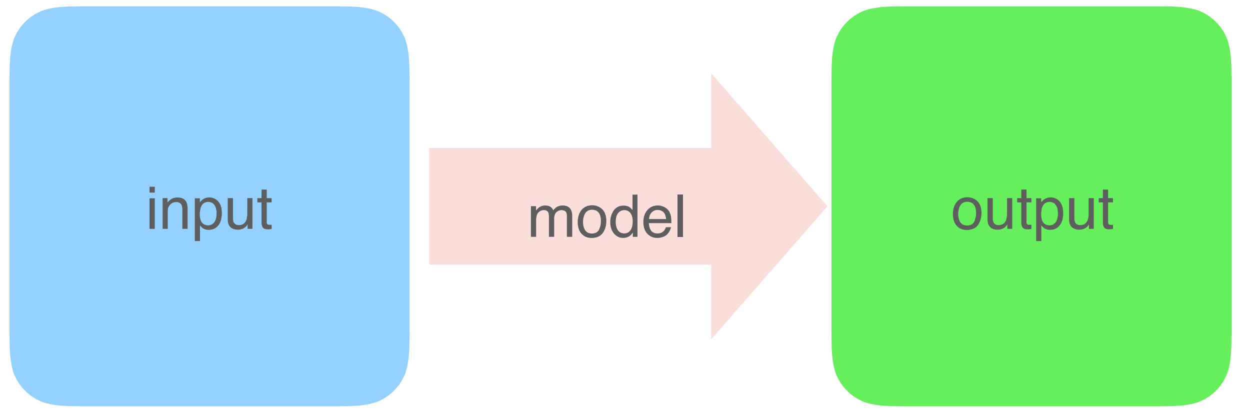
There is no a priori knowledge about the function *f* available.

Data-Driven Models



Small data

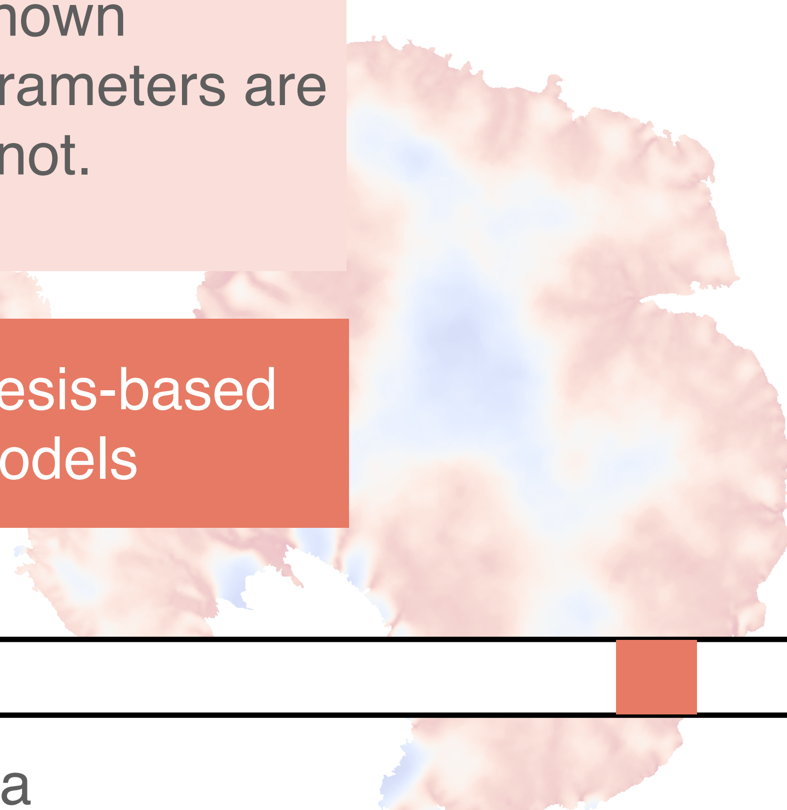
Data-driven Modelling

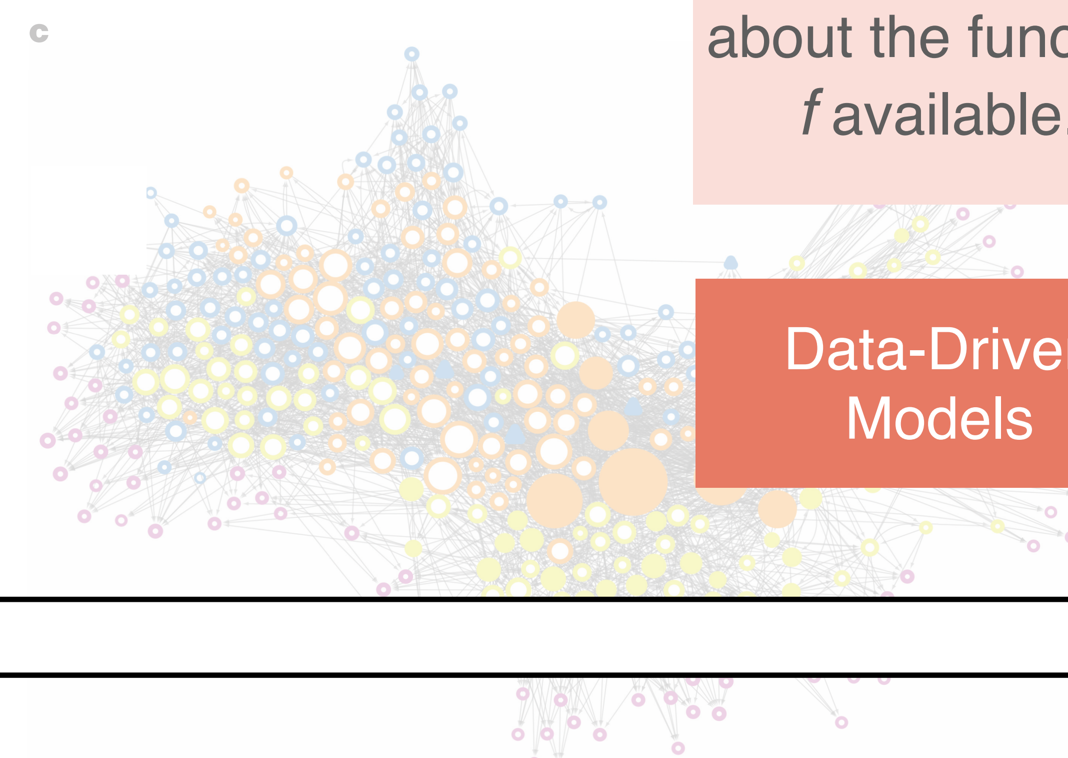


$$f : \mathbf{x} \rightarrow \mathbf{y}$$

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

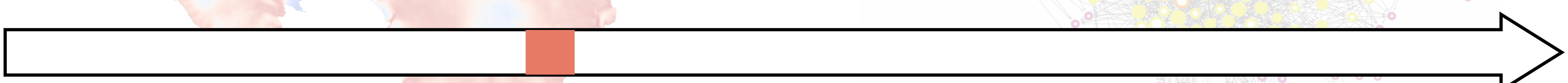
Hypothesis-based Models





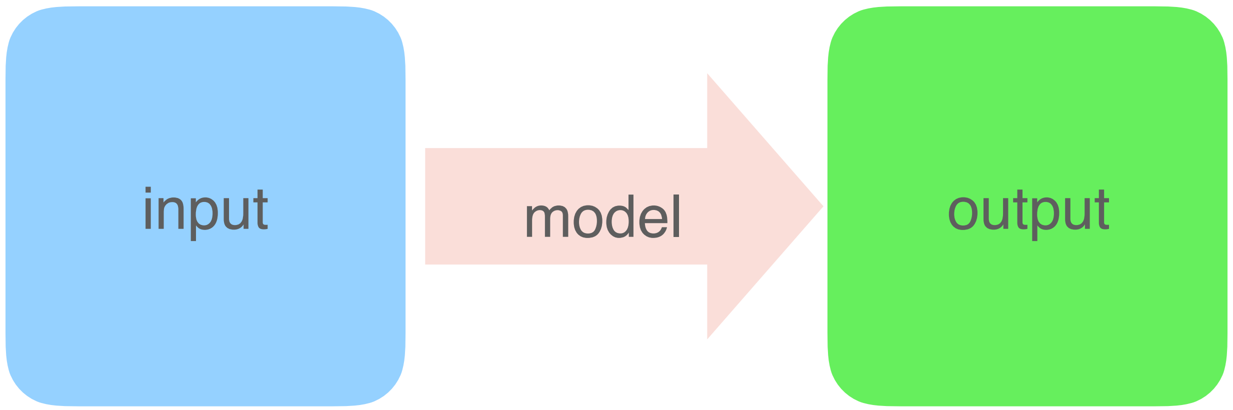
There is no a priori knowledge about the function *f* available.

Data-Driven Models

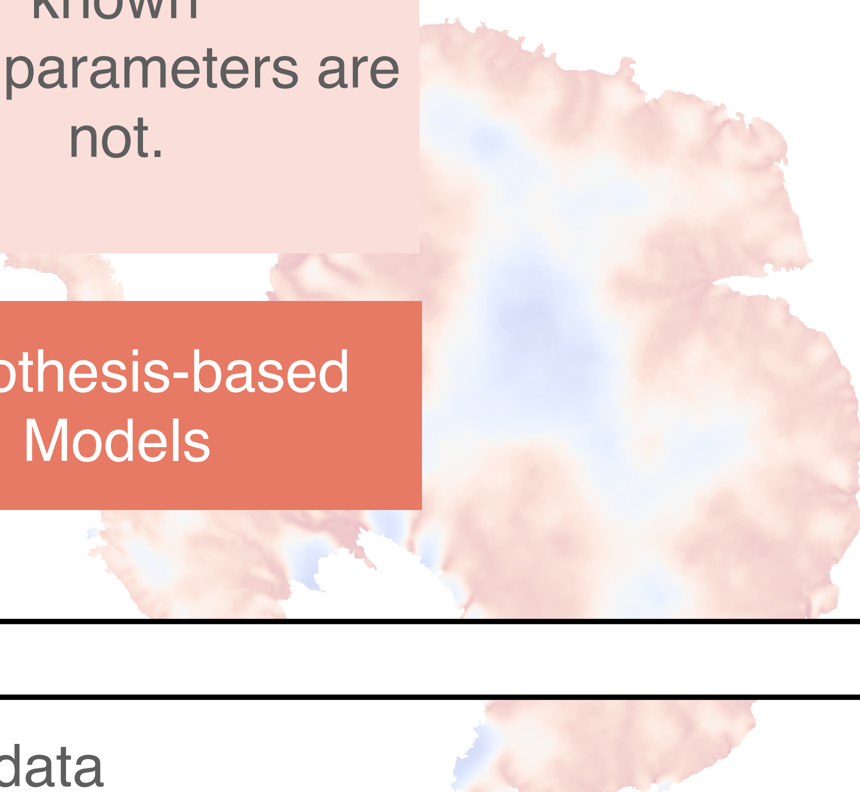


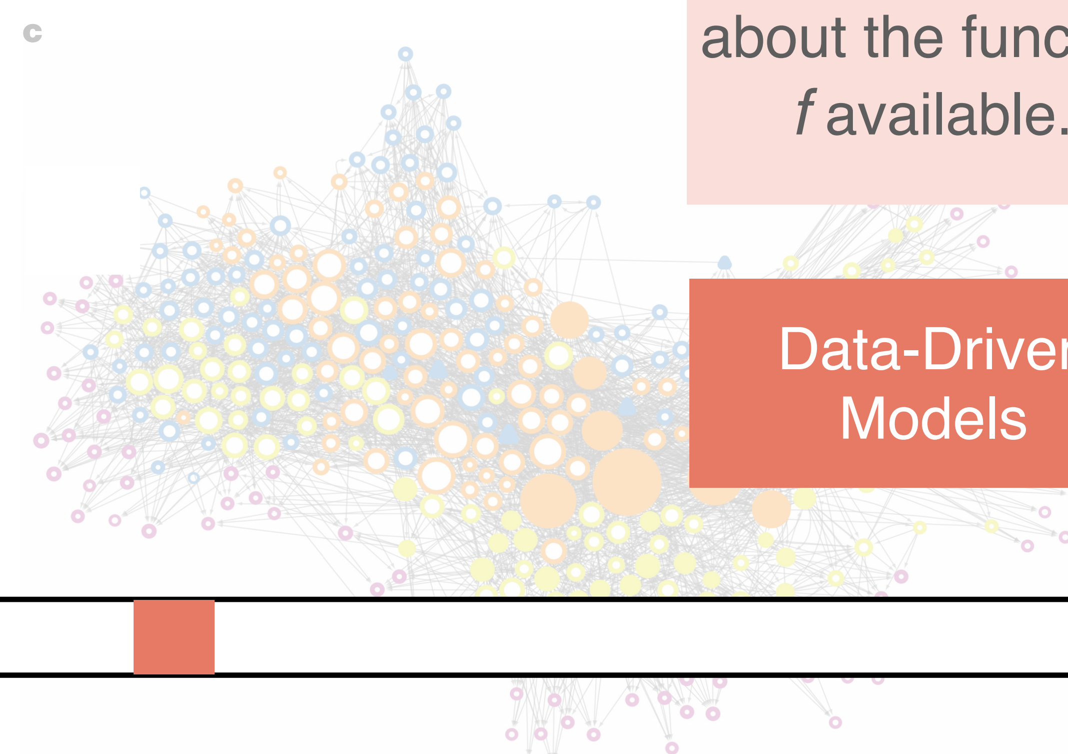
Small data

Data-driven Modelling



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





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

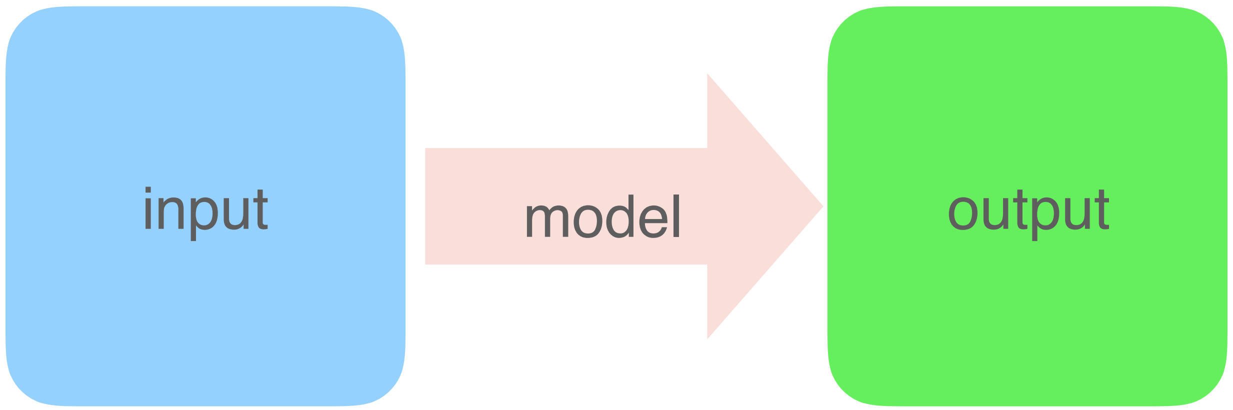
Hypothesis-based Models

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

Data-Driven Models

Small data

Data-driven Modelling



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

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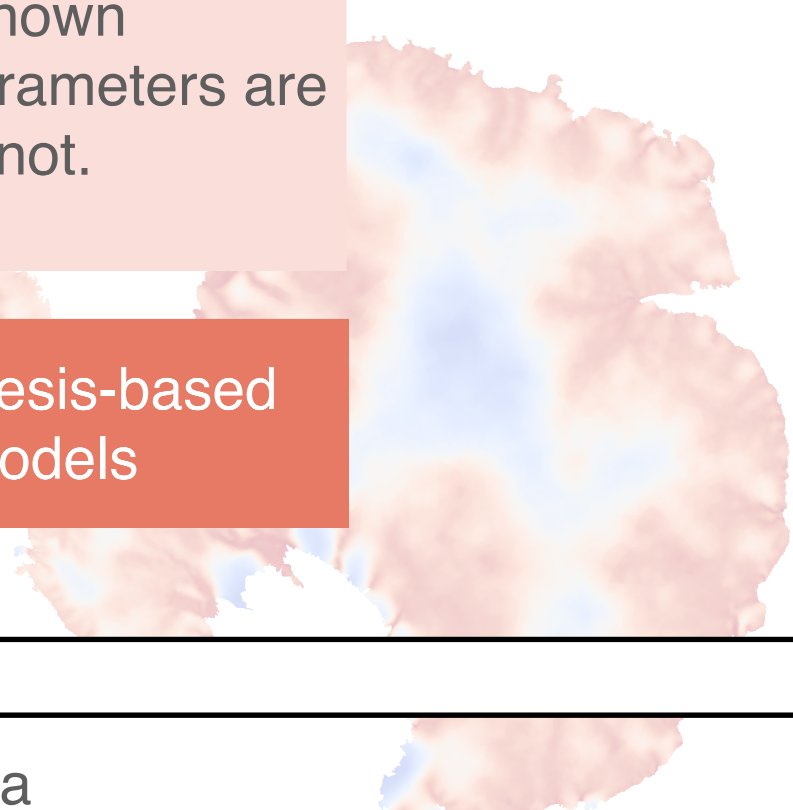
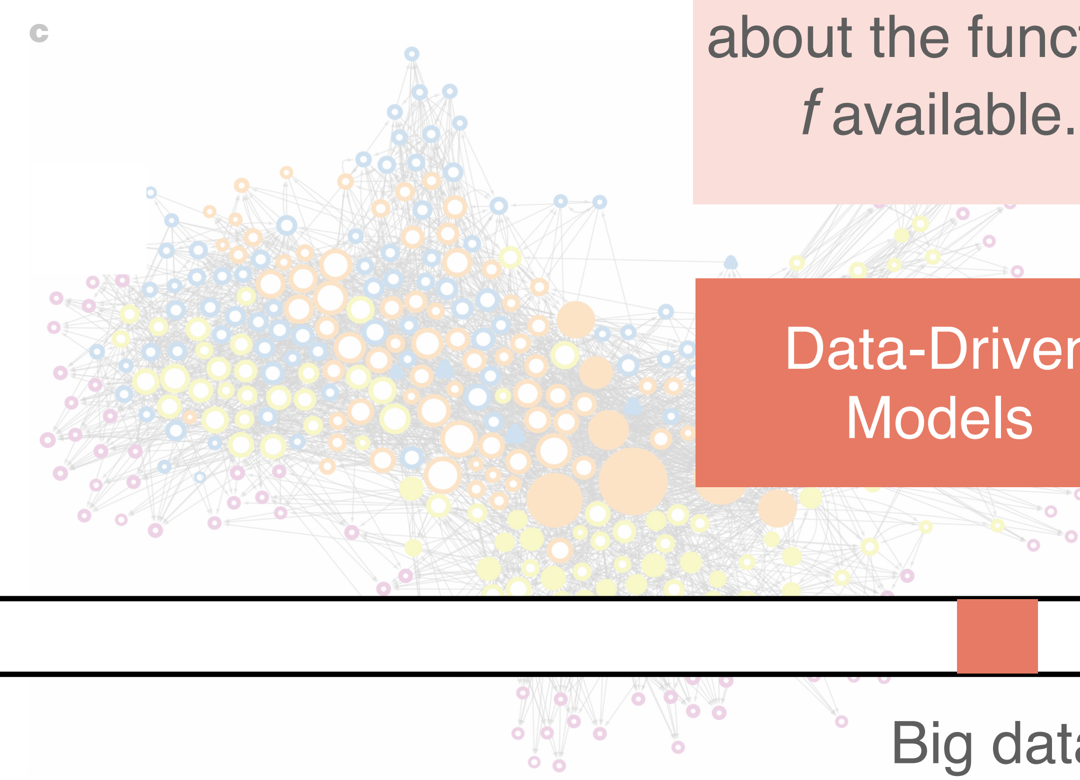
Hypothesis-based Models



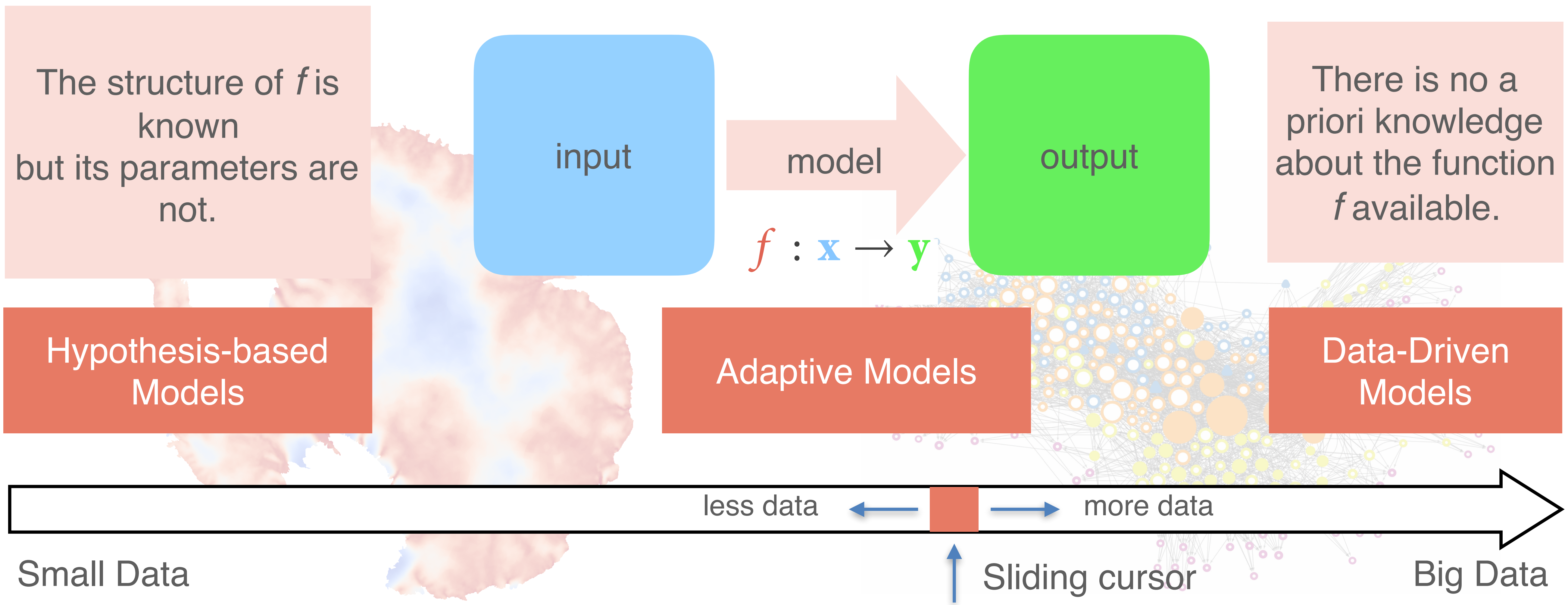


There is no a priori knowledge about the function *f* available.

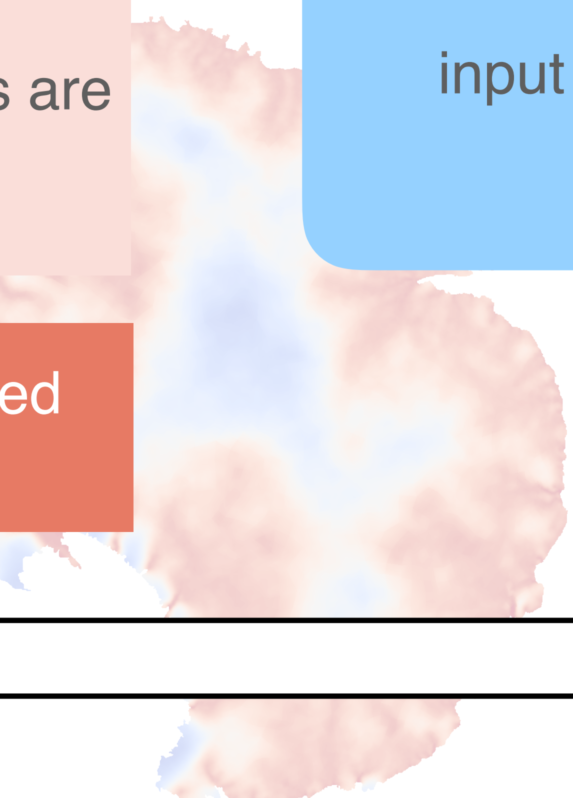
Data-Driven Models

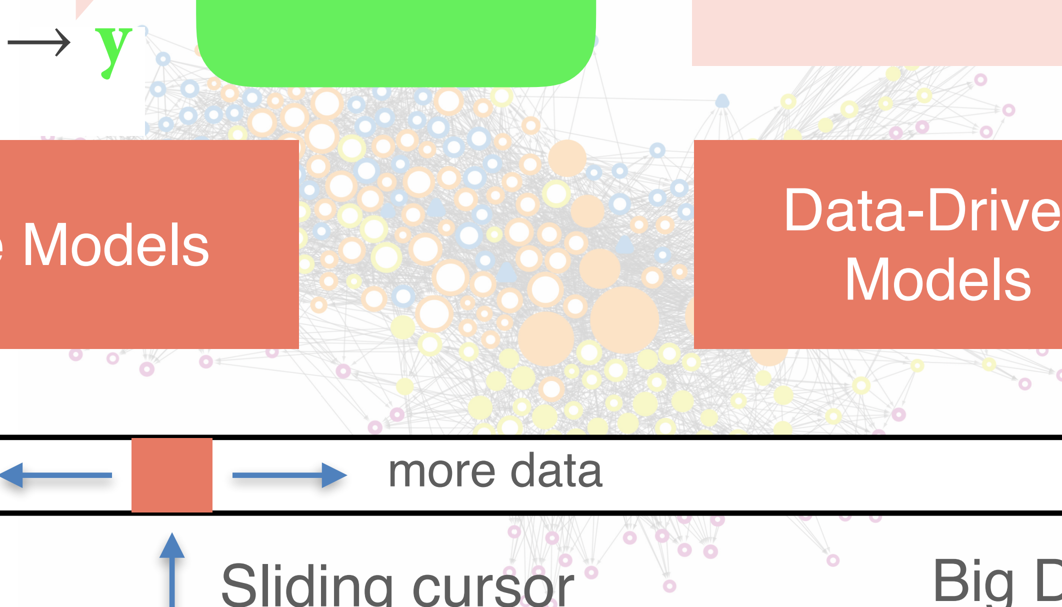
Small data → Big data

Model Discovery



Model Discovery





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

input

model

output

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

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

Hypothesis-based Models

Adaptive Models

Data-Driven Models

less data ← → more data

Small Data

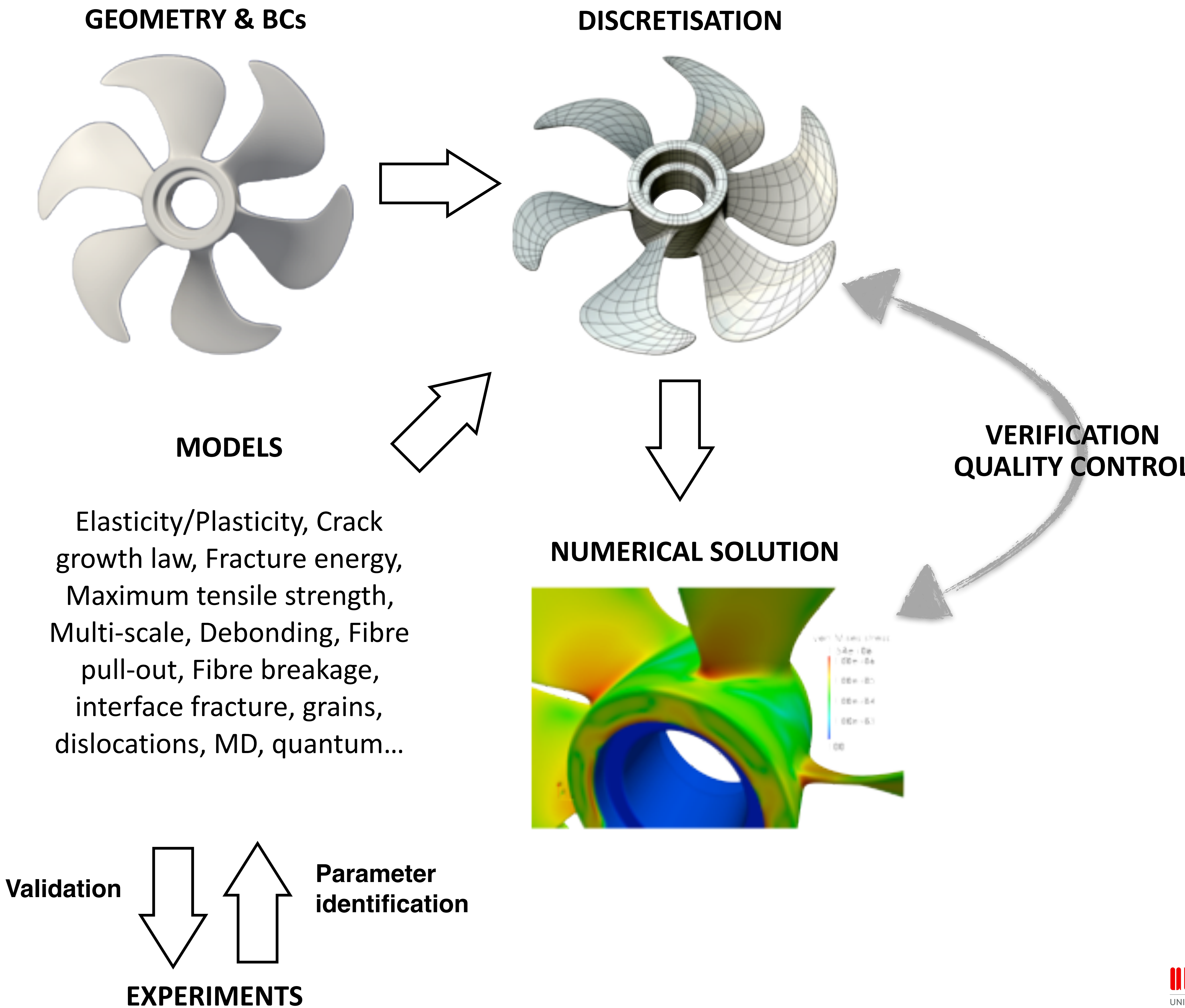
Sliding cursor

Big Data

Computational Engineering Sciences

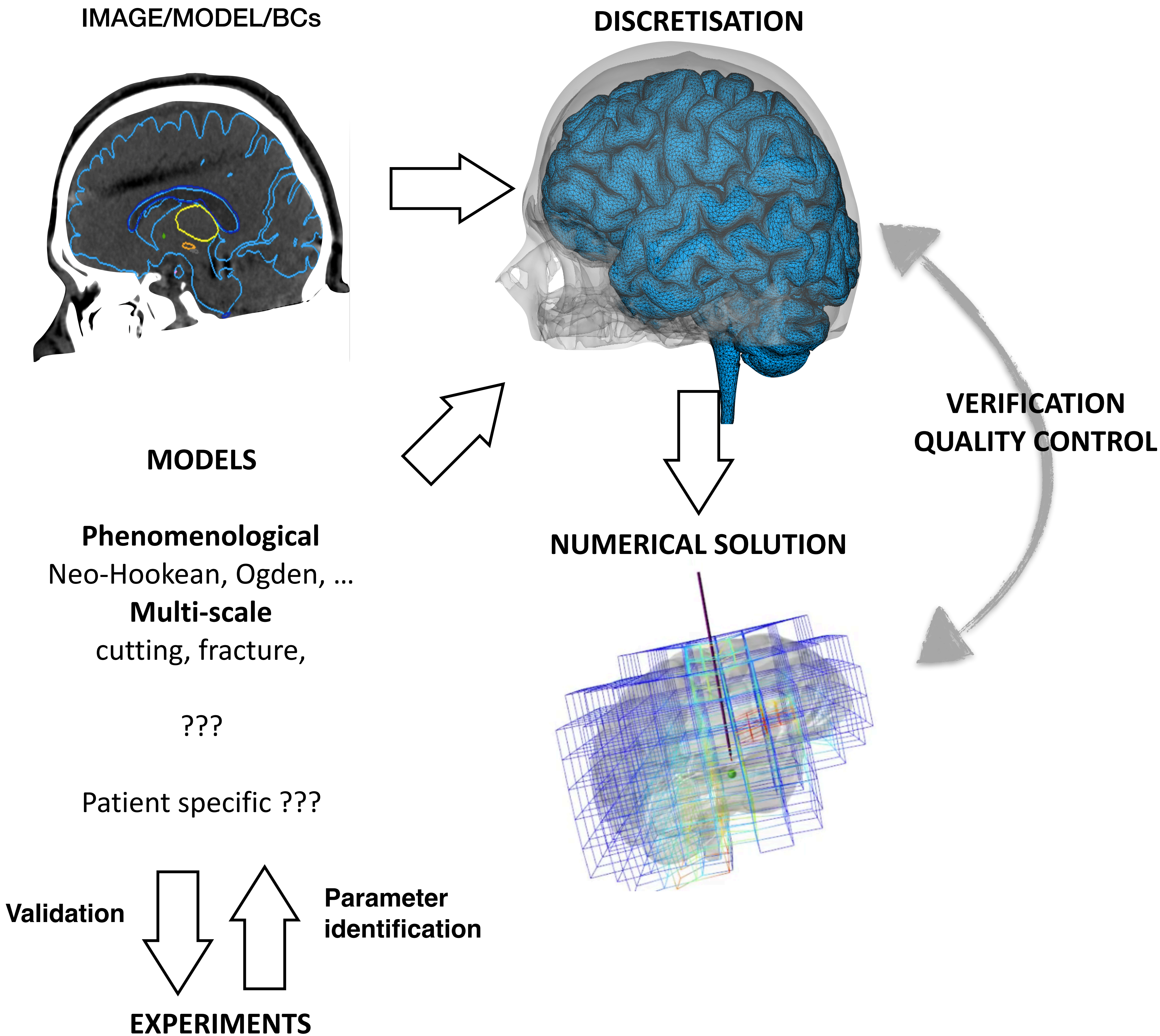
Computational Physics

Mathematics



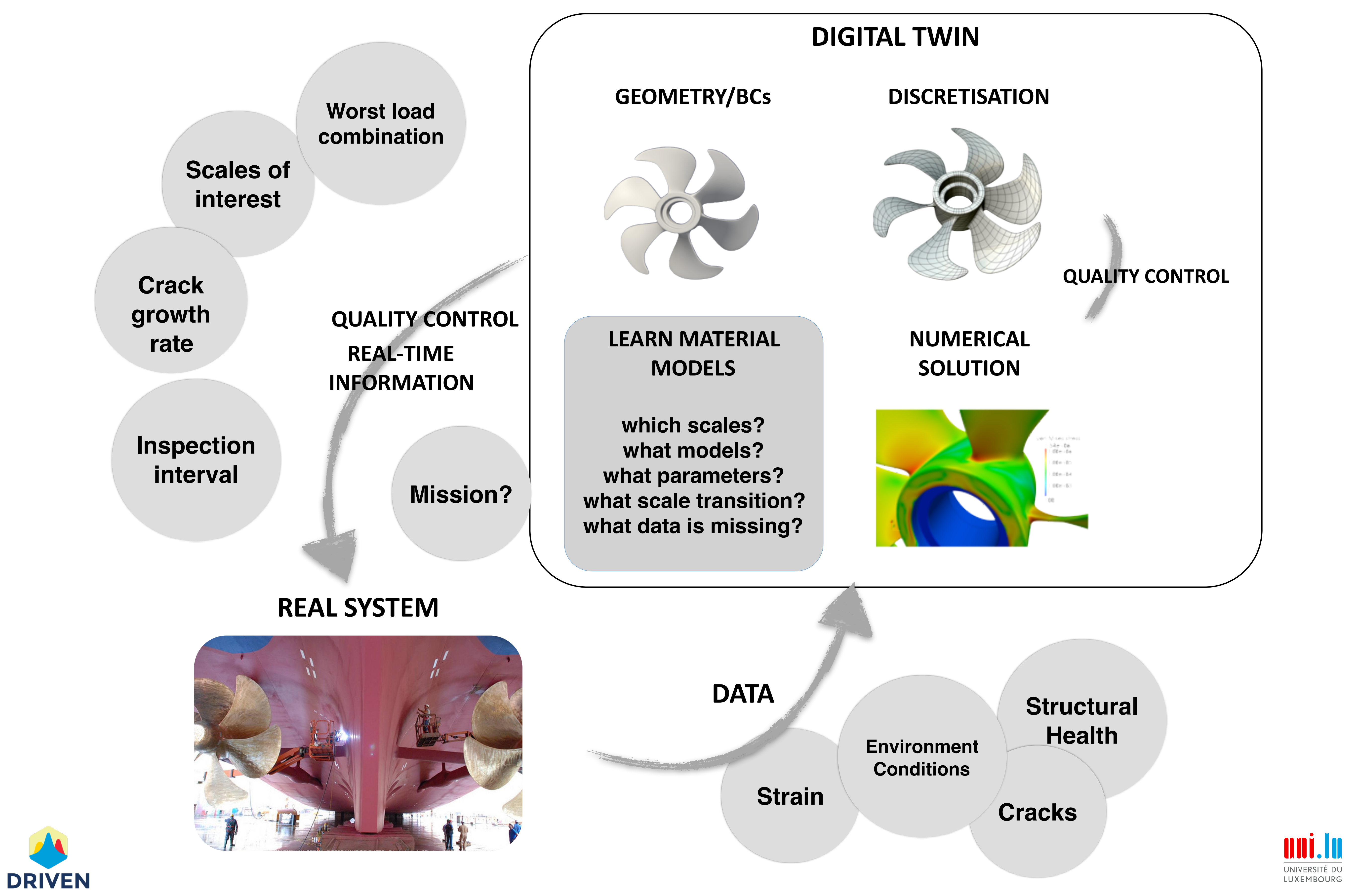
DRIVEN

UNIVERSITÉ DU LUXEMBOURG



DRIVEN

UNIVERSITÉ DU LUXEMBOURG



DIGITAL TWIN
GEOMETRY/BCs
DISCRETISATION
QUALITY CONTROL
LEARN MATERIAL MODELS
which scales?
what models?
what parameters?
what scale transition?
what data is missing?
NUMERICAL SOLUTION
Worst load combination
Scales of interest
Crack growth rate
Inspection interval
Mission?
QUALITY CONTROL
REAL-TIME INFORMATION
REAL SYSTEM
DATA
Strain
Environment Conditions
Structural Health
Cracks
DRIVEN
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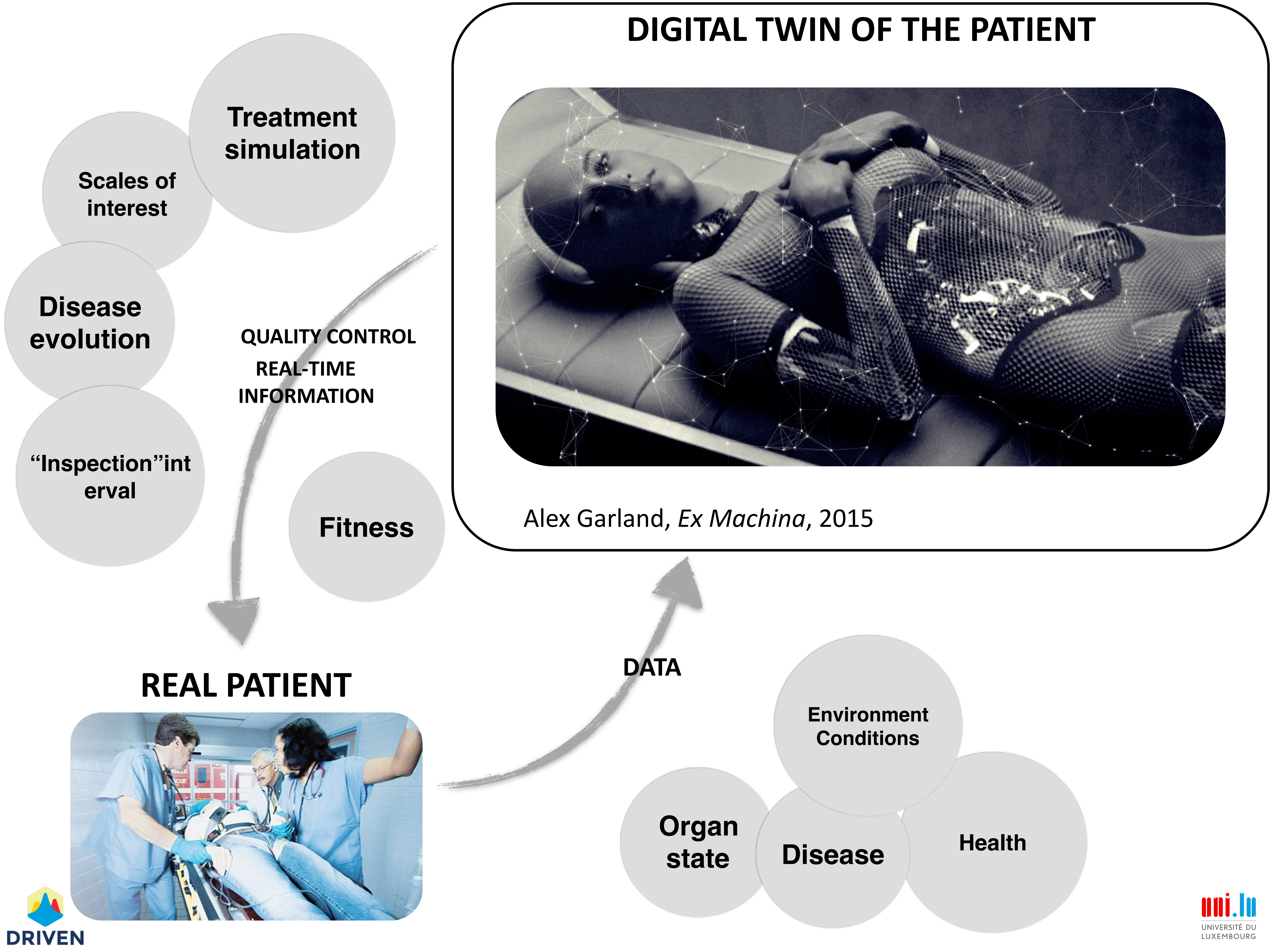
DIGITAL TWIN OF THE PATIENT
Alex Garland, *Ex Machina*, 2015
Treatment simulation
Scales of interest
Disease evolution
“Inspection”interval
Fitness
QUALITY CONTROL
REAL-TIME INFORMATION
REAL PATIENT
DATA
Environment Conditions
Organ state
Disease
Health
DRIVEN
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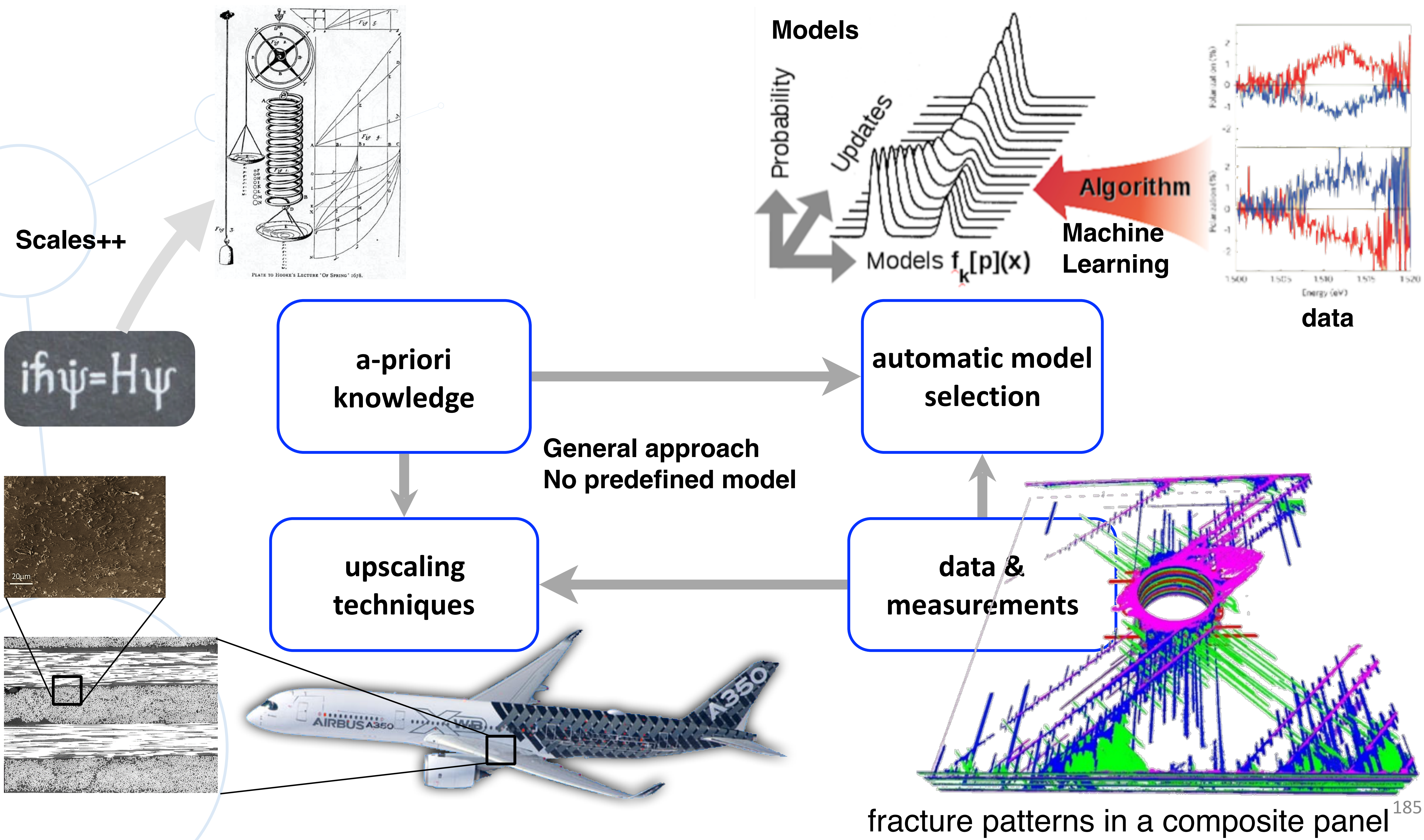
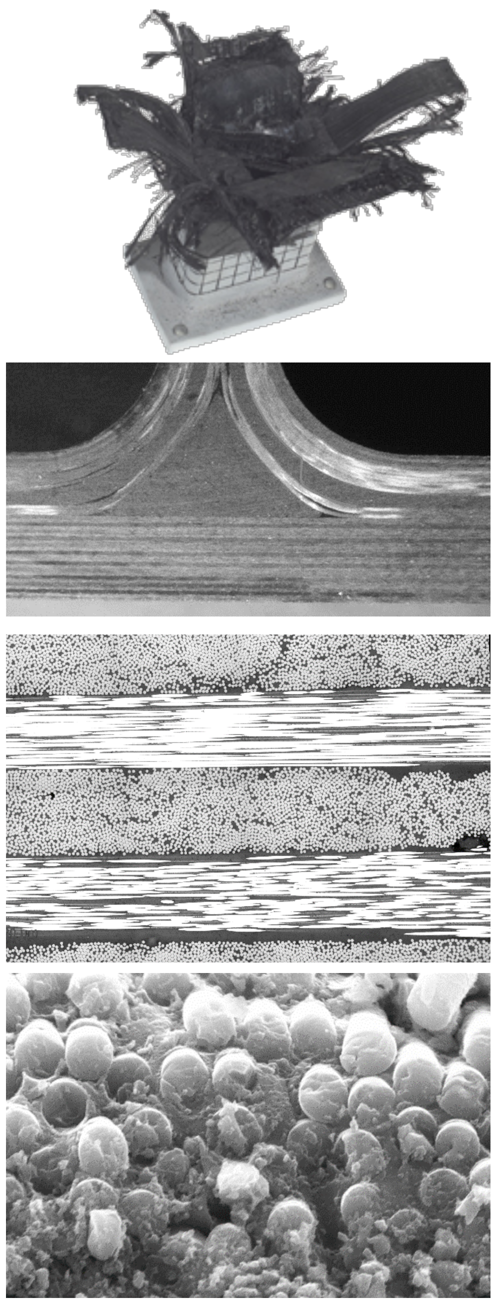
VISION

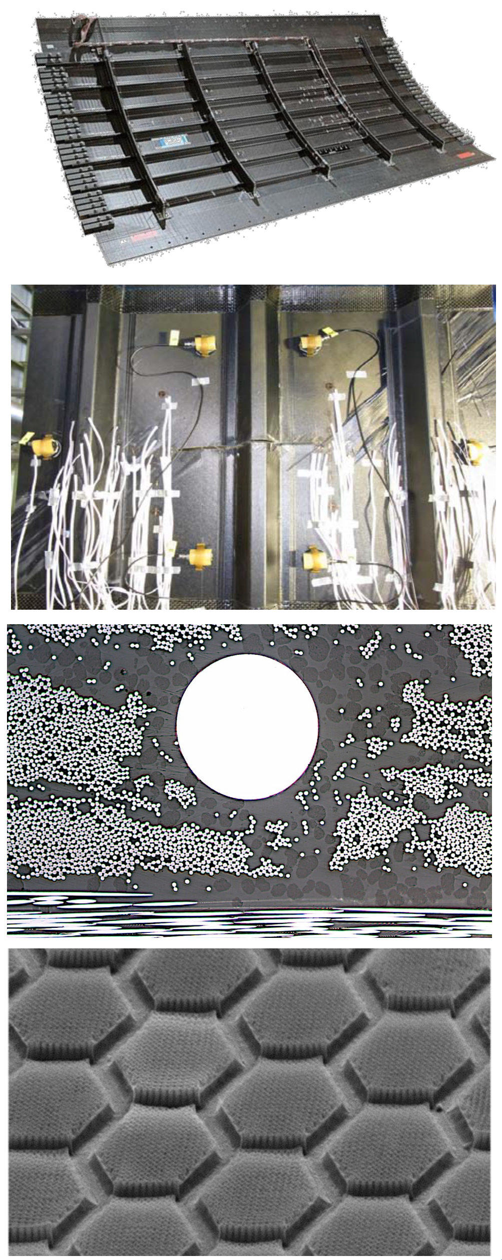

Scales++
iħψ=Hψ
20μm
Models
Probability
Updates
Models f_k[p](x)
Algorithm
Machine Learning
data
a-priori knowledge
automatic model selection
General approach
No predefined model
upscaling techniques
data & measurements
AIRBUS A350
A350
fracture patterns in a composite panel

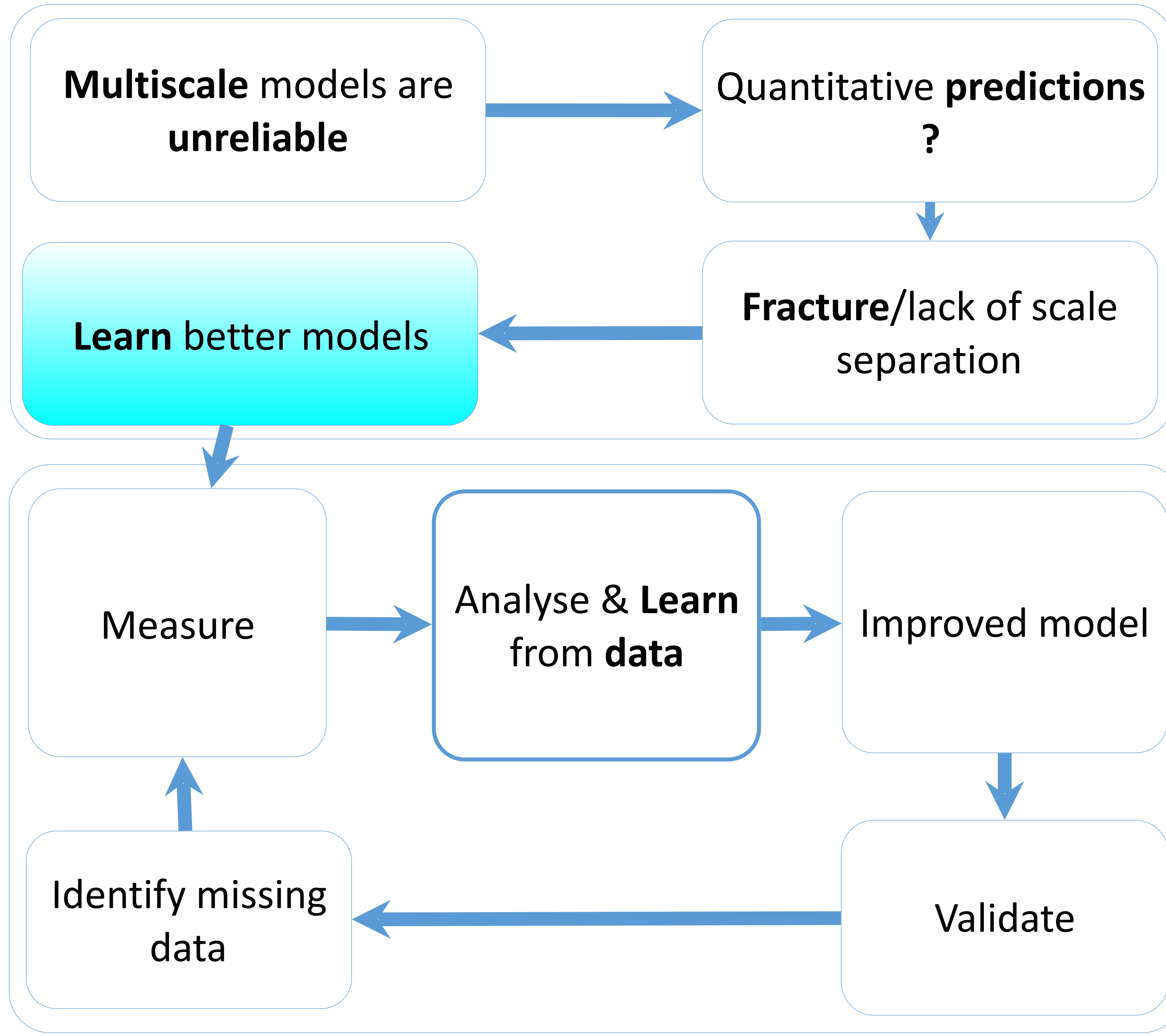
Digital Twins...

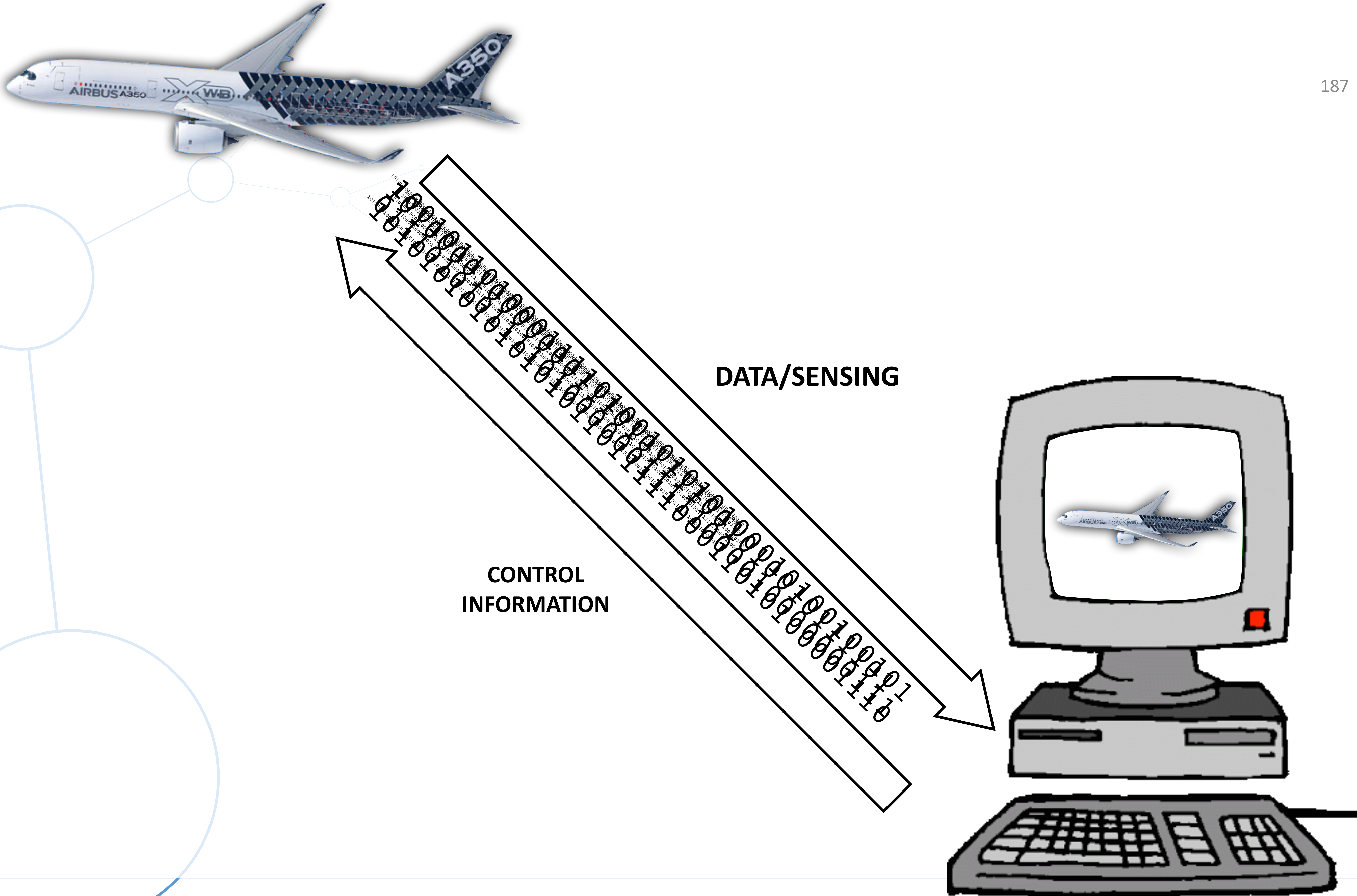
Characterisation



Monitoring






DATA/SENSING
CONTROL
INFORMATION


www.imagespk.com www.imagespk.com www.imagespk.com www.imagespk.com

Prior Knowledge

Prior Knowledge

Hypothesis

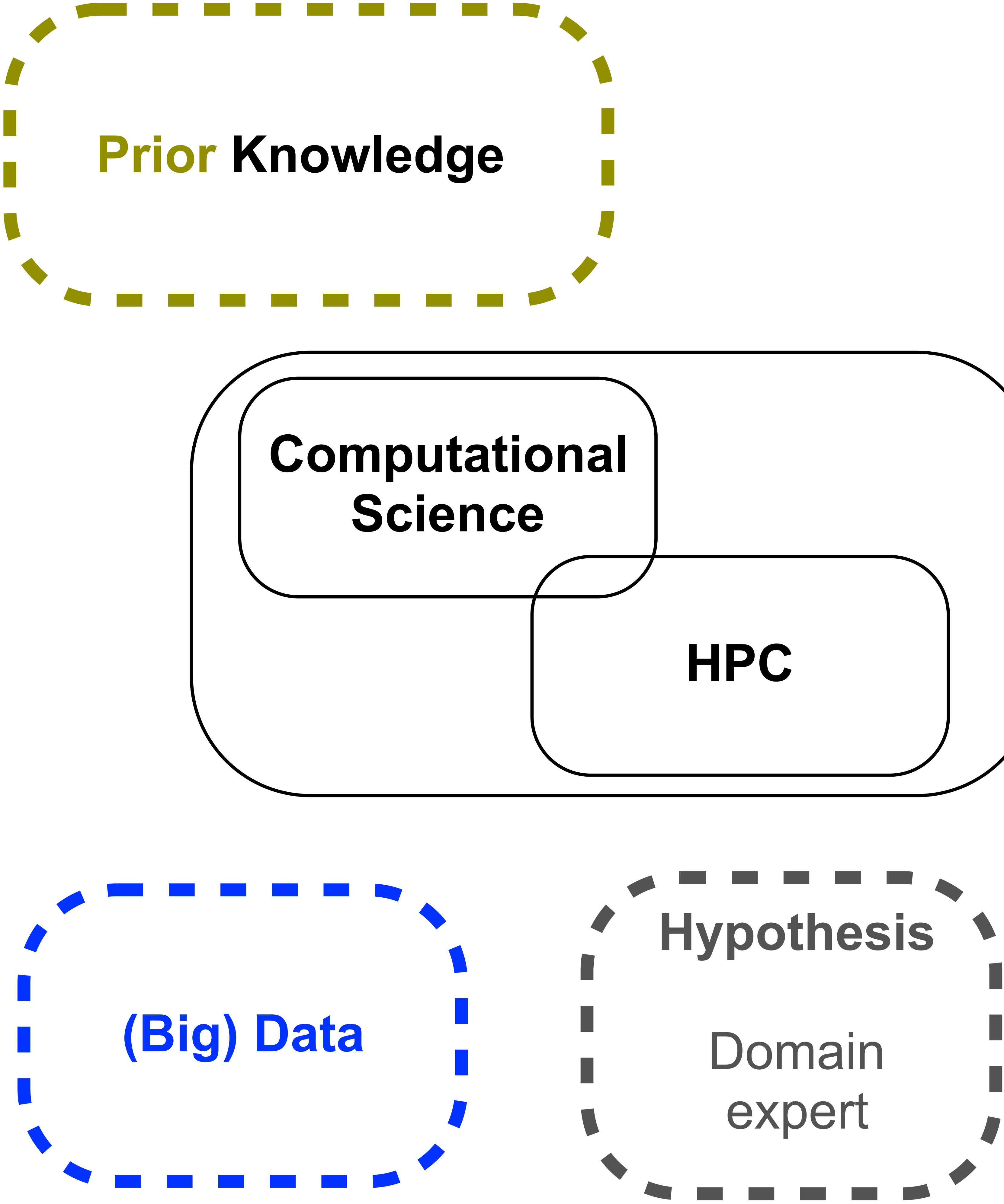
Domain expert

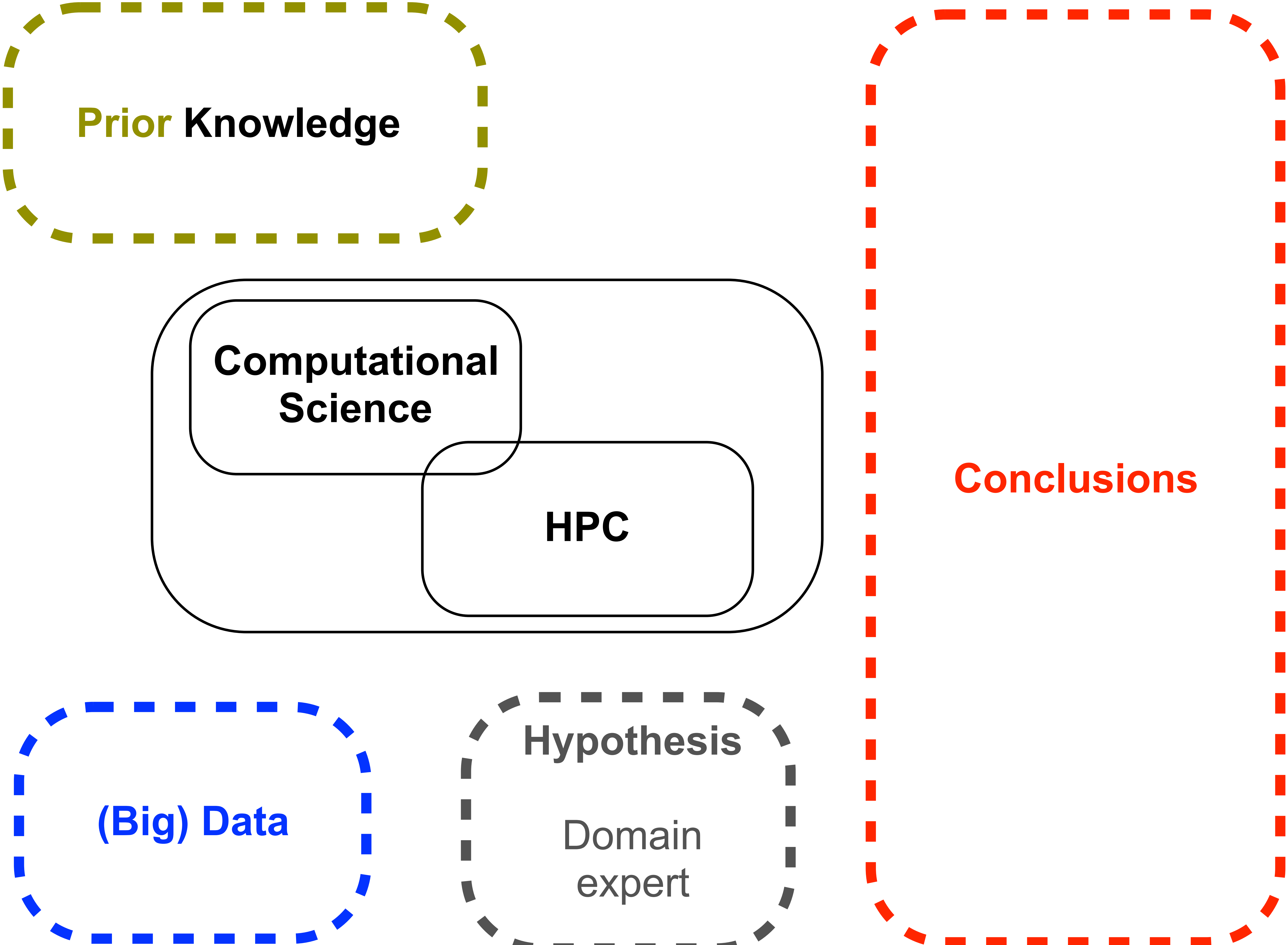
Prior Knowledge

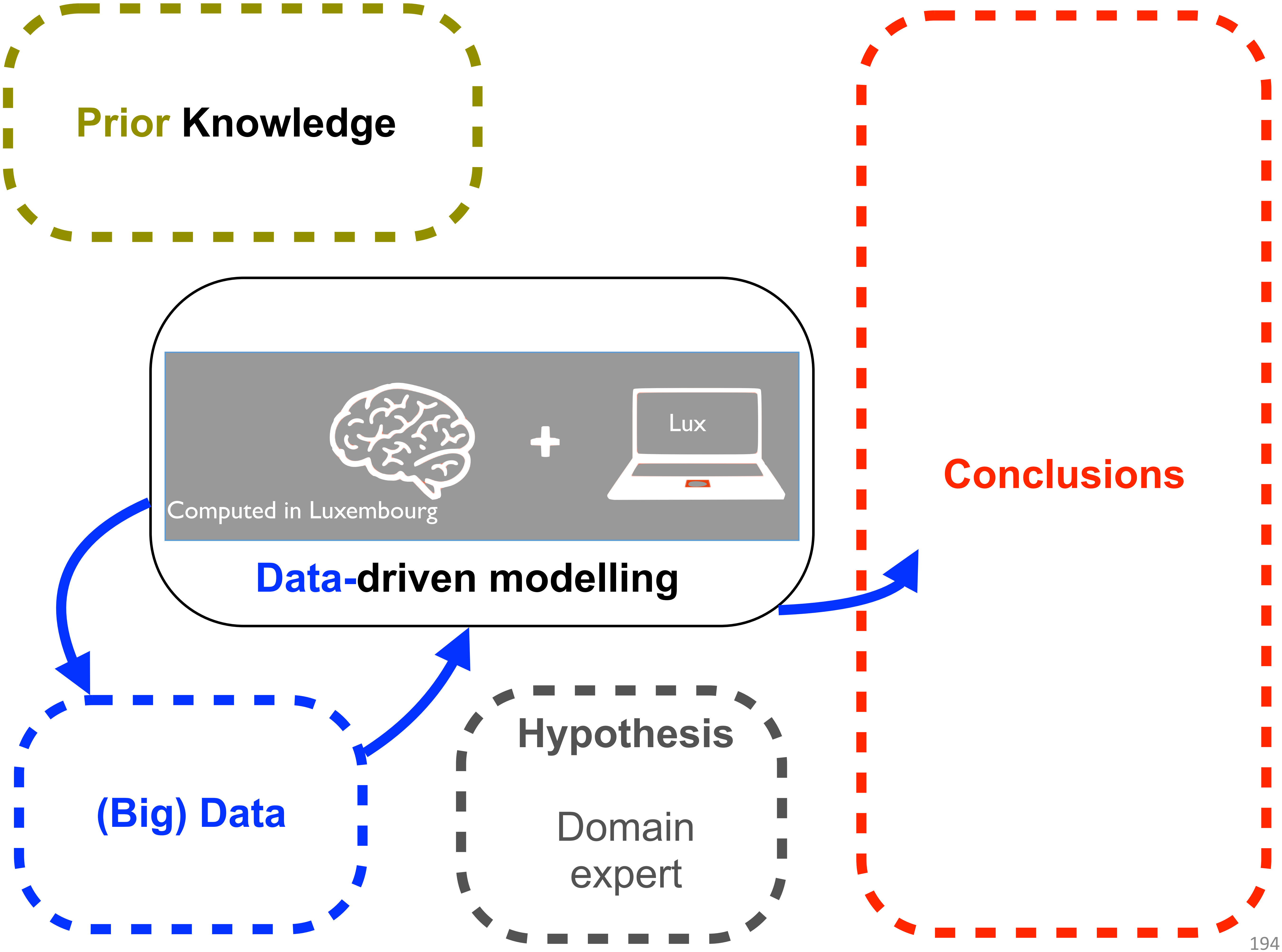
(Big) Data

Hypothesis

Domain expert


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


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


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

Patient-specific material models

1. Prior

Prior knowledge

Material parameters inc. distribution from general population

Noise

- Model (e.g. additive)
- Distribution (Gauss)
- Characterisation

Constitutive model

$$\psi^{\mathrm{eq}}(\mathbf{F}) = \frac{\mu}{2}\left(\frac{(\mathrm{tr}\,\mathbf{B})}{J^{2/3}} - 3\right) + \frac{1}{2}K(J-1)^2$$

Patient-specific material models

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Data assimilator

Bayesian inference

$$\Pr(M|D) = \frac{\Pr(D|M)\Pr(M)}{\Pr(D)}.$$

Patient-specific material models

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$$\Pr(M|D) = \frac{\Pr(D|M)\Pr(M)}{\Pr(D)}.$$

MRI

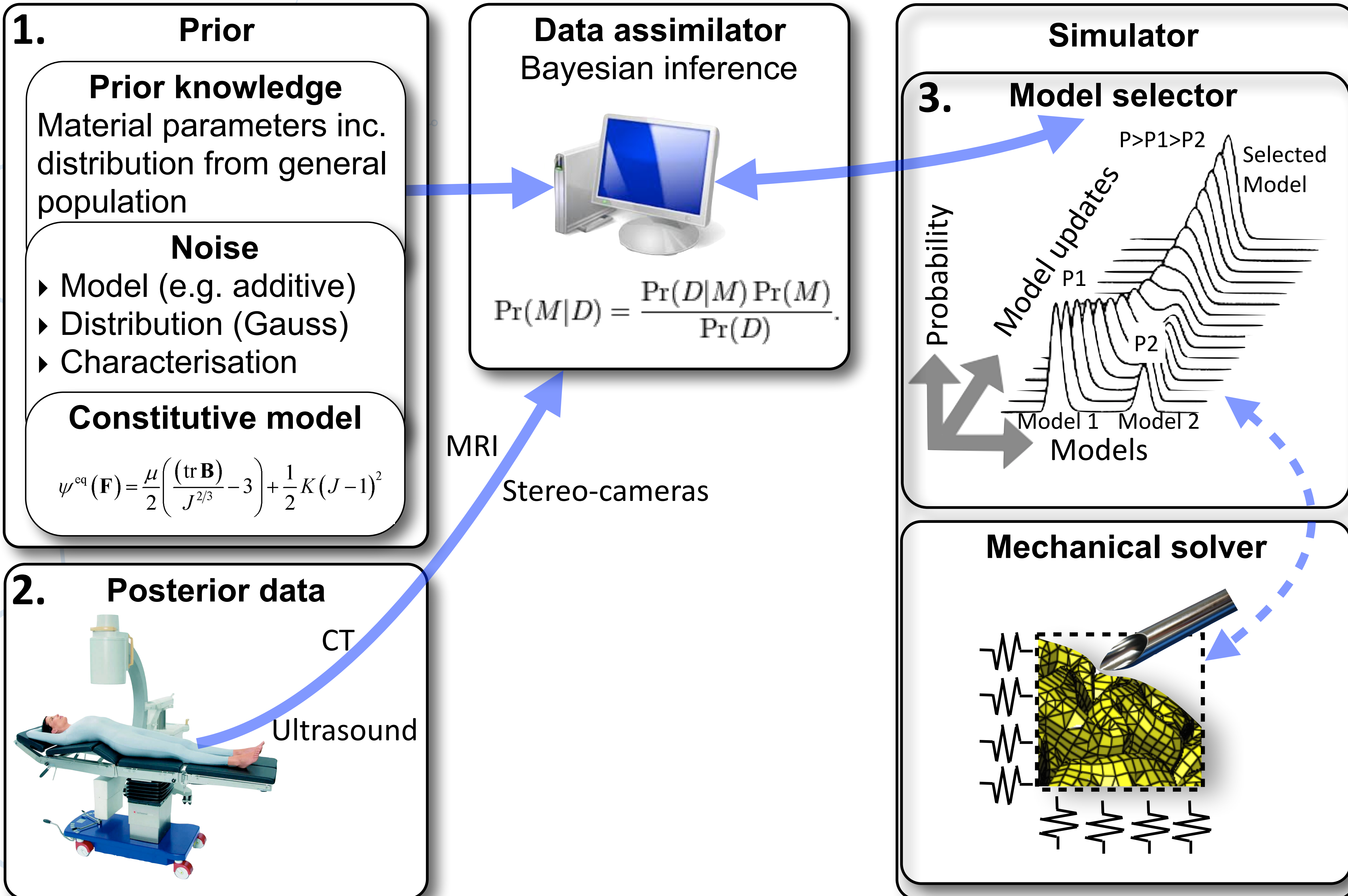
Stereo-cameras

2. Posterior data

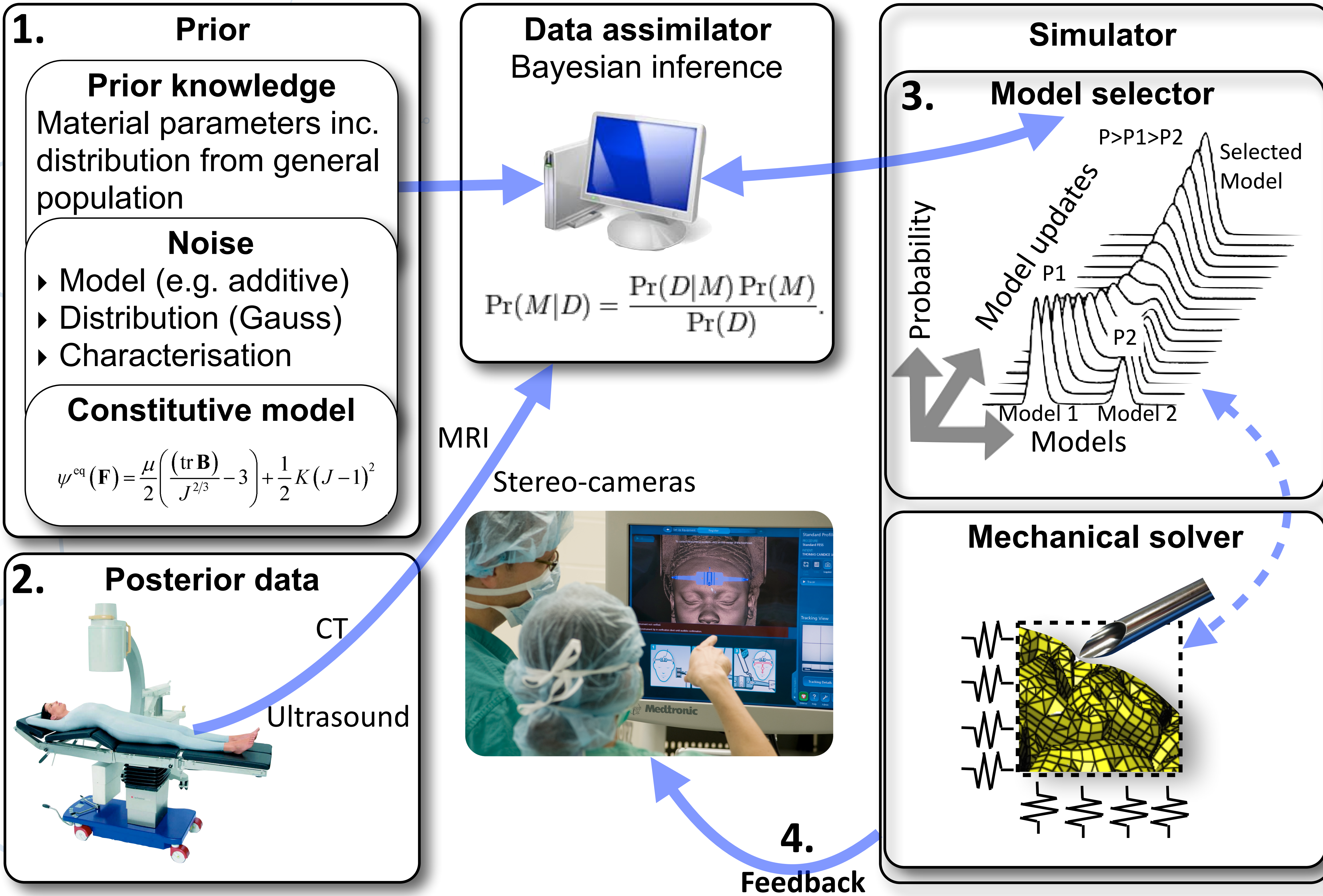
CT

Ultrasound

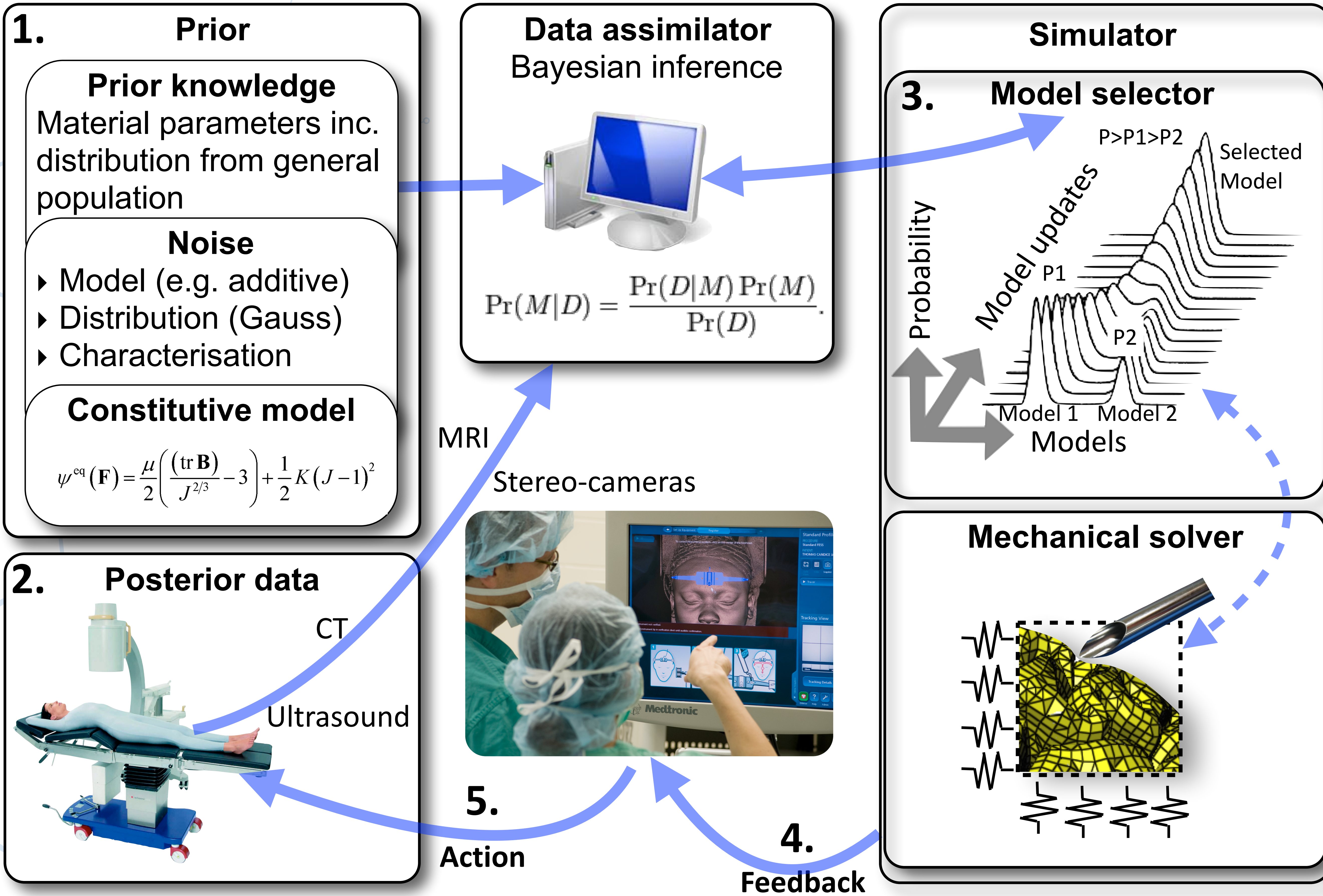
Patient-specific material models



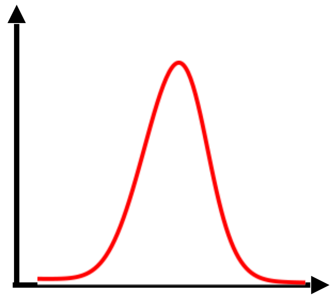
Patient-specific material models

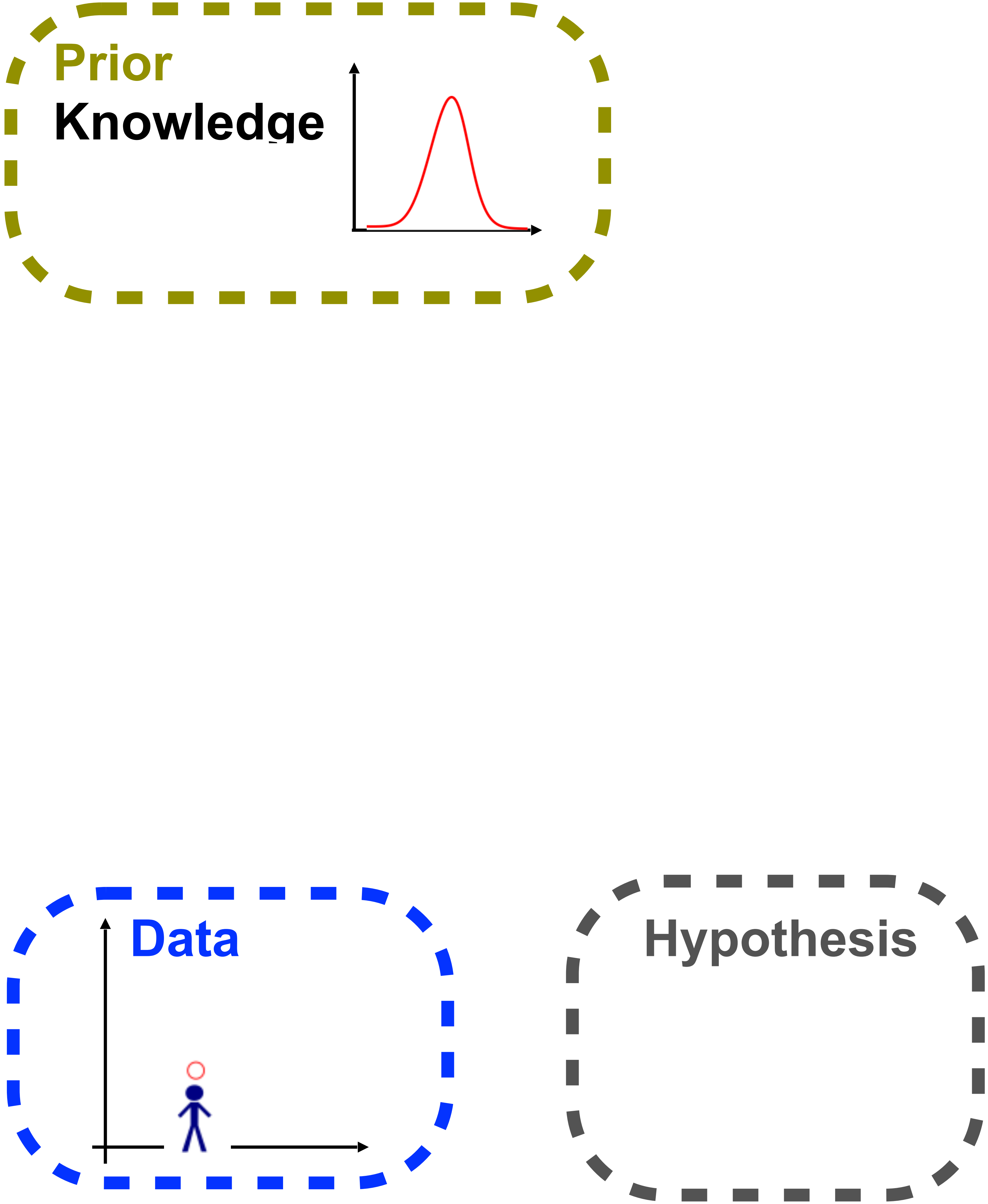


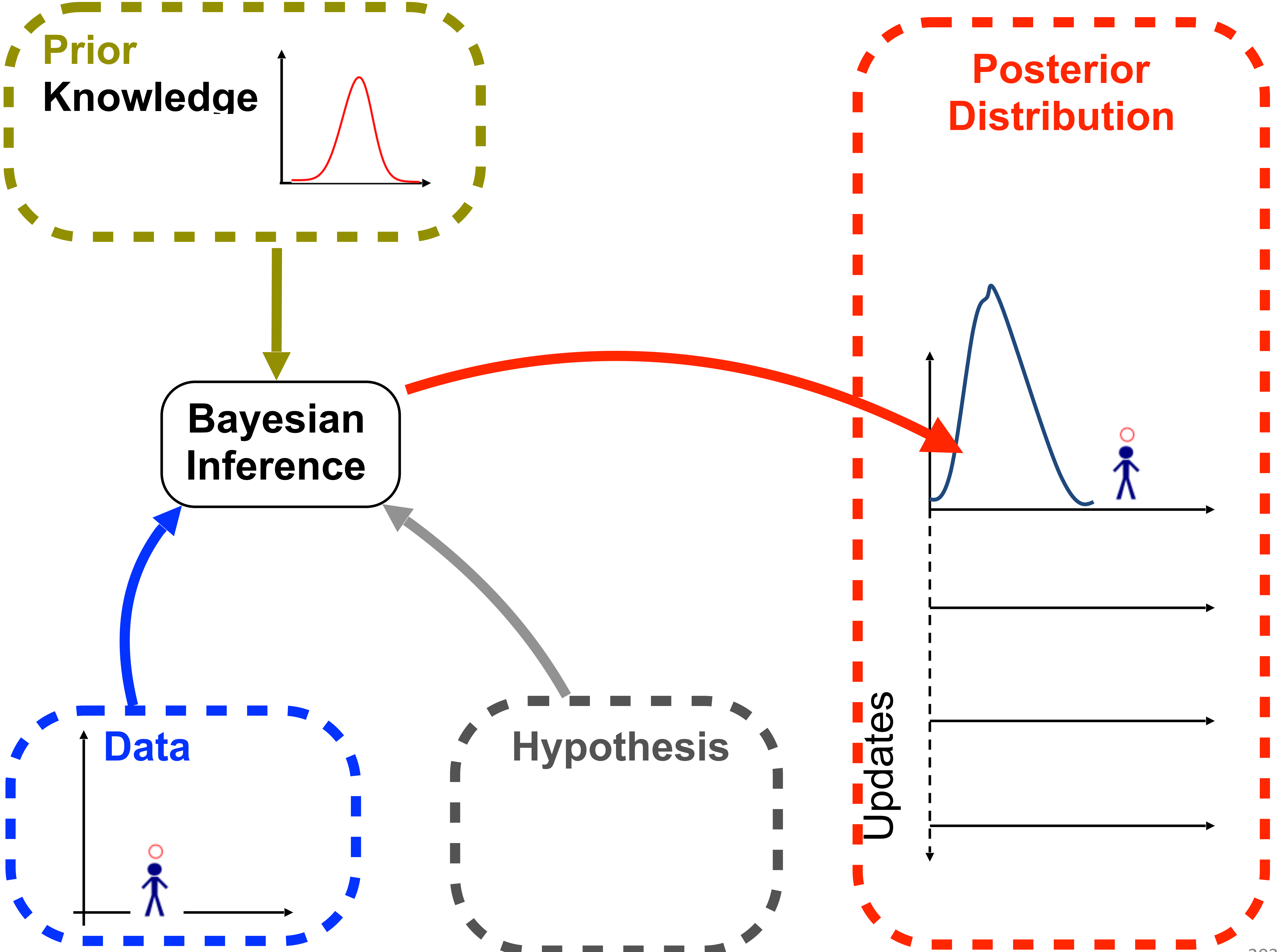
Patient-specific material models

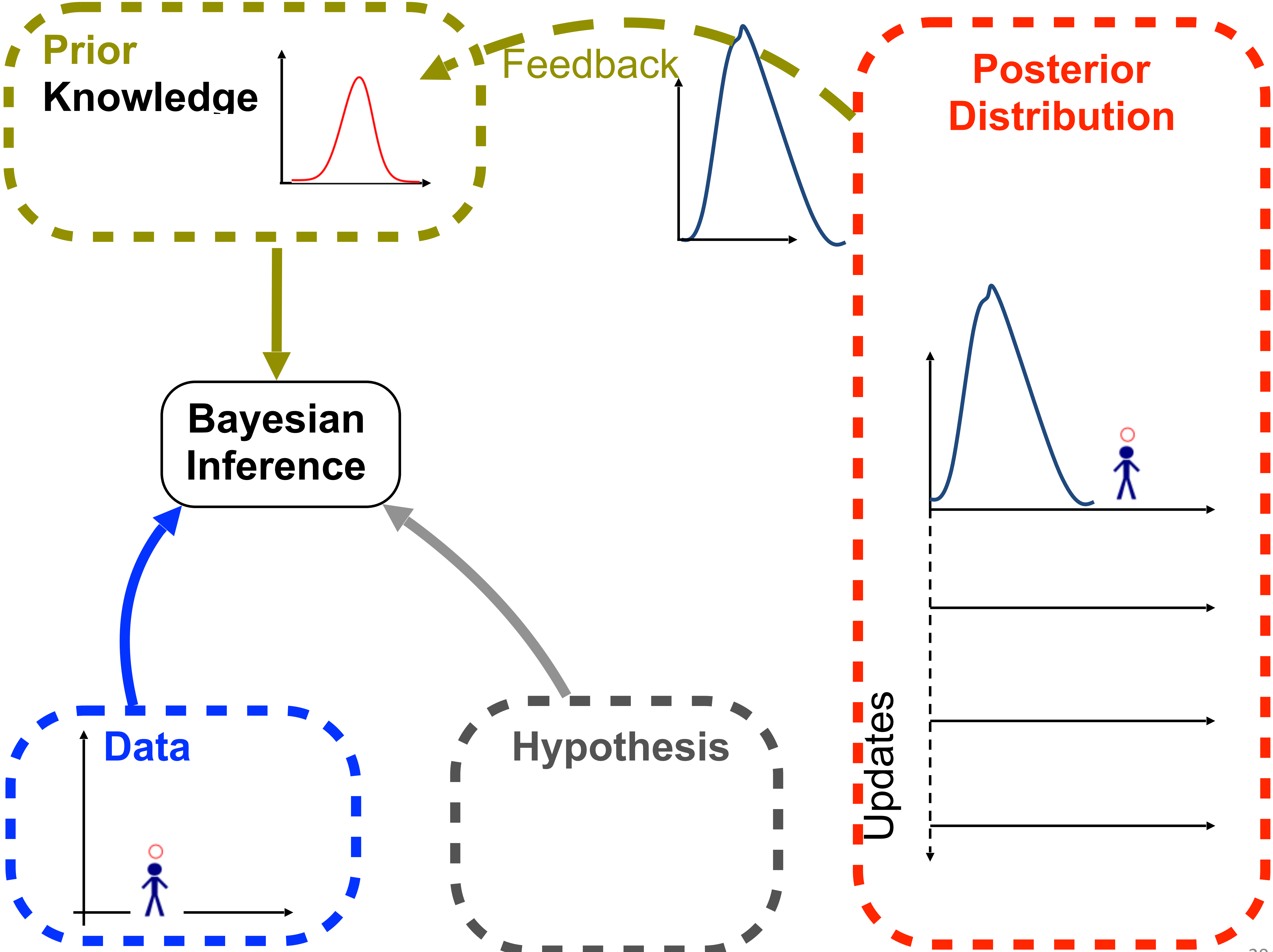


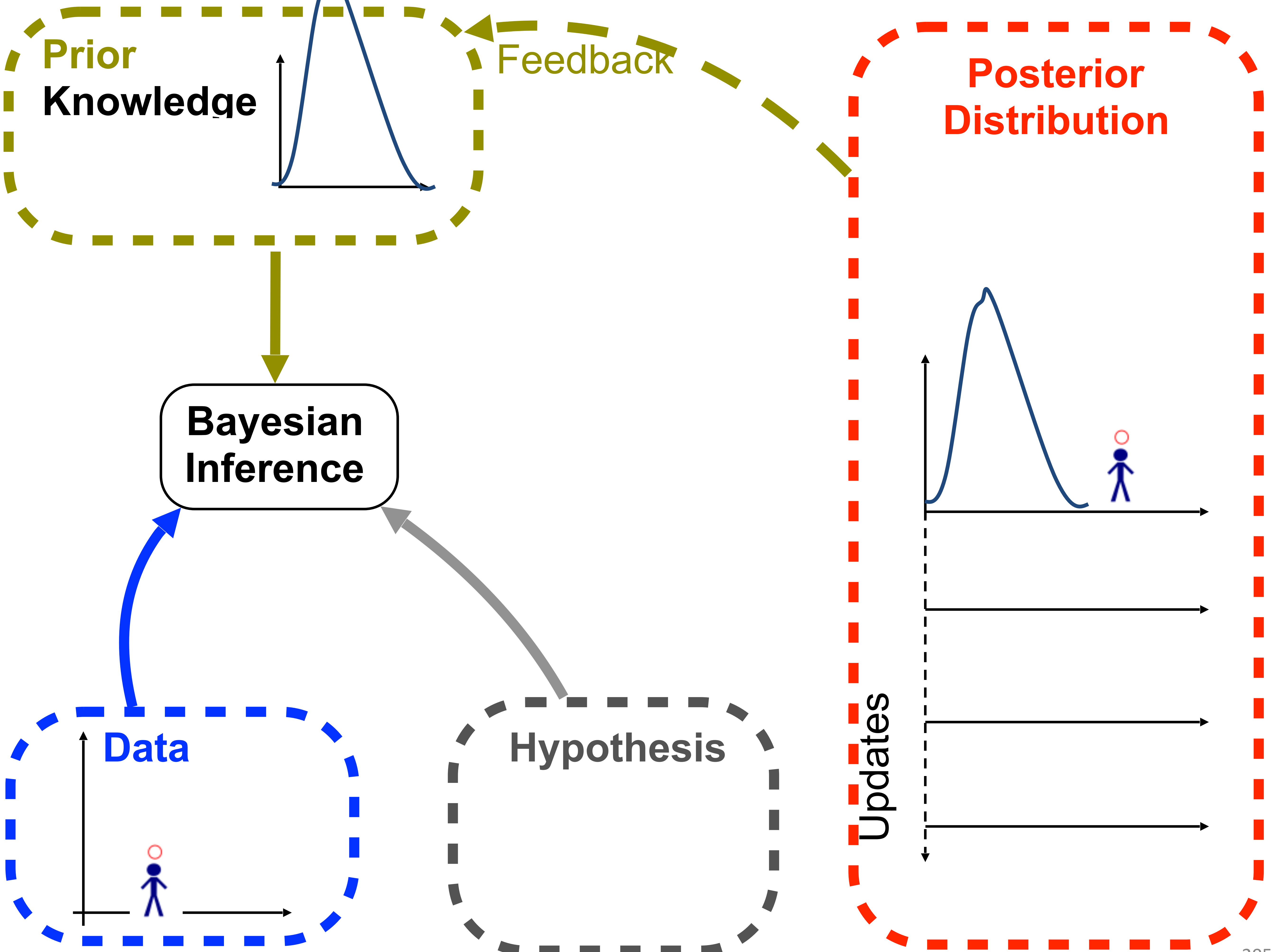
Prior
Knowledge




Prior
Knowledge
Data
Hypothesis


Prior
Knowledge
Bayesian
Inference
Posterior
Distribution
Updates
Data
Hypothesis


Prior
Knowledge
Feedback
Posterior
Distribution
Bayesian
Inference
Data
Hypothesis
Updates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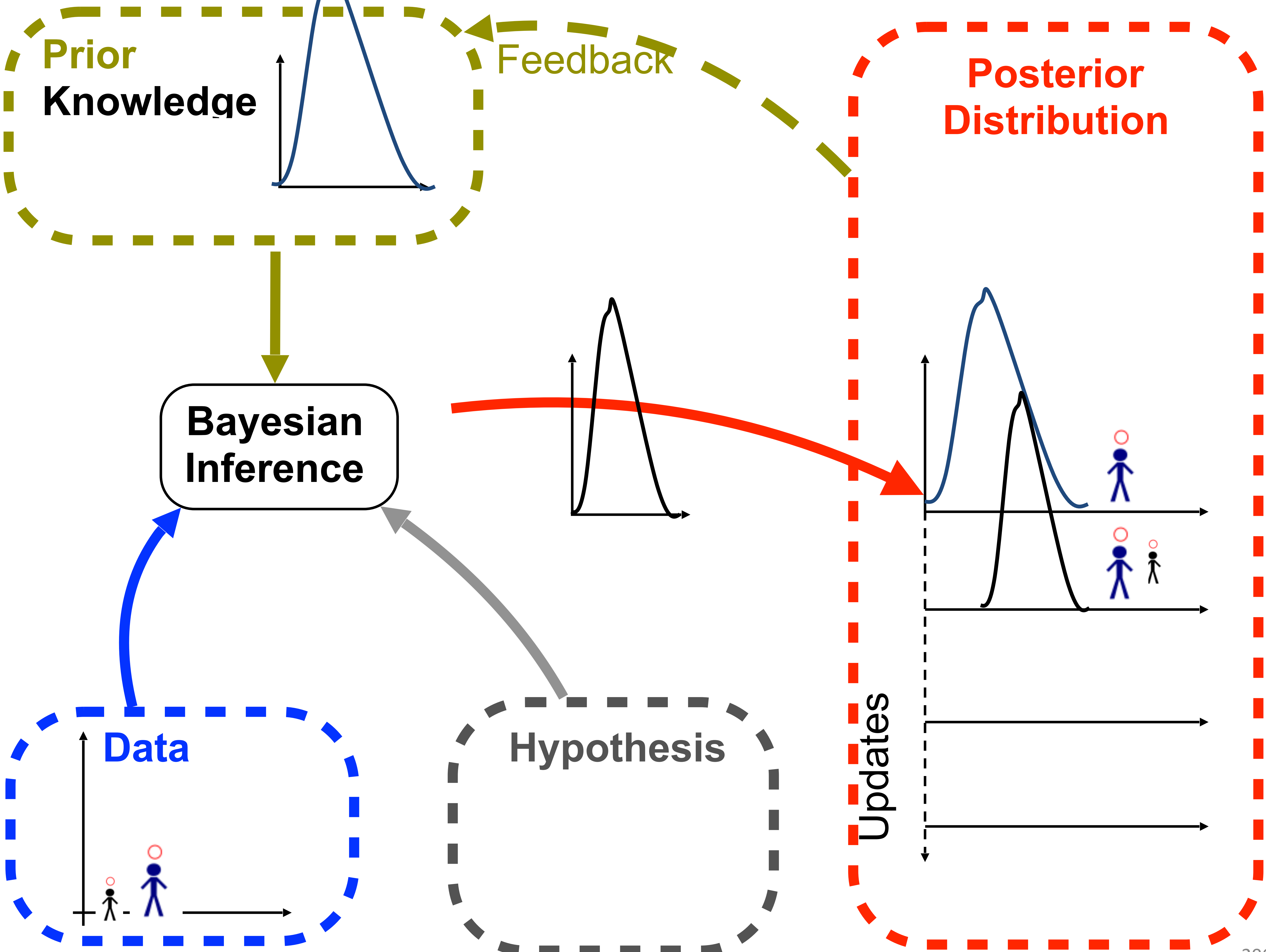
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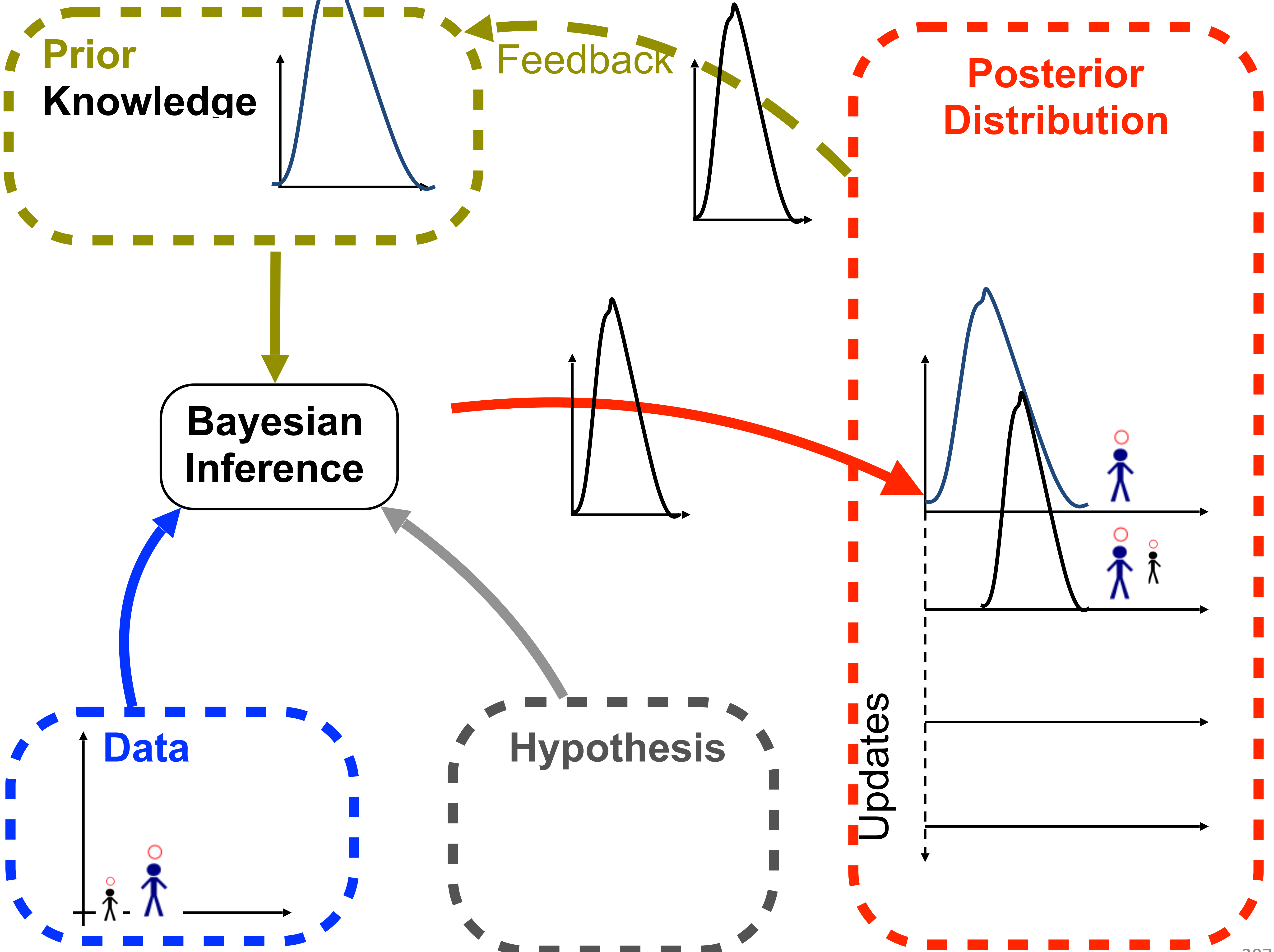
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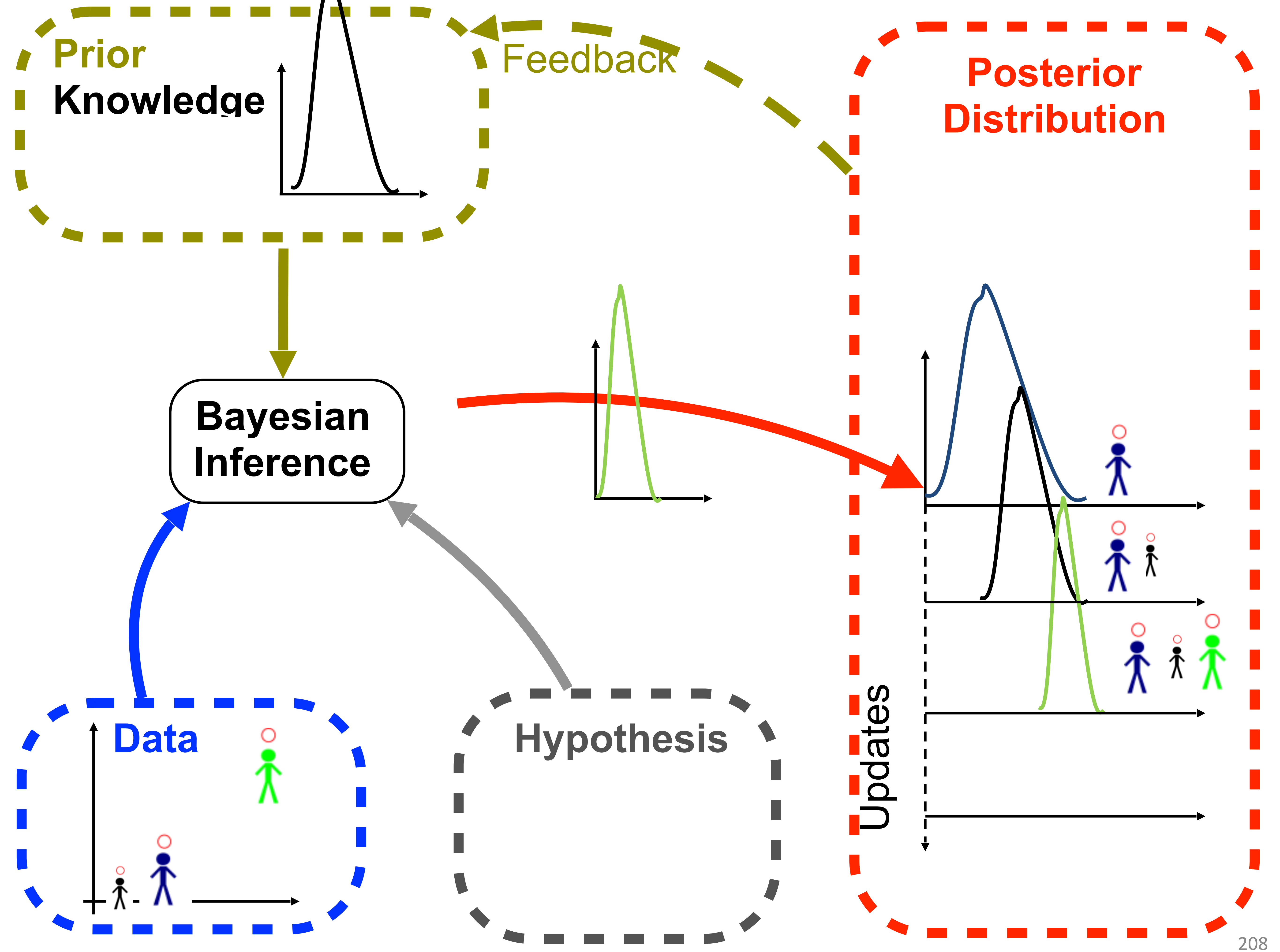

Prior
Knowledge
Feedback
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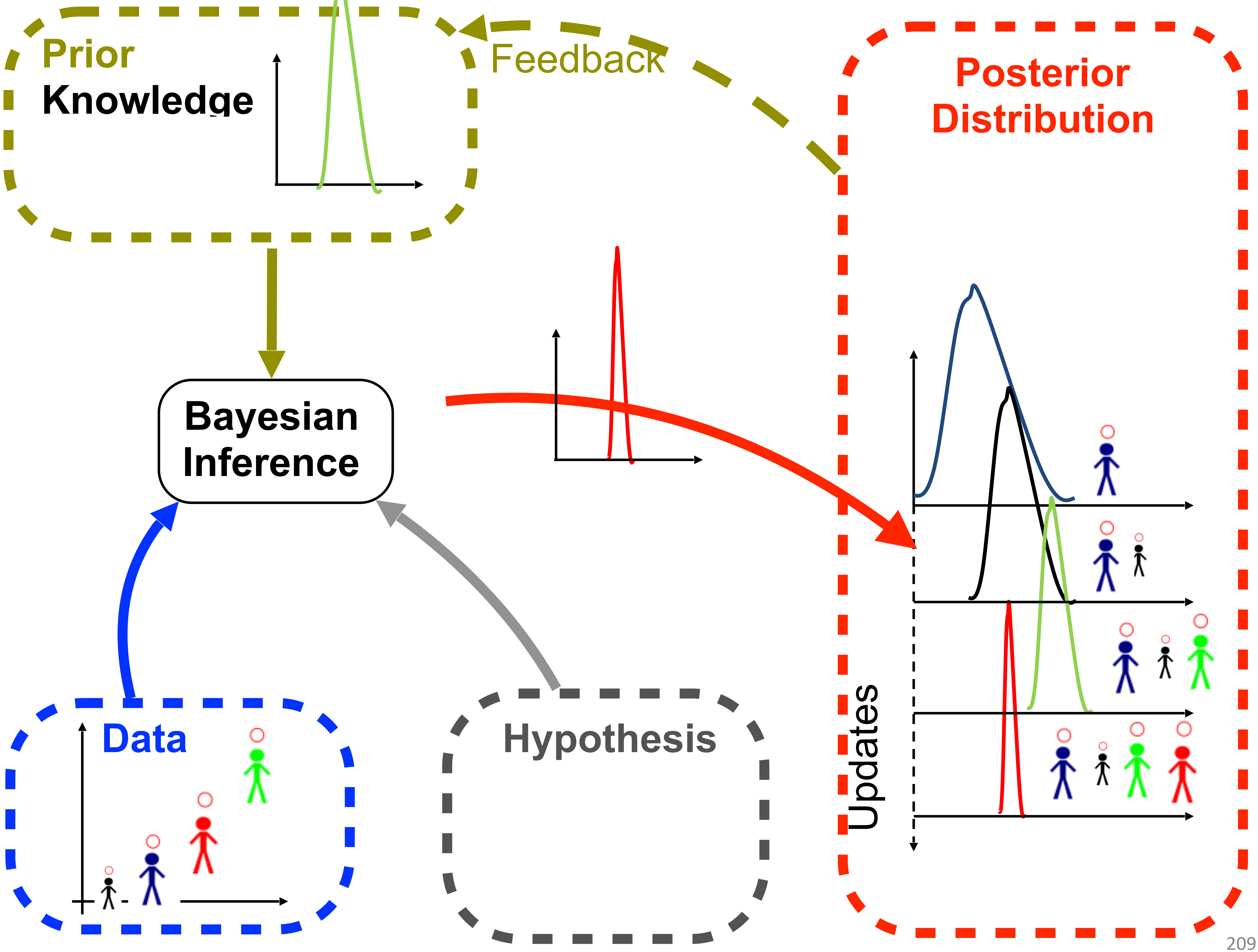
Data
Hypothesis


Prior
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Feedback
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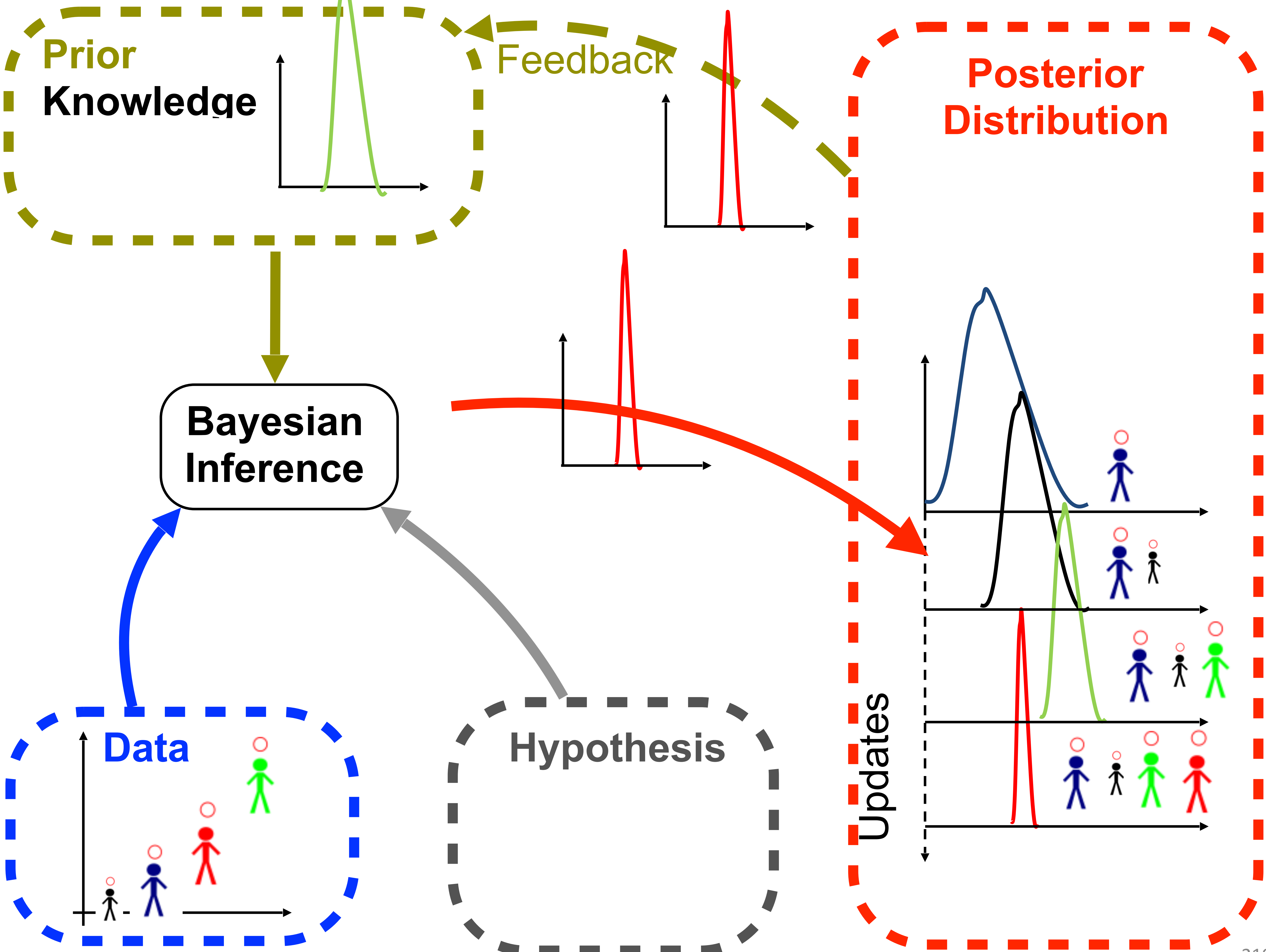
Distribution
Bayesian
Inference
Updates
Data
Hypothesis



Prior
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Feedback
Posterior
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Bayesian
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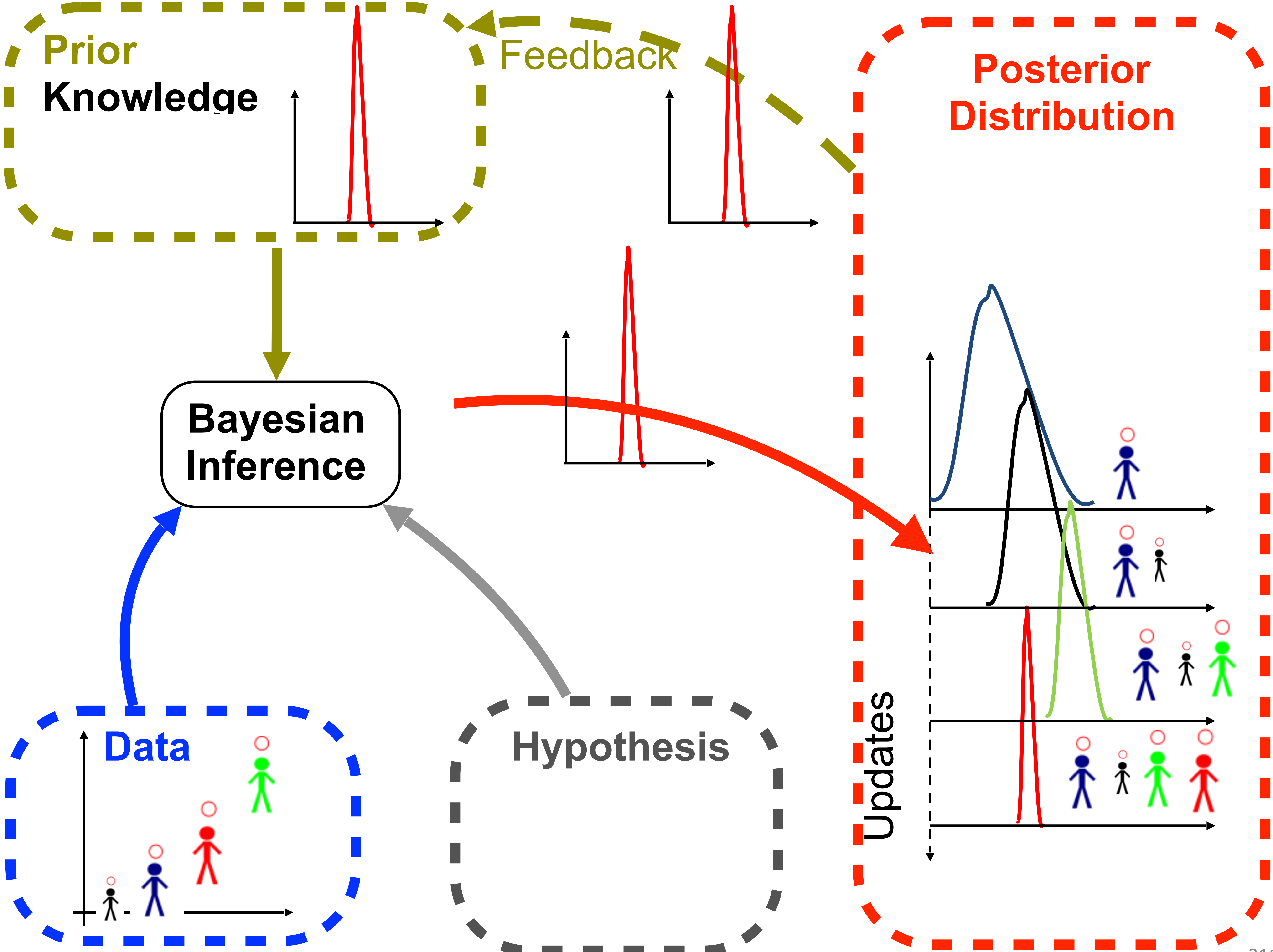
Data
Hypothesis


Prior
Knowledge
Feedback
Posterior
Distribution
Bayesian
Inference
Data
Hypothesis
Updates

Some applications

- Focus on the finite element method
- Applications in materials science
- Applications in fluid dynamics
- Applications in manufacturing
- Applications in biomechanics
- Applications in real-time simulation for surgical training and surgical guidance

Cut Finite Element Methods for Contact Problems

Susanne Claus

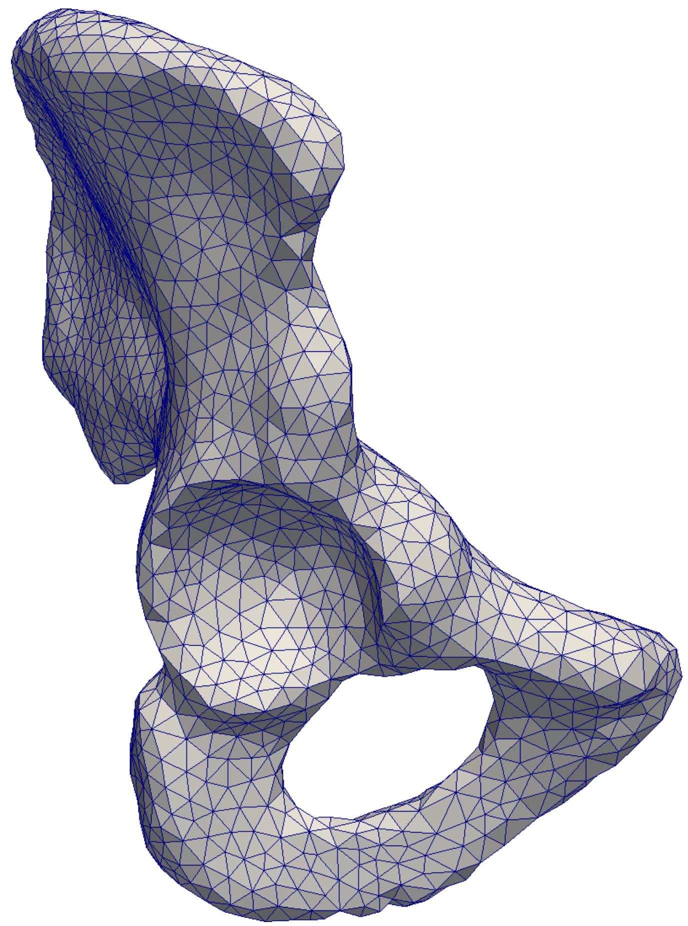
Department of Computer Science, University of Copenhagen, Denmark.

AI Seminar Series, Copenhagen, Jan 2019

THE ALFRED BENZON FOUNDATION

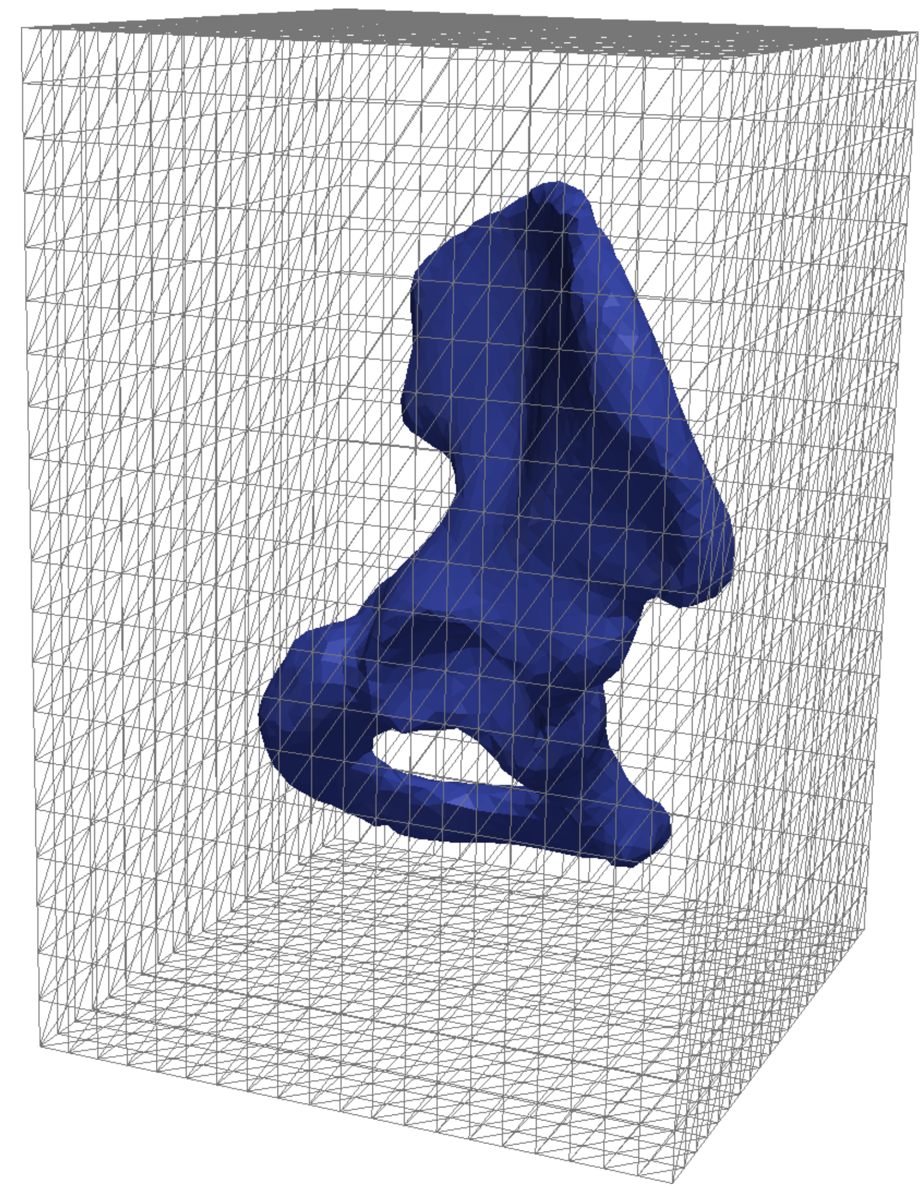
Geometry Discretisation in Finite Element Methods

Classical FEM



Geometry is meshed

CutFEM



Geometry is embedded in fixed background grid and described by a function (e.g. level set function)

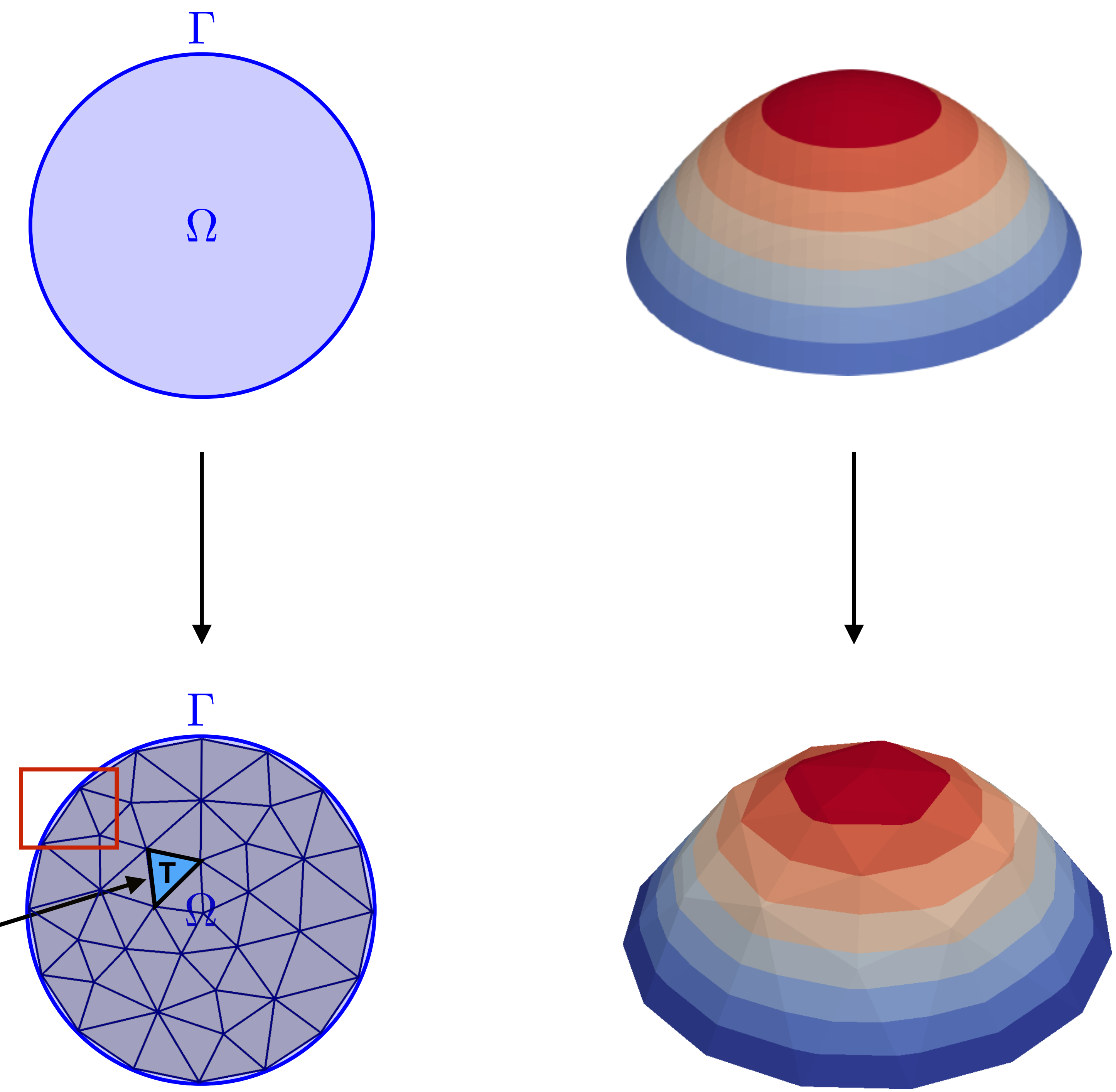
Finite Element Methods

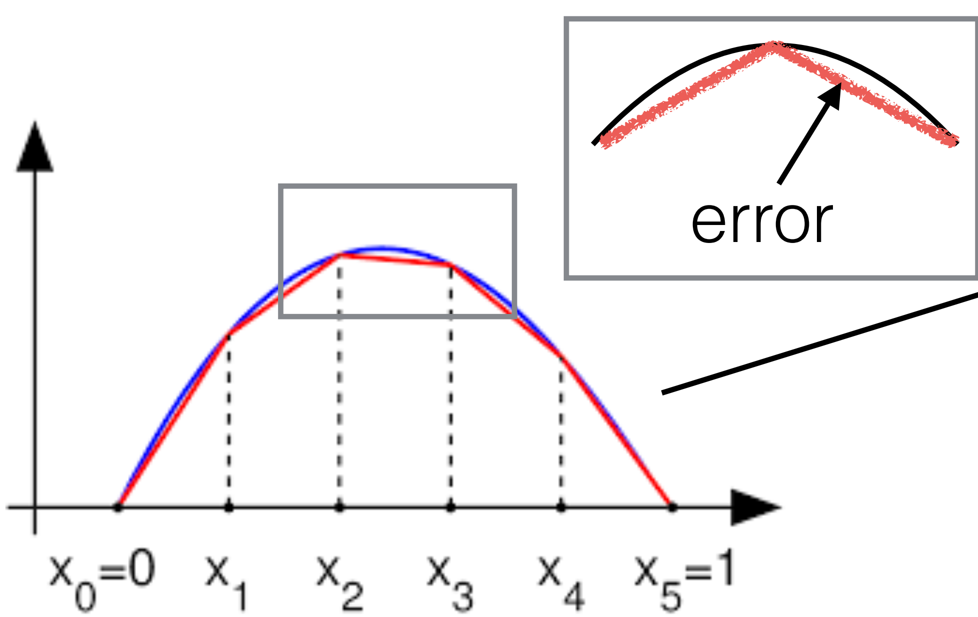
Consider the following diffusion partial differential equation (PDE)

$$-\Delta u = f \text{ in } \Omega$$
$$u = 0 \text{ on } \Gamma$$

Find $u \in V$ such that

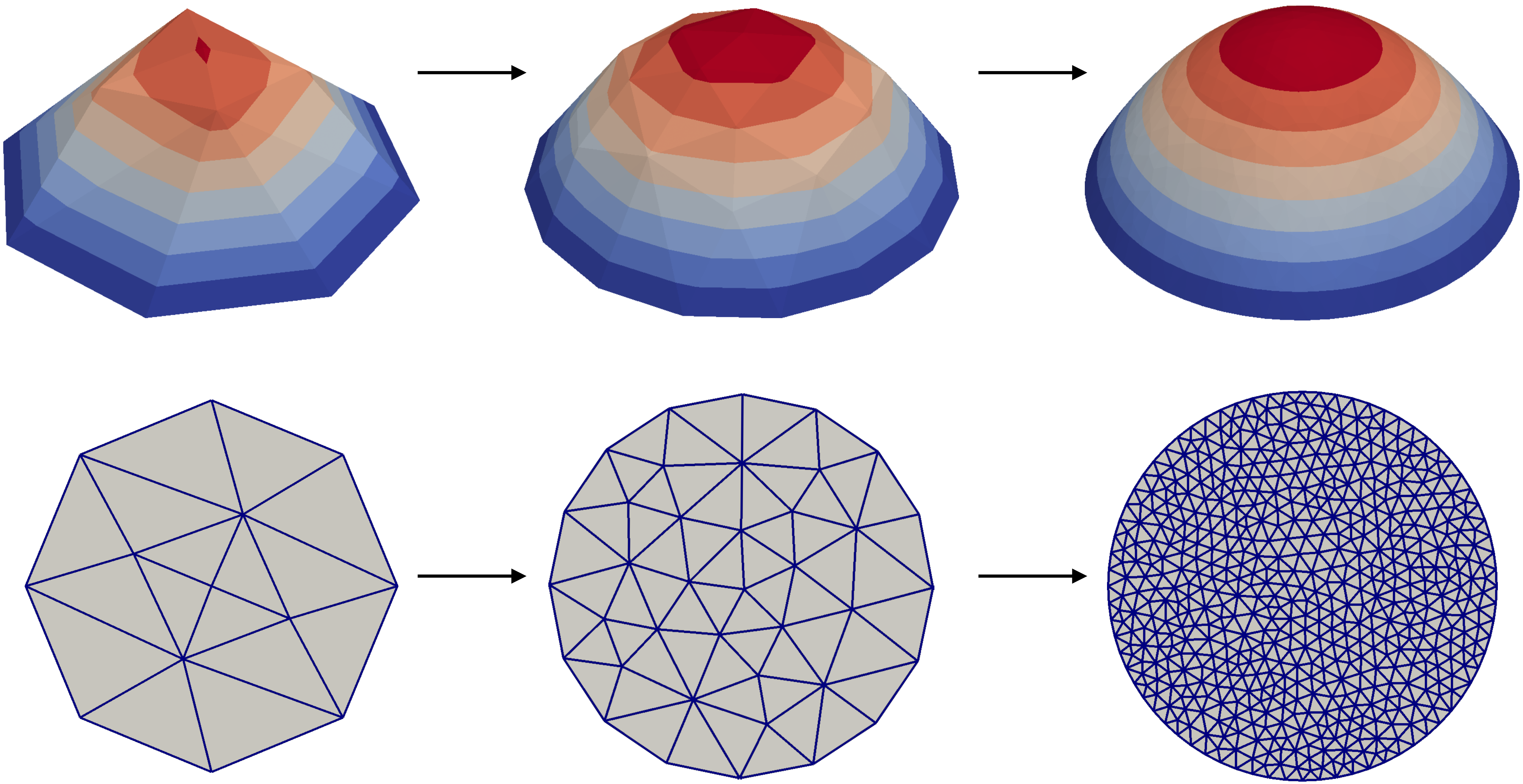
$$\int_\Omega \nabla u \cdot \nabla v dx = \int_\Omega f v dx \quad \forall v \in V$$





Convergence with mesh refinement

The error decreases with mesh refinement. However, how fast the error decreases with mesh refinement (convergence order) depends on multiple factors.



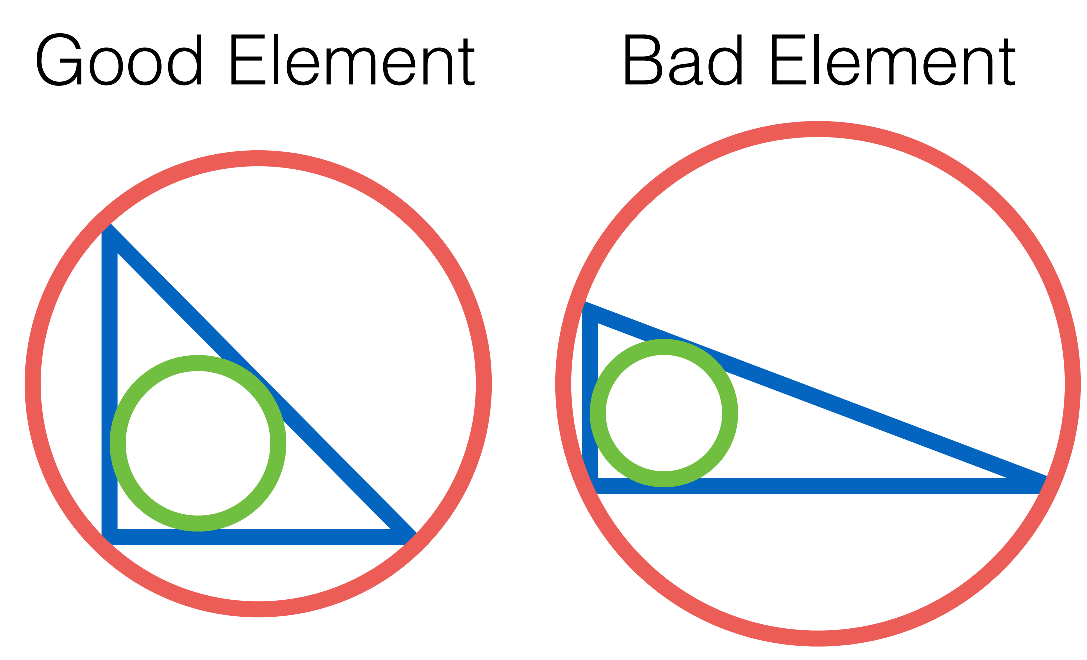
Convergence strongly depends on

Accuracy

- **Numerical error**: error from piecewise polynomial approximation of the solution and of the geometry.
- **Mesh Quality:** The quality and size of the mesh has a significant impact on the accuracy of the solution

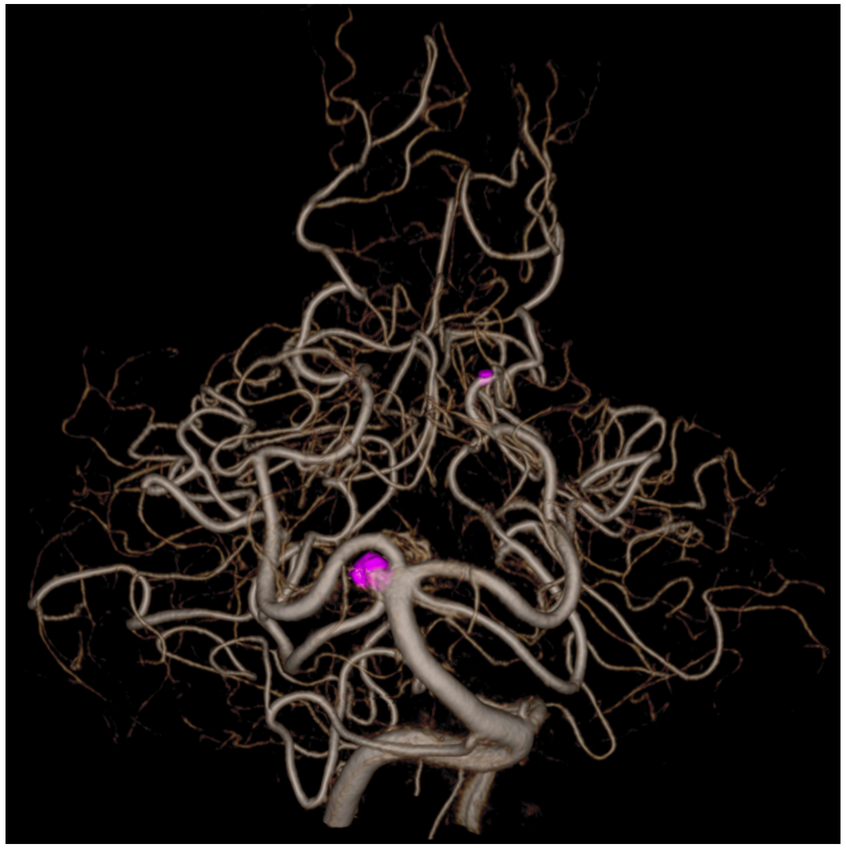
Stability

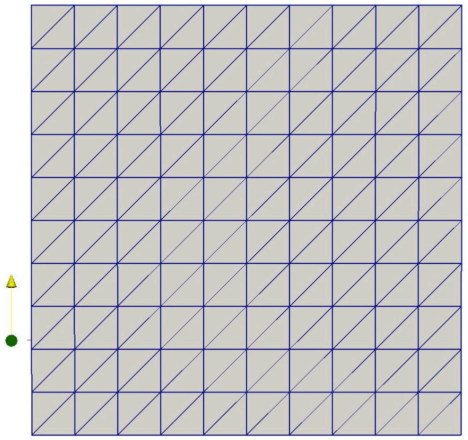
- **Instabilities** frequently occur in **simulations as numerical errors can grow in the solution process. Numerical error growth needs to be controlled and stabilised** carefully. Too much stabilisation leads to inaccuracies.

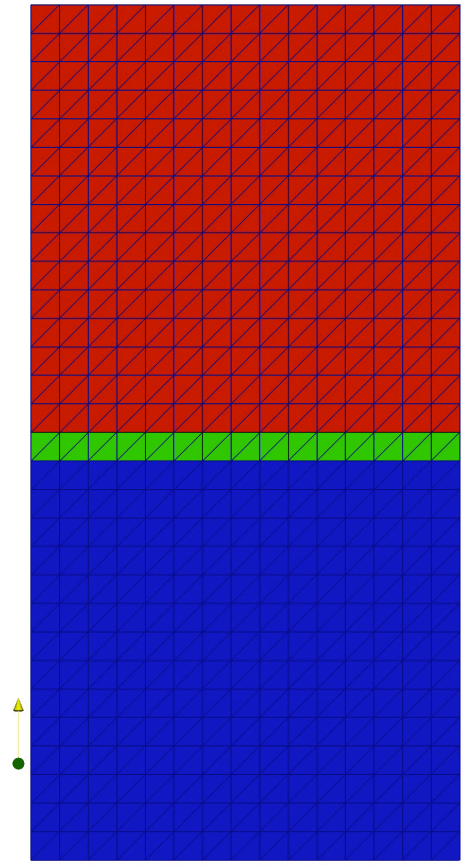


Convergence = Accuracy + Stability

Difficulty of maintaining a high quality mesh







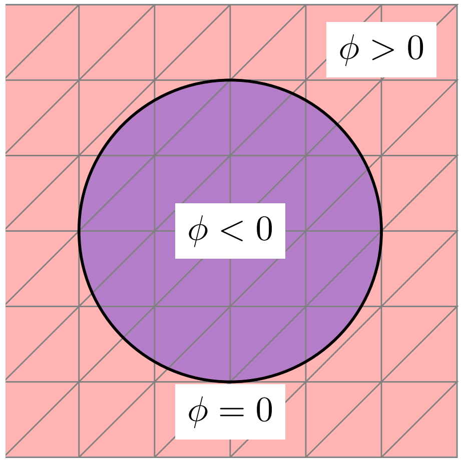
Advantages of Mesh Independent Geometry Descriptions

1. reduces the computational cost for preprocessing or transformation of acquired geometry descriptions
2. efficient and robust for problems involving evolving geometries undergoing large deformations

Important aspects of implicit geometry/cut finite element methods

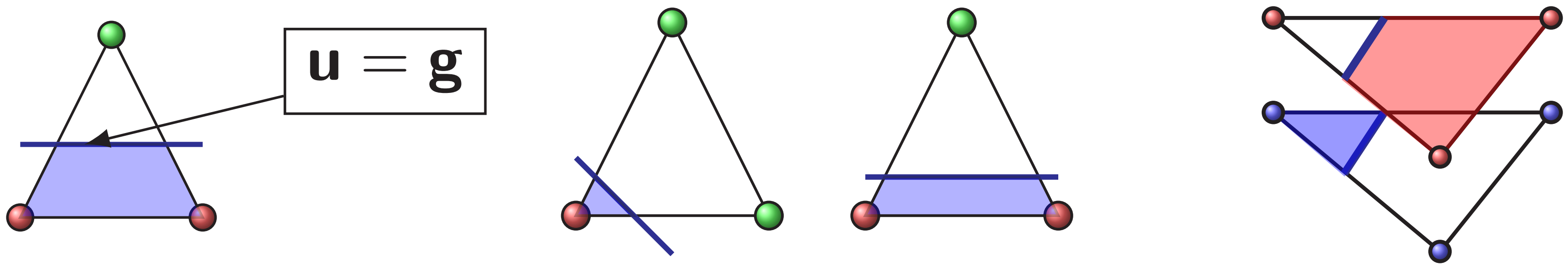
Geometry Algorithms

Discretisation of the geometry based on implicit interface description



Accuracy and Stabilisation

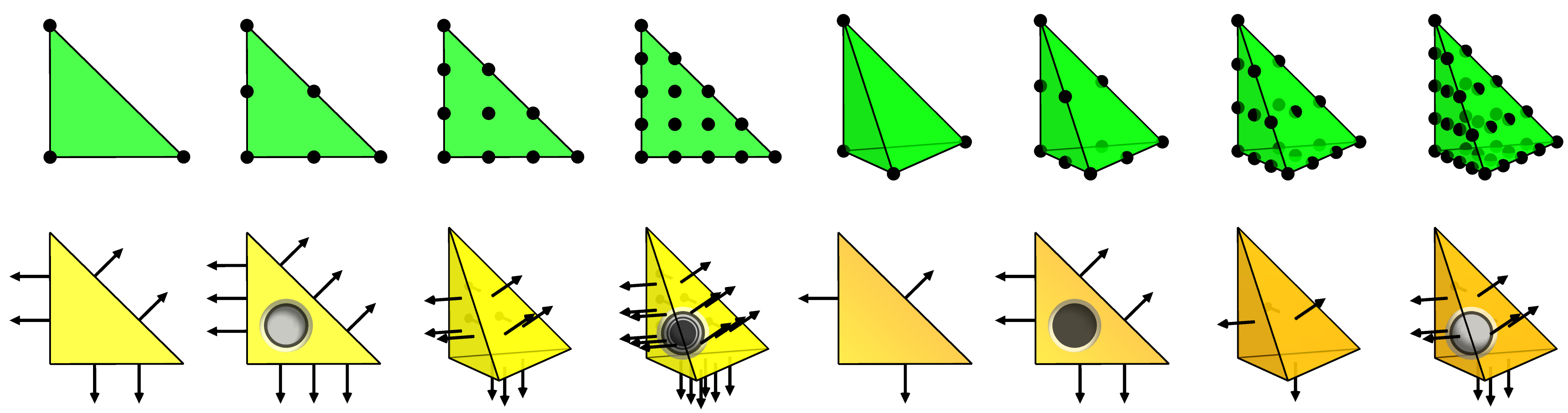
Construction of stable and accurate finite element methods independent of how the interface intersects the mesh.



FEniCS

Open Source Finite Element Library for the Automated Solution of PDEs

- high level mathematical input language
- generates efficient C++ code from these mathematical inputs
- supports a wide range of different finite element types
- supports simulations in 2D and 3D
- fully parallelised
- active world wide developer community, e.g. Simula Research Laboratory, University of Cambridge, University of Chicago, University of Texas at Austin, KTH Royal Institute of Technology, Chalmers University of Technology.



http://fenicsproject.org

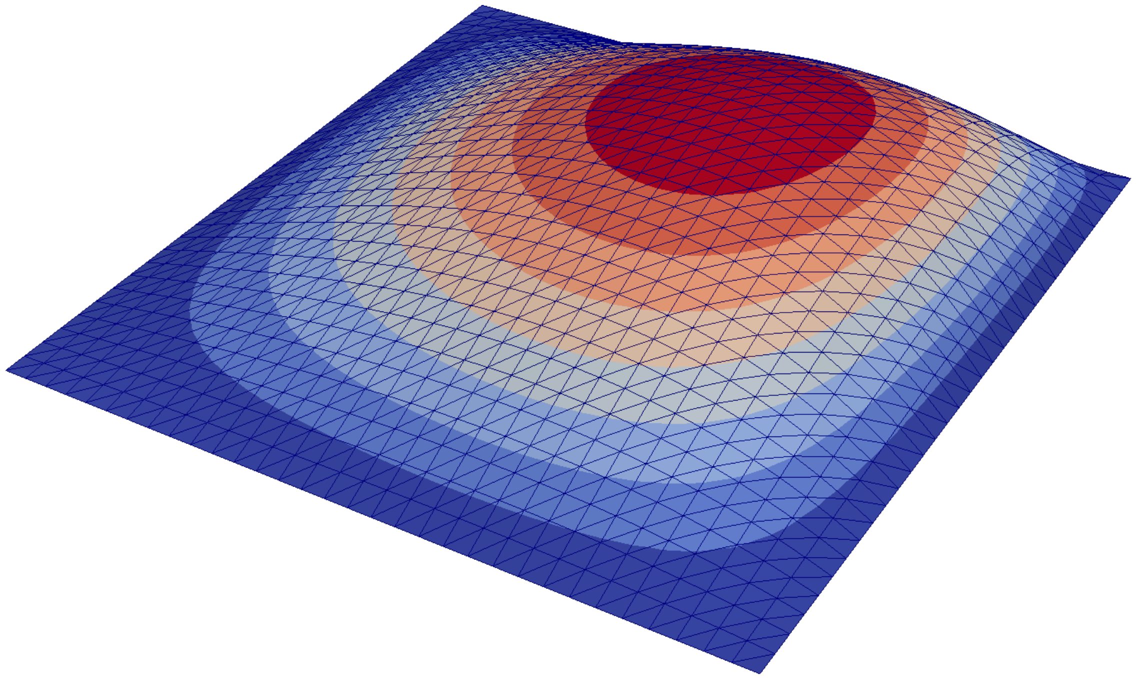
FEniCS Example: Poisson Equation

Consider the elliptic problem

$$\begin{aligned} -\Delta u &= f \text{ in } \Omega, \\ u &= 0 \text{ on } \Gamma. \end{aligned}$$

Find $u \in V$ such that

$$\int_\Omega \nabla u \cdot \nabla v dx = \int_\Omega f v dx \quad \forall v \in V$$



```python
from dolfin import *

# Create mesh and define function space
mesh = UnitSquareMesh(32, 32)
V = FunctionSpace(mesh, "CG", 1)

# Define boundary condition
bc = DirichletBC(V, 0.0, DomainBoundary())

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("x[0]*x[1]")

a = inner(grad(u), grad(v))*dx
L = f*v*dx

# Compute solution
u = Function(V)
solve(a == L, u, bc)
```

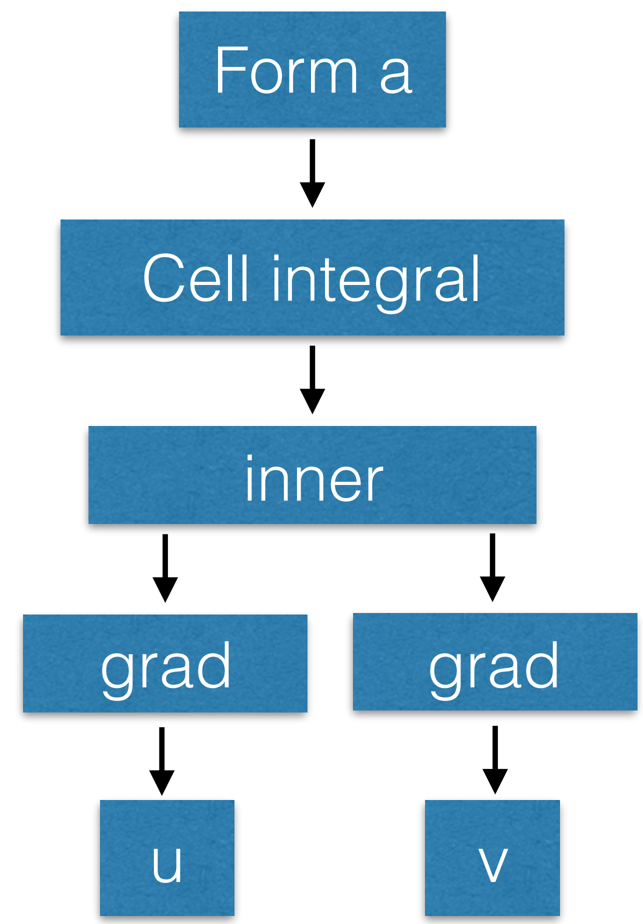
FEniCS: Under The Hood

Input: File in Python and Unified From Language

→ **Unified Form Language (UFL)**
Interprets expressions close to mathematical notation

```
a=inner(grad(u), grad(v))*dx
```

$$a(u,v) = \int \nabla u \nabla v \, dx$$



FEniCS: Under The Hood

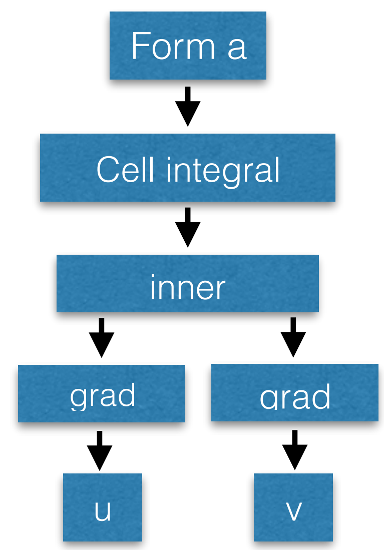
Input: File in Python and Unified From Language

a=inner(grad(u), grad(v))*dx

$$a(u,v) = \int \nabla u \nabla v \, dx$$

Unified Form Language (UFL)
Interprets expressions close to mathematical notation

FEniCS Form Compiler (FFC)
Generates Header file with information about
Elemental matrices (form)
Degrees of Freedom Map (element)



Poisson.h

```
/// Evaluate basis function i at given point x in cell
_evaluate_basis(std::size_t i, double* values, const double* x, const double* coordinate_dofs)

 /// Tabulate the tensor for the contribution from a local cell
virtual void tabulate_tensor(double*  A, const double * const *  w, const double* coordinate_dofs)
```

DOLFIN
(Mesh, Communicator and Assembler)

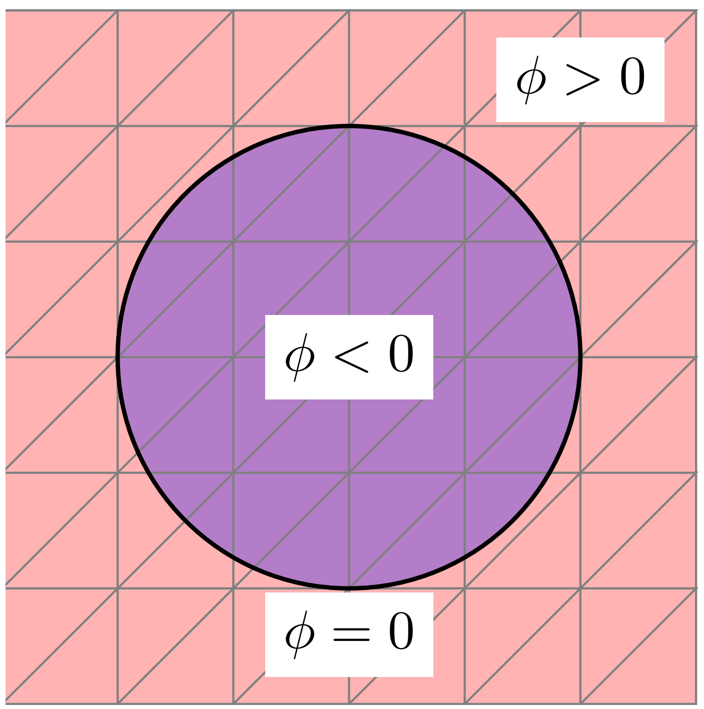
LibCutFEM

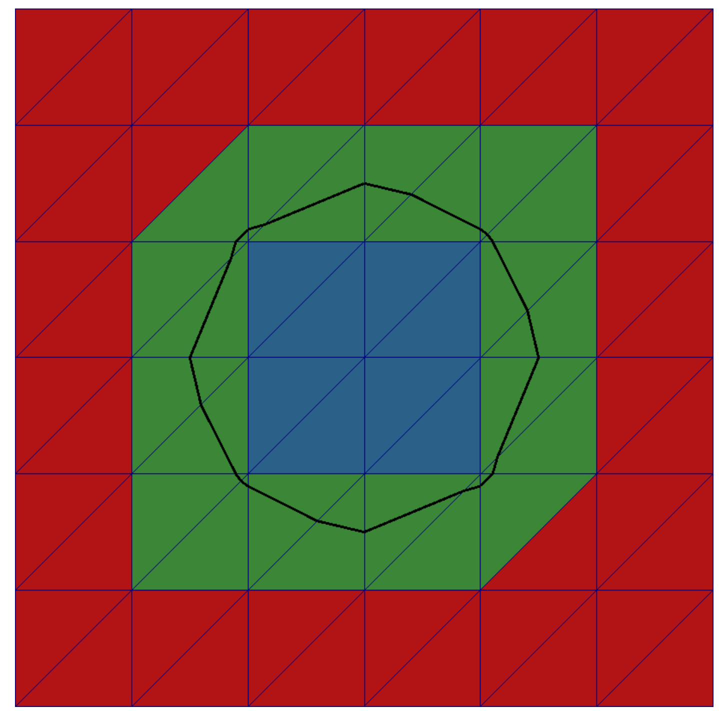
Geometry Algorithm

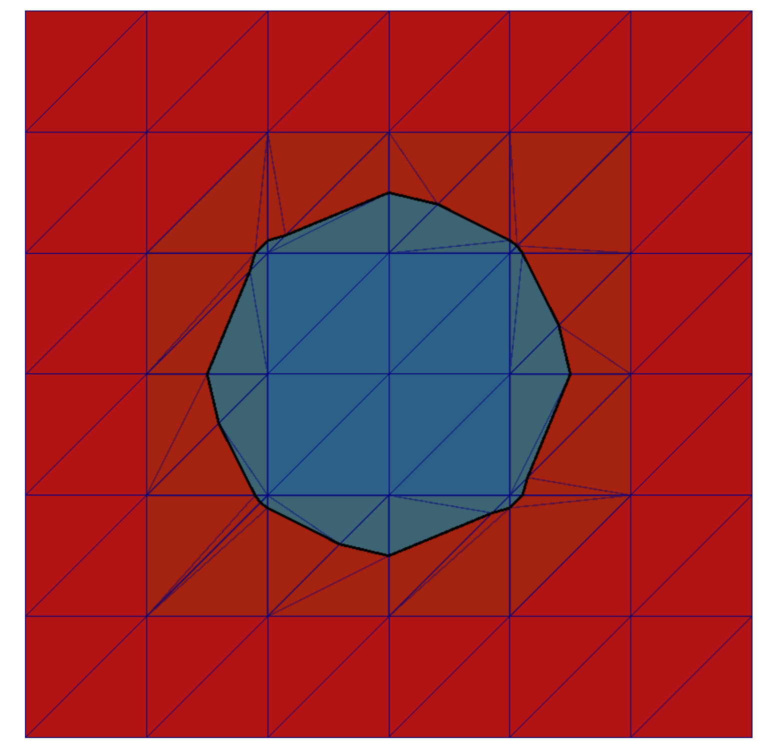
Level Set Function

Finite Element Approximation

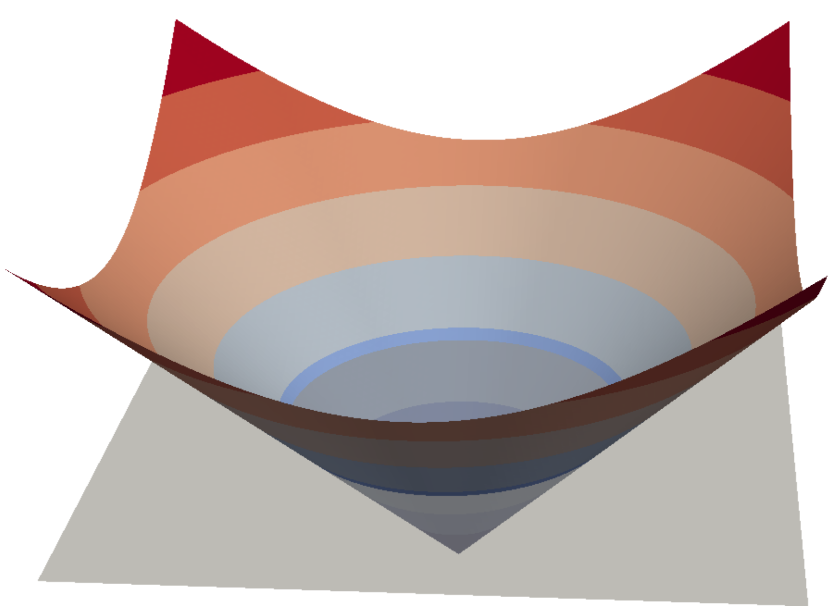
Mesh/Levelset intersection for integration

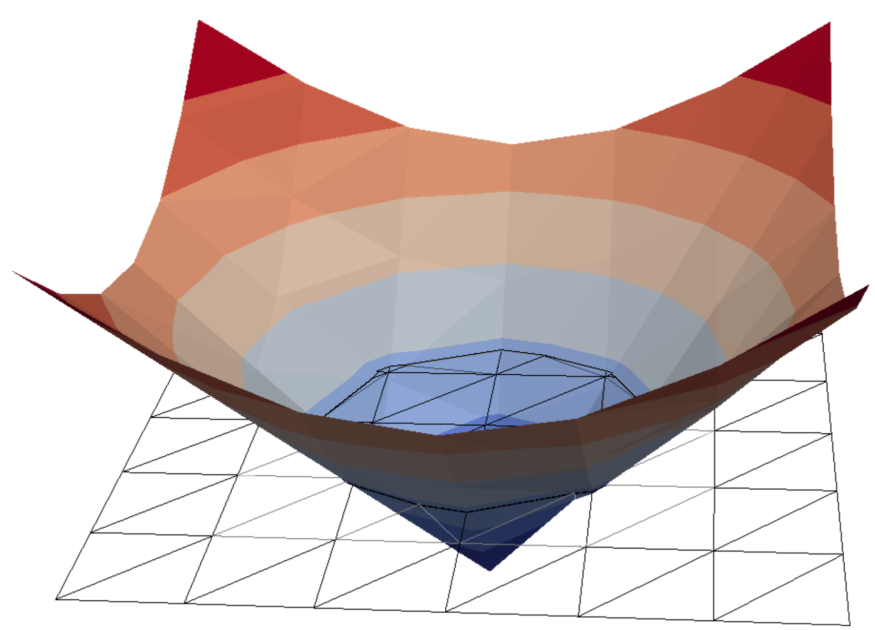


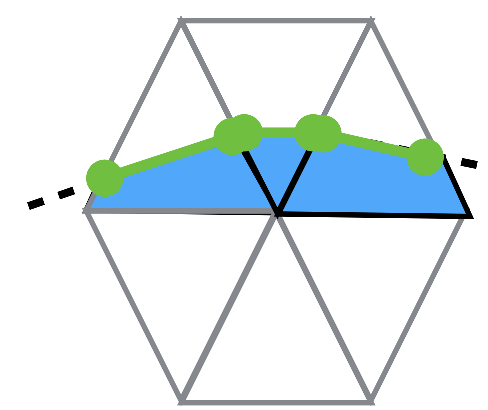


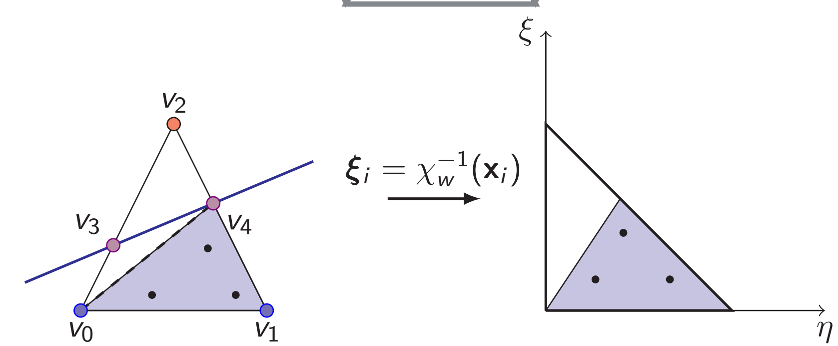


Signed Distance Function

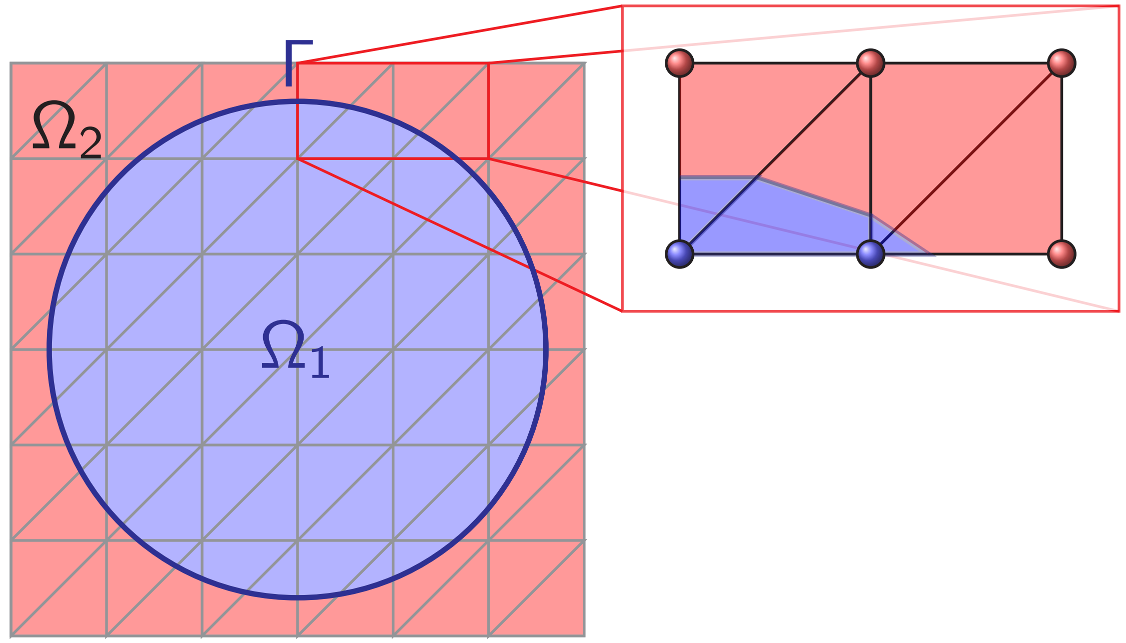




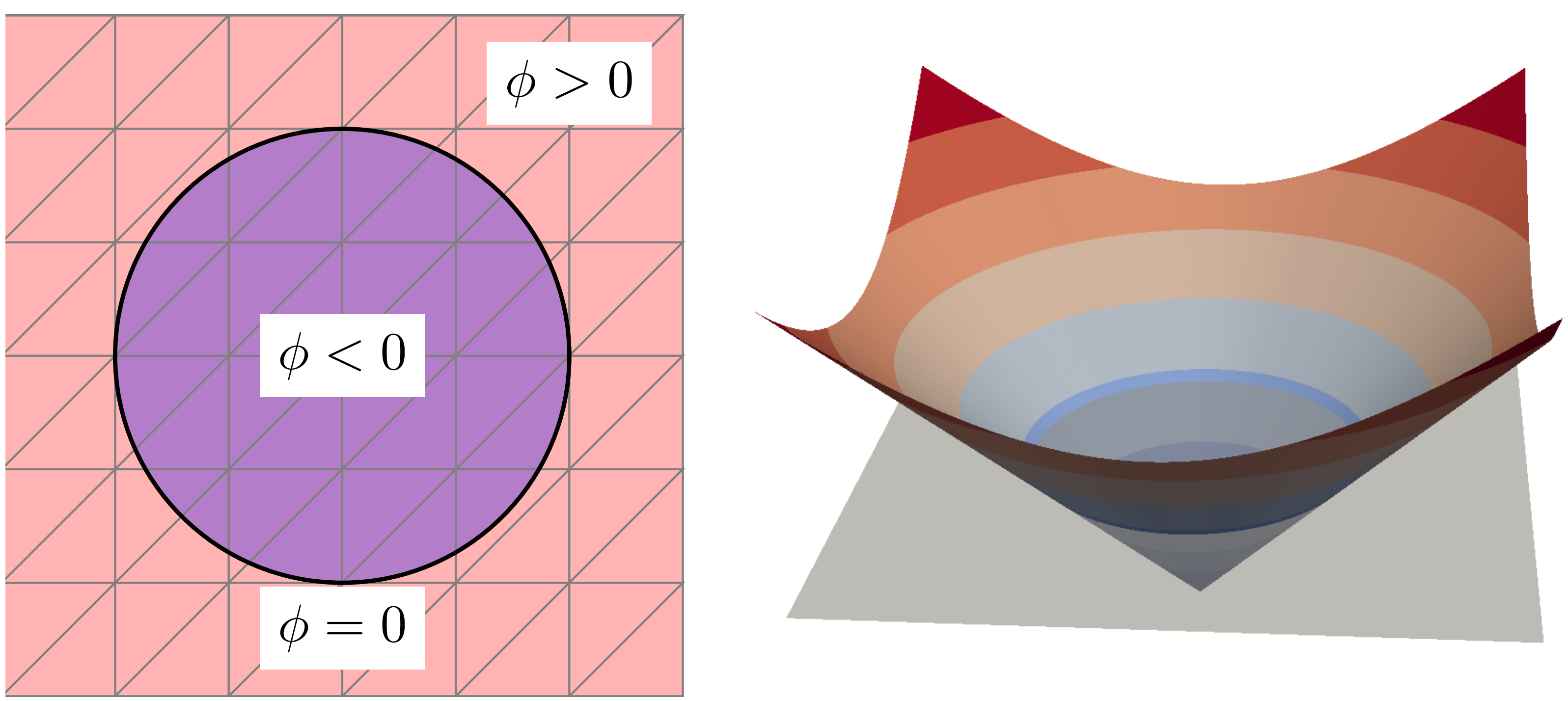




Level Set Geometry Description



Describe geometry using Level-Set Function



Normal

$$\mathbf{n}_\Gamma = \frac{\nabla\phi}{||\nabla\phi||_0}$$

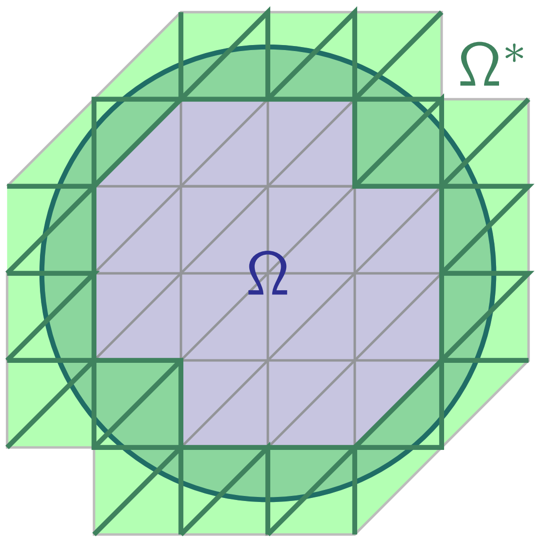
Curvature

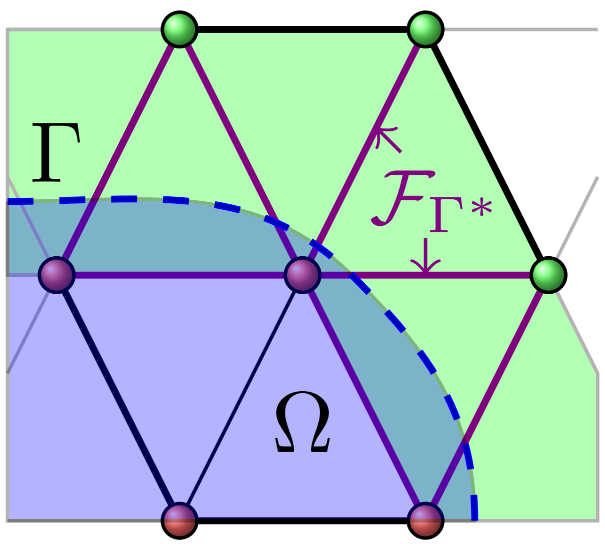
$$\kappa = \nabla \cdot \mathbf{n}$$

Sense of Vicinity

$$|\phi(x)| < \delta$$

Fictitious Domain Poisson Problem





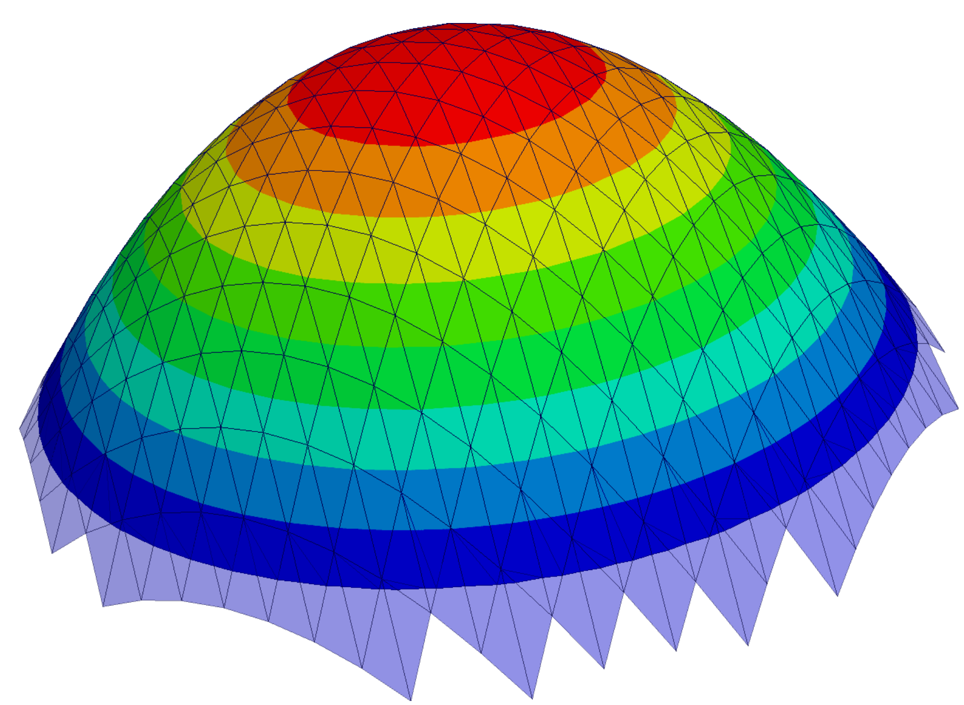
Find $u_h \in V_h$ such that for all $v_h \in V_h$

$$A(u_h, v_h) = a(u_h, v_h) + j(u_h, v_h) = L(v_h)$$

$$a(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \,\mathrm{d}x + \int_\Gamma \Big(-\underbrace{\nabla u_h \cdot n v_h}_{\text{consistency}} - \underbrace{\nabla v_h \cdot n u_h}_{\text{symmetry}} + \underbrace{\frac{\gamma}{h} u_h v_h}_{\text{coercivity}}\Big)\,\mathrm{d}s$$

$$L(v_h) = \int_\Omega f\, v_h \,\mathrm{d}x + \int_\Gamma \Big(-g\, \nabla v_h \cdot n + \frac{\gamma}{h} g\, v_h\Big)\,\mathrm{d}s$$

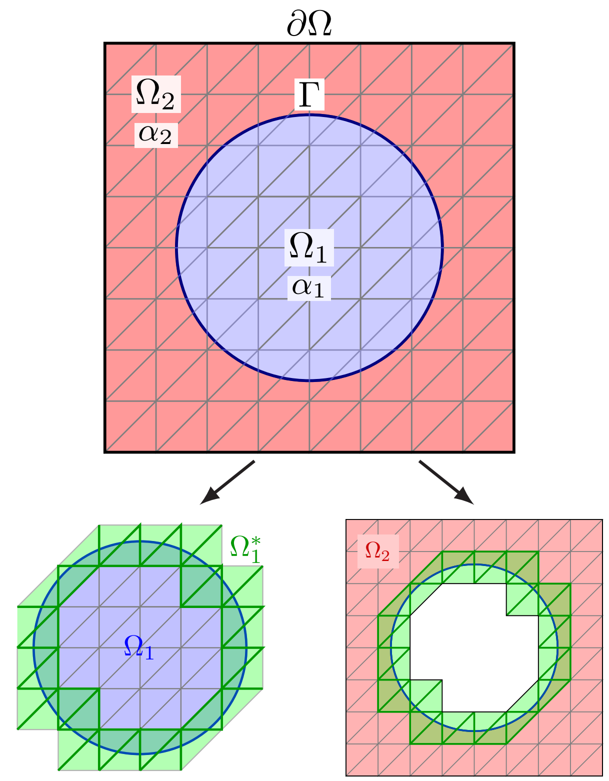
$$j(u_h, v_h) = \gamma_1 \sum_{F \in \mathcal{F}_{\Gamma^*}} h_F ([\![\partial_n u_h]\!], [\![\partial_n v_h]\!])_F$$

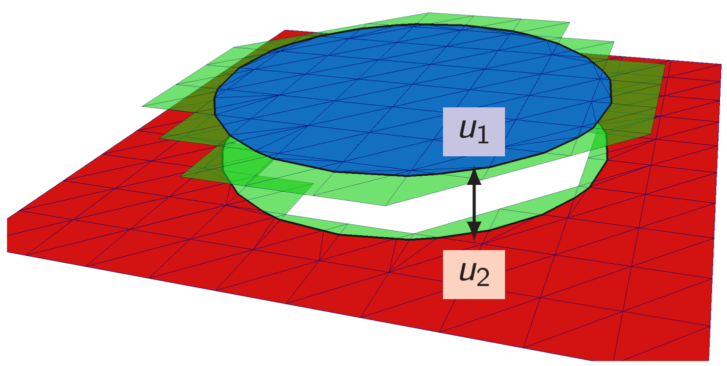


Poisson with contrast in diffusivities

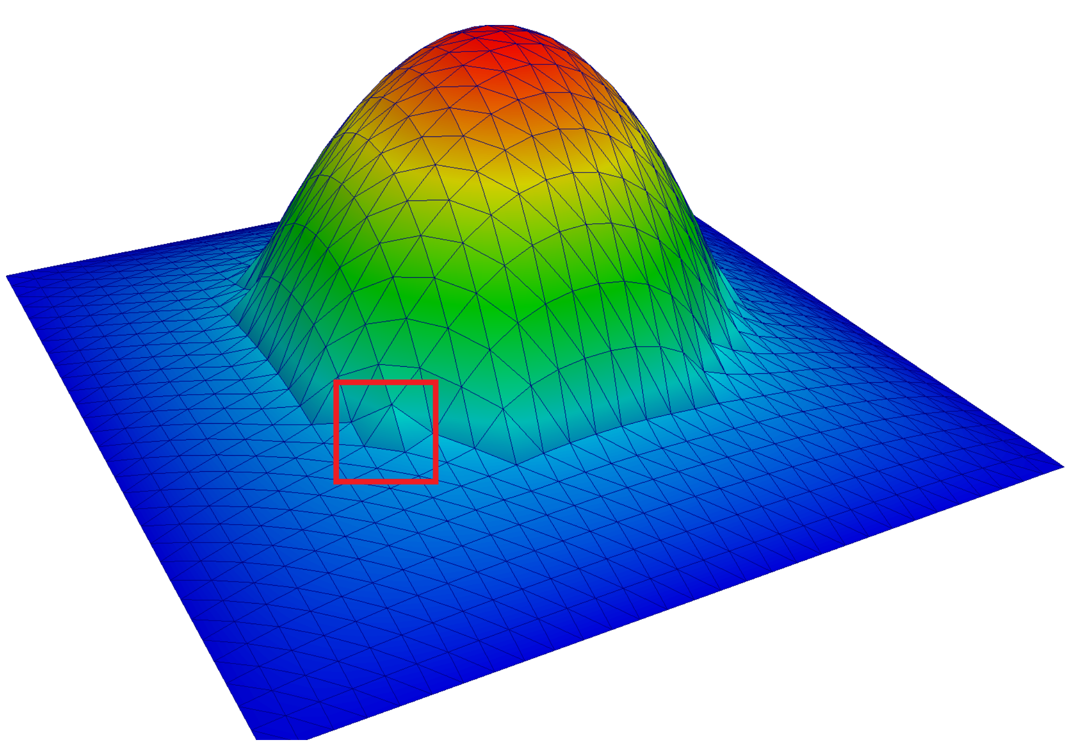
$$
\begin{aligned}
-\nabla \cdot (\alpha \nabla u) &= f && \text{in} && \Omega_1 \cup \Omega_2, \\
u &= 0 && \text{on} && \partial\Omega, \\
[\![u]\!] &= 0 && \text{on} && \Gamma, \\
[\![-\alpha_i \nabla u_i \cdot \mathbf{n}]\!] &= 0 && \text{on} && \Gamma.
\end{aligned}
$$

Choose $\alpha_1 = 1, \alpha_2 = 10, f_1 = f_2 = 1.$

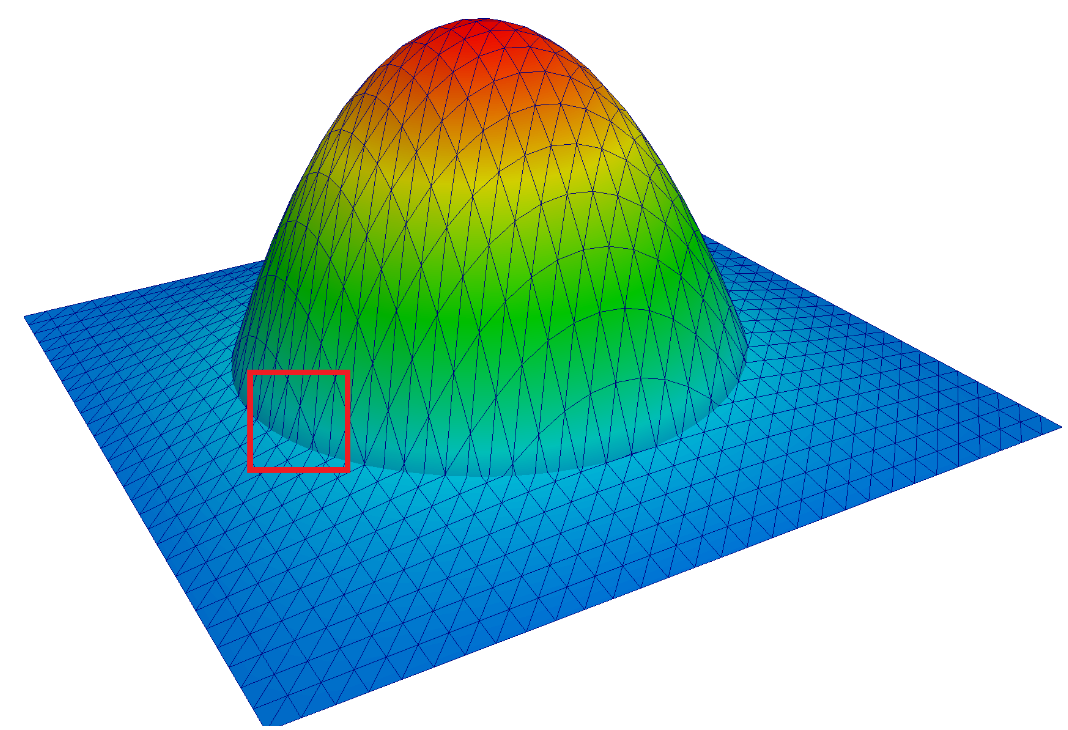


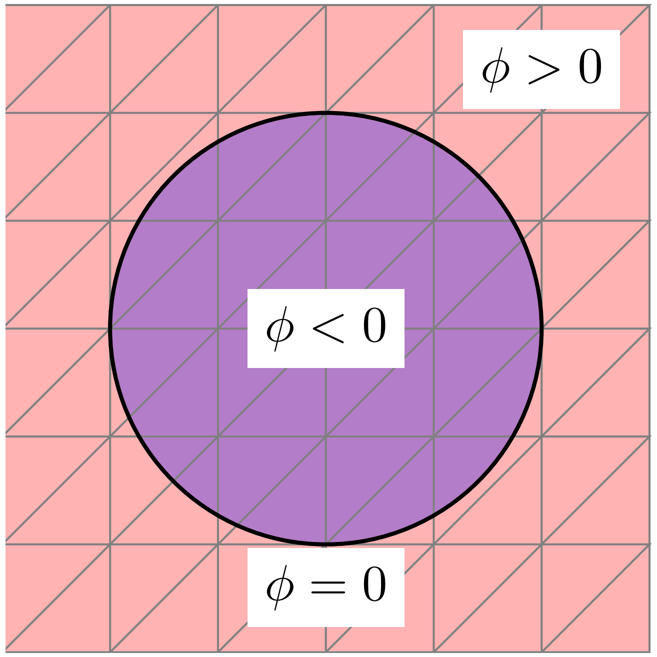


Without Enrichment



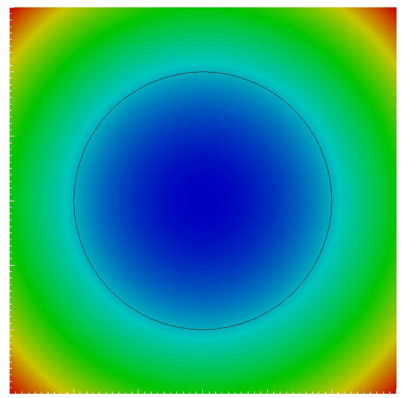
With Enrichment





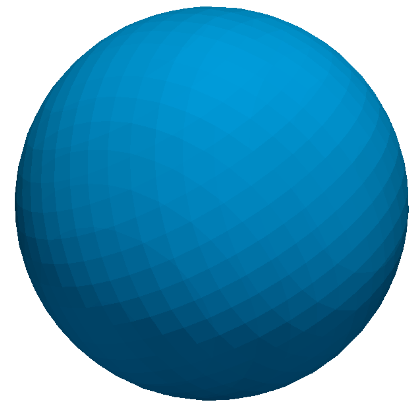
Circle

$$\phi(\boldsymbol{x}) = x^2 + y^2 - 1$$



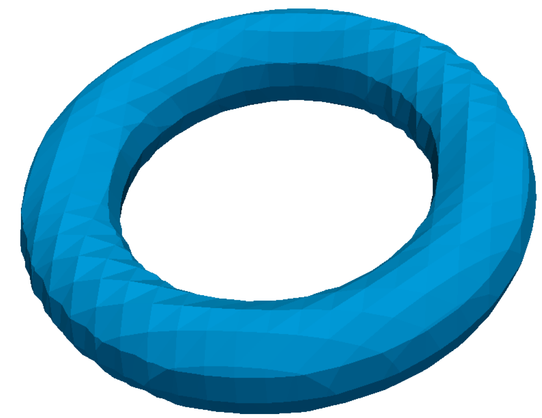
Sphere

$$\phi(\boldsymbol{x}) = x^2+y^2+z^2-1$$

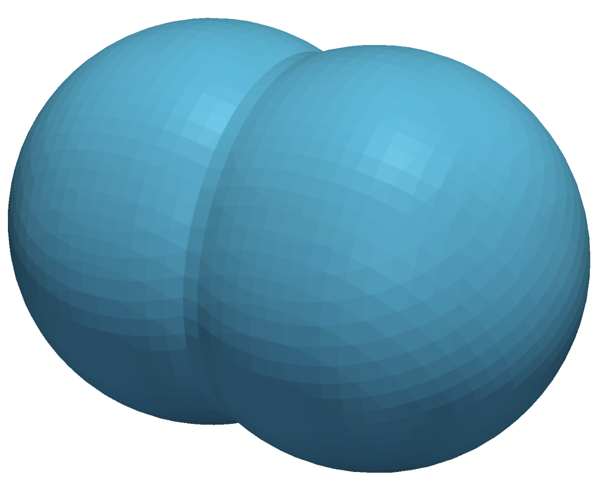


Torus

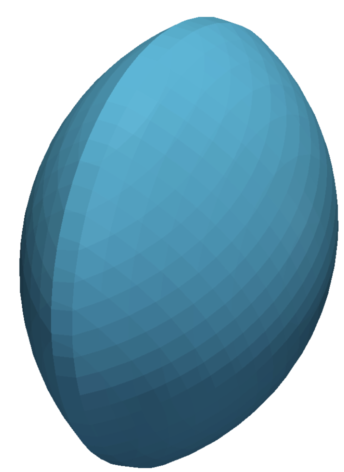
$$\phi(\boldsymbol{x}) = (R-\sqrt{x^2 + y^2})^2+z^2-r^2$$



Union:
$\phi(\boldsymbol{x}) = \min(\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}))$

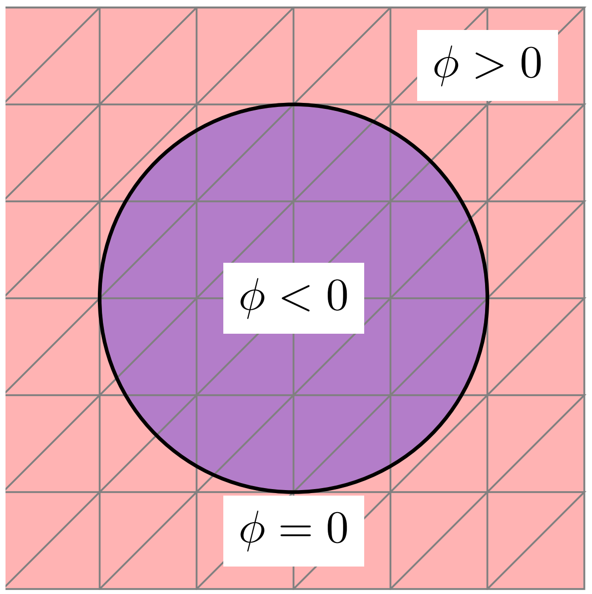


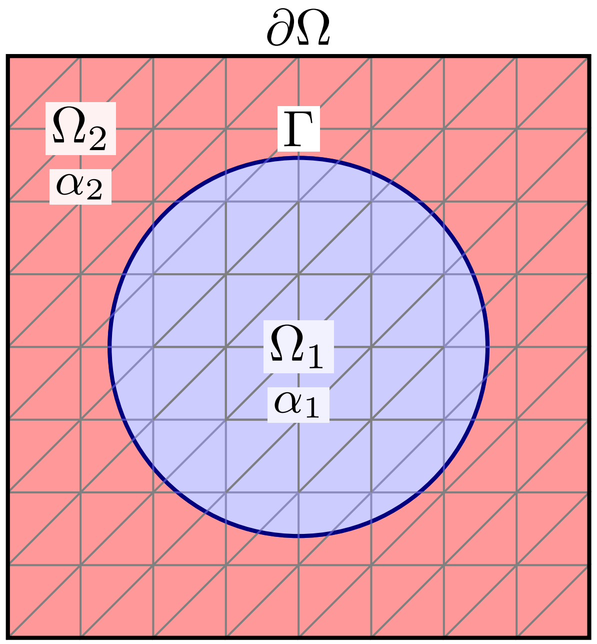
Intersection:
$\phi(\boldsymbol{x}) = \max(\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}))$

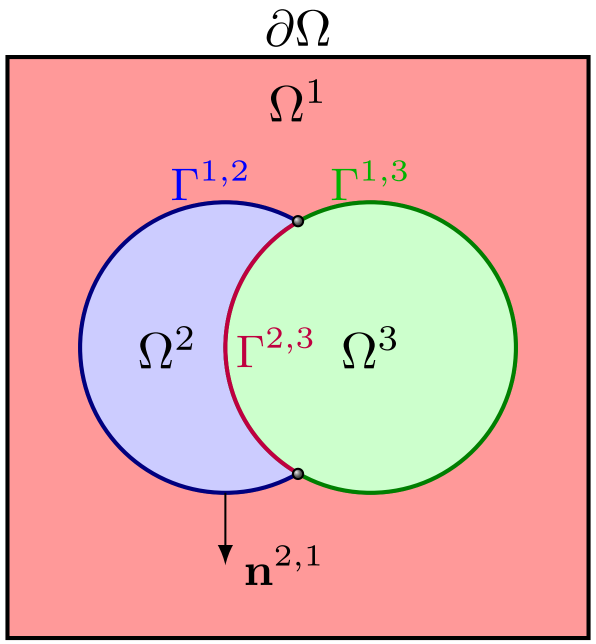


Limitations with single level set function

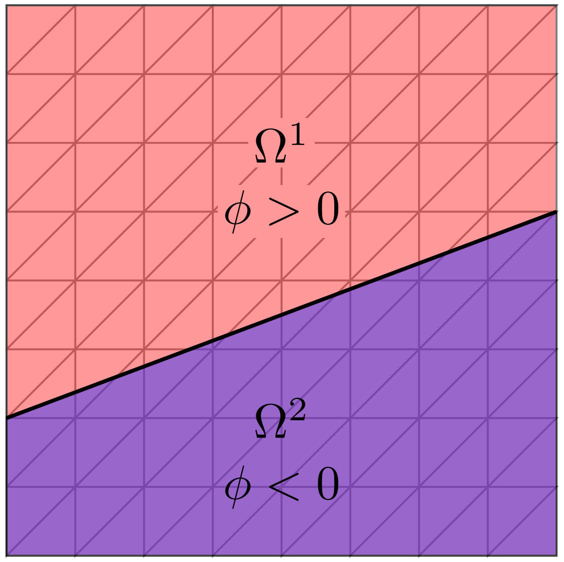
Partitions the domain into one inside and one outside domain (max. 2 different materials)

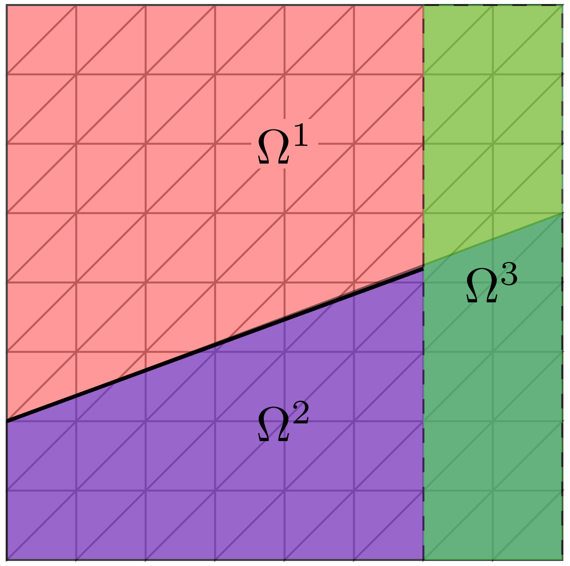






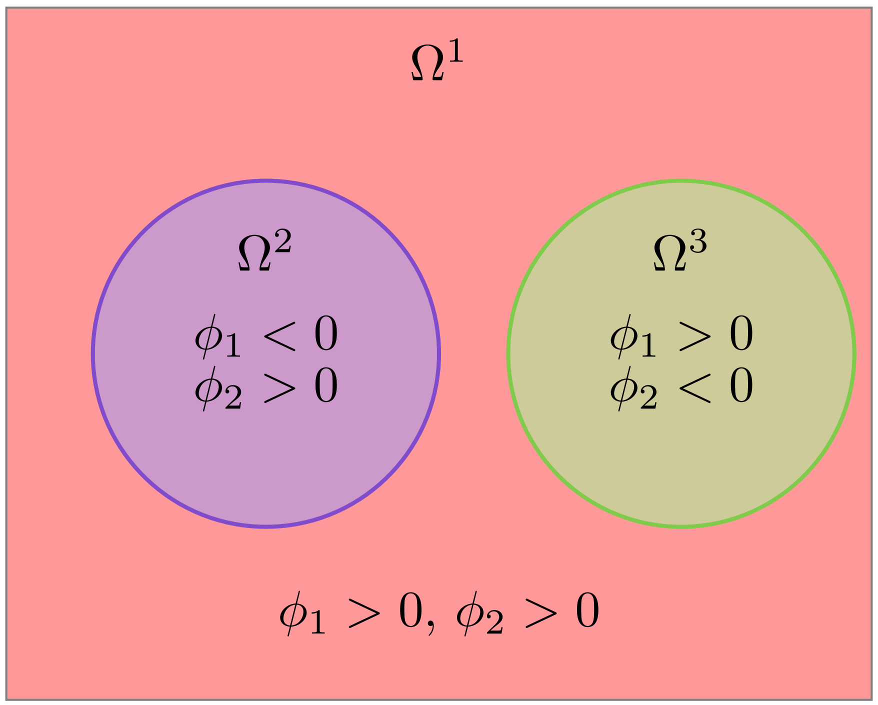
Zero level set surface contour is a closed surface, i.e it is not possible to describe geometries with open boundaries such as cracks

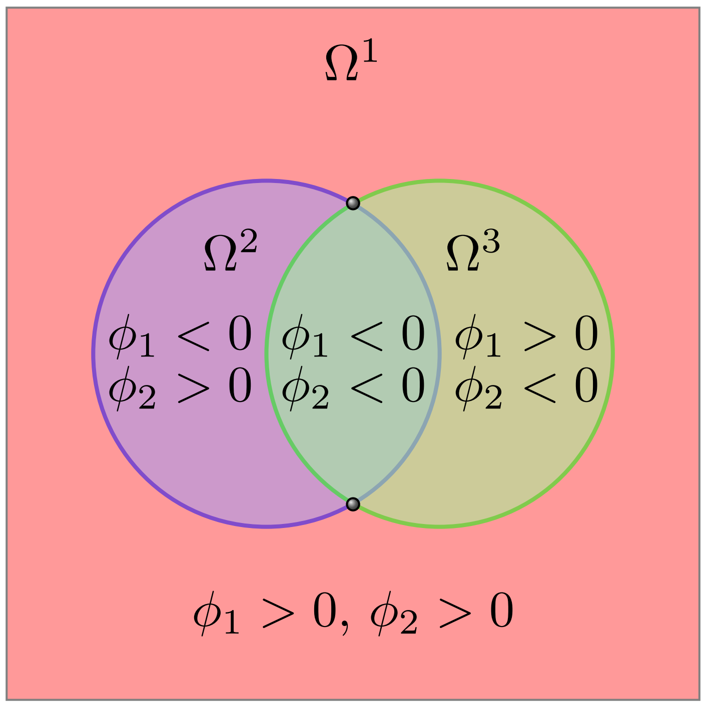


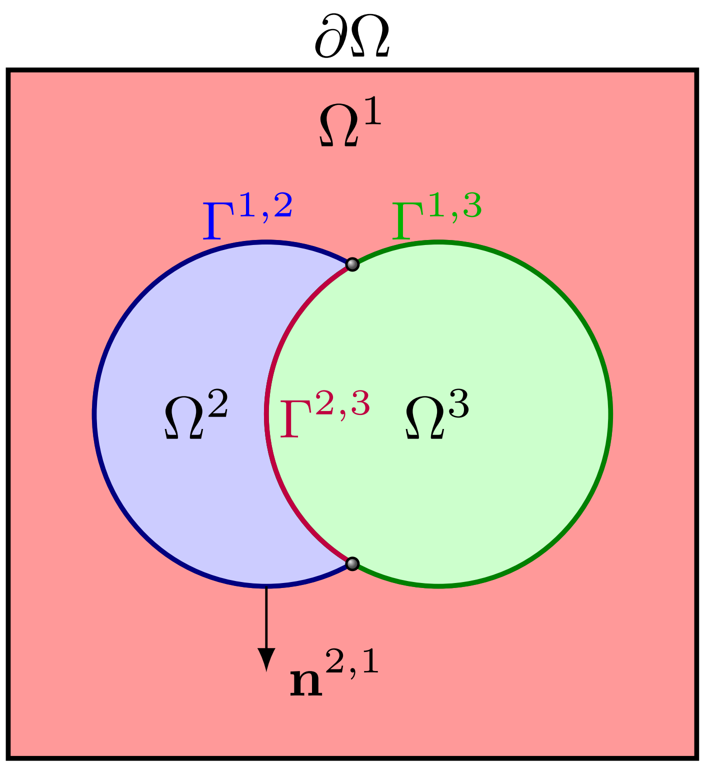


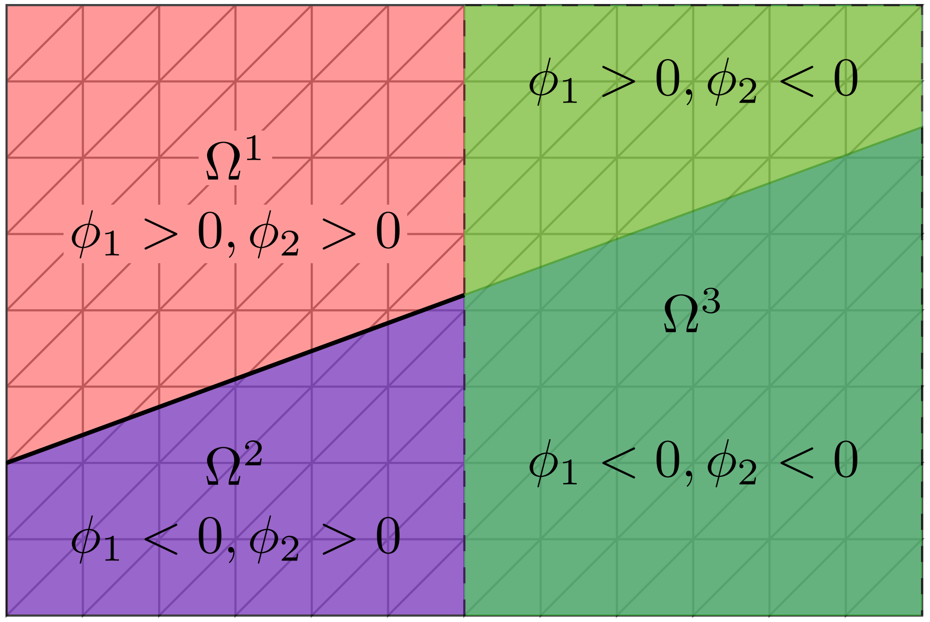
Use multiple level set functions for complex geometries

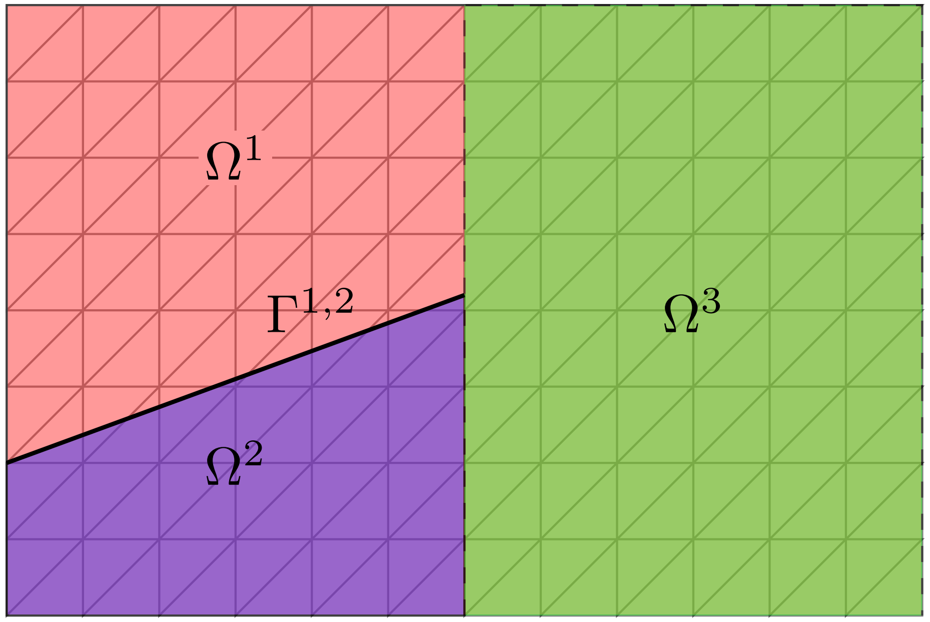
N-1 level set functions can described N different subdomains



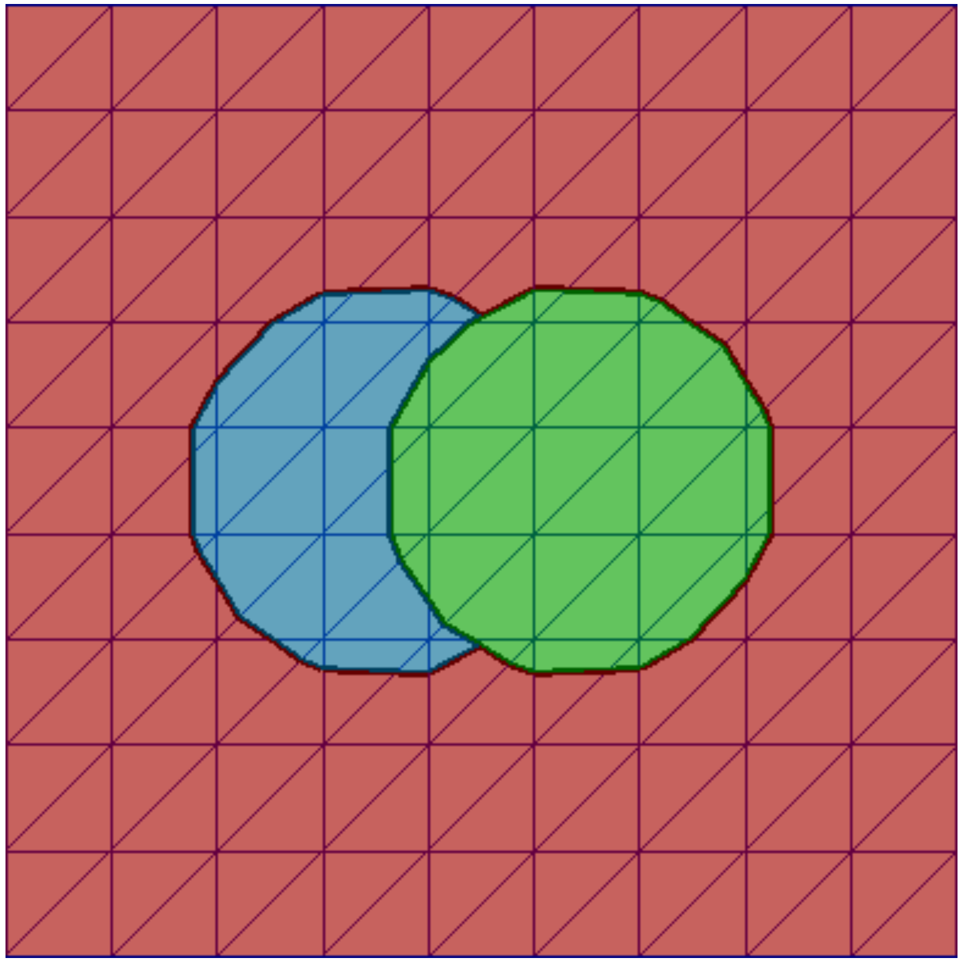


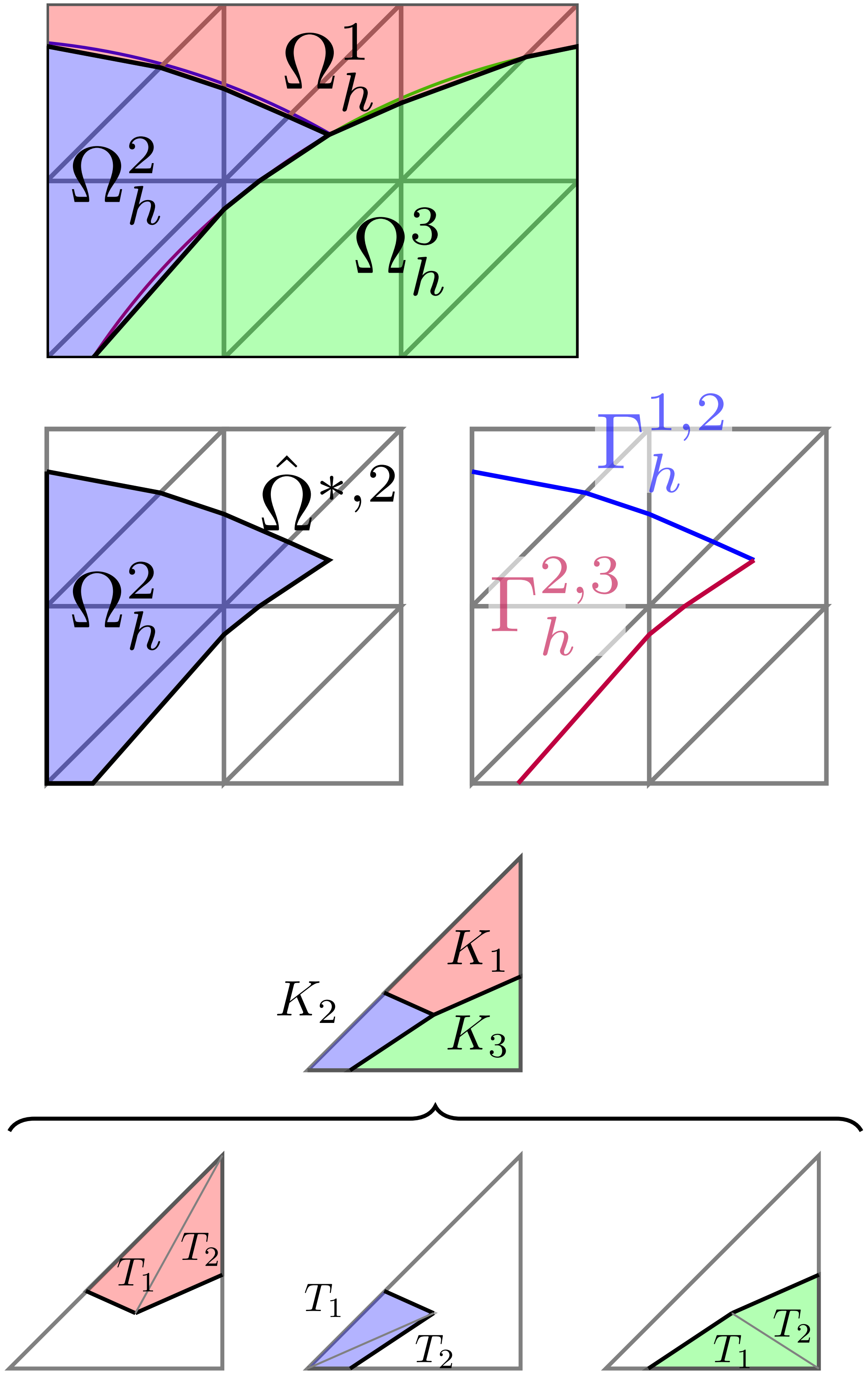




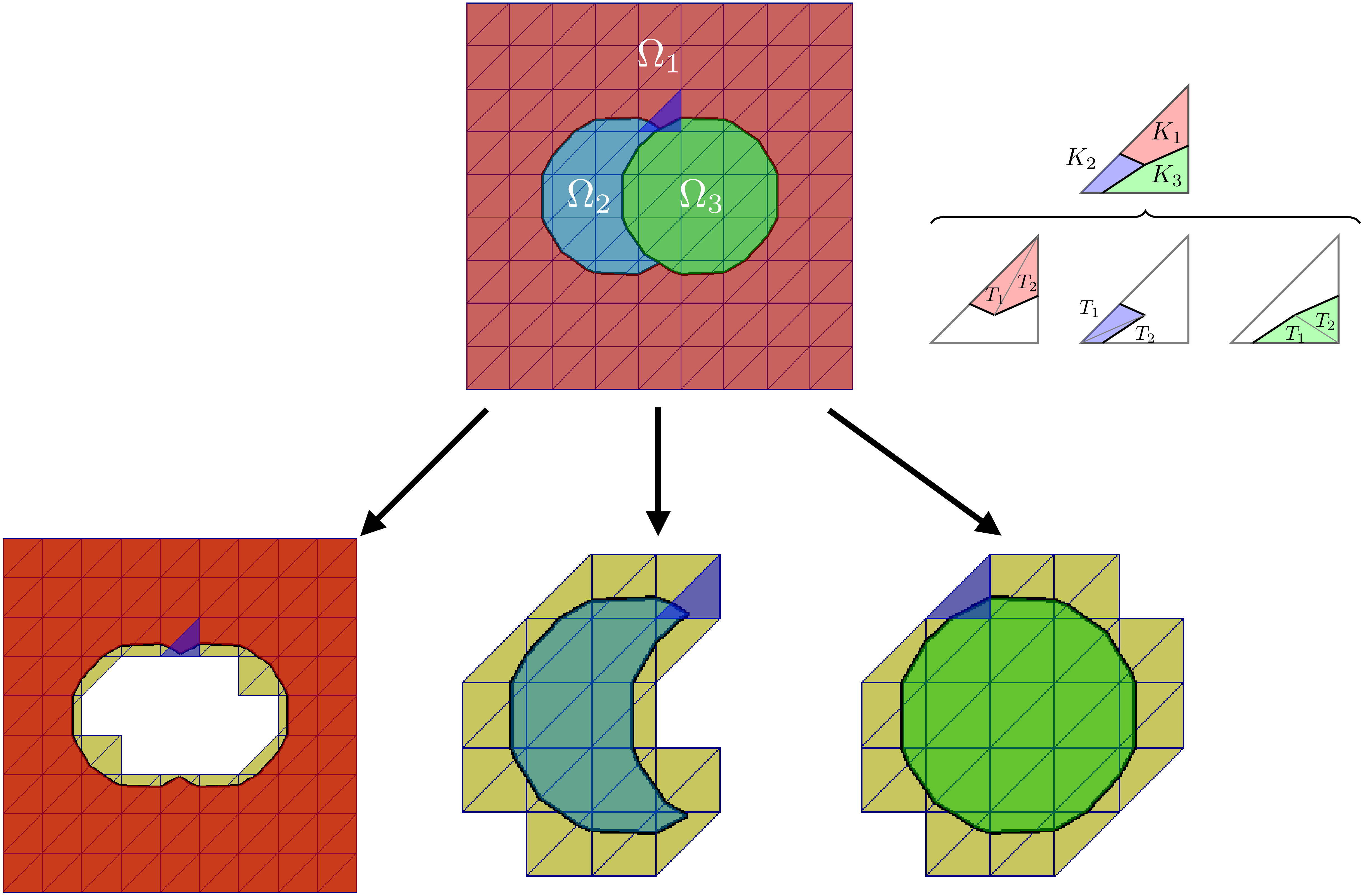


Level Set Mesh Intersection



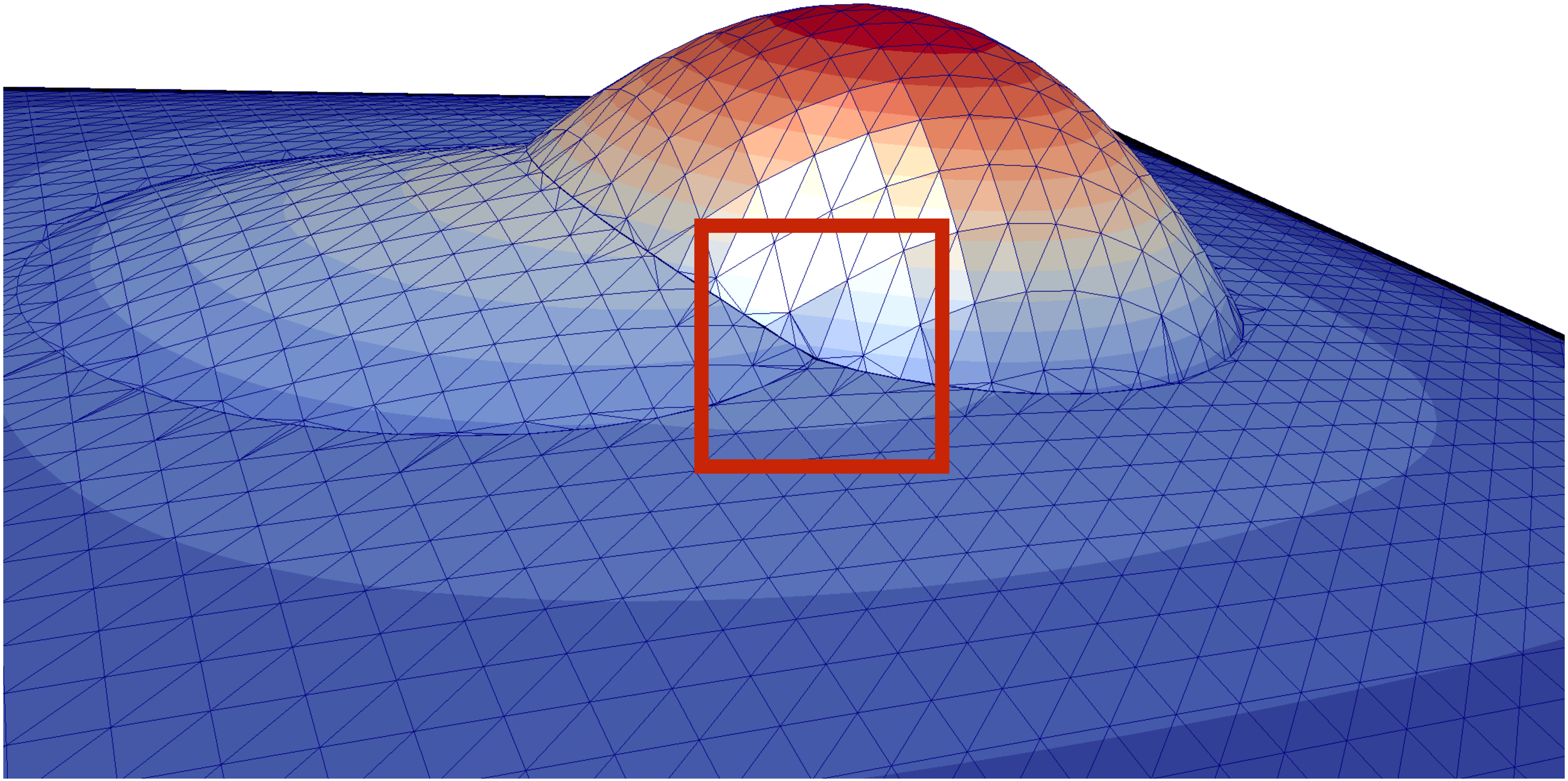


Enrichment for jump and kink representation



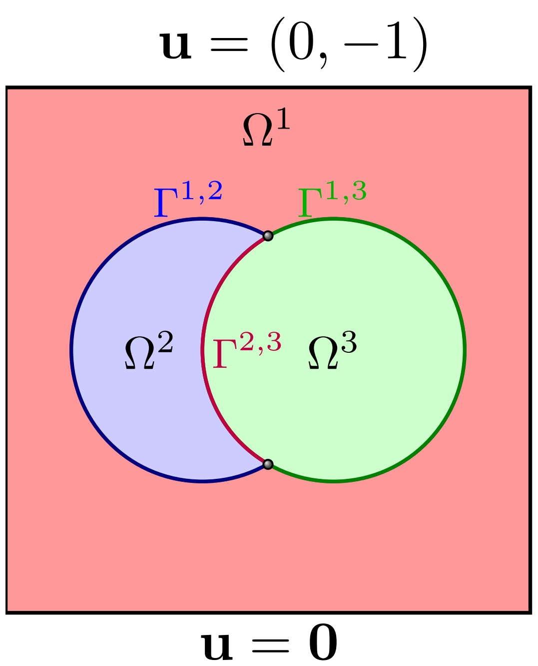
Claus, S., and P. Kerfriden. "A stable and optimally convergent LaTIn-CutFEM algorithm for multiple unilateral contact problems." IJNME 113.6 (2018): 938-966.

Triple Poisson Problem



Contact Problems

Contact Problem in linear Elasticity



Bulk Problem

For all Ω_i, find the displacement fields $\mathbf{u}^i : \Omega_i \to \mathbb{R}$, such that

$$-\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}^i) = \mathbf{f} \qquad \text{in } \Omega_i$$

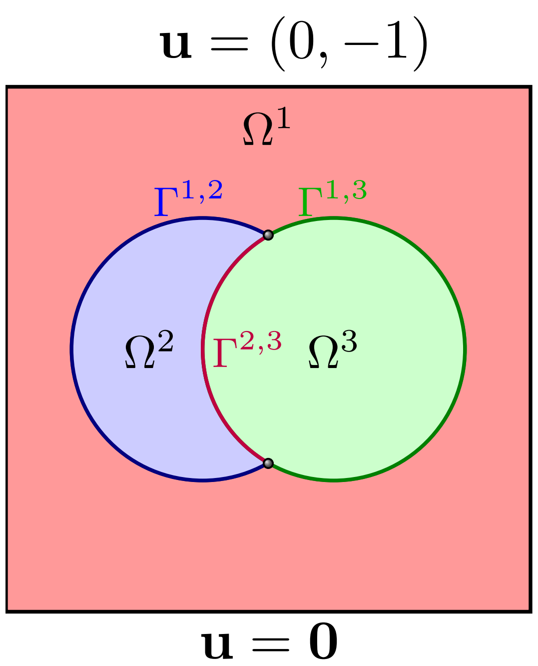
$$\boldsymbol{\sigma}(\mathbf{u}^i) = \lambda^i \operatorname{tr}(\boldsymbol{\epsilon}(\mathbf{u}^i))\, \boldsymbol{I} + 2\, \mu_i\, \boldsymbol{\epsilon}(\mathbf{u}^i) \qquad \text{in } \Omega_i$$

$$\mathbf{u}^i = \mathbf{g} \text{ on } \partial\Omega_D\,,\ \boldsymbol{\sigma}(\mathbf{u}_i) \cdot \mathbf{n} = \mathbf{F_N} \text{ on } \partial\Omega_N$$

Here, $\boldsymbol{\epsilon}(\mathbf{u}) = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)$ is the strain tensor, $\mathbf{f}$ is the body force, $\mathbf{F_N}$ is the surface load, $\mathbf{g}$ the Dirichlet boundary condition, λ^i and μ^i are the two Lamé coefficients (E^i is the Young's modulus, $\nu = 0.3$ is the Poisson's ratio)

$$\mu^i = \frac{E^i}{2(1+\nu)}, \quad \lambda^i = \frac{E^i \nu}{(1+\nu)(1-2\nu)}.$$

Unilateral contact for isotropic linear elasticity



Contact Conditions

For any displacement field $\mathbf{u}_i$, we decompose the surface traction $\mathbf{F}^i = \boldsymbol{\sigma}(\mathbf{u}_i) \cdot \mathbf{n}^{i,j}$ on the interface $\Gamma^{i,j}$ into its normal and tangential components

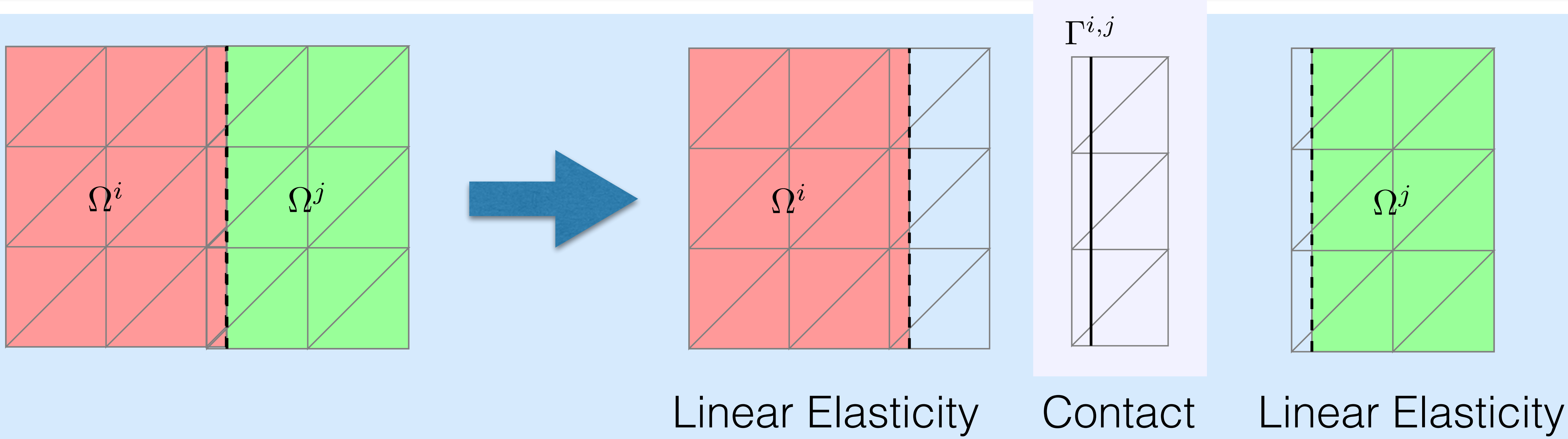
$$\mathbf{F}^i = \mathbf{F_n}^i + \mathbf{F_t}^i .$$

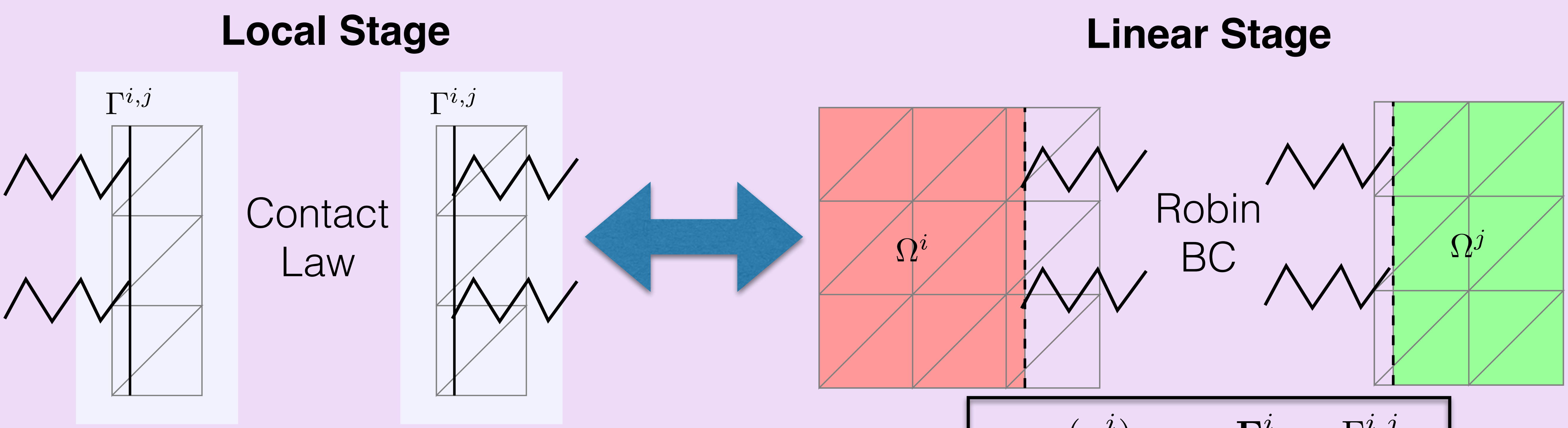
Then, the conditions of contact with Coulomb friction reads

$$\begin{aligned}
\left(\mathbf{u}^j - \mathbf{u}^i\right) \cdot \mathbf{n}^{i,j} &\geq 0\,, \\
\mathbf{F}^i \cdot \mathbf{n}^{i,j} &\leq 0\,, \\
\left(\left(\mathbf{u}^j - \mathbf{u}^i\right) \cdot \mathbf{n}^{i,j}\right) \cdot \left(\mathbf{F}^i \cdot \mathbf{n}^{i,j}\right) &= 0\,, \\
\|\mathbf{F_t}^i\| &\leq c\,\mathbf{F}^i \cdot \mathbf{n}^{i,j} && \text{if } \|\hat{\mathbf{g}}_t^i\|_2 = 0 \\
\mathbf{F_t}^i &= -c\,\mathbf{F}^i \cdot \mathbf{n}^{i,j} \frac{\hat{\mathbf{g}}_t^i}{\|\hat{\mathbf{g}}_t^i\|_2} && \text{if } \|\hat{\mathbf{g}}_t^i\|_2 > 0
\end{aligned}$$

Here, $\mathbf{n}^{i,j}$ is the normal pointing from Ω_i to Ω_j, c is the Coulomb friction coefficient, and $\hat{\mathbf{g}}_t^i := (\mathbf{I} - \mathbf{n}^{i,j} \otimes \mathbf{n}^{i,j}) \cdot (\dot{\mathbf{u}}^j - \dot{\mathbf{u}}^i)$ is the relative tangential velocity

LaTIn Algorithm



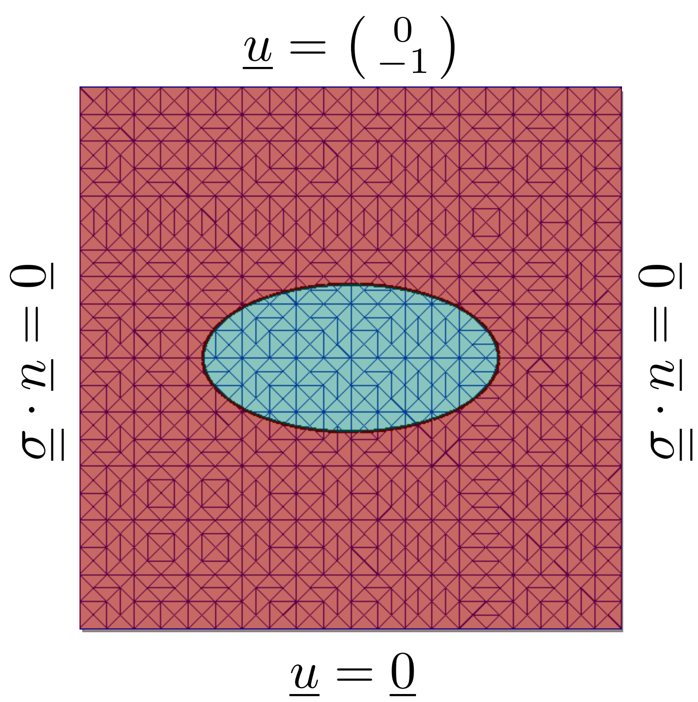


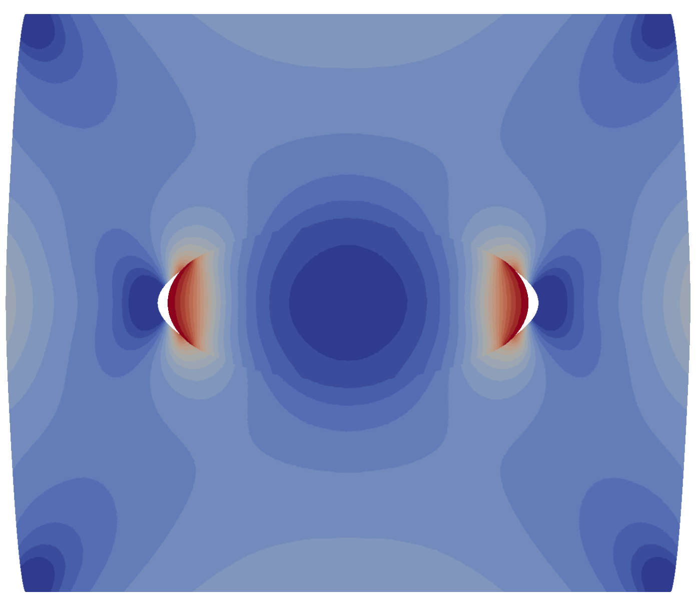
$$\hat{\mathbf{F}}^i - k^+\hat{\mathbf{w}}^i = \mathbf{F}^i - k^+\mathbf{w}^i$$

where $\hat{\mathbf{F}}^i$ and $\hat{\mathbf{w}}^i$ satisfy contact

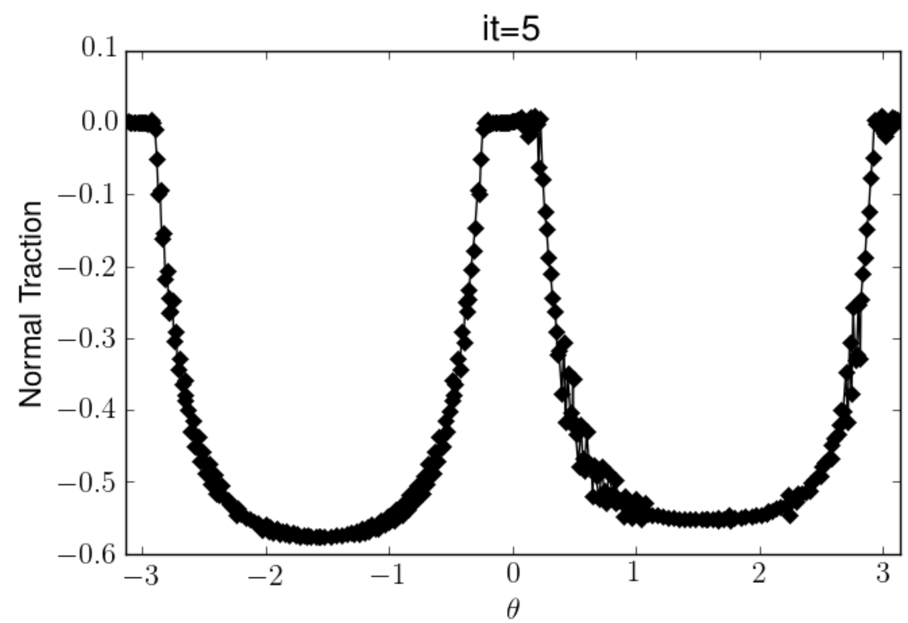
$$\boldsymbol{\sigma}(\mathbf{u}^i)\cdot\mathbf{n} = \mathbf{F}^i \text{ on } \Gamma^{i,j}$$
$$\mathbf{u}^i = \mathbf{w}^i \text{ on } \Gamma^{i,j}$$
$$\mathbf{F}^i + k^-\mathbf{w}^i = \hat{\mathbf{F}}^i + k^-\hat{\mathbf{w}}^i$$

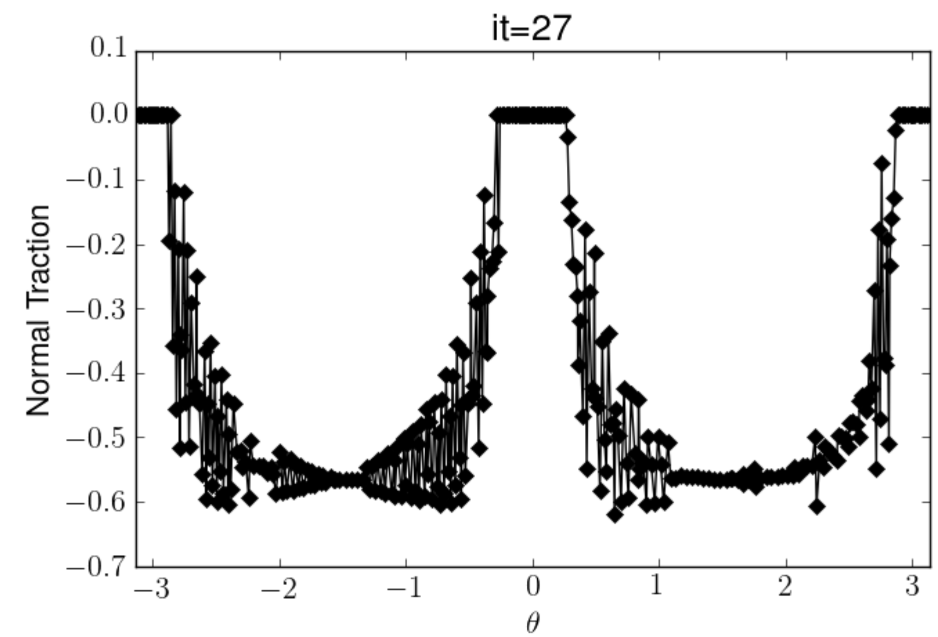
LaTIn Algorithm: Stability

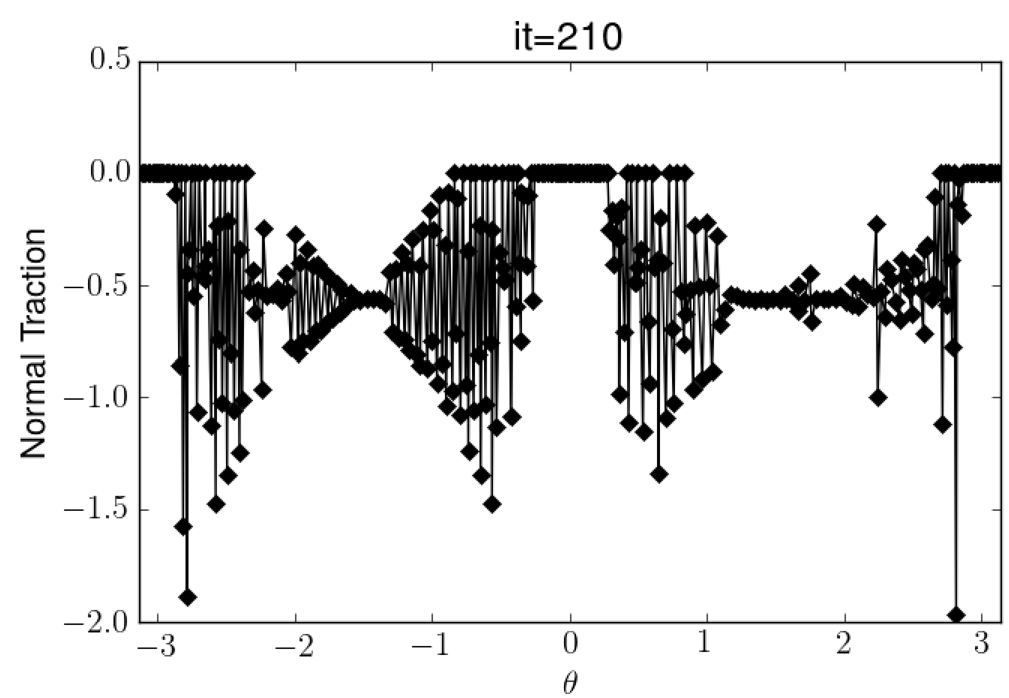




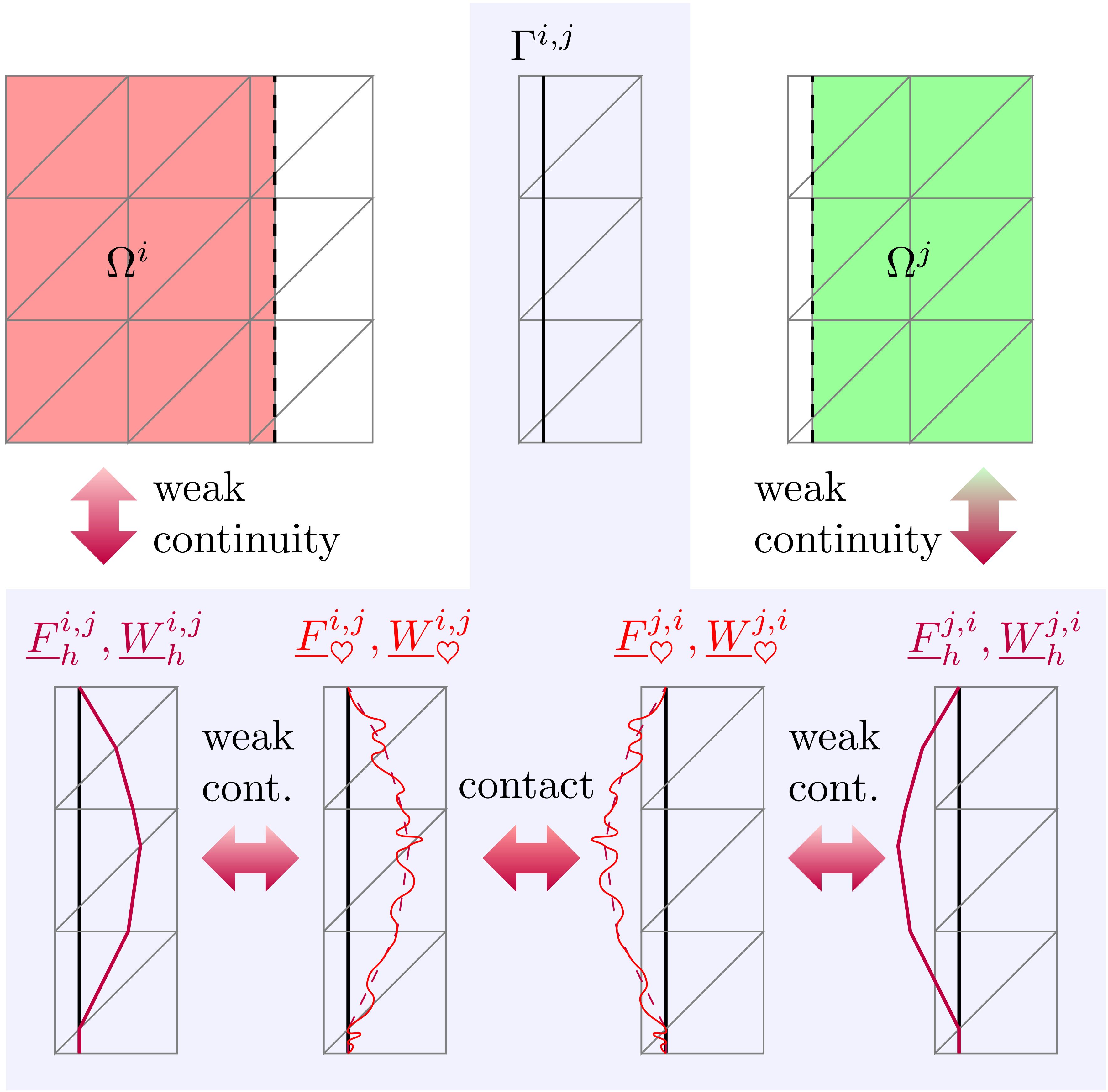
P1/P0 scheme polluted $\mathbf{F}^i$



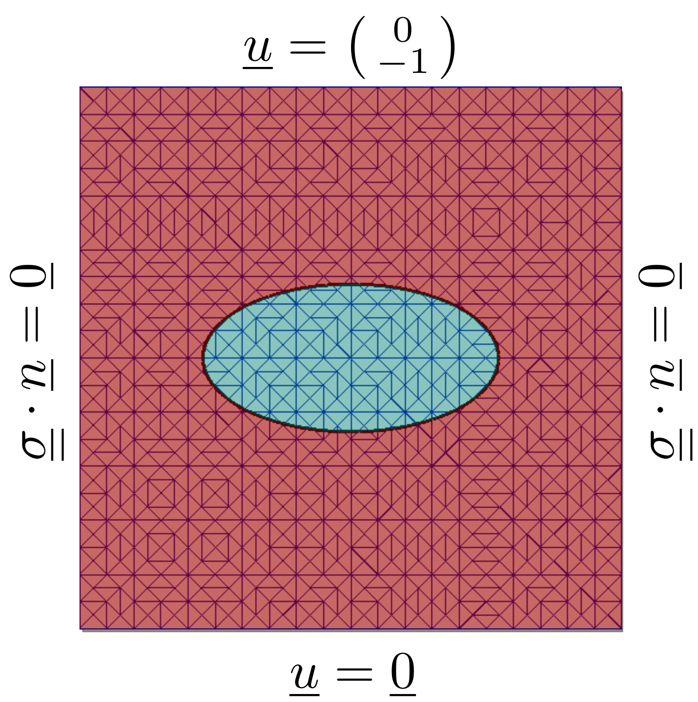




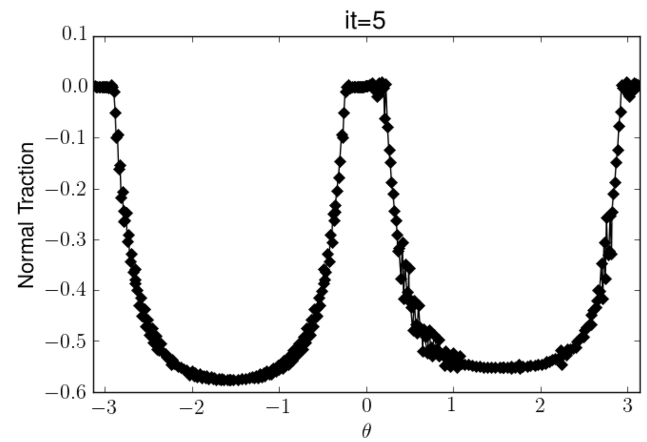
P1/P1 Stabilised Projection



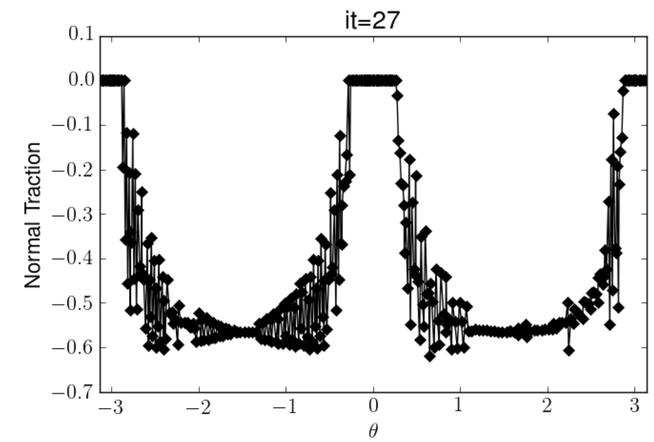
LaTIn Algorithm: Stability



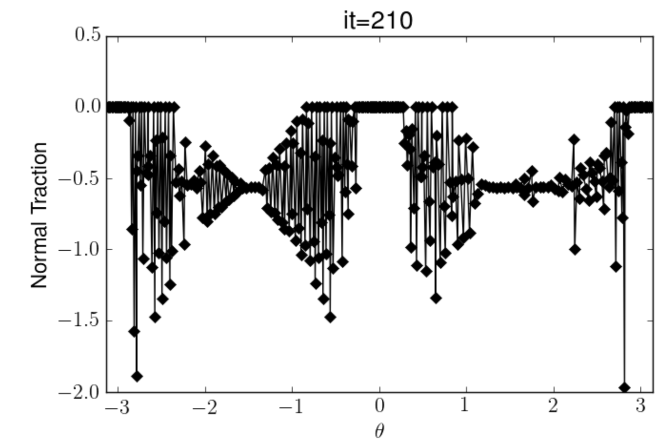
P1/P0 scheme polluted



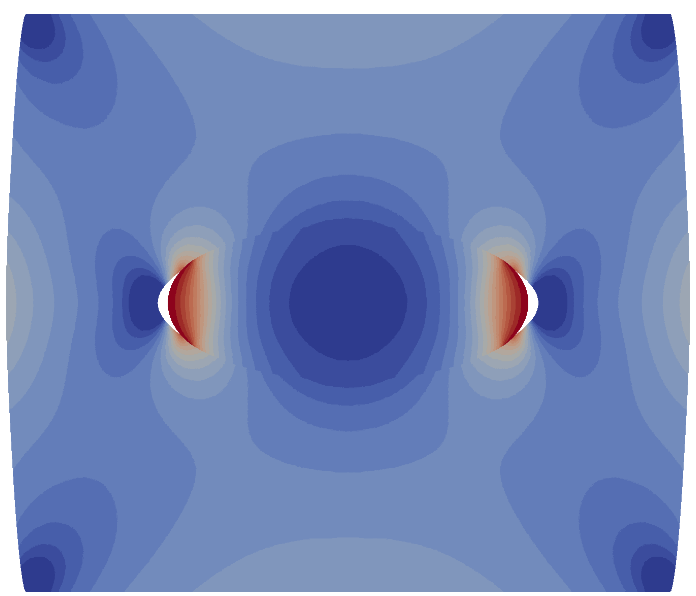
(a) P1/P0



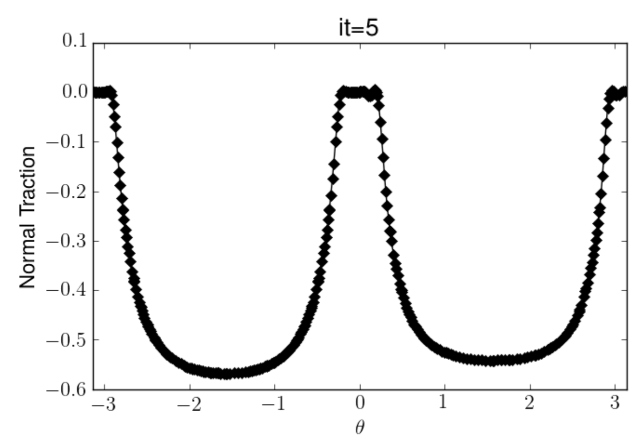
(b) P1/P0



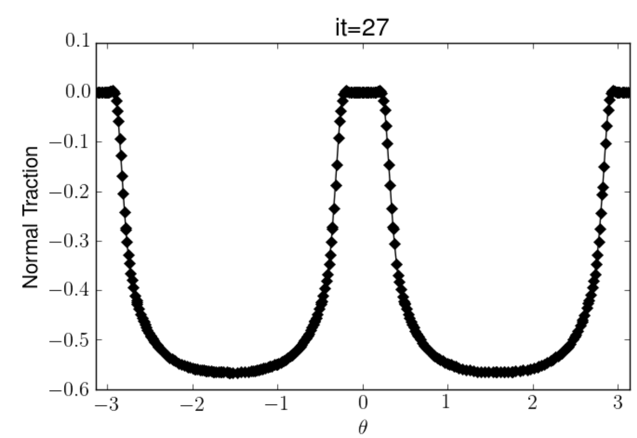
(c) P1/P0



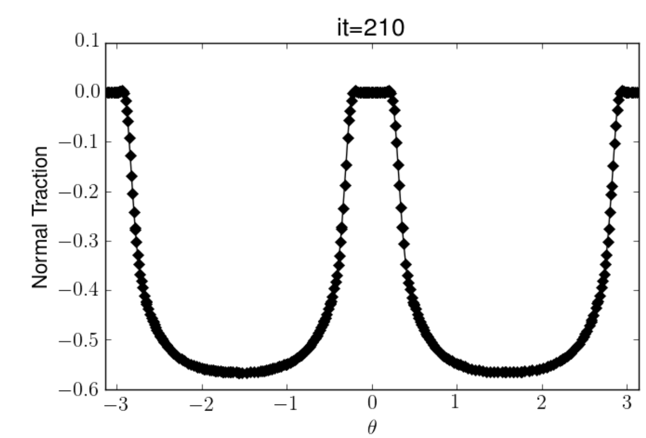
Proposed Solution: P1/P1 scheme with stabilisation



(d) P1/P1

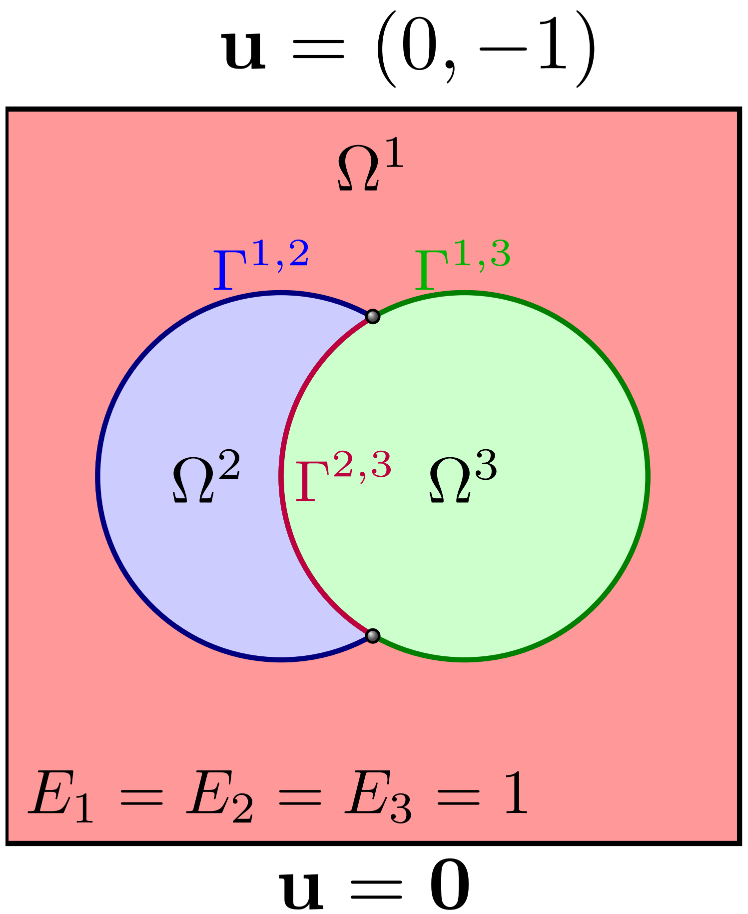


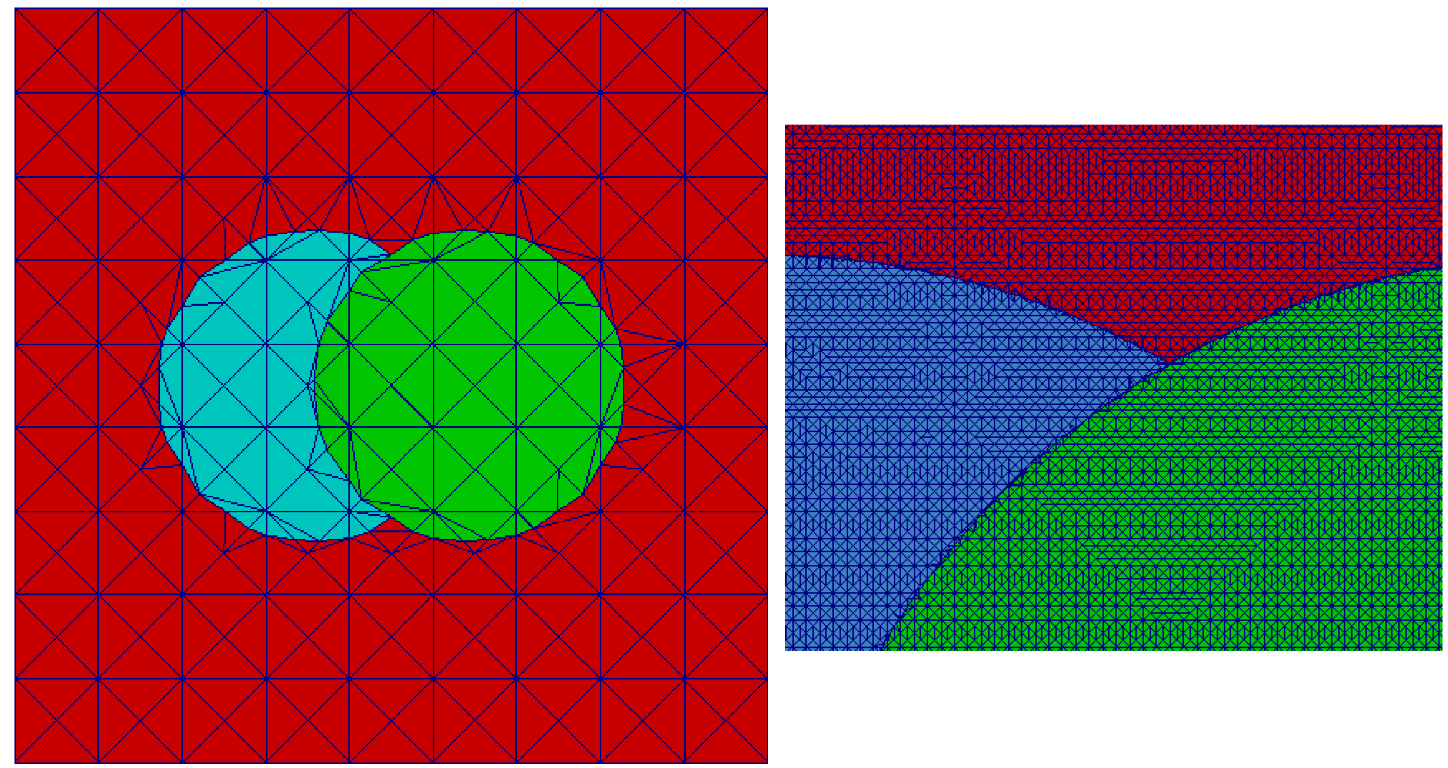
(e) P1/P1

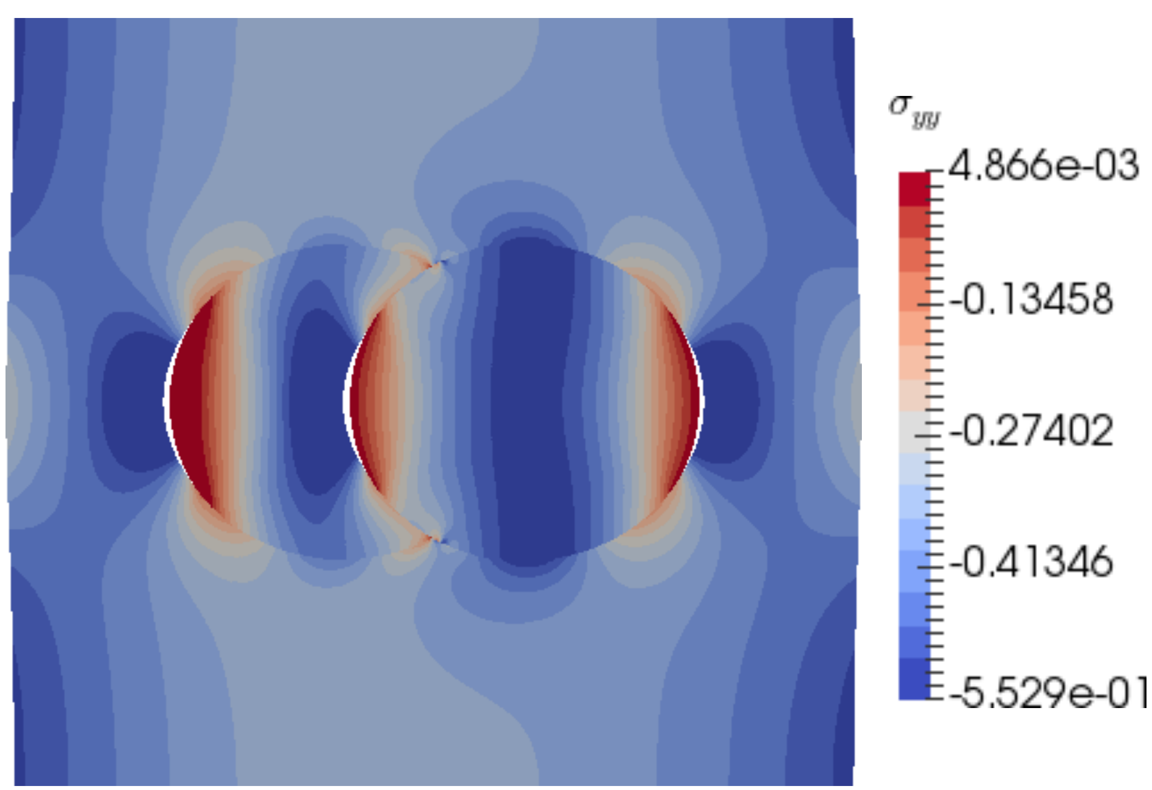


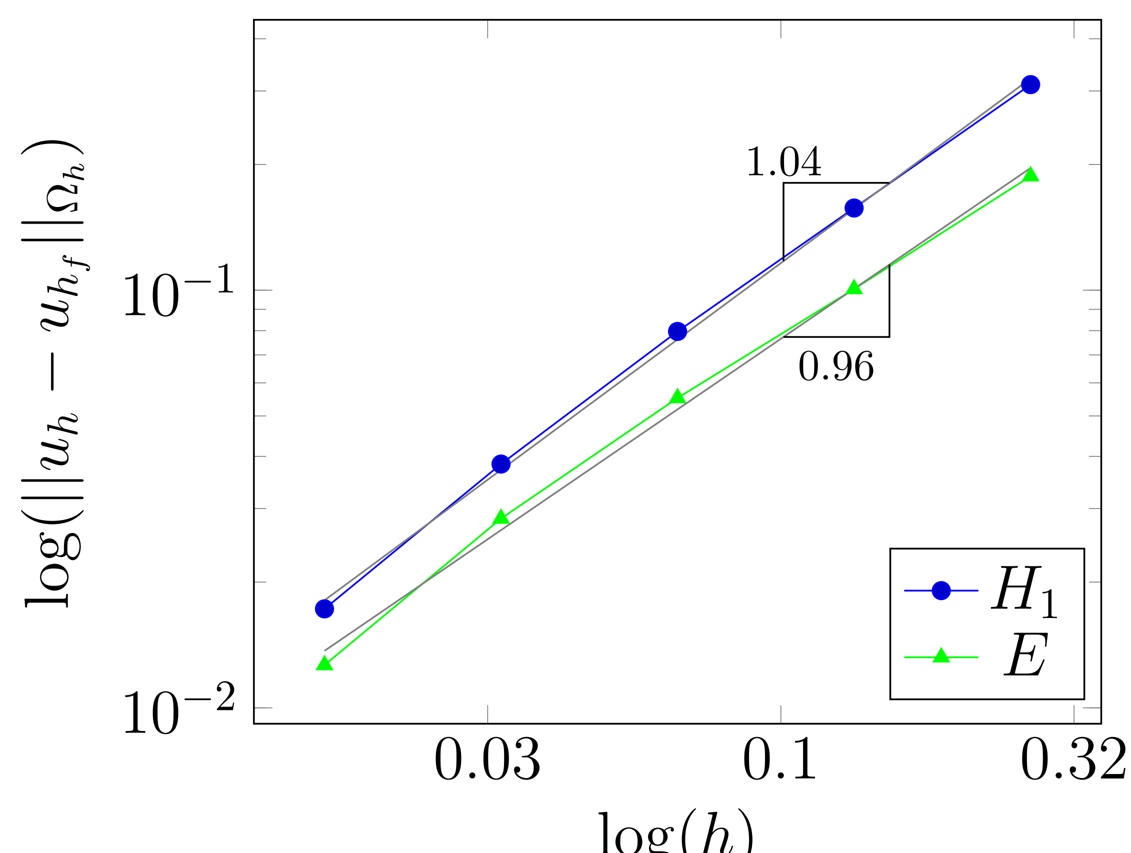
(f) P1/P1

Two Inclusions Frictionless Contact



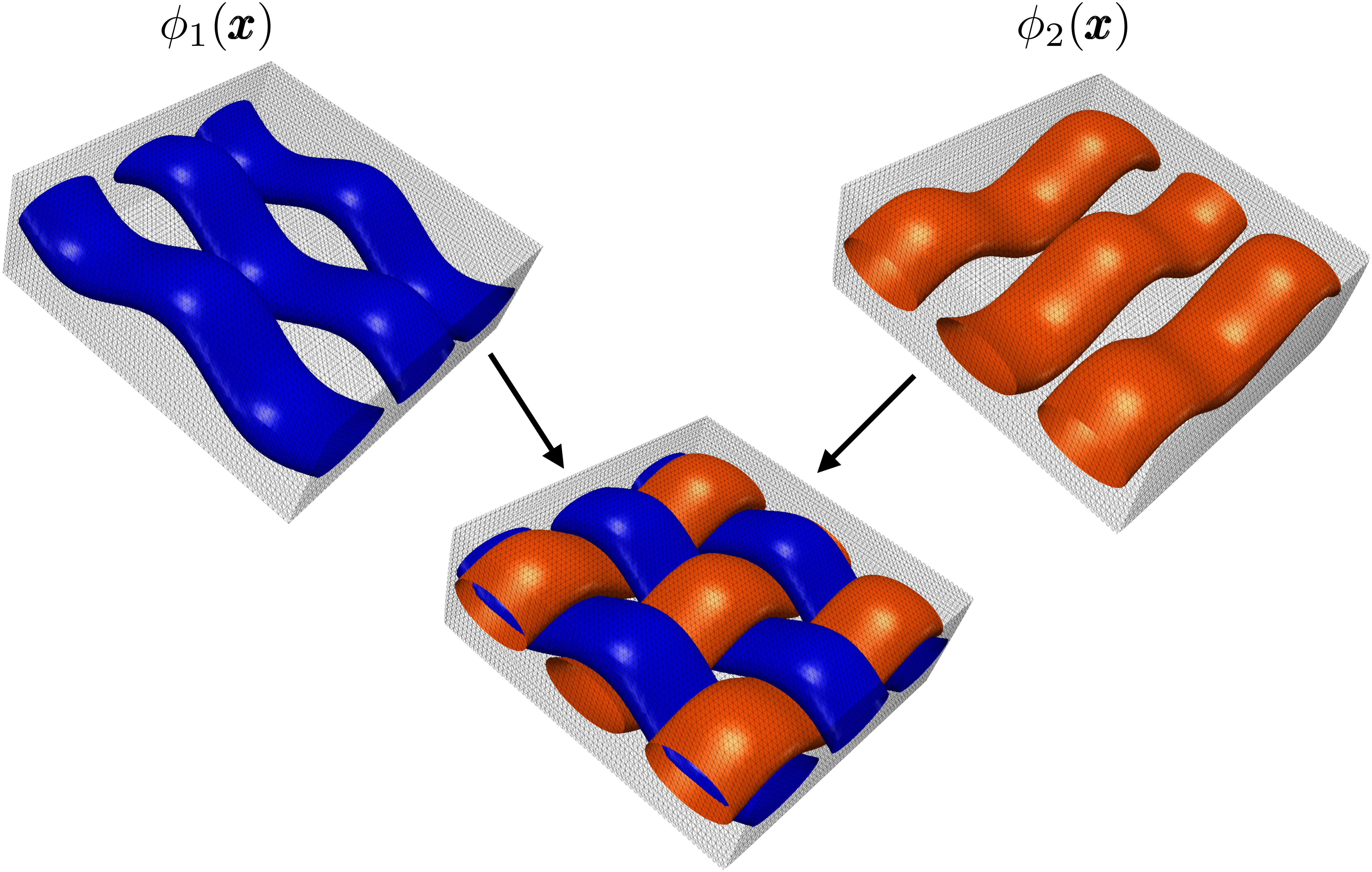






Applications in Engineering

Braided Composite



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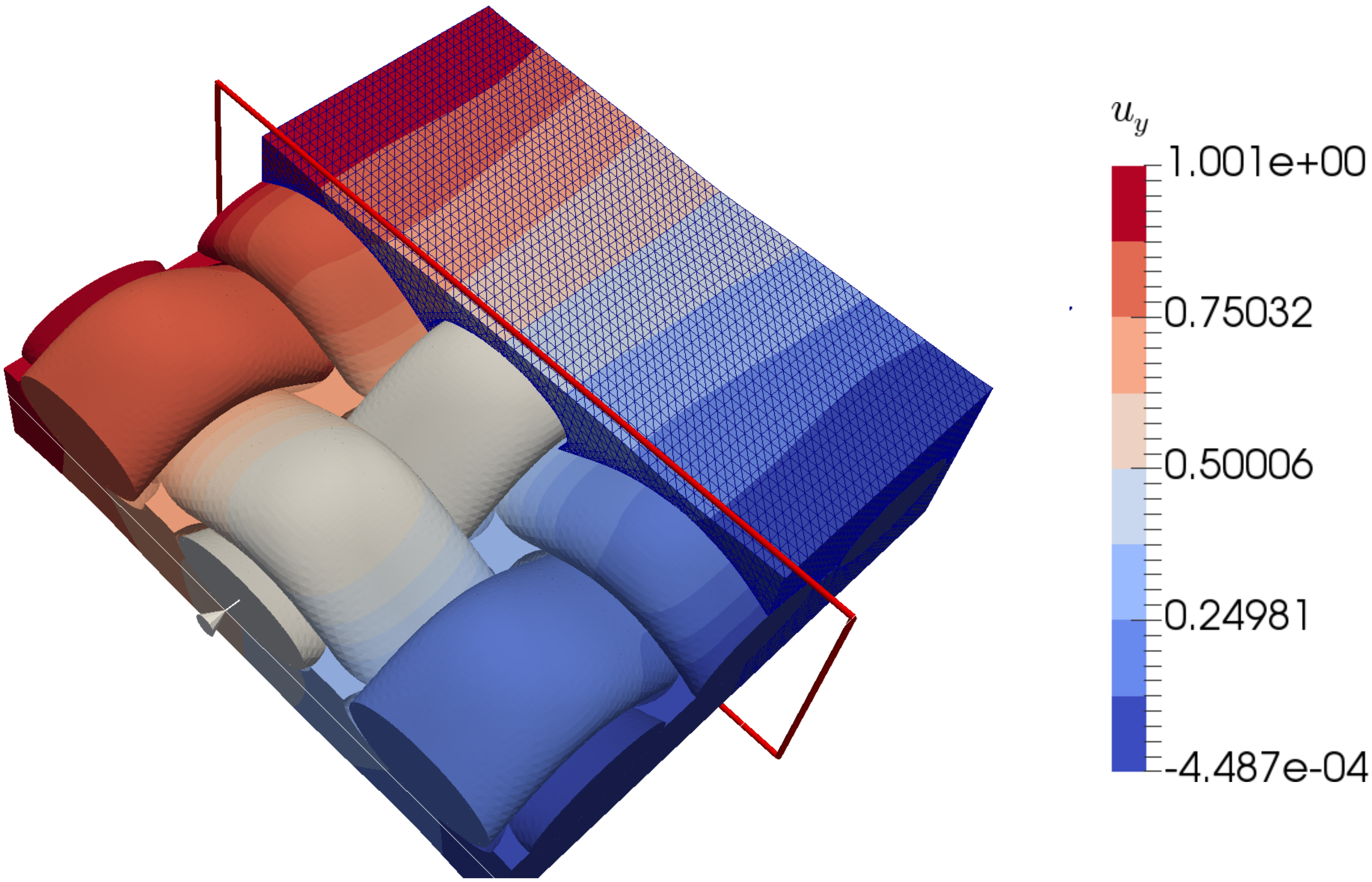

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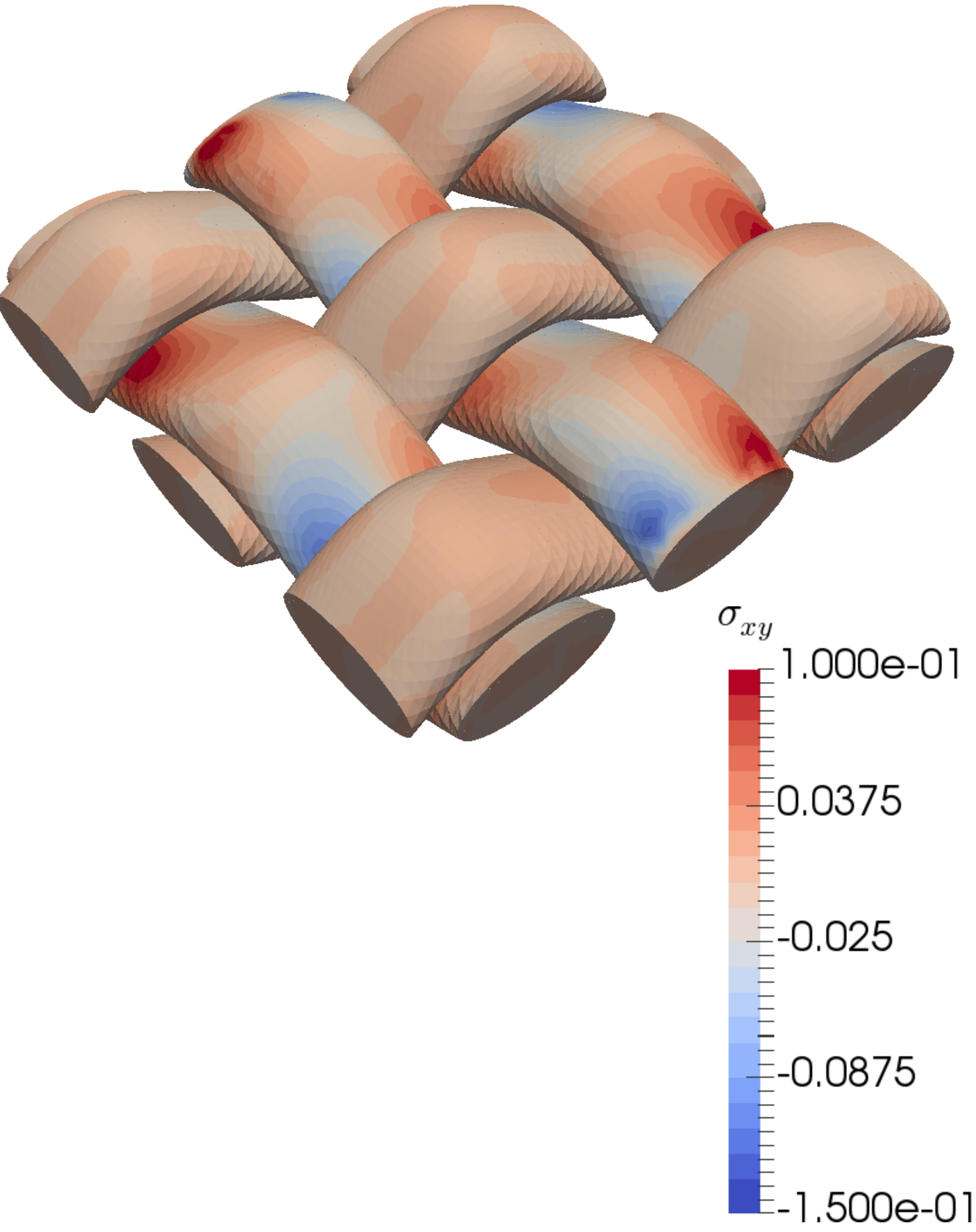

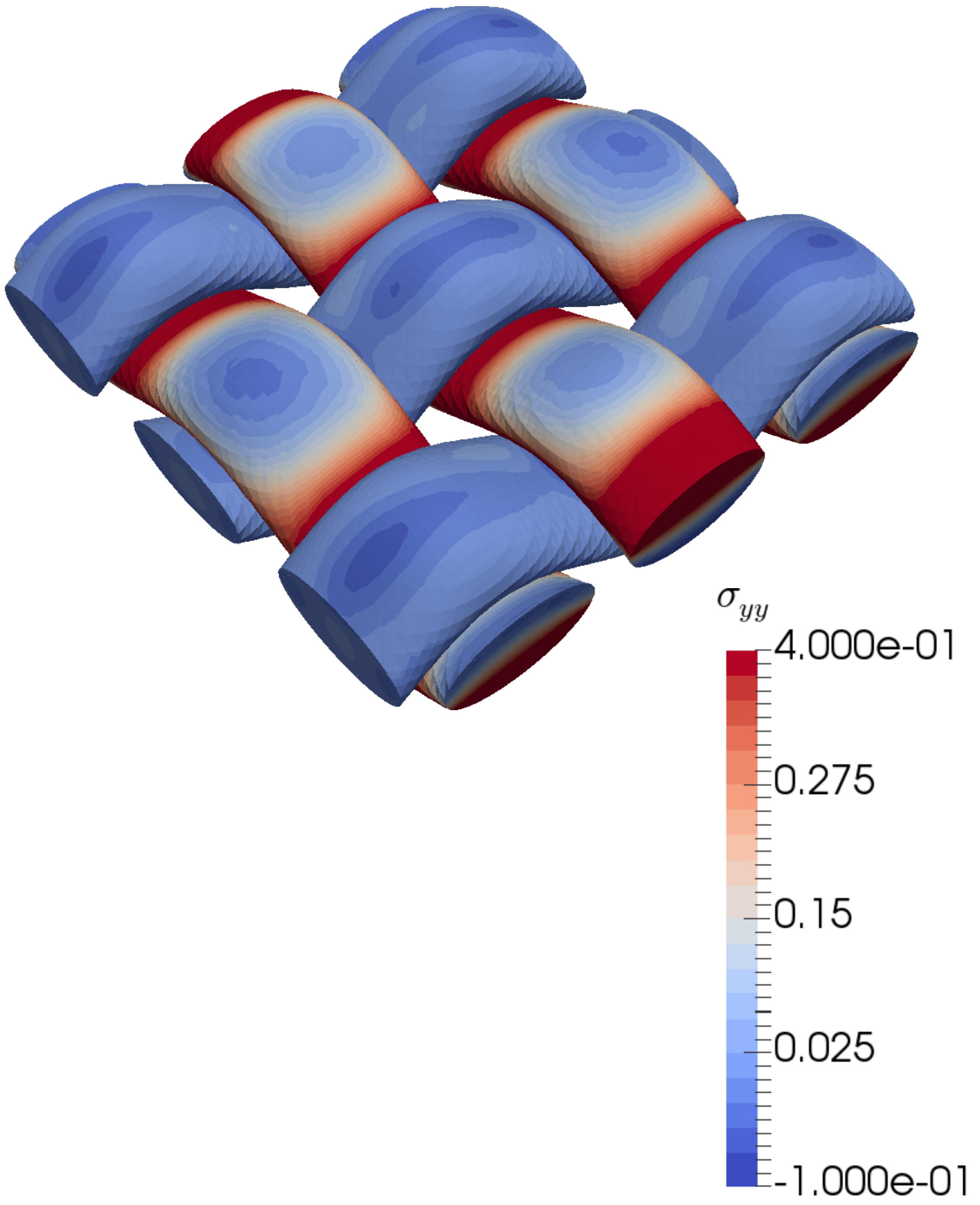

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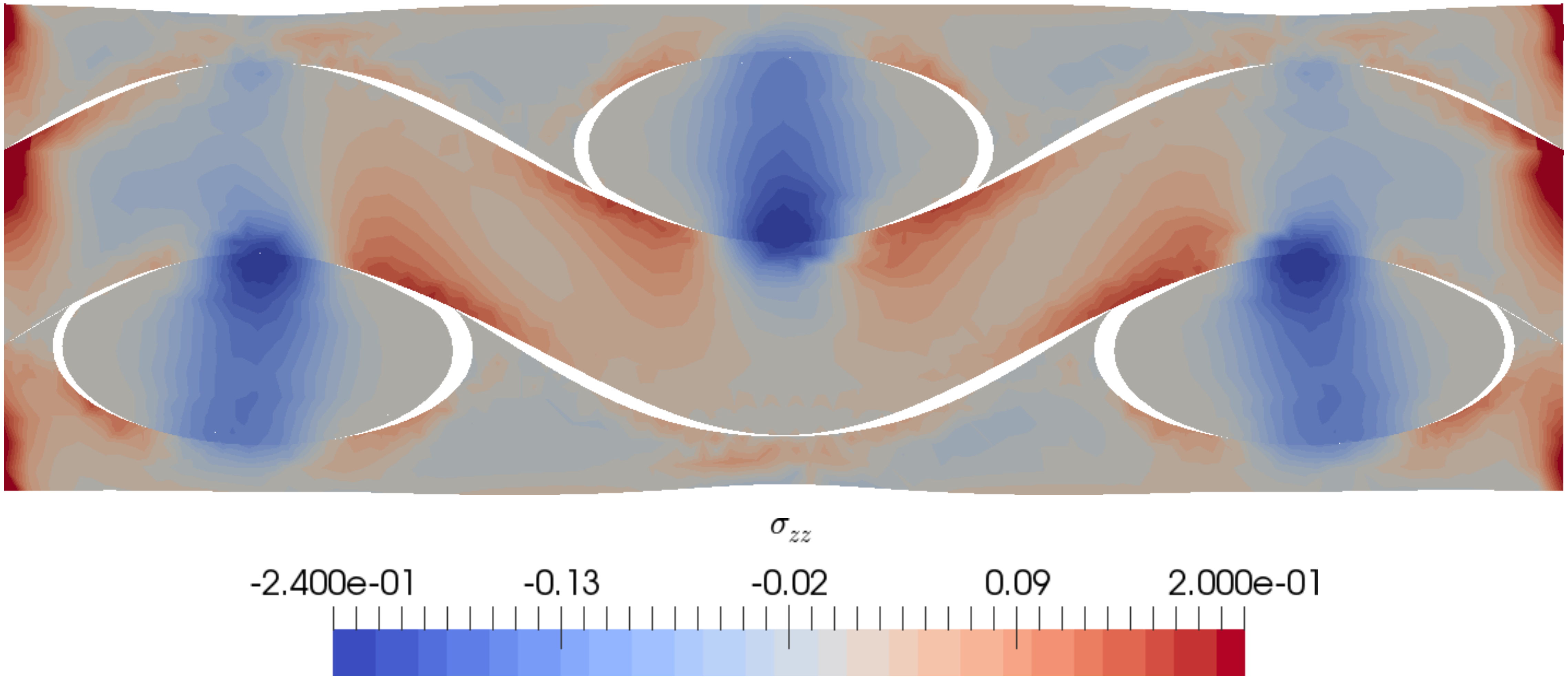
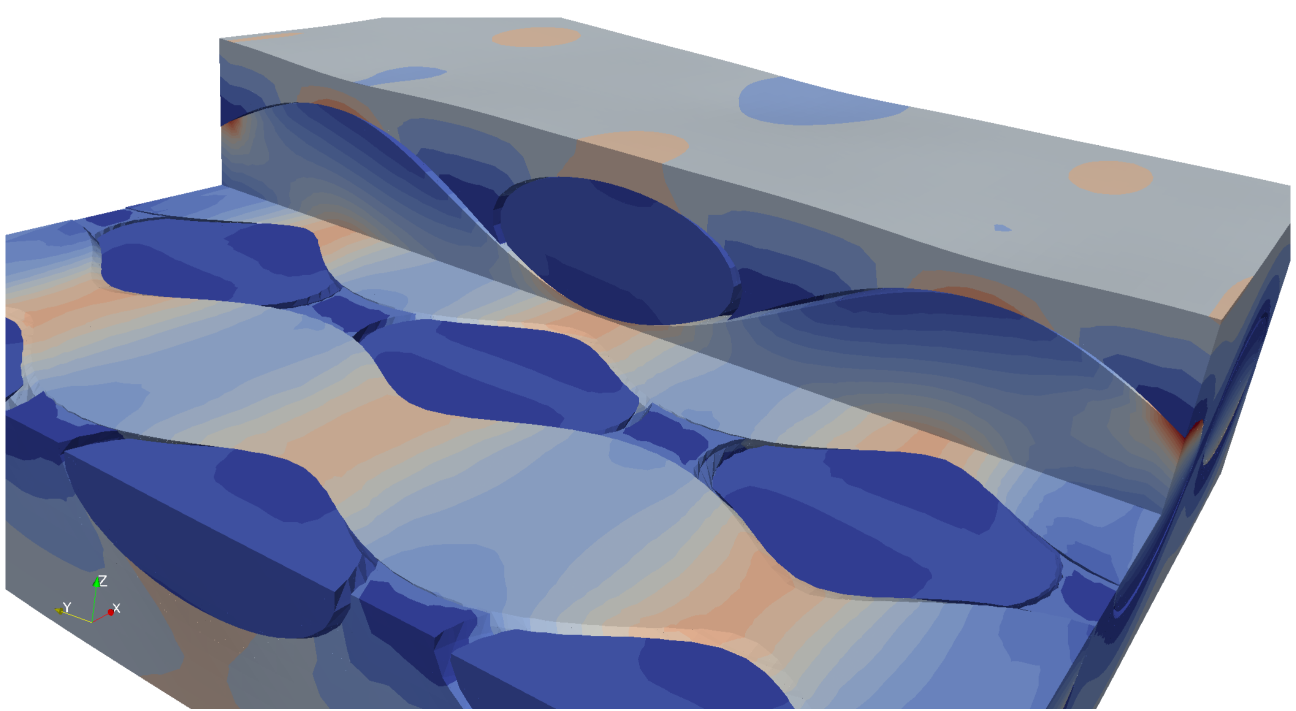
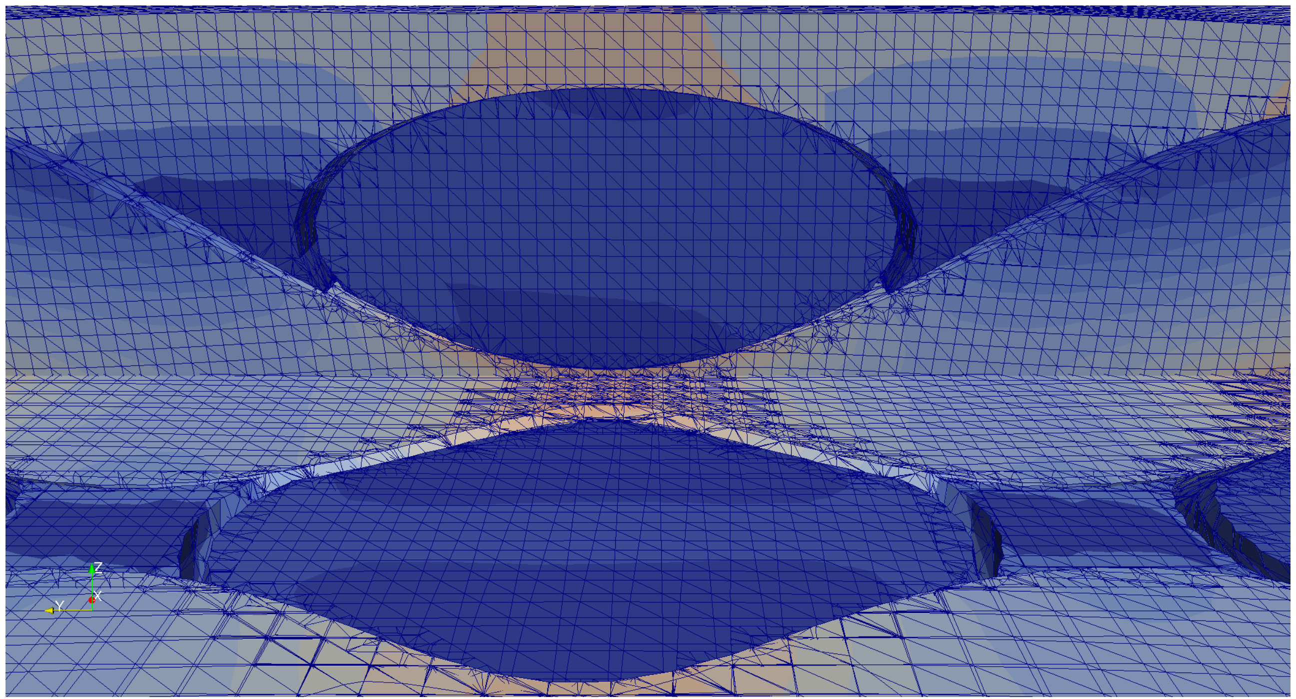
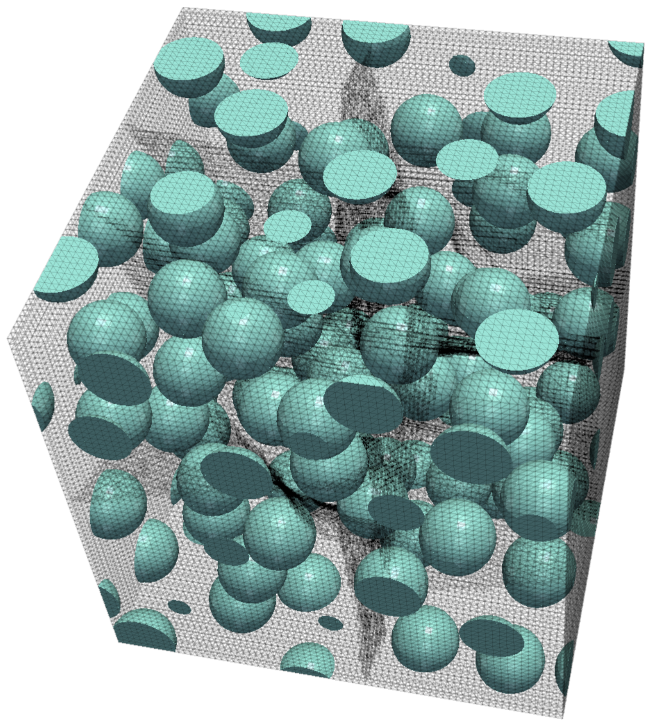
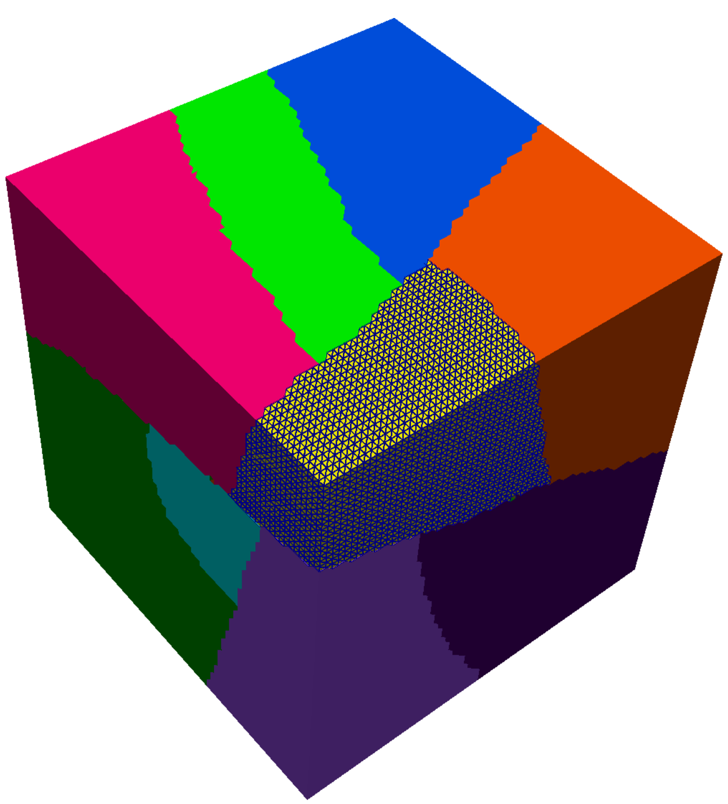




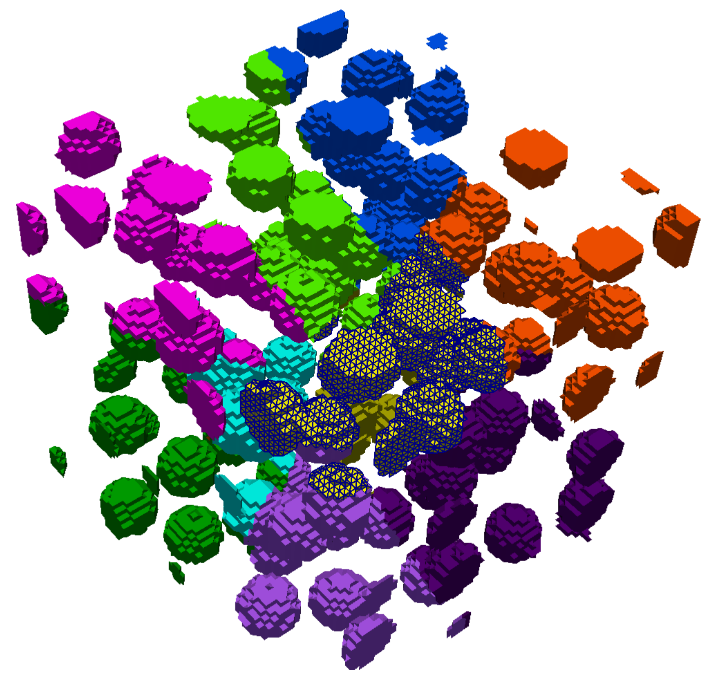


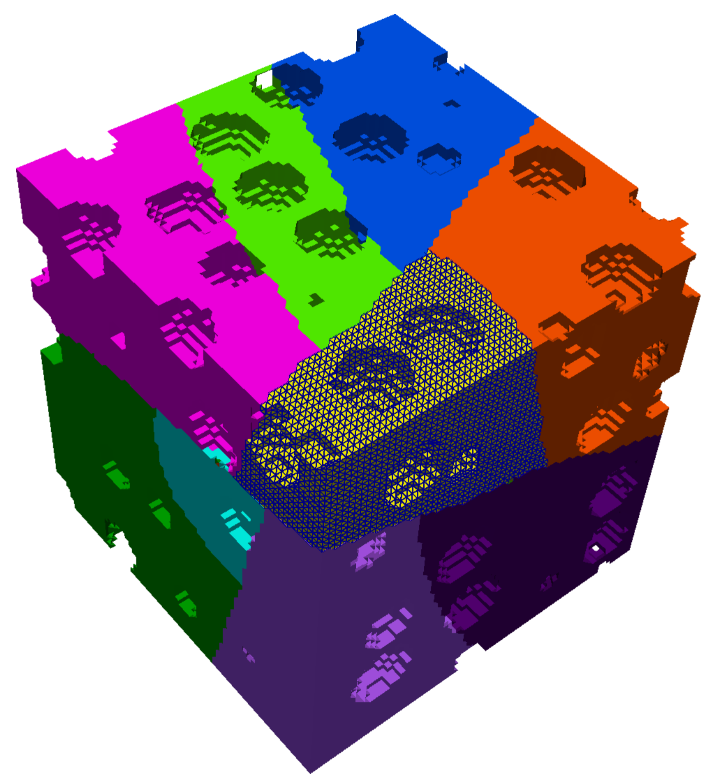
Damage in Concrete: Parallelisation

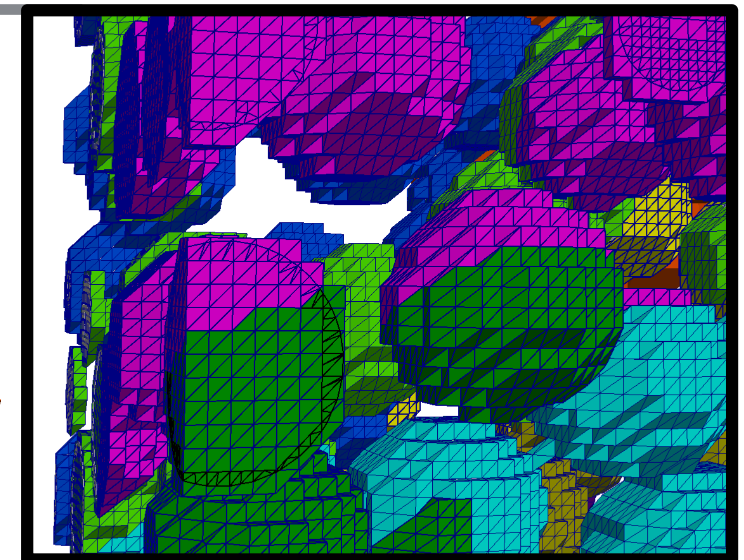




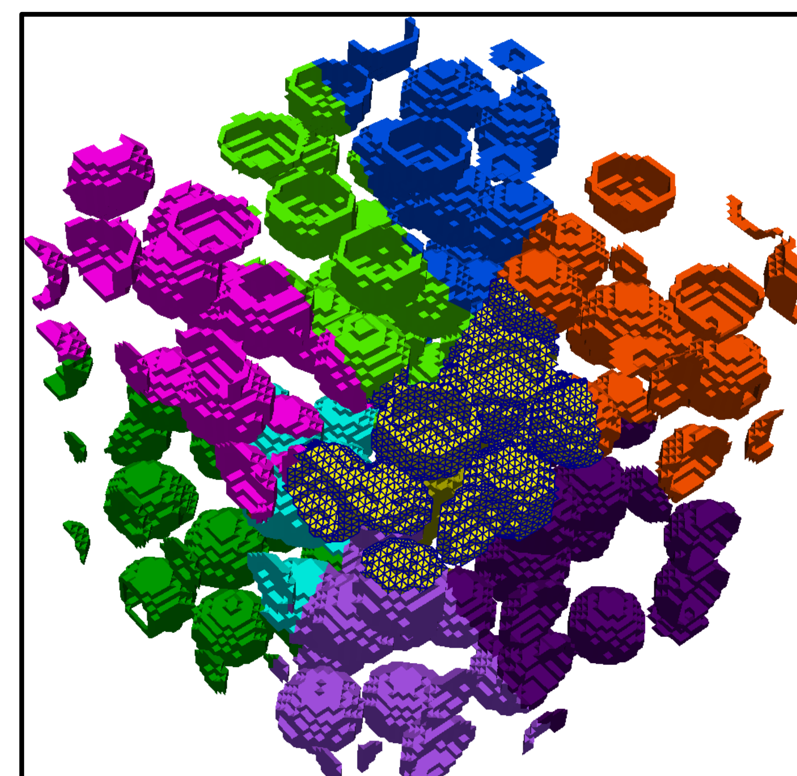
Linear Stage



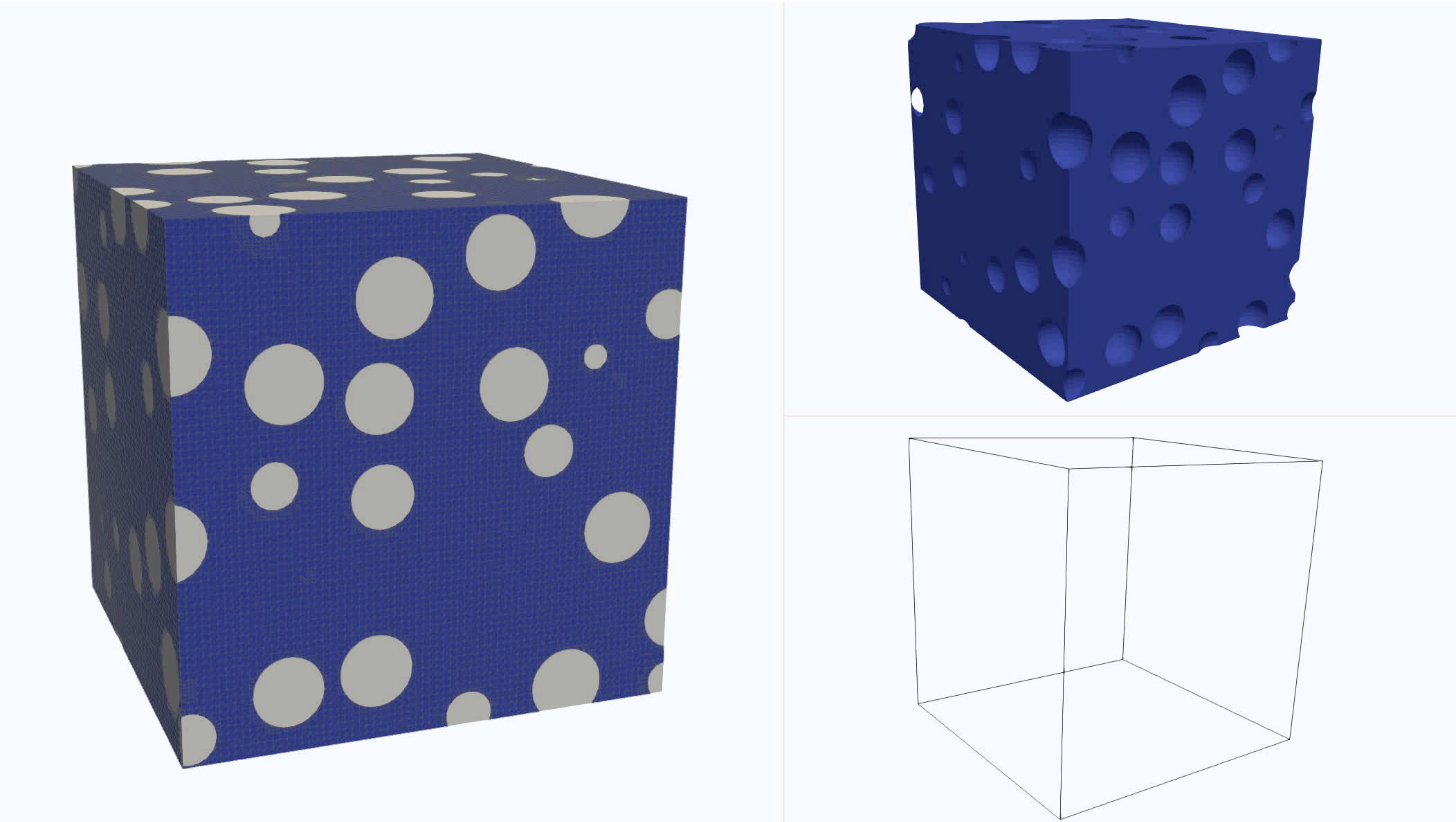


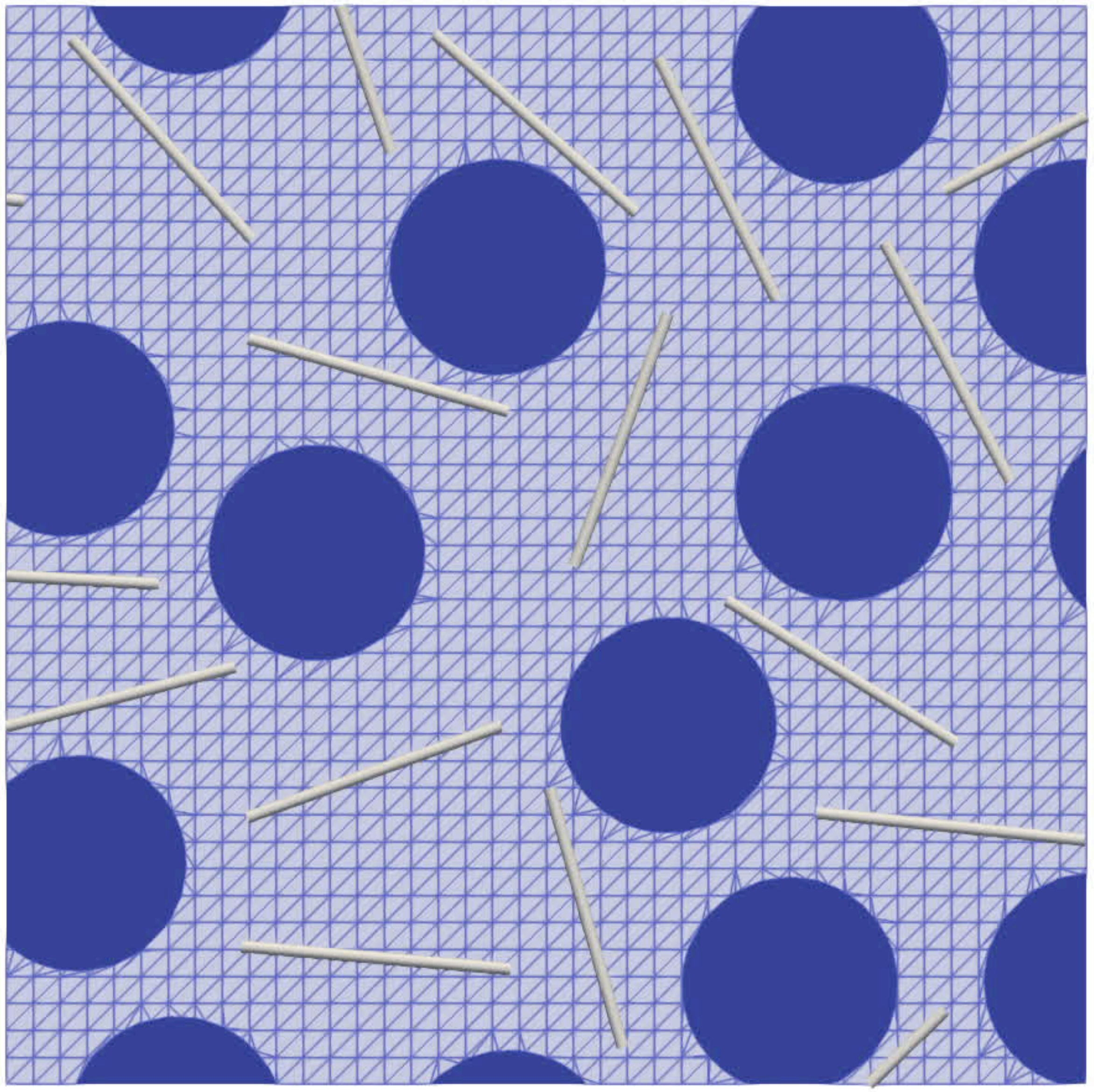


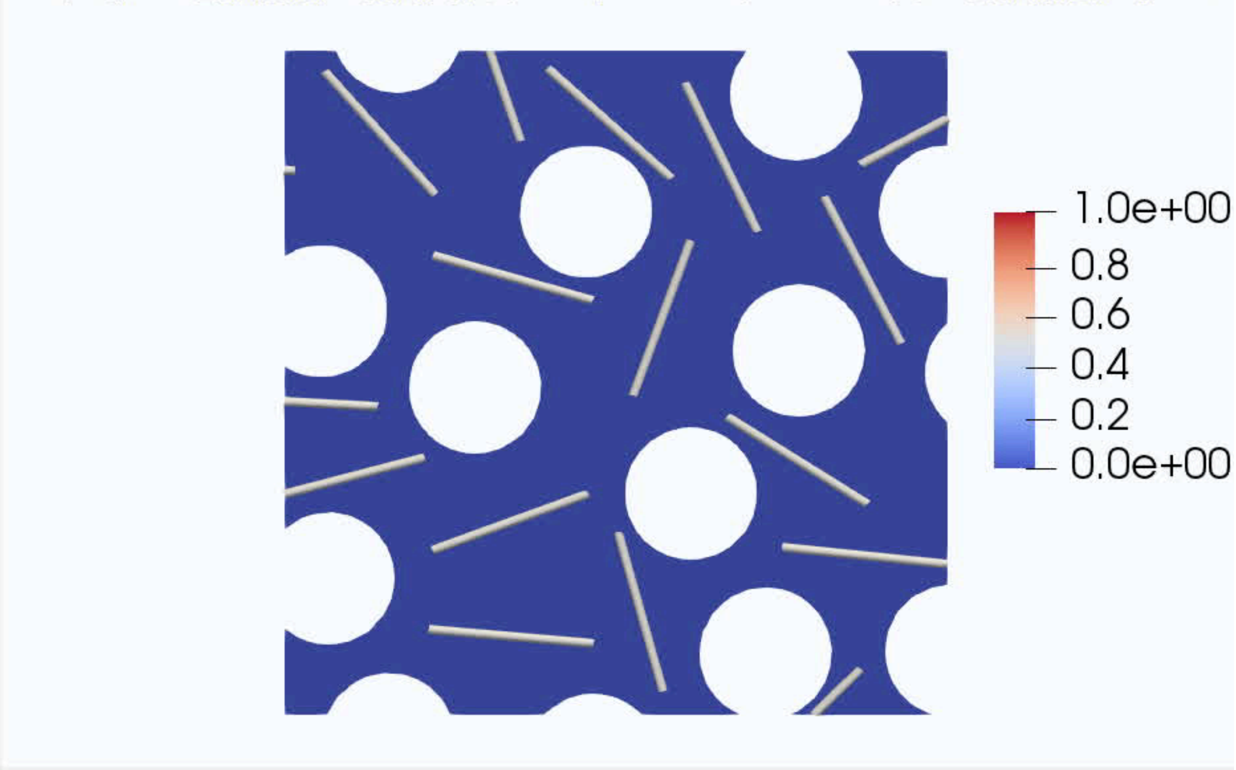
Local Stage



Damage in Concrete



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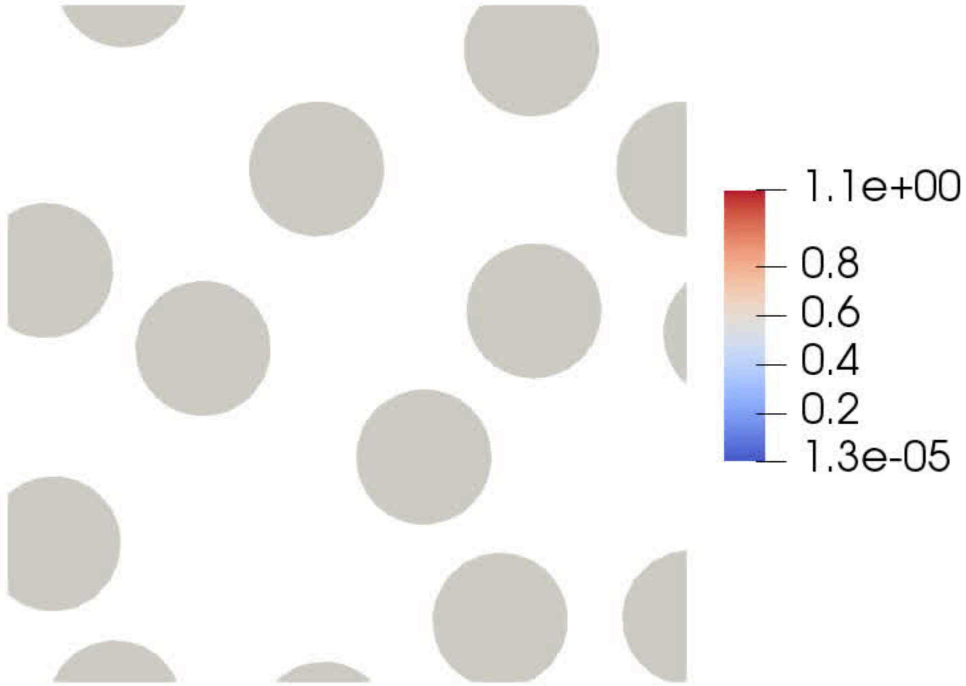
1.1e+00
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0.2
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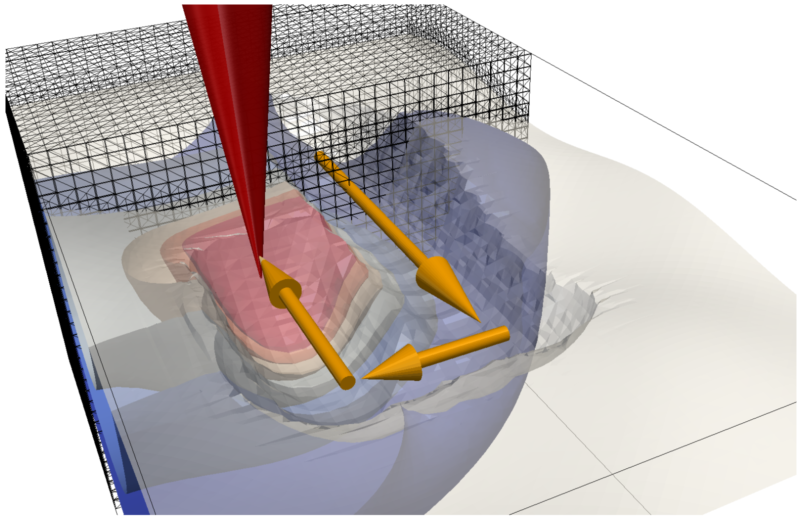
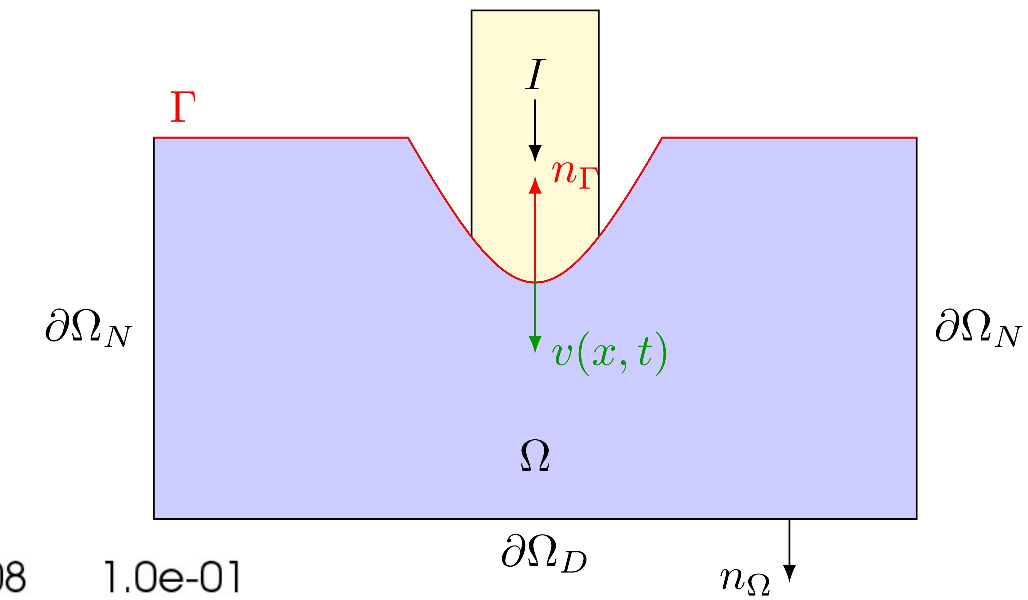
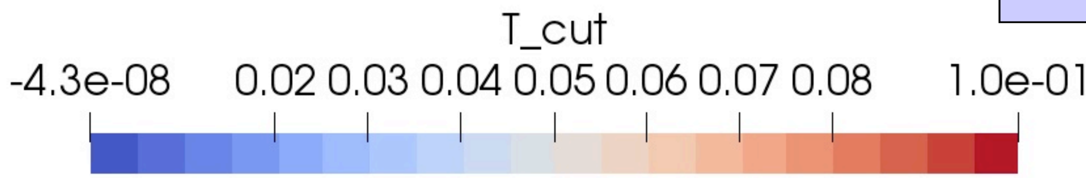
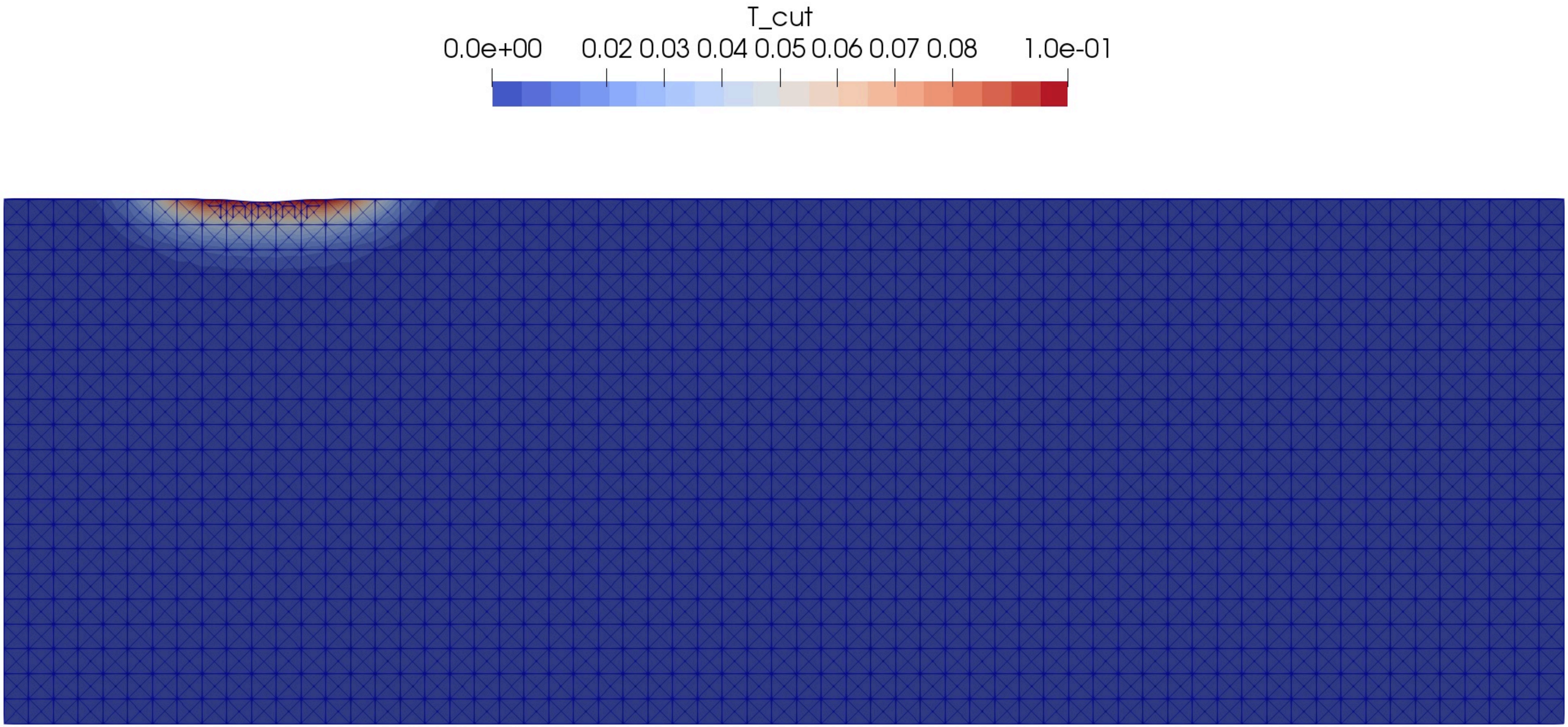
Pulsed Thermal Ablation



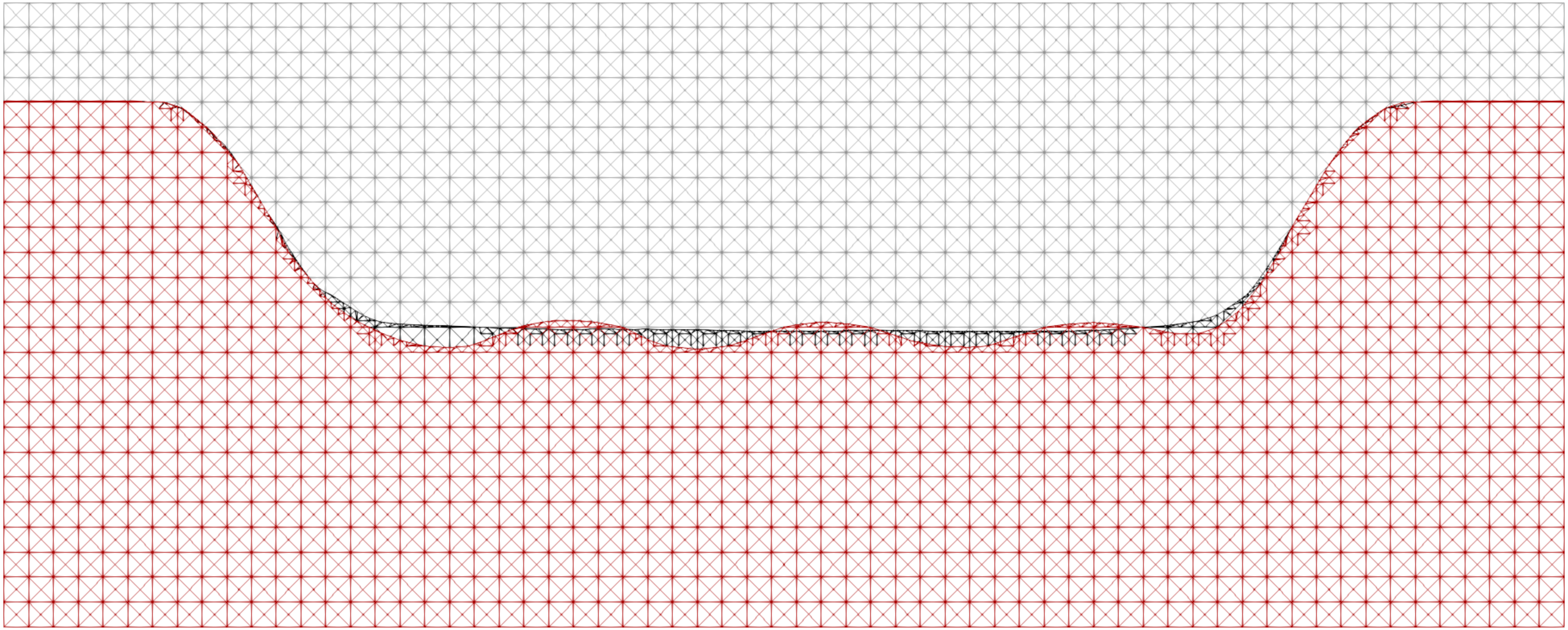




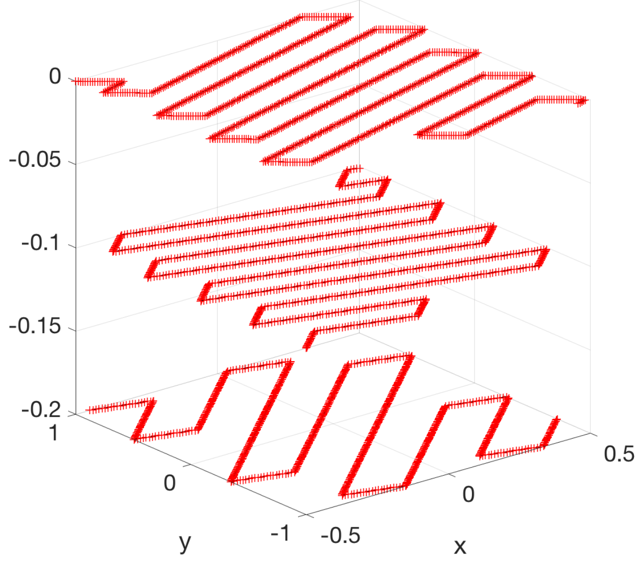
Pulsed Thermal Ablation

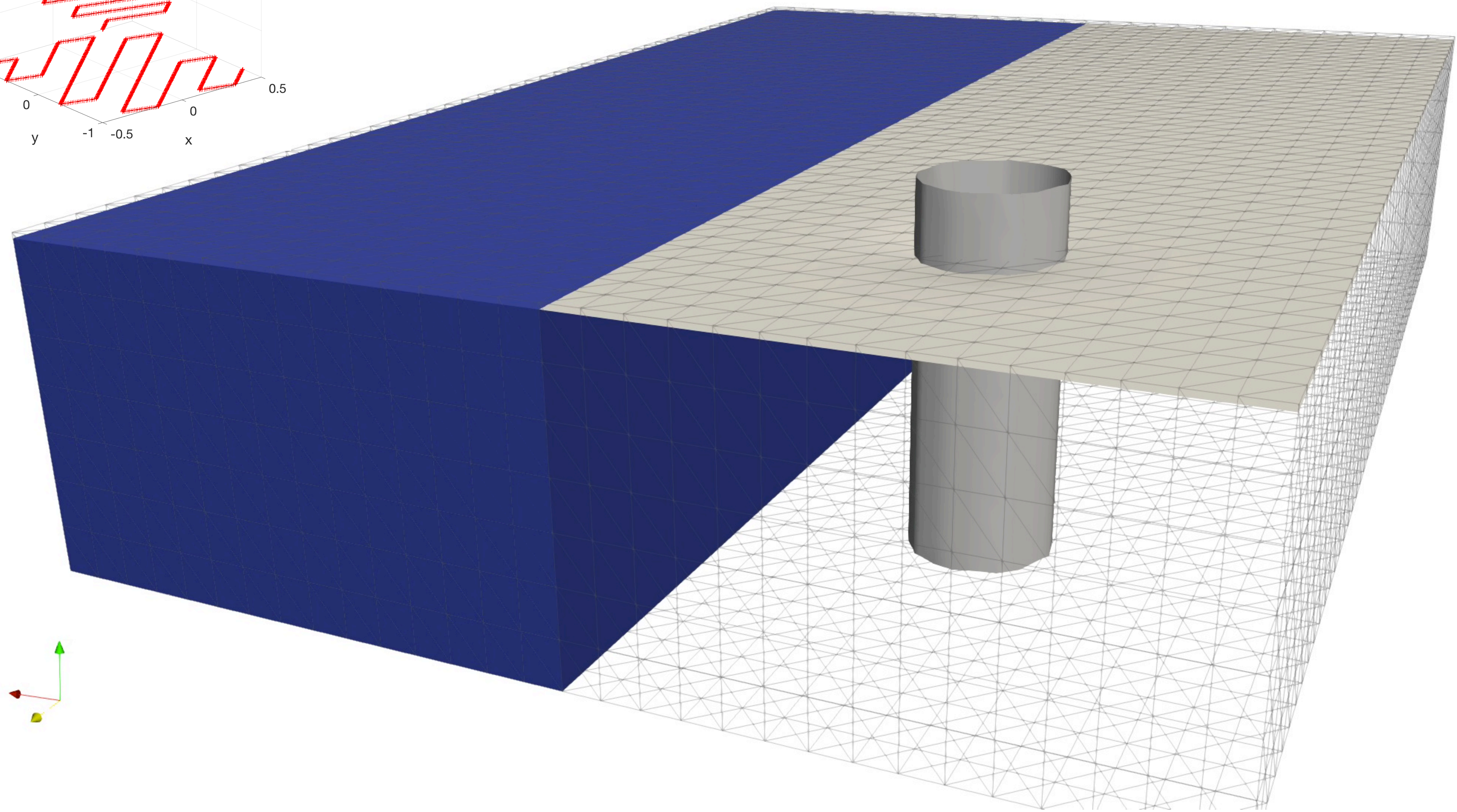


Pulsed Thermal Ablation



3D Machining Path





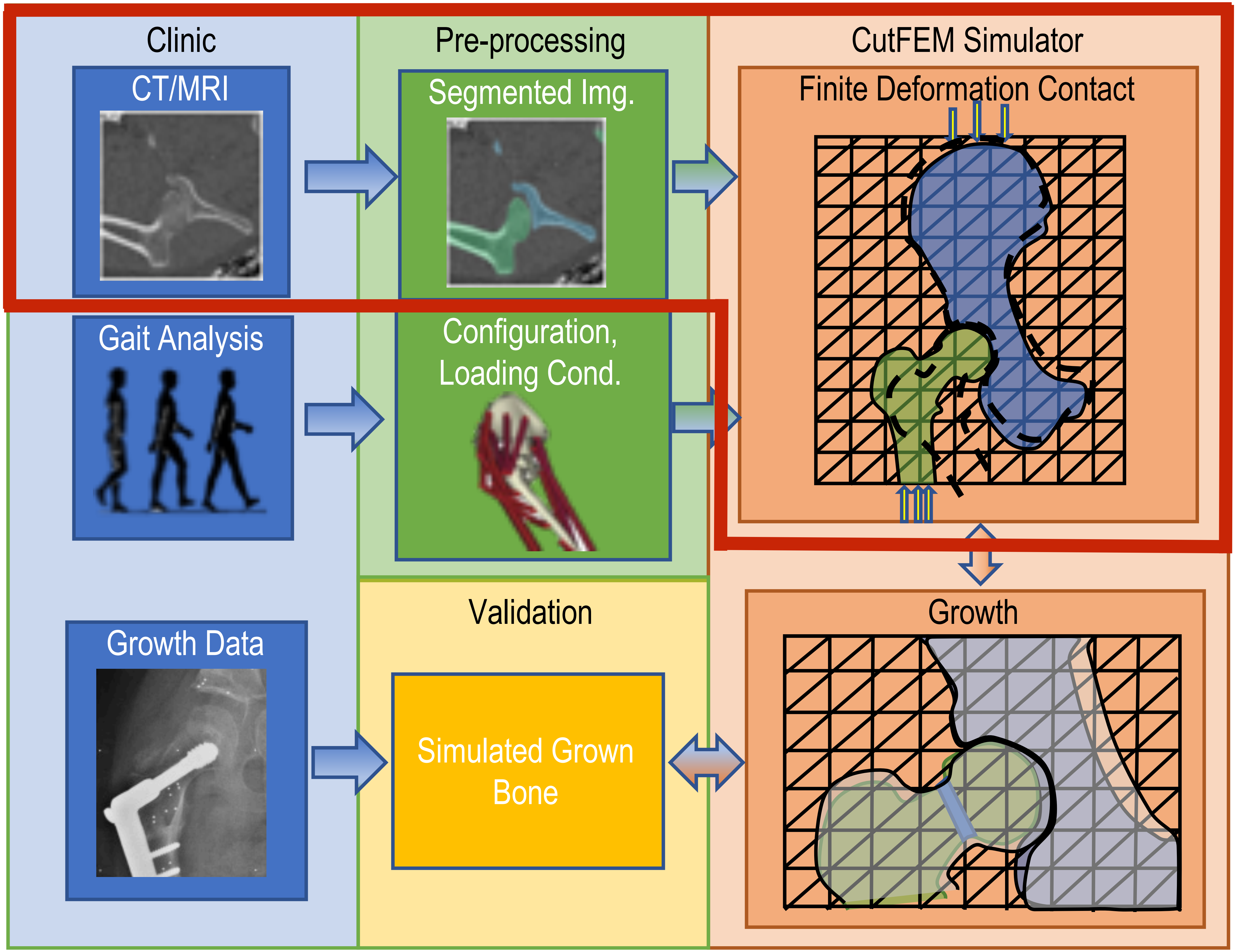
Applications in Biomechanics

Cut Finite Element Hip Modelling Motivation

Treatment options for hip malformations: (left) untreated hip deformity of a 4-year-old child, (middle) well-formed hip 8 years post guided growth surgery[1], i.e. insertion of one screw through the growth plate of the femur bones, (right) well-formed hip after an invasive femur and hip osteotomy, i.e. cutting through the bones and insertion of screws and plates.

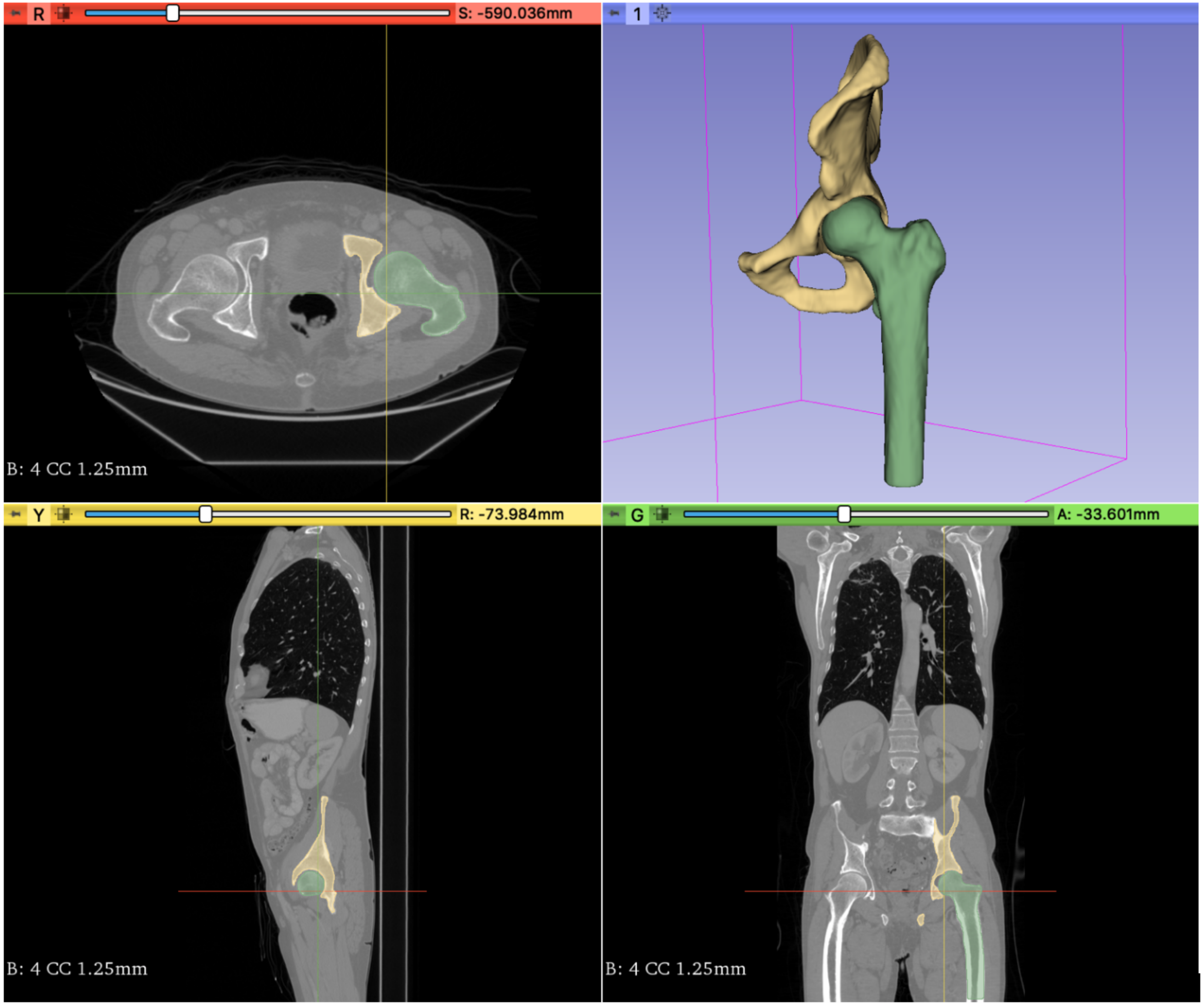
Study stress in hip joint using FE Modelling to enhance understanding of bone growth and bone shape changes

[1] Lee, W-C et al. "Guided growth of the proximal femur for hip displacement in children with cerebral palsy." *Journal of Pediatric Orthopaedics* 36.5, 511-515, (2016).

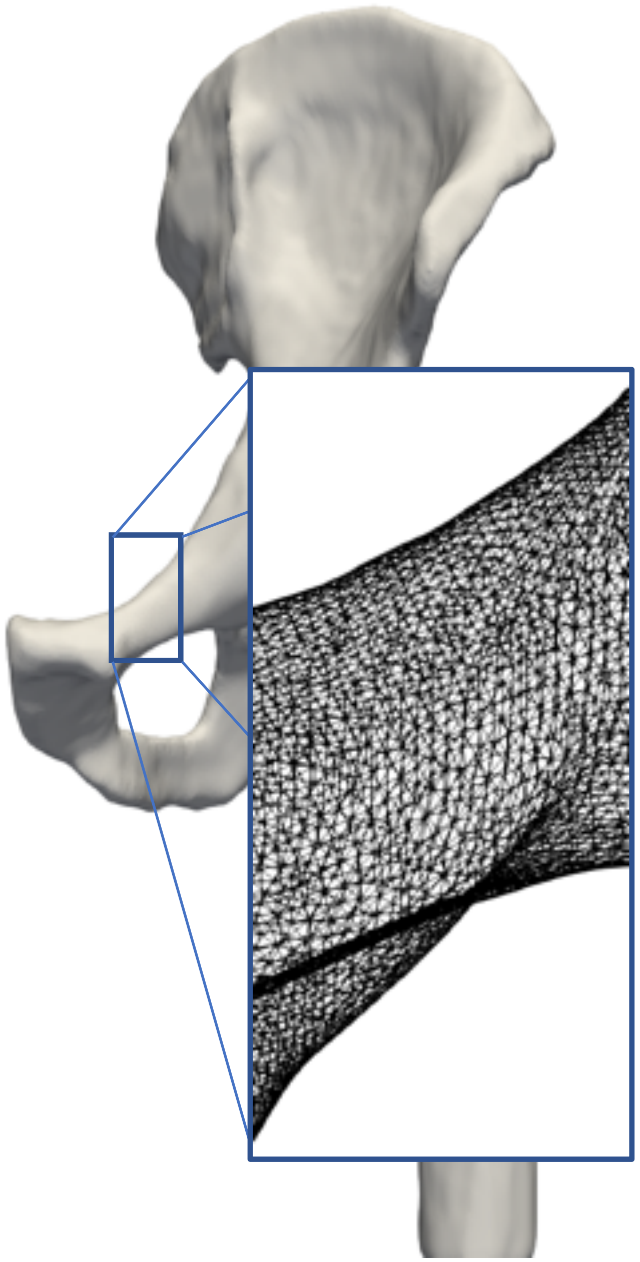

Clinic
CT/MRI
Gait Analysis
Growth Data
Pre-processing
Segmented Img.
Configuration,
Loading Cond.
Validation
Simulated Grown
Bone
CutFEM Simulator
Finite Deformation Contact
Growth

Surface Triangulation to CutFEM pipeline

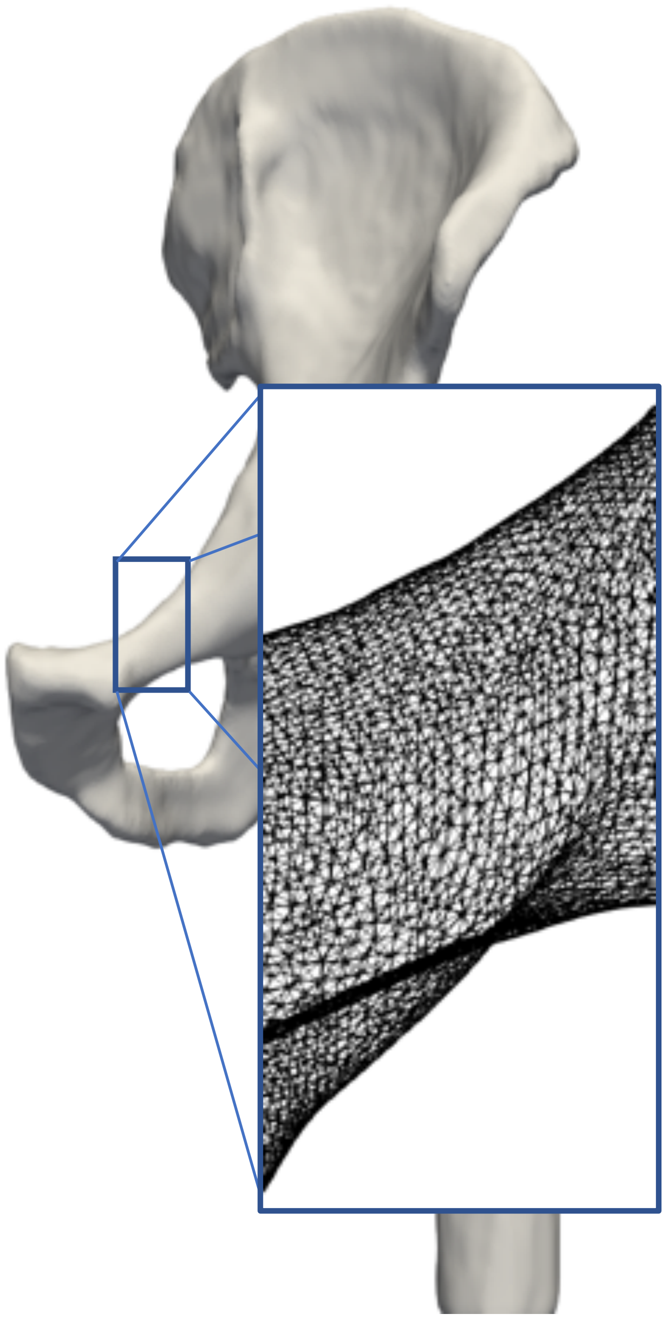
Segmentation with 3D Slicer (Faezeh Moshfeghifar) of CT-image from the cancer imaging archive (TCIA)

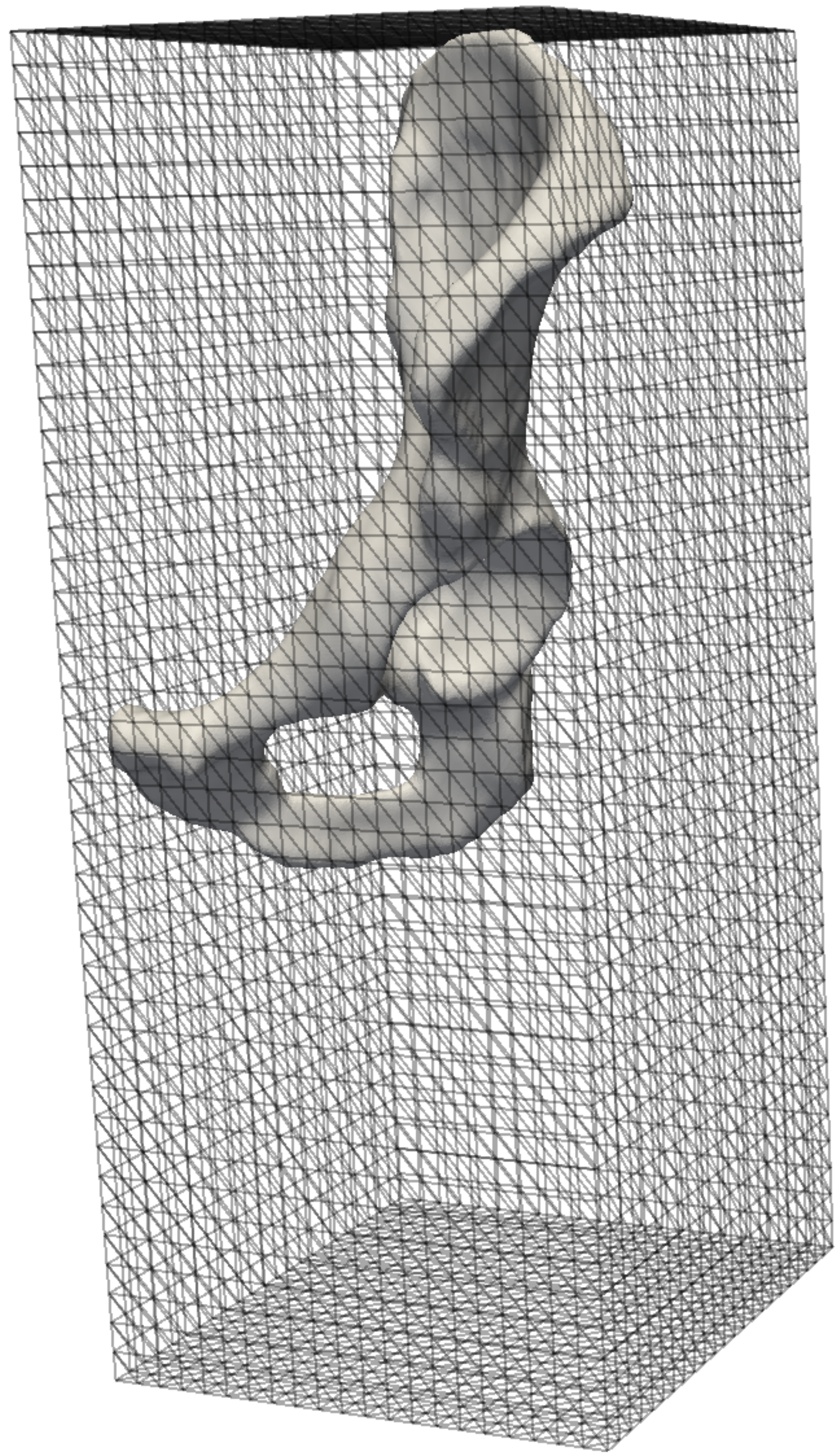


Surface triangulation

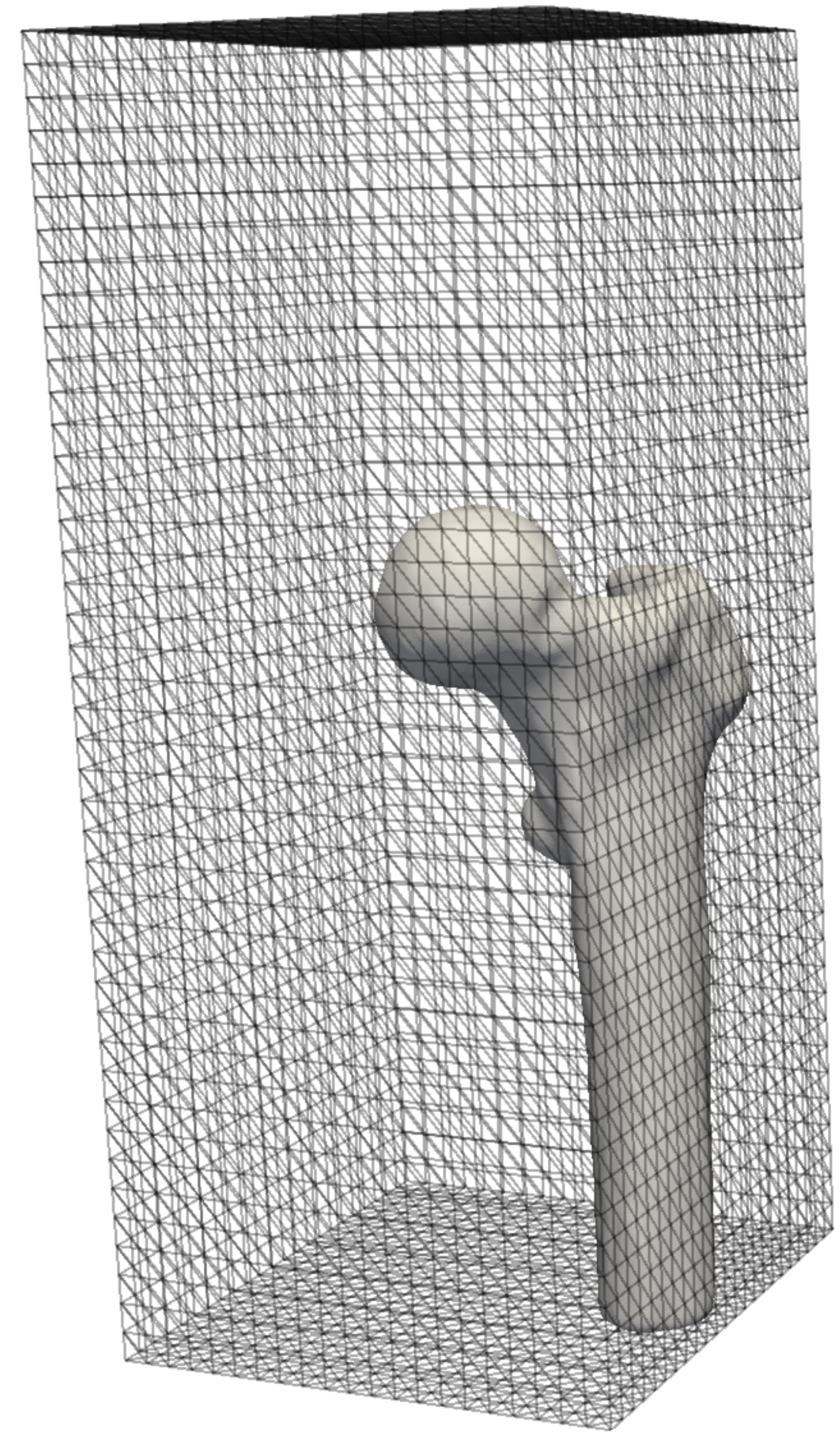


Create Regular Background mesh



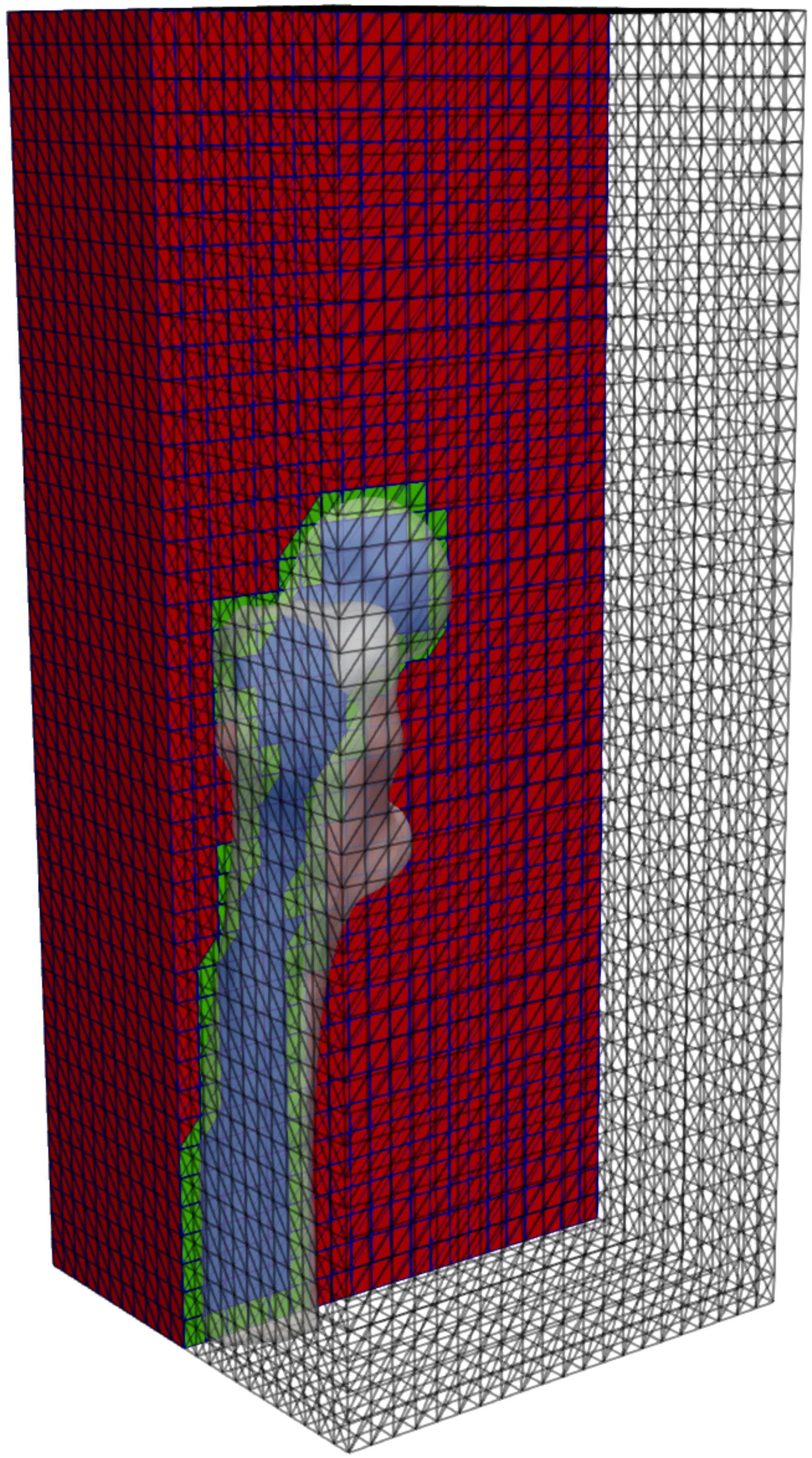


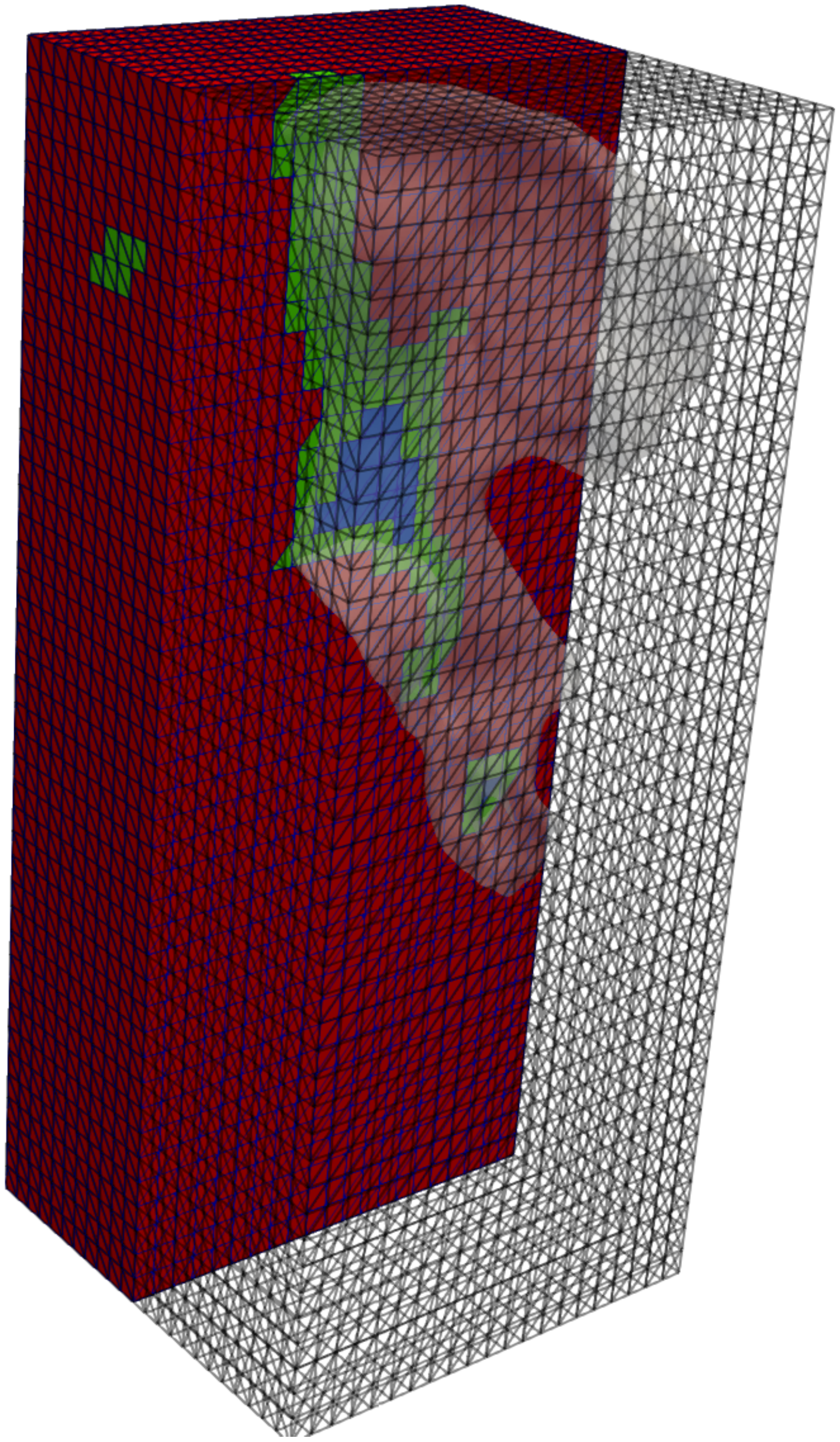
Hip bone surface triangulation embedded in regular background mesh



Femur bone surface triangulation embedded in regular background mesh

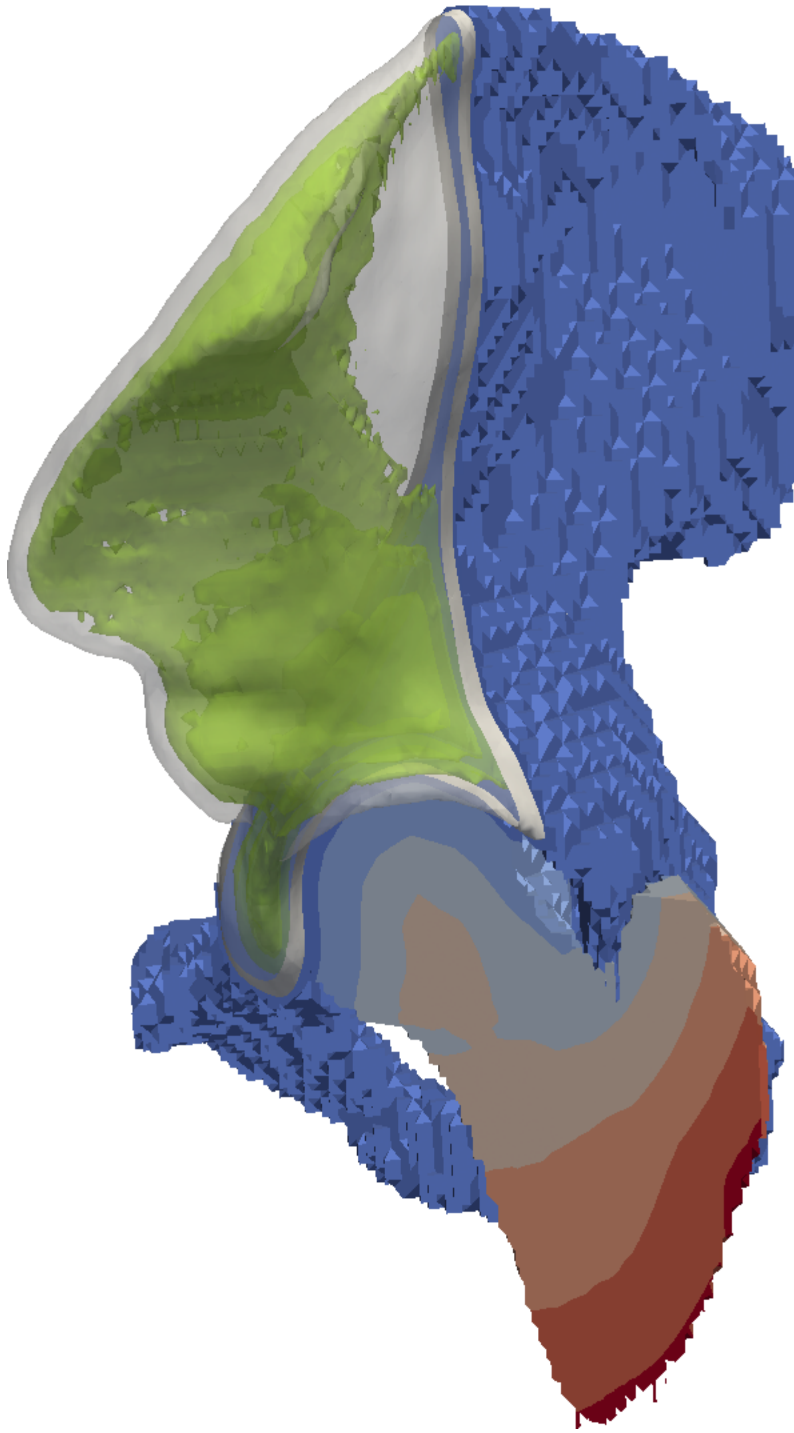
Determine inside, outside and intersected cells



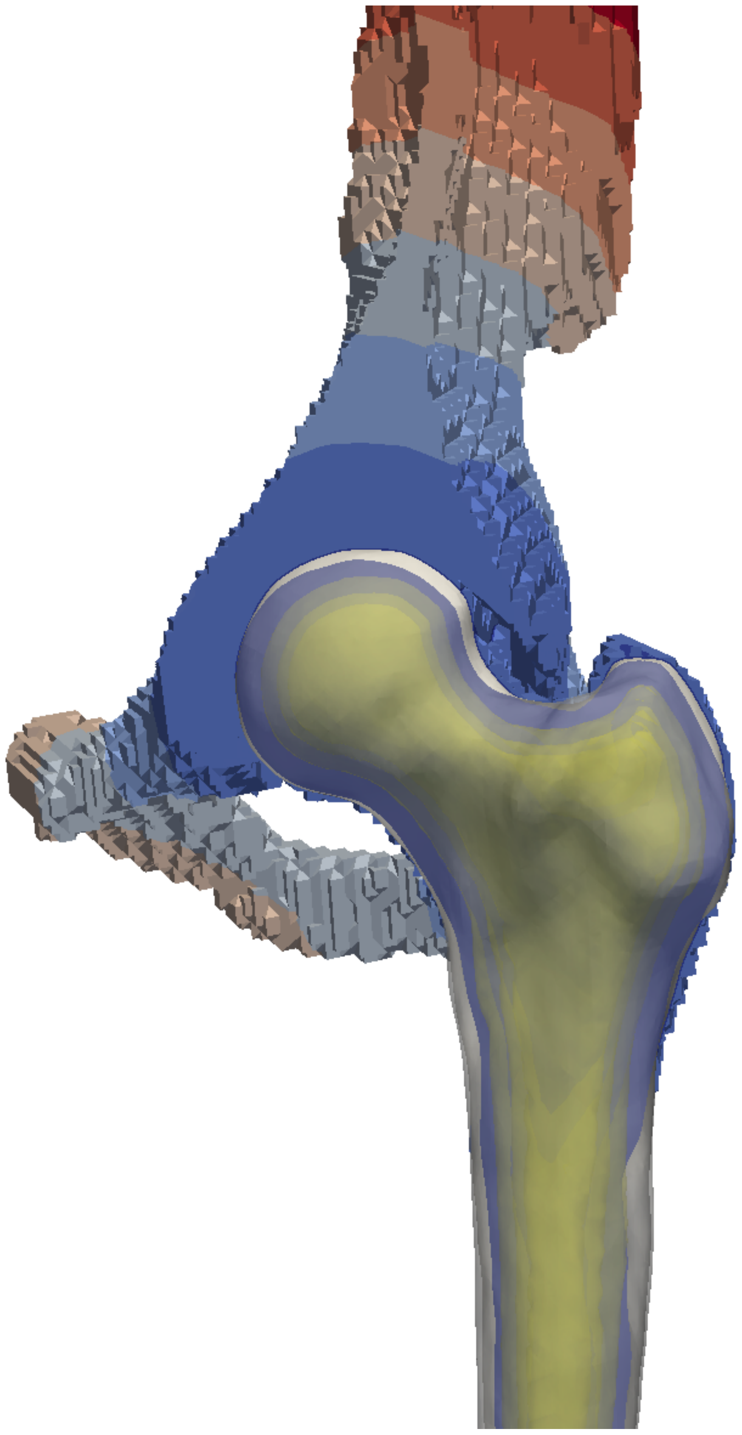


Compute signed distance function for each bone

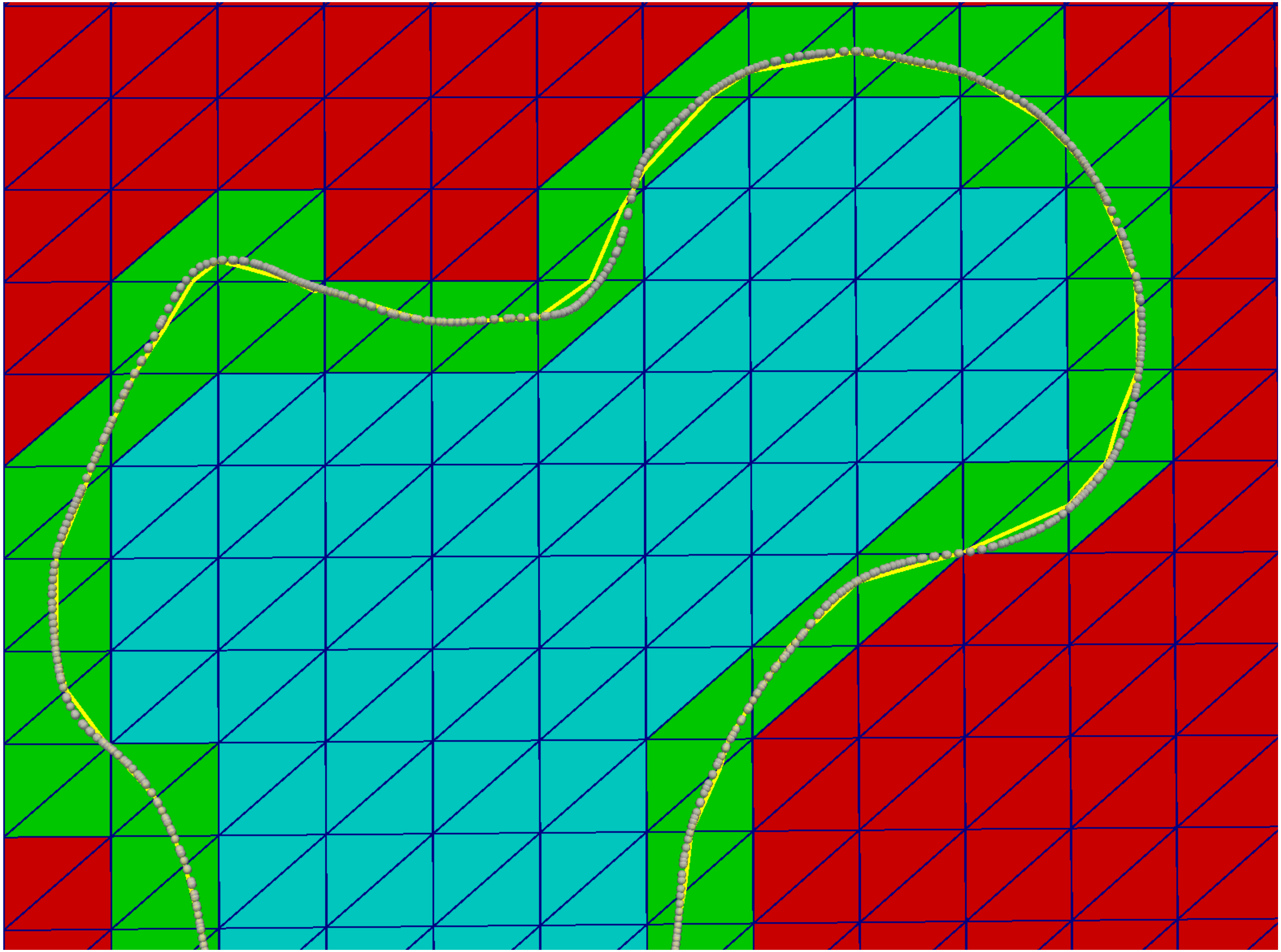
ϕ_1



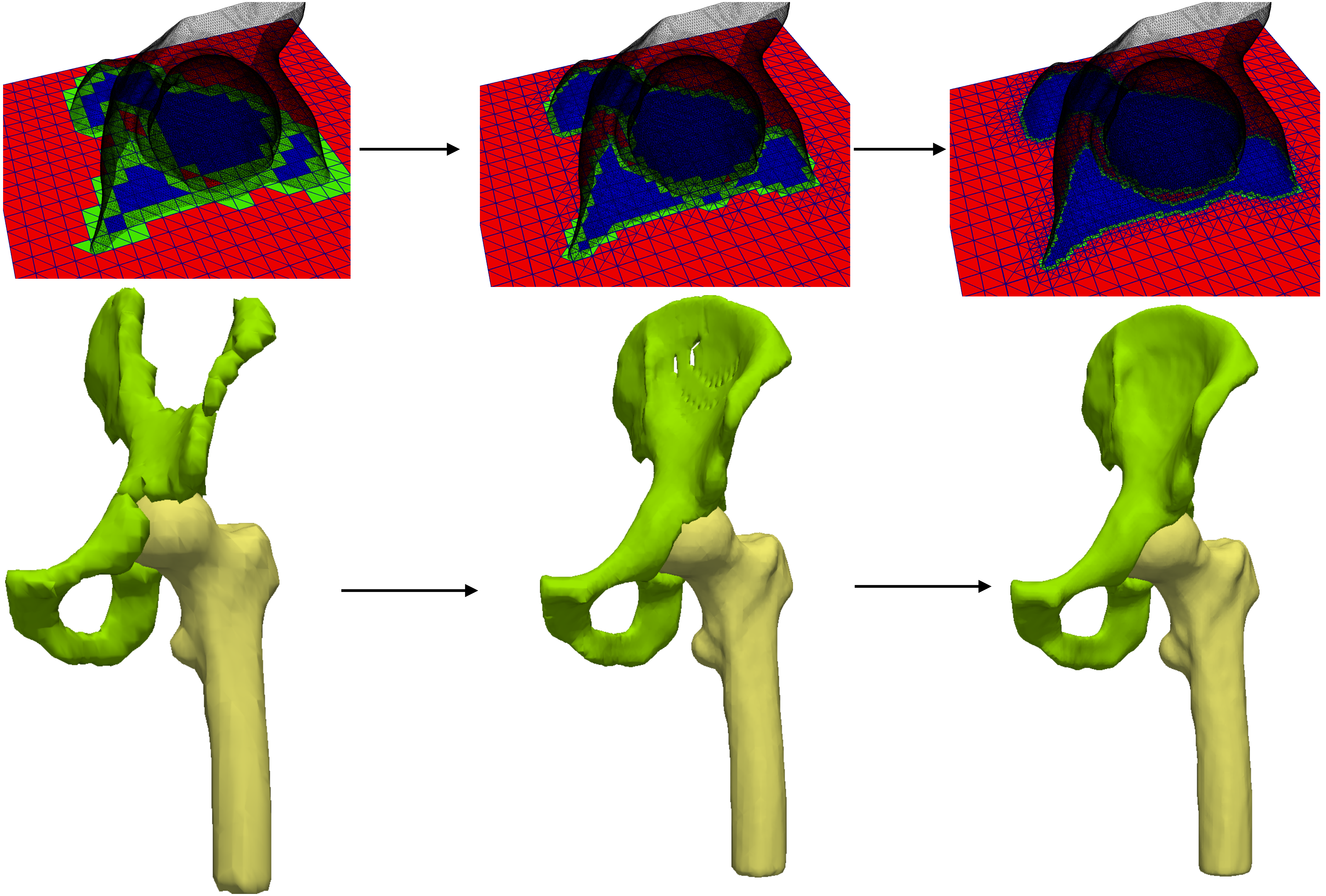
ϕ_2



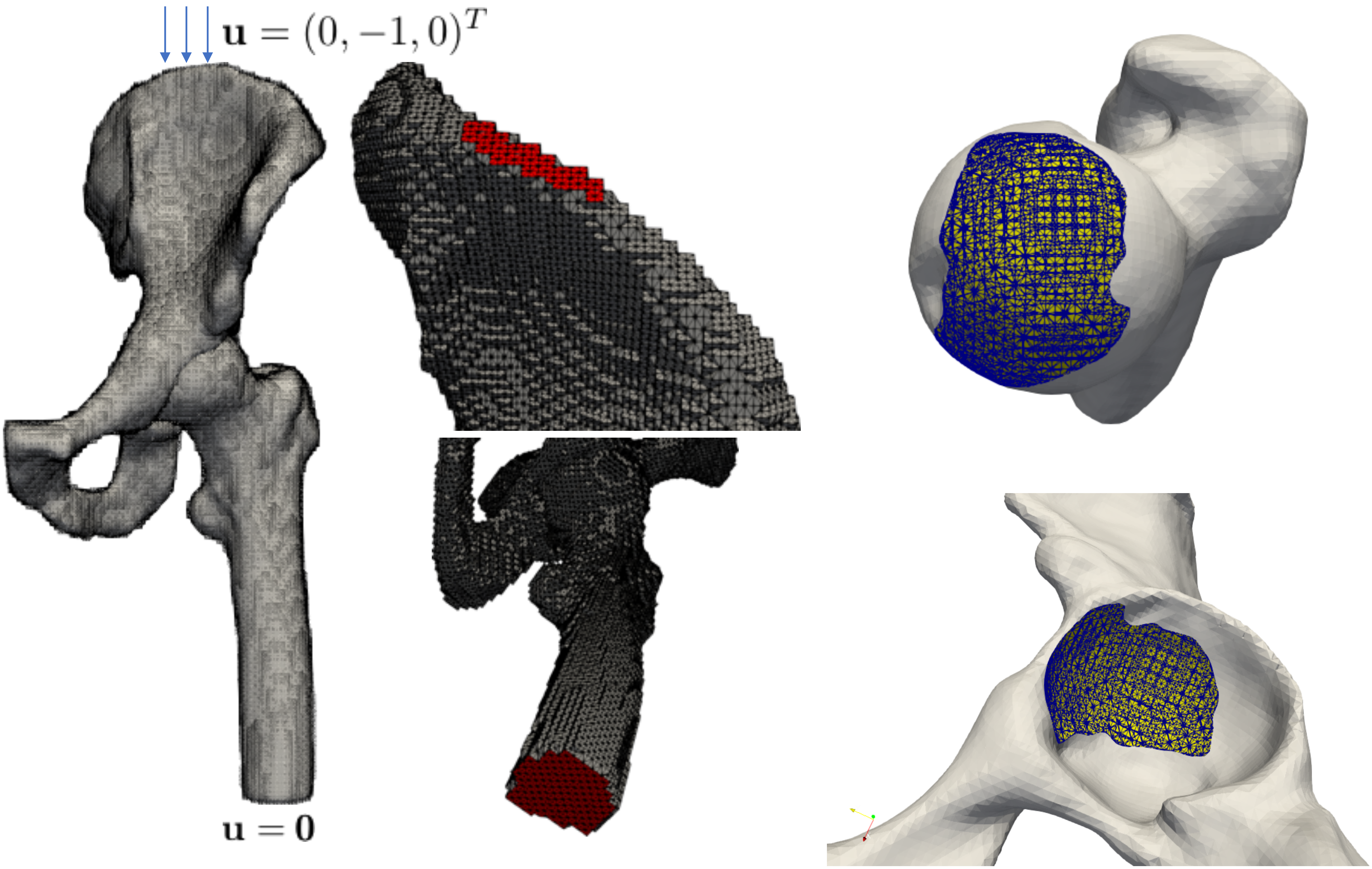
Geometrical Error (Linear Approximation)



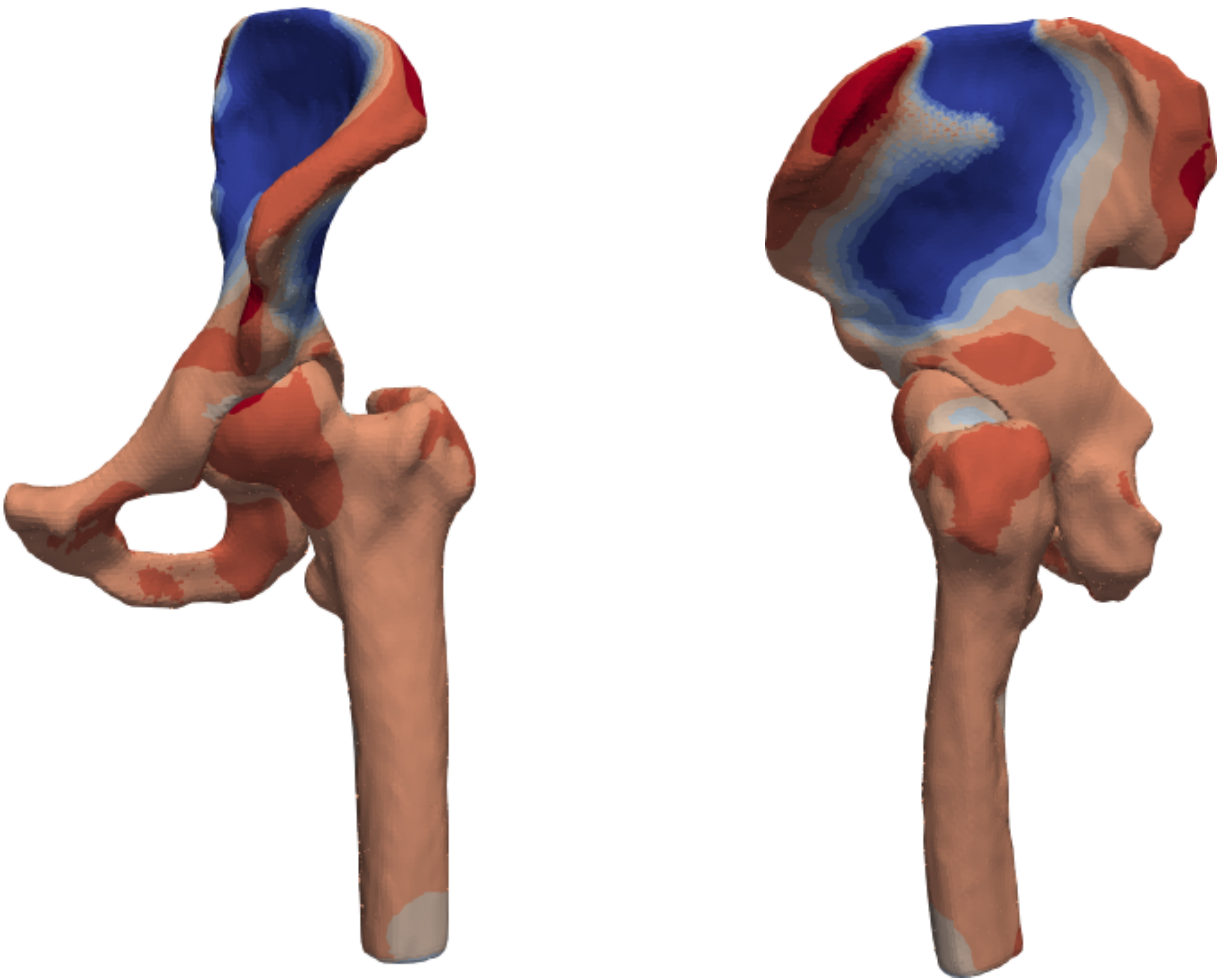
Refine elements that are intersected by surface triangulation



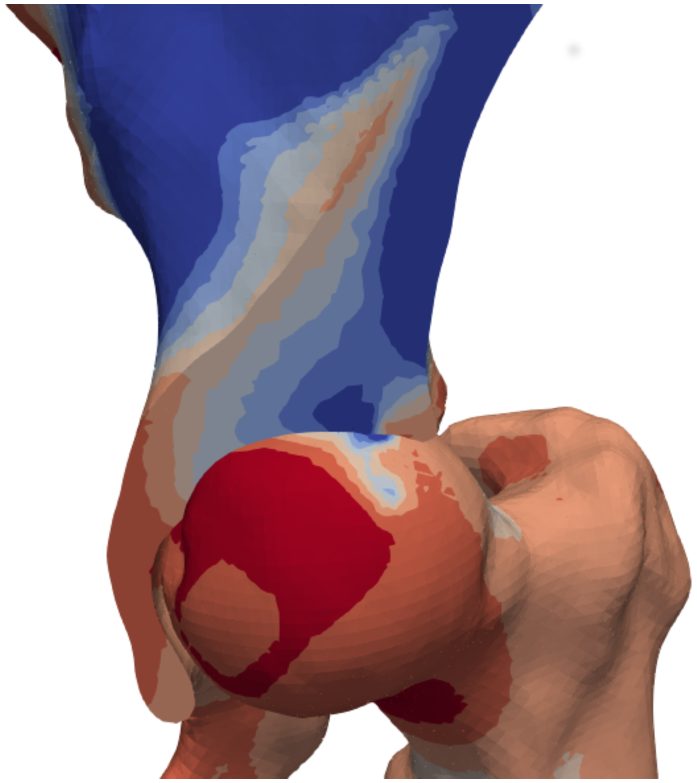
Extract elements and set boundary conditions

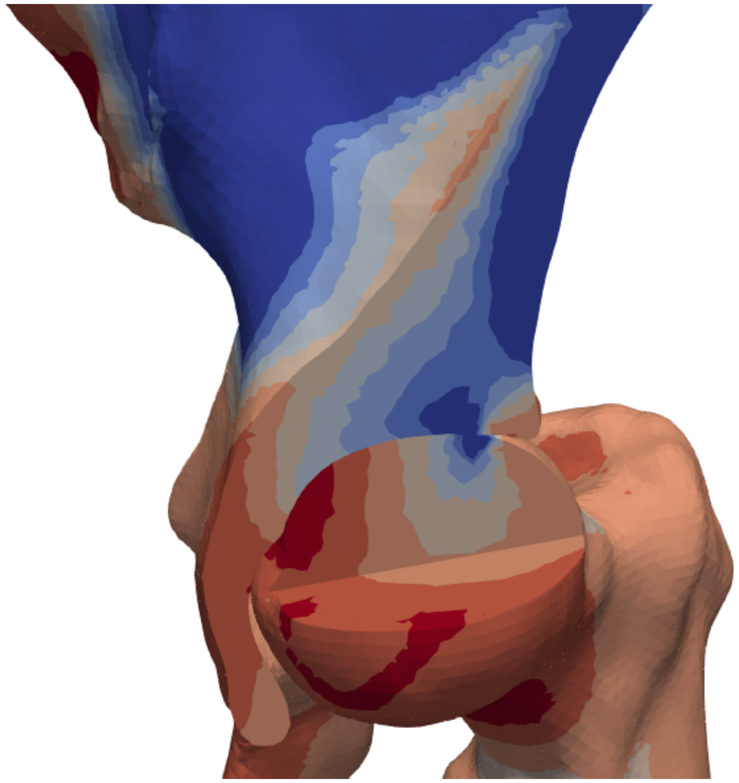


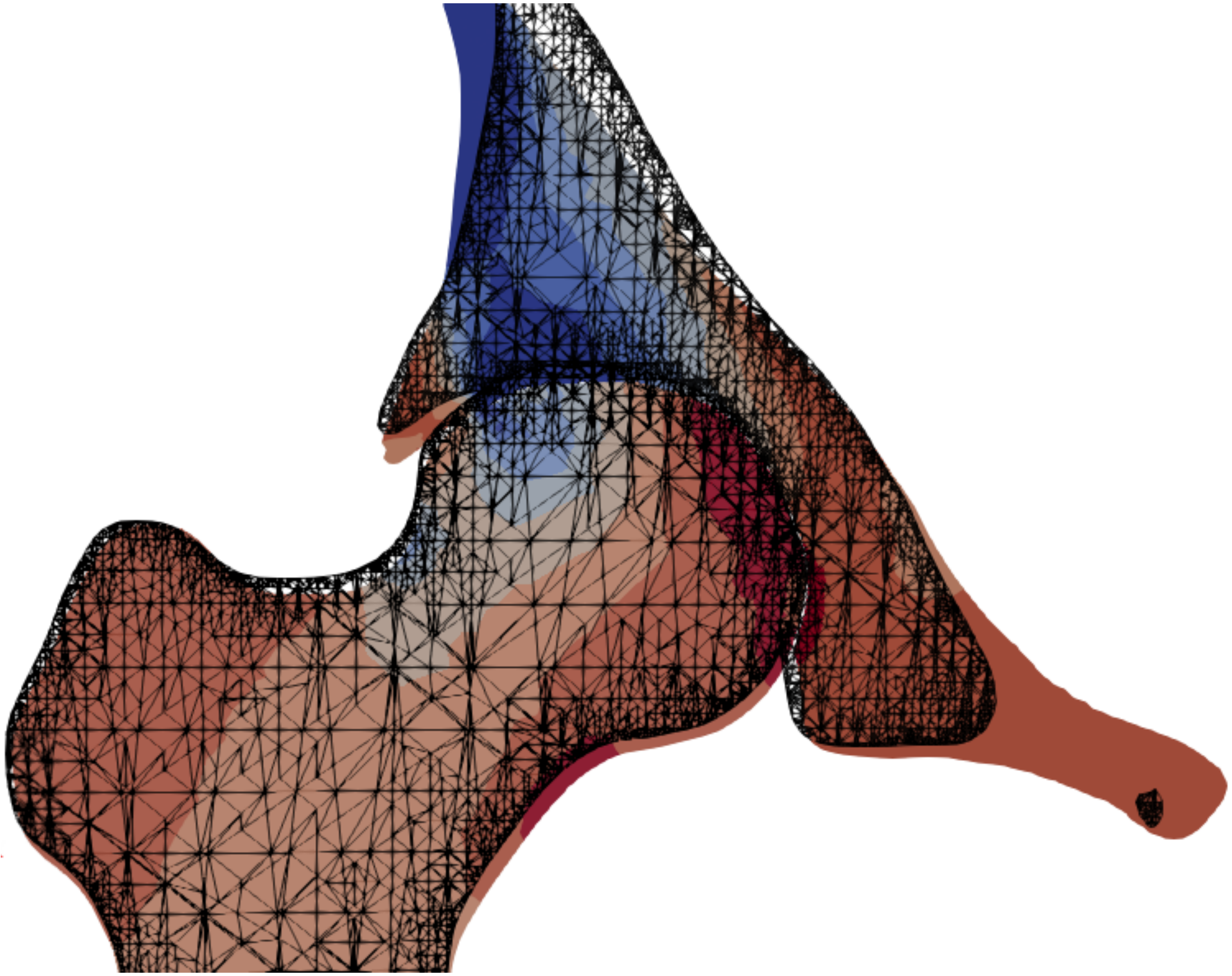
Stress Profile σ_{yy}

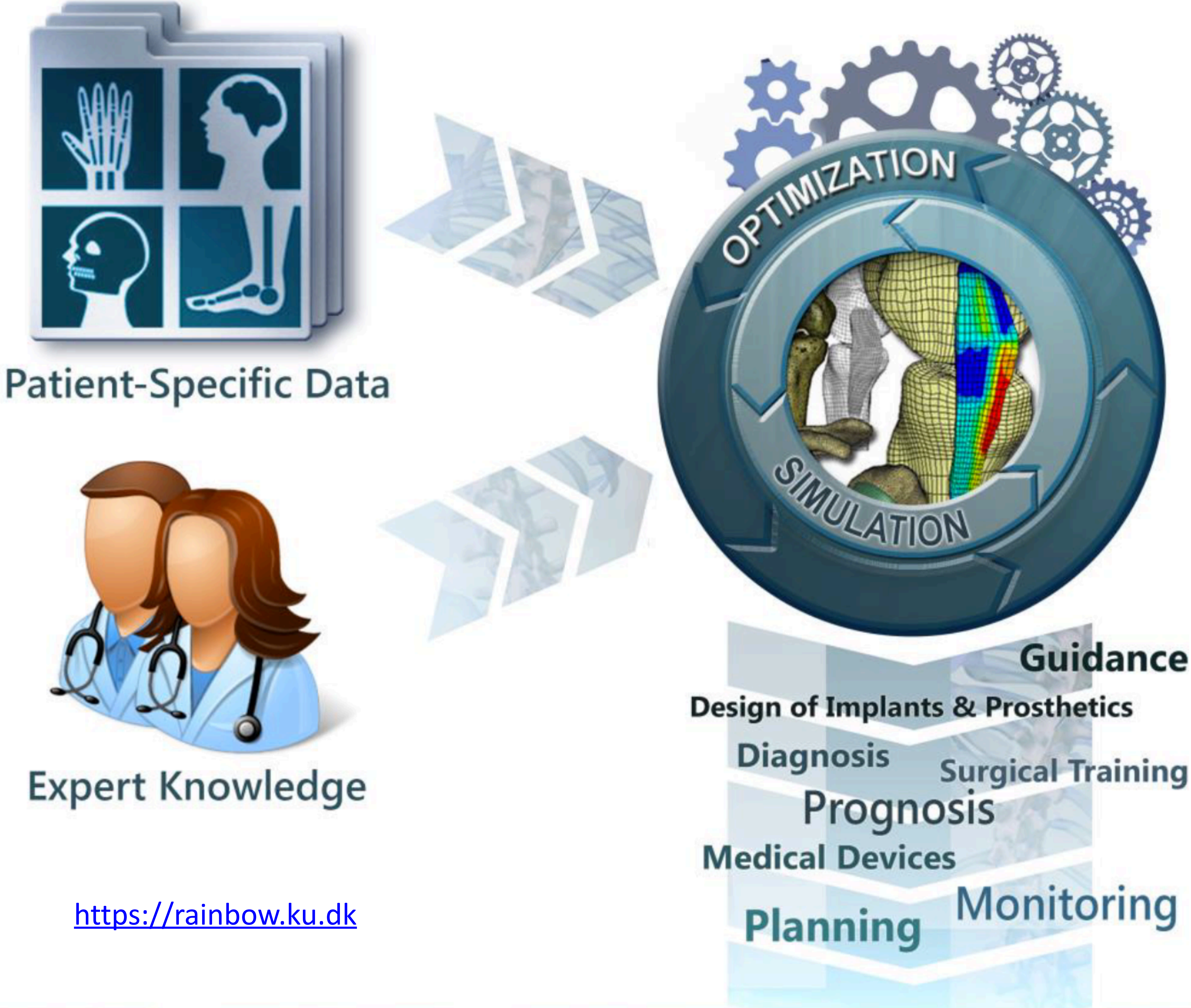


Stress Profile σ_{yy}

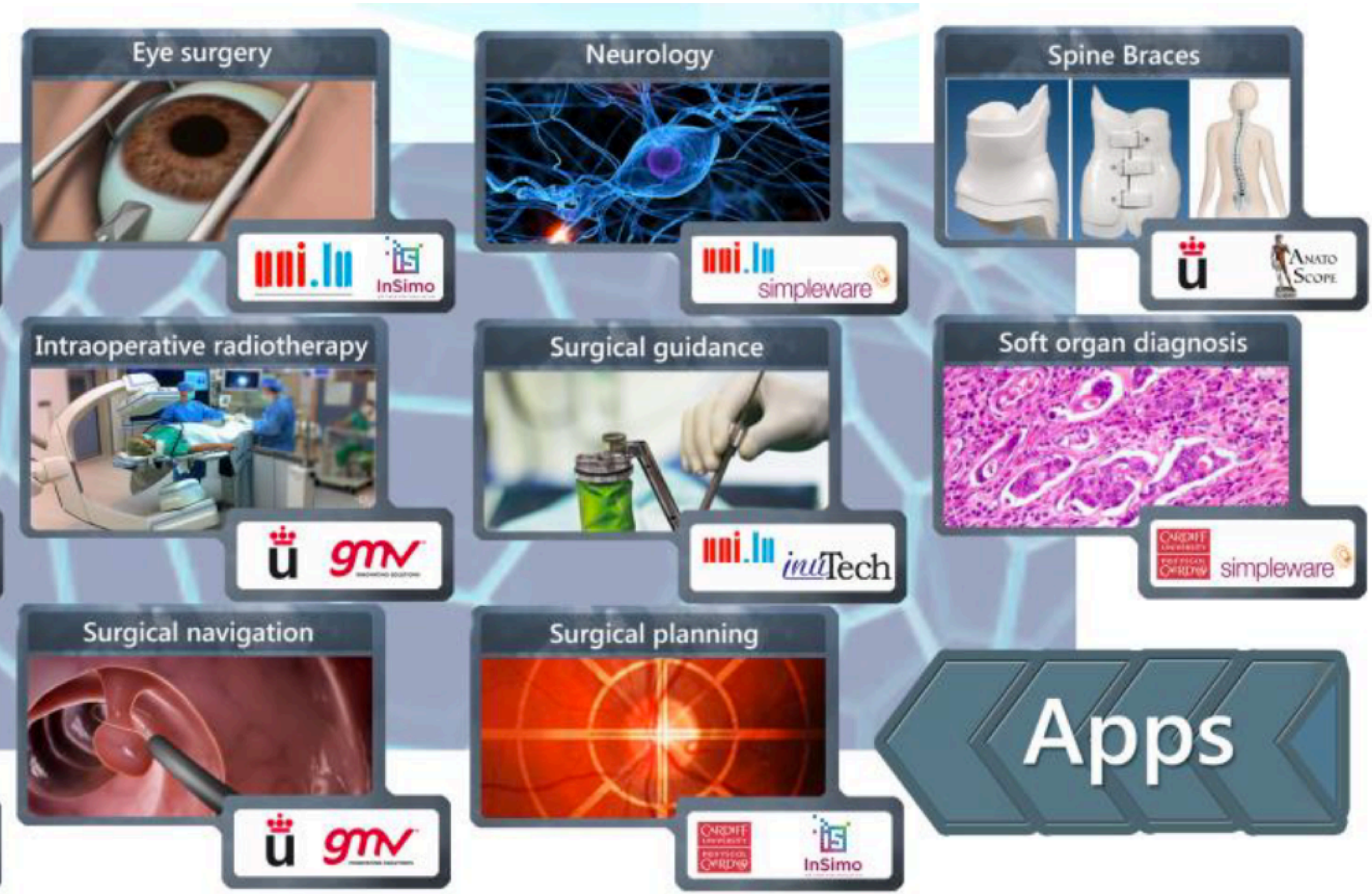








https://rainbow.ku.dk



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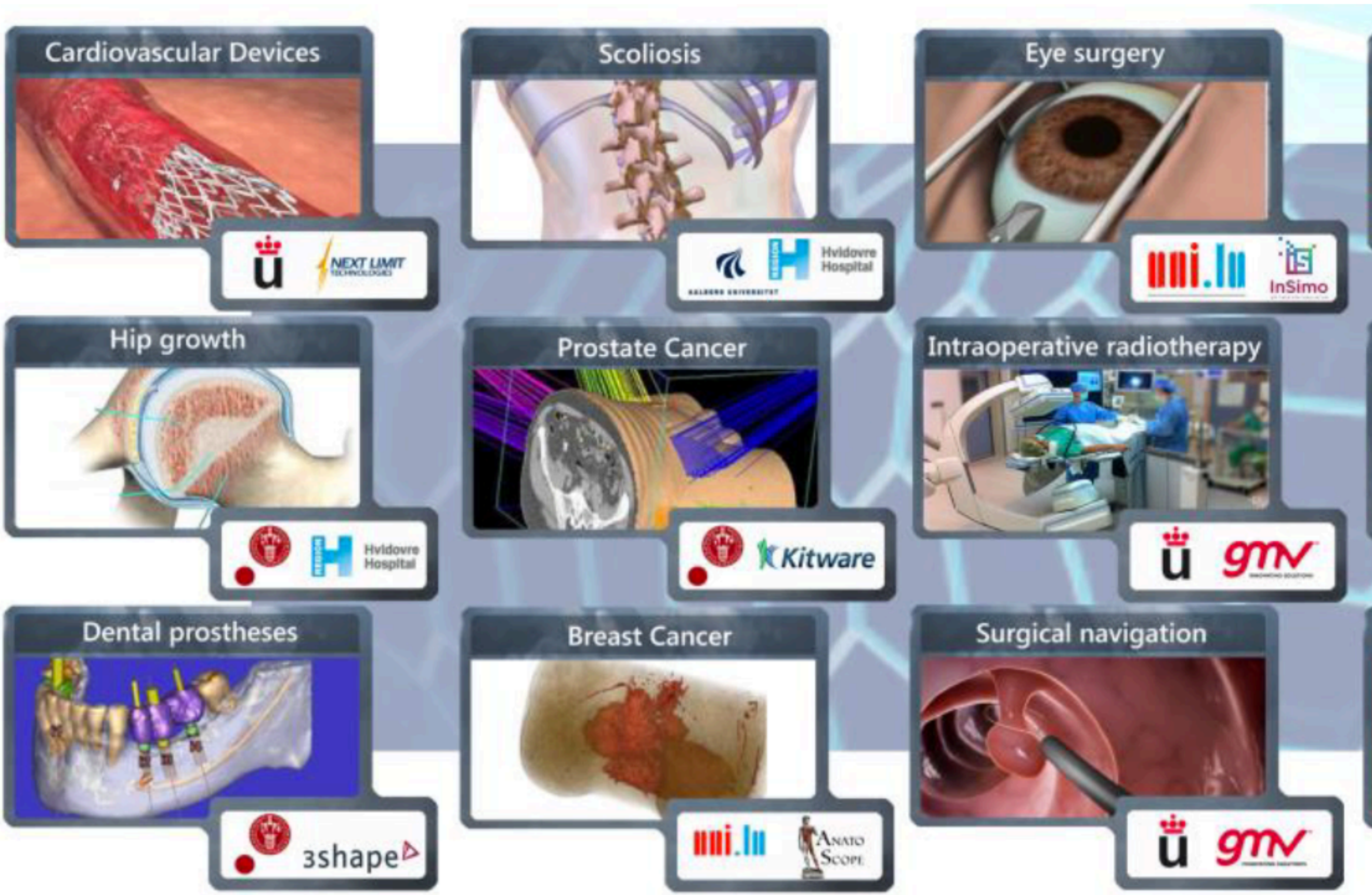
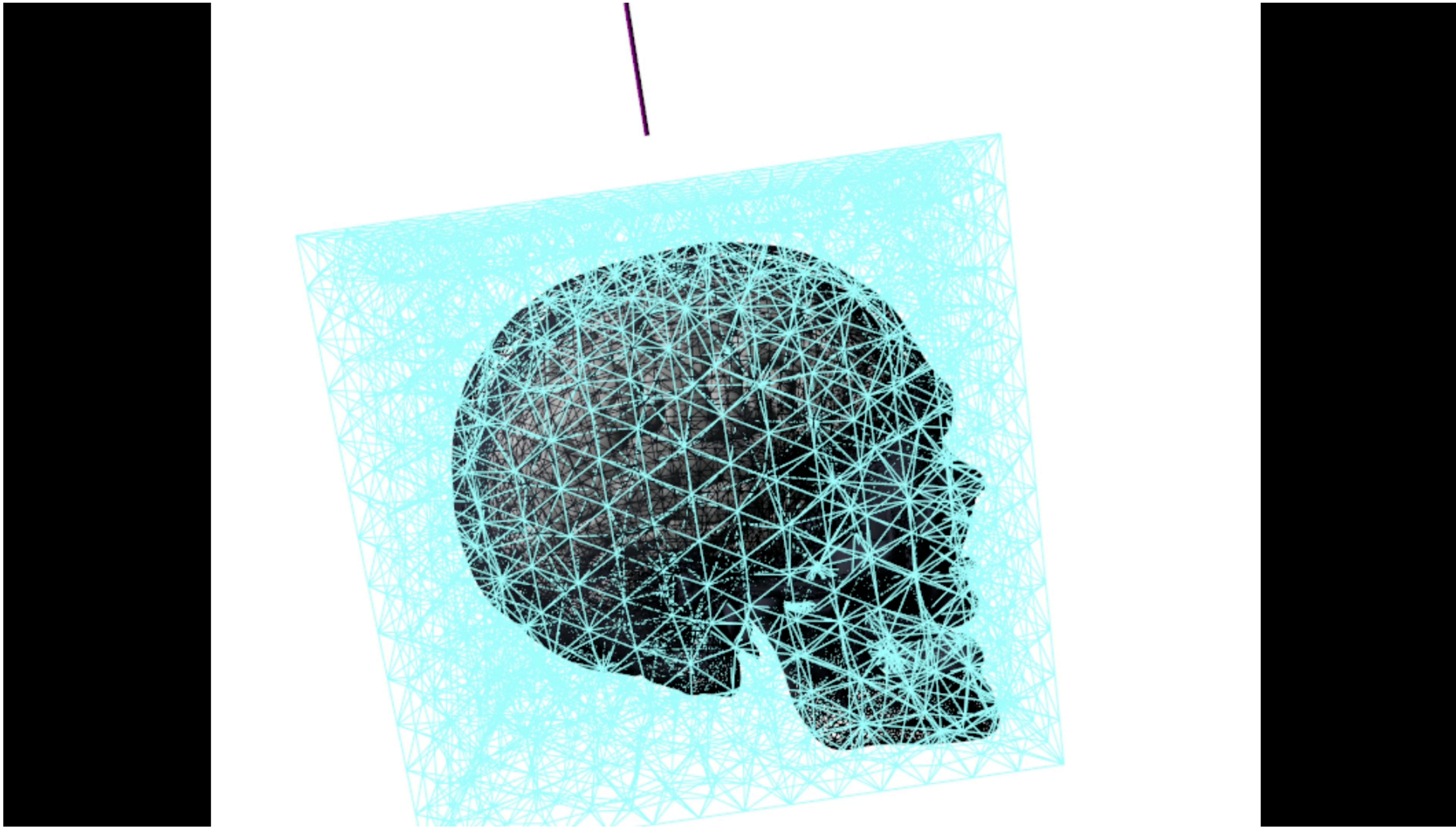


https://rainbow.ku.dk

Brain shift and electrode implantation



Controlling the Error on Target Motion through Real-time Mesh Adaptation: Applications to Deep Brain Stimulation, HP Bui et al, Int J Numer Meth Bio, 2017.

Error estimation and adaptivity

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Superconvergence recovery

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

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

Controlling the Error on Target Motion through Real-time Mesh Adaptation: Applications to Deep Brain Stimulation, HP Bui et al, Int J Numer Meth Bio, 2017.

Goal-oriented error estimate

$$Q(\mathbf{u}) = \frac{1}{|\omega|} \int_{\omega} \nabla \mathbf{u} d\omega$$

$$Q(\mathbf{u}) - Q(\mathbf{u}_h)$$

$$|Q(\mathbf{u}) - Q(\mathbf{u}_h)| \leq \epsilon$$

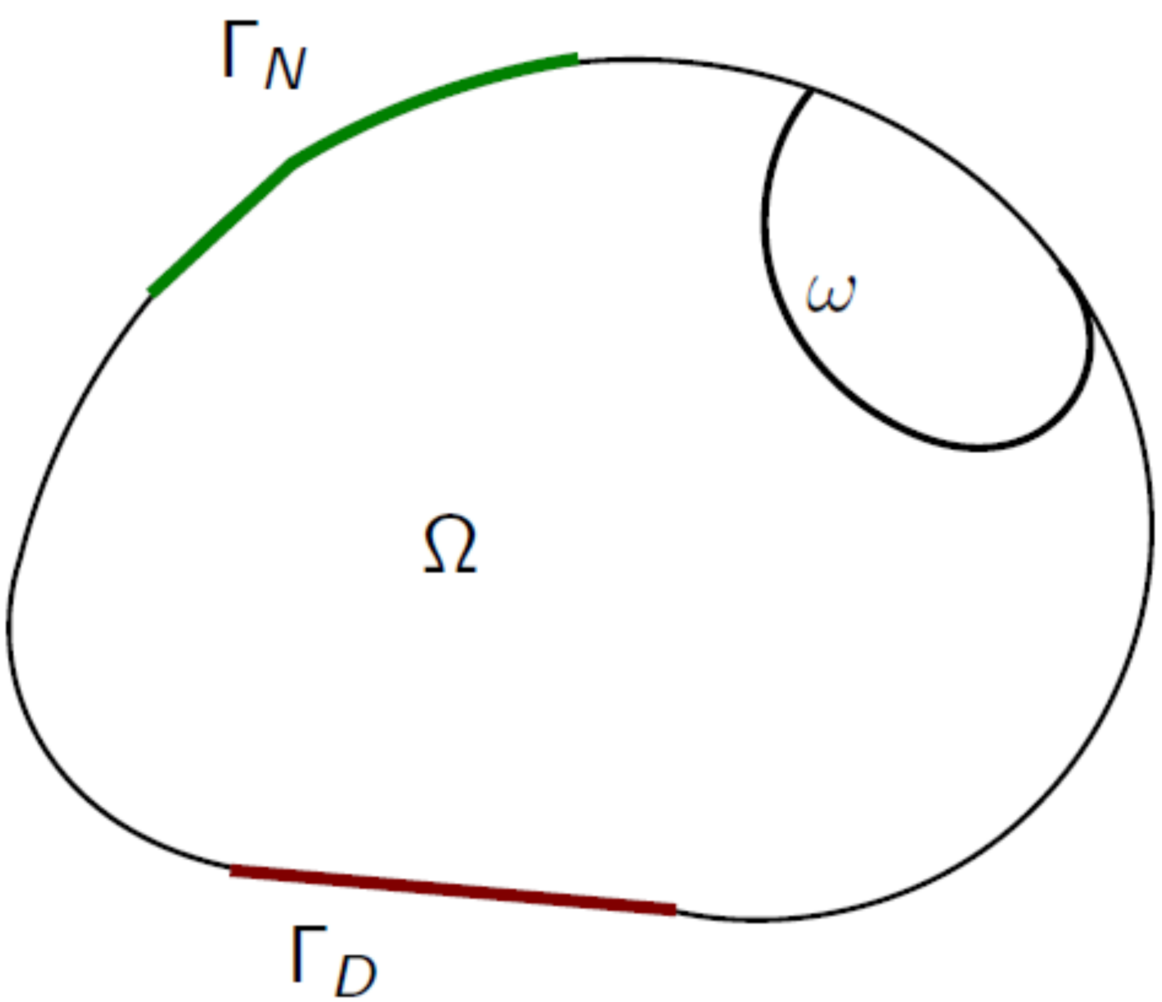

Figure 1: If we are interested in some quantity of interest defined on a subdomain ω, what is the optimal mesh?

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Goal-oriented error estimate

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

Solve by FEM: $a(\mathbf{u}_h, \mathbf{v}_h) = l(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in \mathbf{V}_h$

→ $\mathbf{u}_h$

Weak residual: $r(\mathbf{v}) = l(\mathbf{v}) - a(\mathbf{u}_h, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V}$

If we define a dual problem:

Find $\mathbf{z} \in \mathbf{V}$ such that $a(\mathbf{v}, \mathbf{z}) = Q(\mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V}$

We observe:

$$Q(\mathbf{u}) - Q(\mathbf{u}_h) = a(\mathbf{u}, \mathbf{z}) - a(\mathbf{u}_h, \mathbf{z}) = l(\mathbf{z}) - a(\mathbf{u}_h, \mathbf{z}) = r(\mathbf{z})$$

Corotational Cut Finite Element Method for real-time surgical simulation: application to needle insertion simulation, HP Bui et al, arXiv:1712.03052[cs.CE]

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Hyperelasticity

Equilibrium equations in initial configuration:

$$-\mathrm{div}\boldsymbol{\Pi} = \boldsymbol{B} \quad \text{in } \Omega^0$$
$$\boldsymbol{u} = \boldsymbol{0} \quad \text{on } \Gamma_D^0$$
$$\boldsymbol{\Pi} \cdot \boldsymbol{N} = \boldsymbol{T} \quad \text{on } \Gamma_N^0$$

- $\boldsymbol{\Pi} = \boldsymbol{\Pi}(\boldsymbol{u})$ is the first Piola-Kirchhoff stress tensor
- $\boldsymbol{B}$ is a given body force per unit volume
- $\boldsymbol{u}$ is the displacement
- $\boldsymbol{T}$ is a given boundary traction

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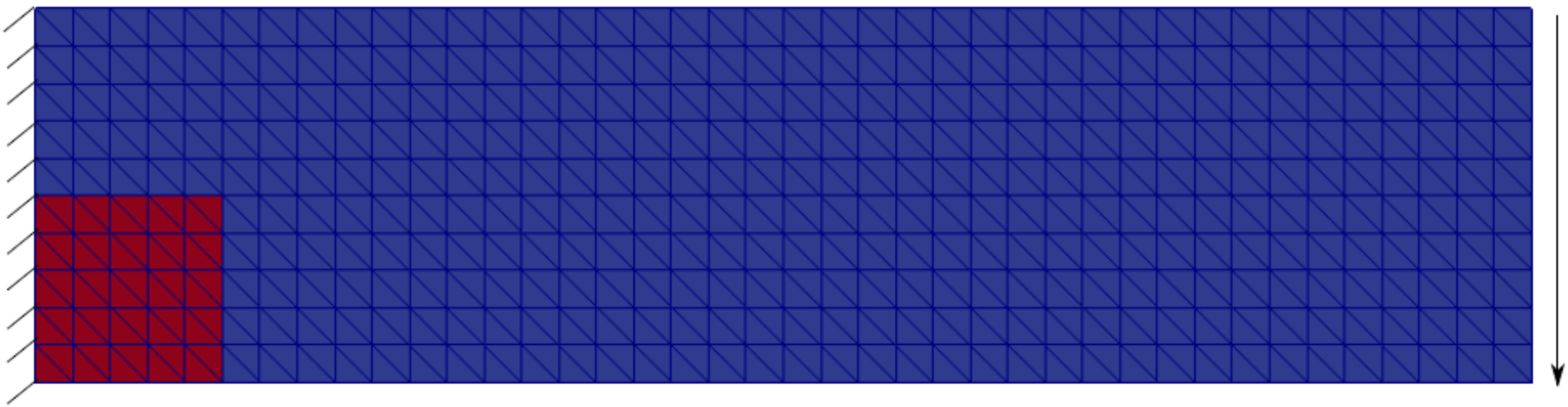
Cantilever beam

Parameters

Saint Venant-Kirchhoff material: $E = 1000$, $\nu = 0.4$



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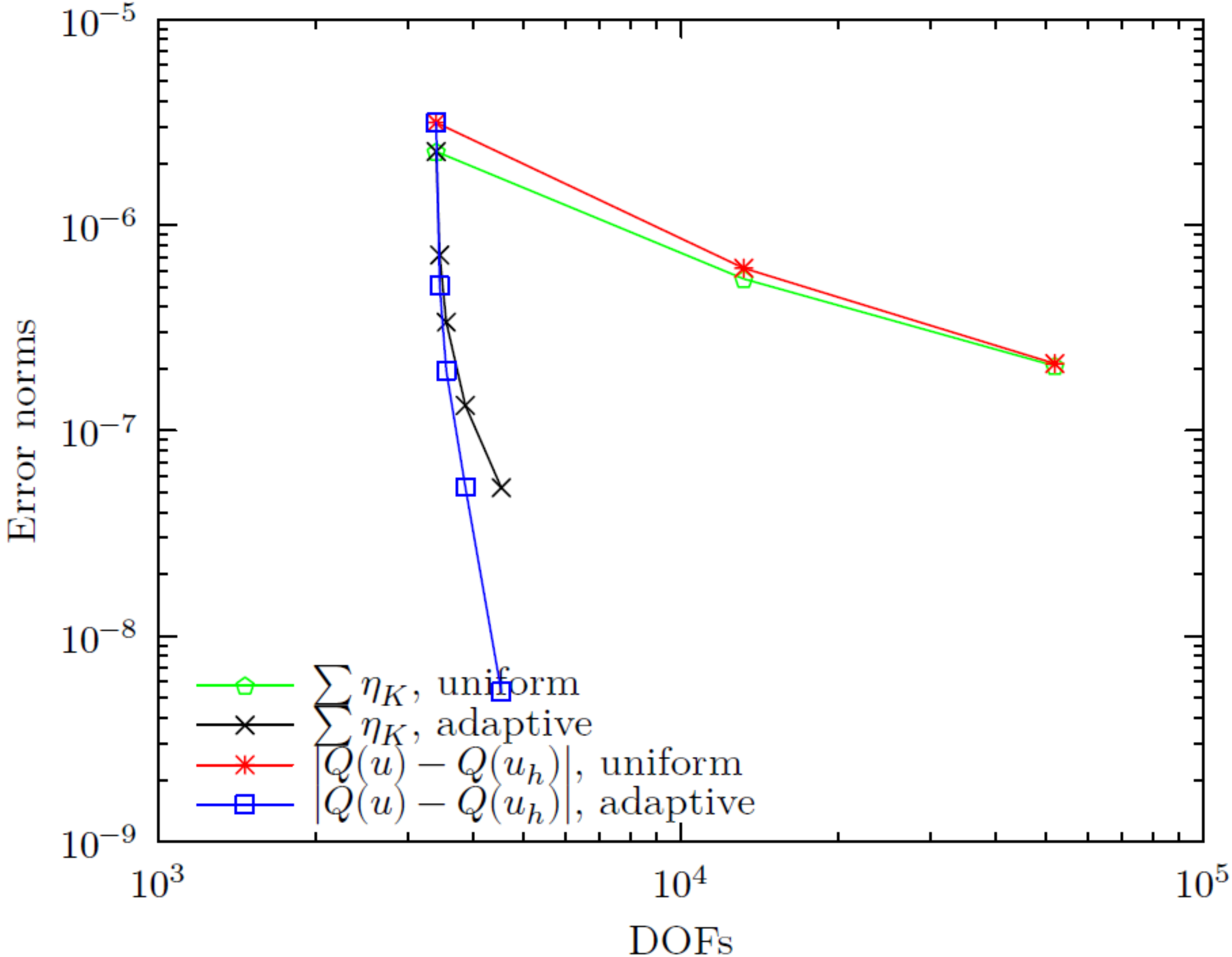
Cantilever beam (2)



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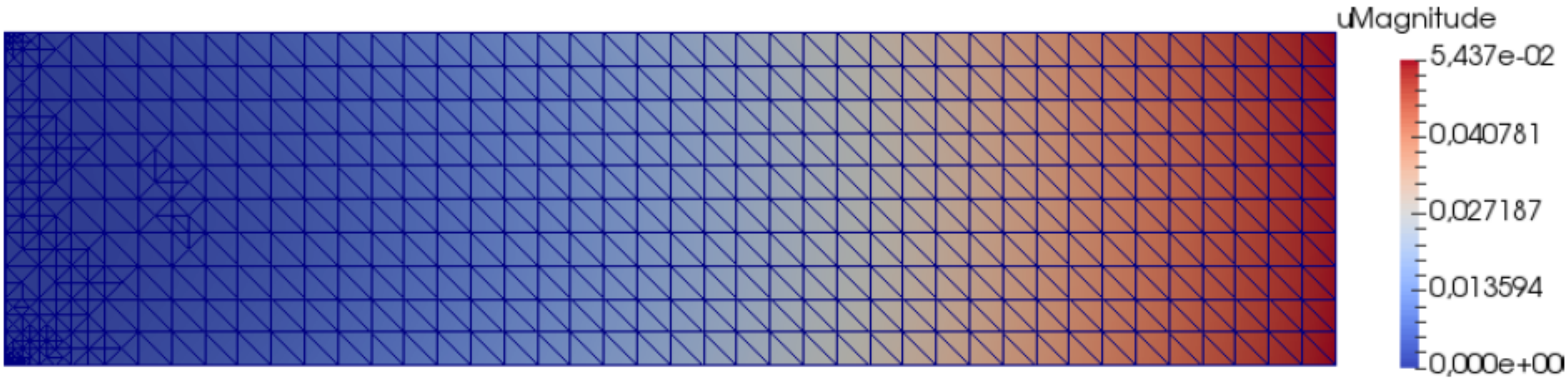
Cantilever beam (3)



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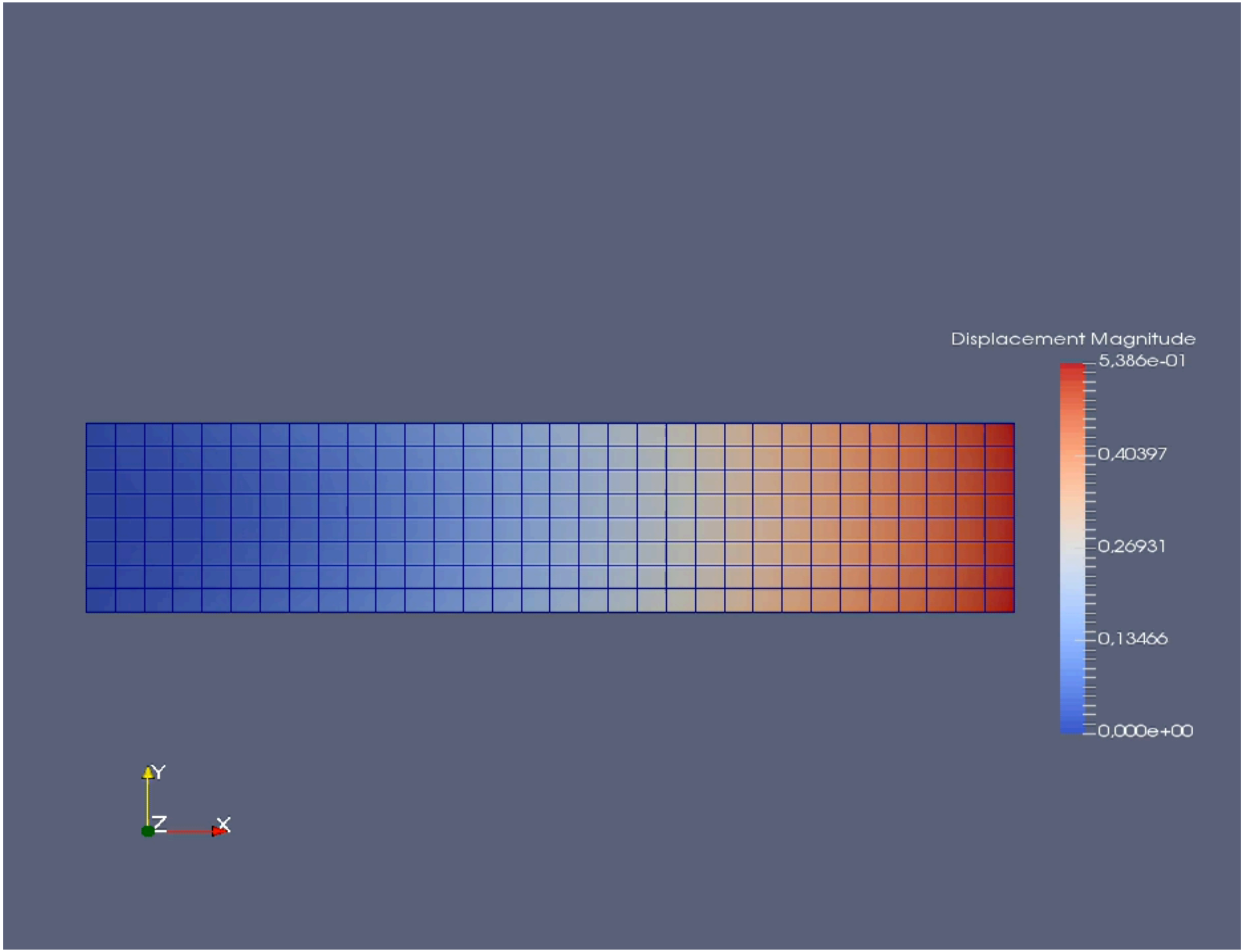
Adaptivity using quadrilaterals



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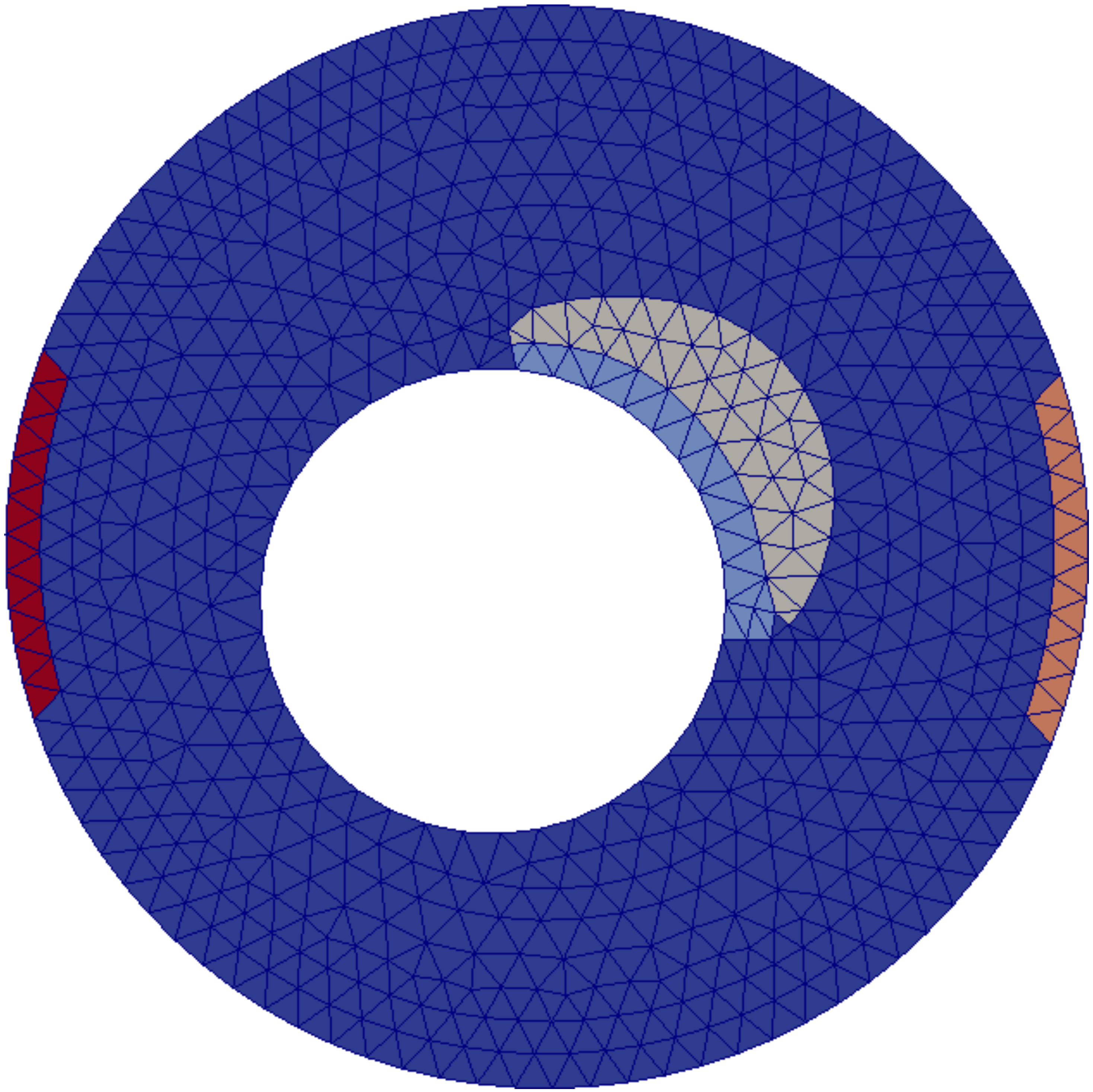
RealTCut

Human artery



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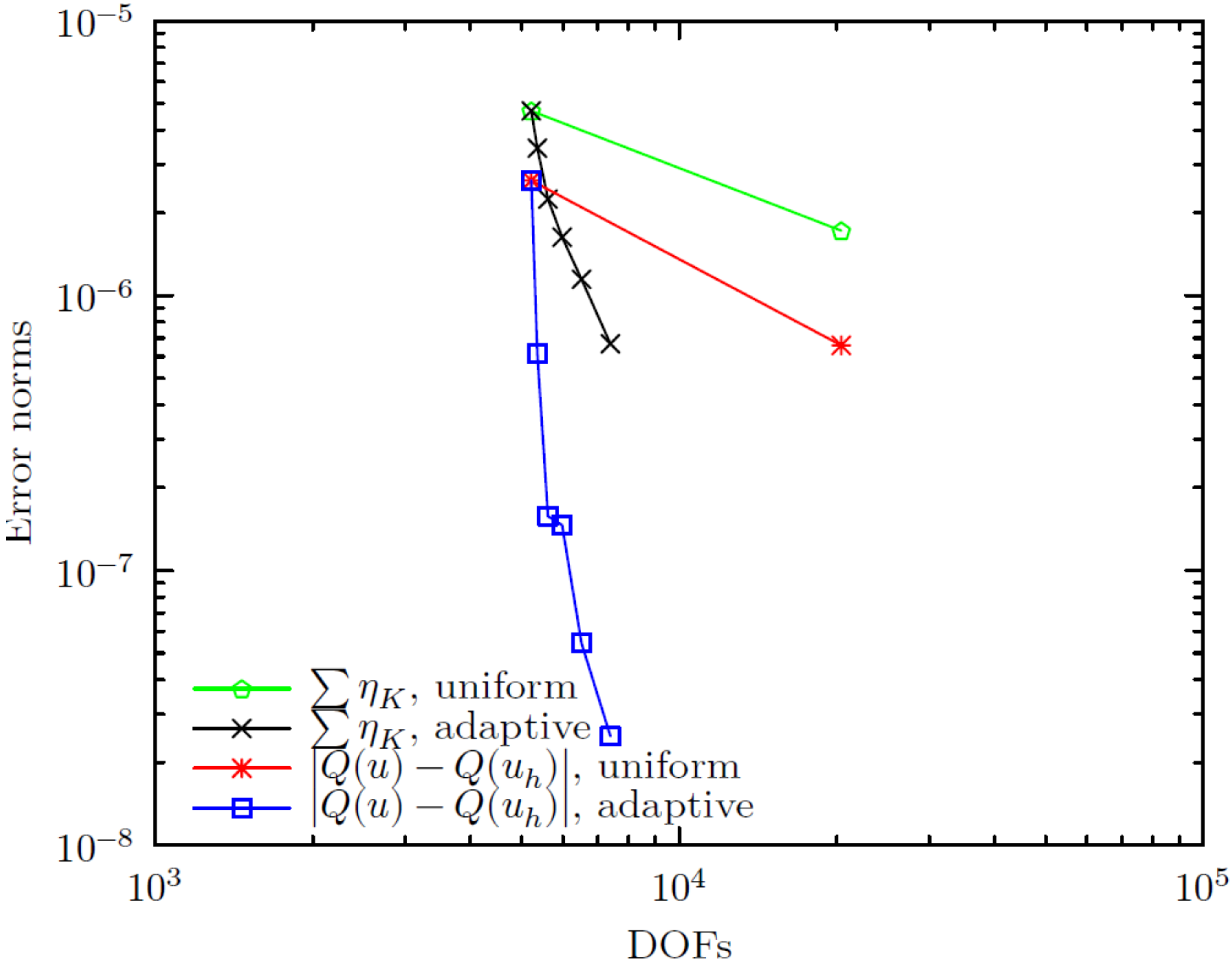
Human artery



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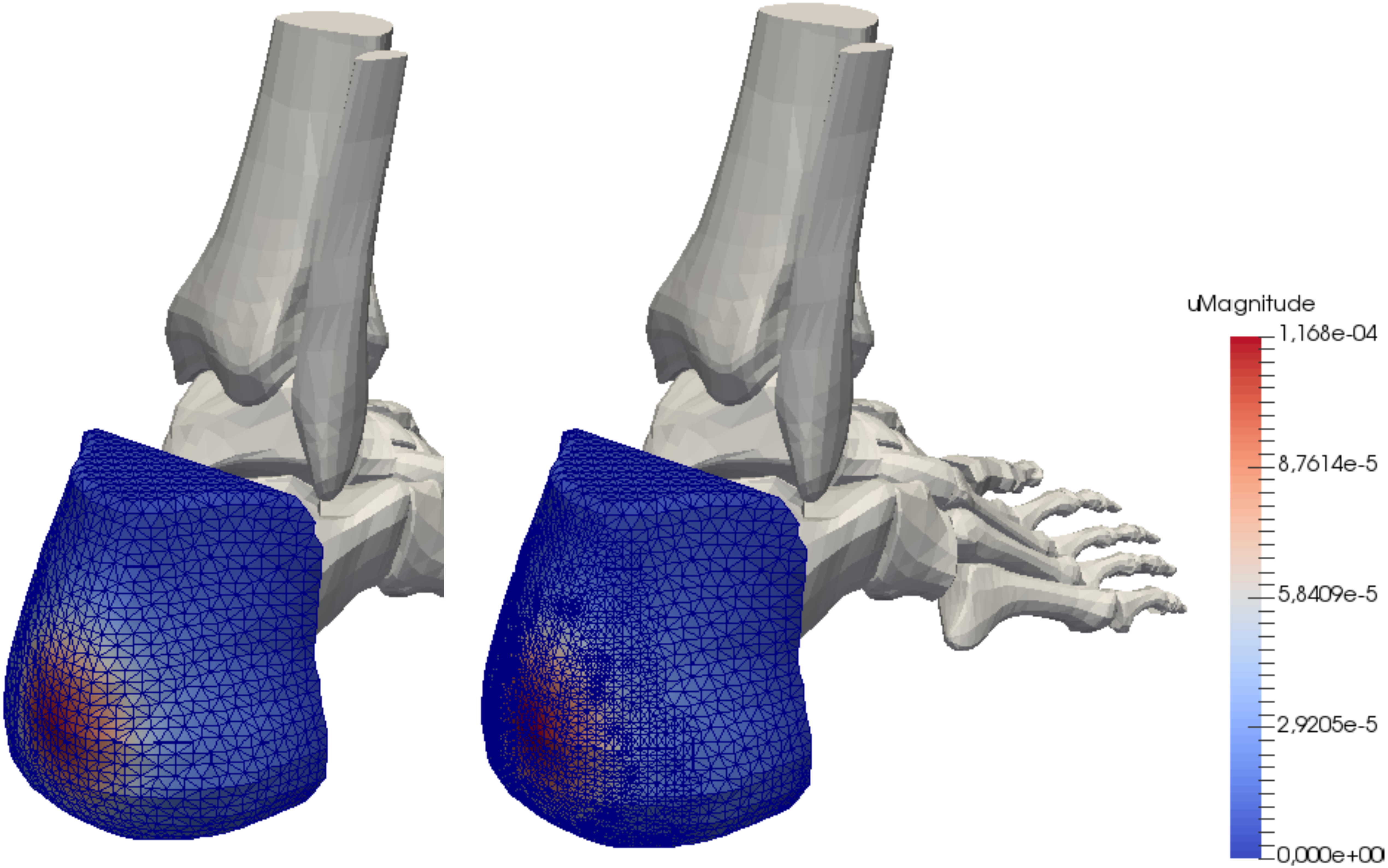
Human heel



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Conclusions

Cut FEM/XFEM for surgical simulations with complex geometries

Making the discretization as independent as possible from geometric description

Verification of convergences with optimal rates

Cut FEM is suitable for real-time and patient specific simulations

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Perspectives

Higher order cut elements

Alexei Lozinski and Franz Chouly: avoid integration on cut elements

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References

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H.P. Bui

RealTCut

Acknowledgements

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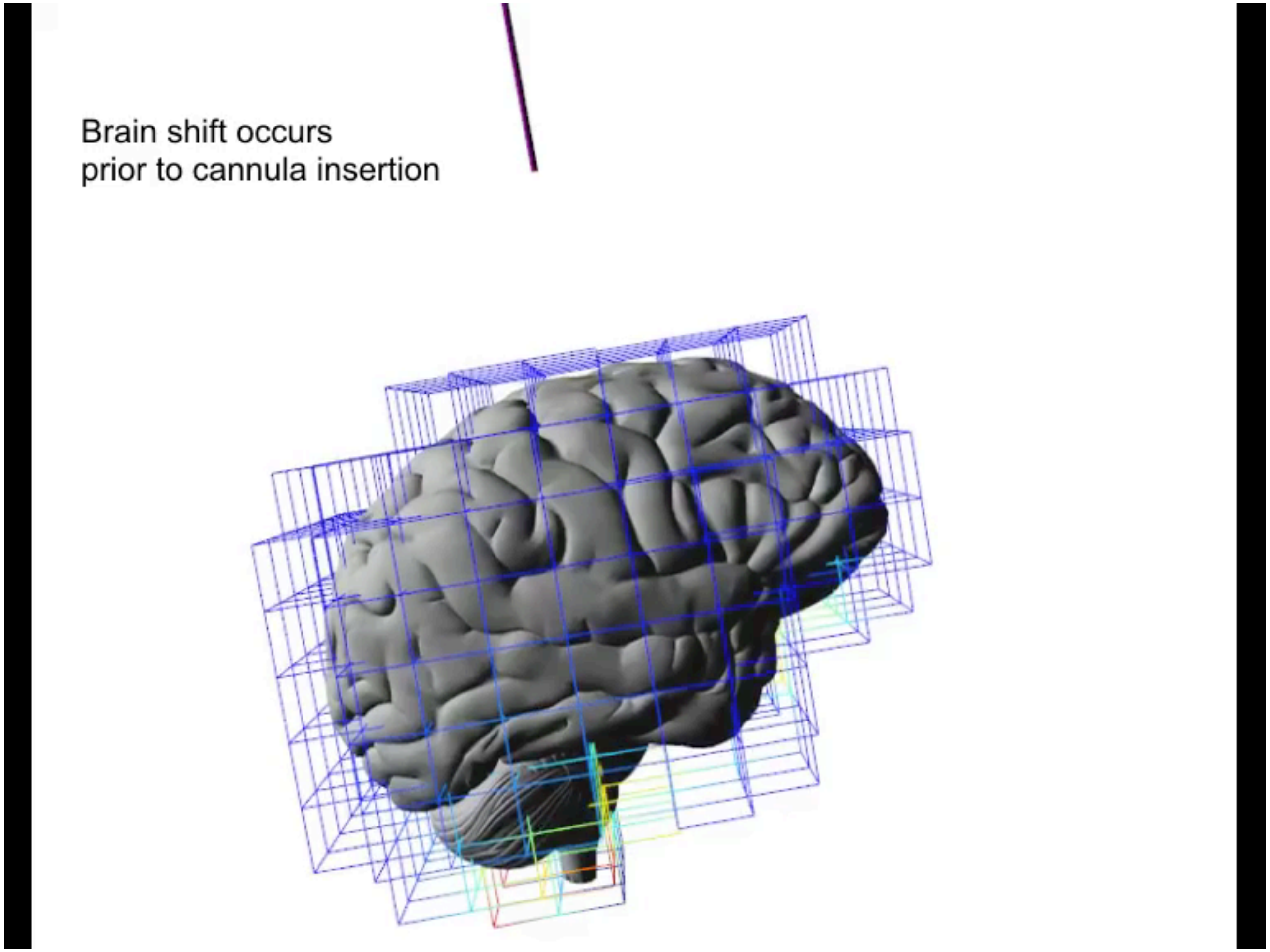
Legato team (Luxembourg) and MIMESIS team (Strasbourg)

SOFA community

AMIES

LmB, University of Franche-Comté, CNRS

Real-time needle steering



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Corotational Cut Finite Element Method for real-time surgical simulation: application to needle insertion simulation, HP Bui et al, arXiv:1712.03052[cs.CE]