Lack of separation of scales

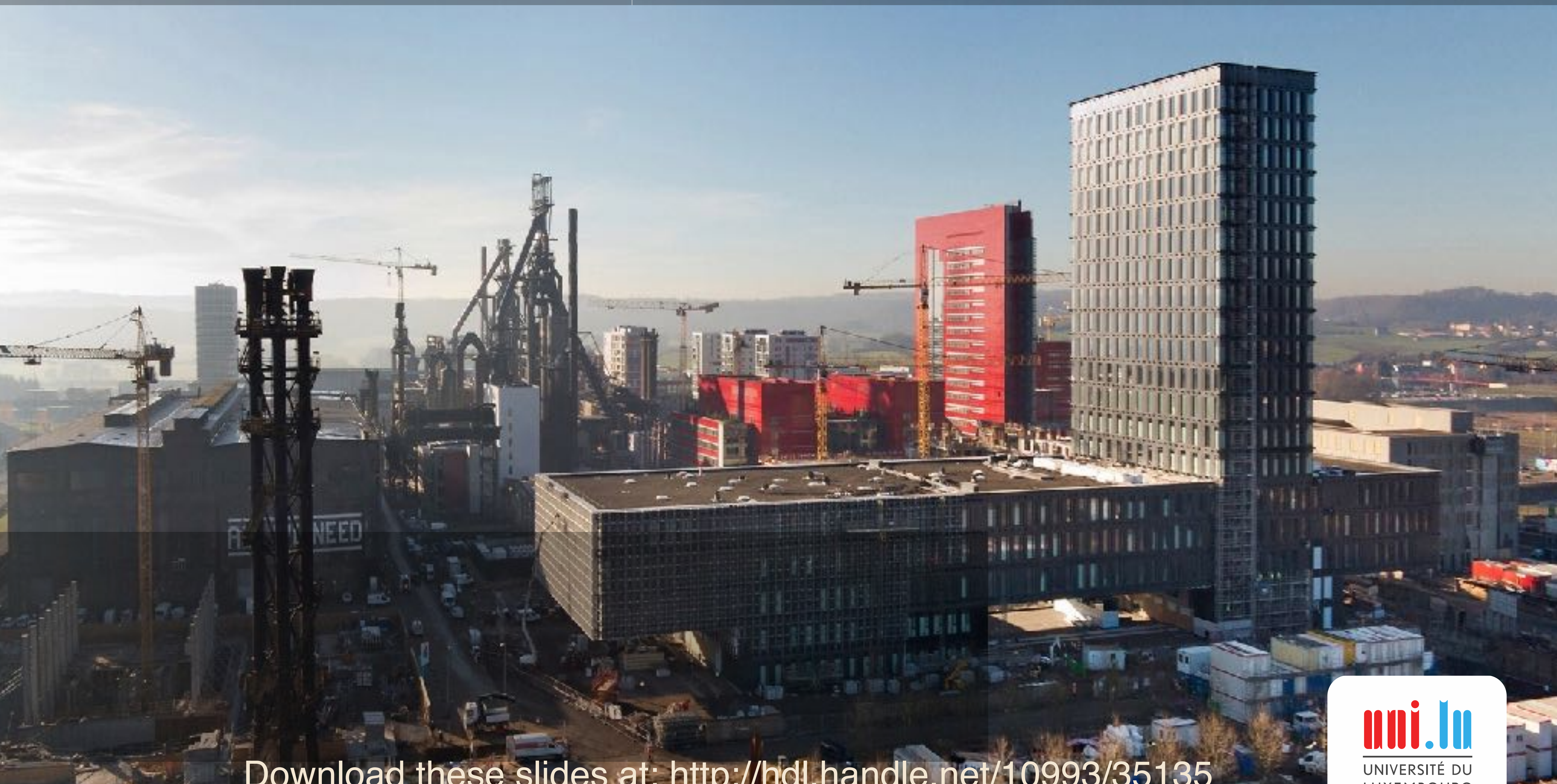
A view from reduced order modelling and homogenisation

Joint work with Pierre Kerfriden
Ahmad Akbari, Olivier Goury, Hussein Rappel
Paul Hauseux, Jack Hale

Stéphane P.A. Bordas, University of Luxembourg and Cardiff University
Nottingham SafeFly Summer School Seminar 2018 09 19 organised by Savvas Triantafyllou

Computed in Luxembourg

Computational Sciences Luxembourg



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10 km
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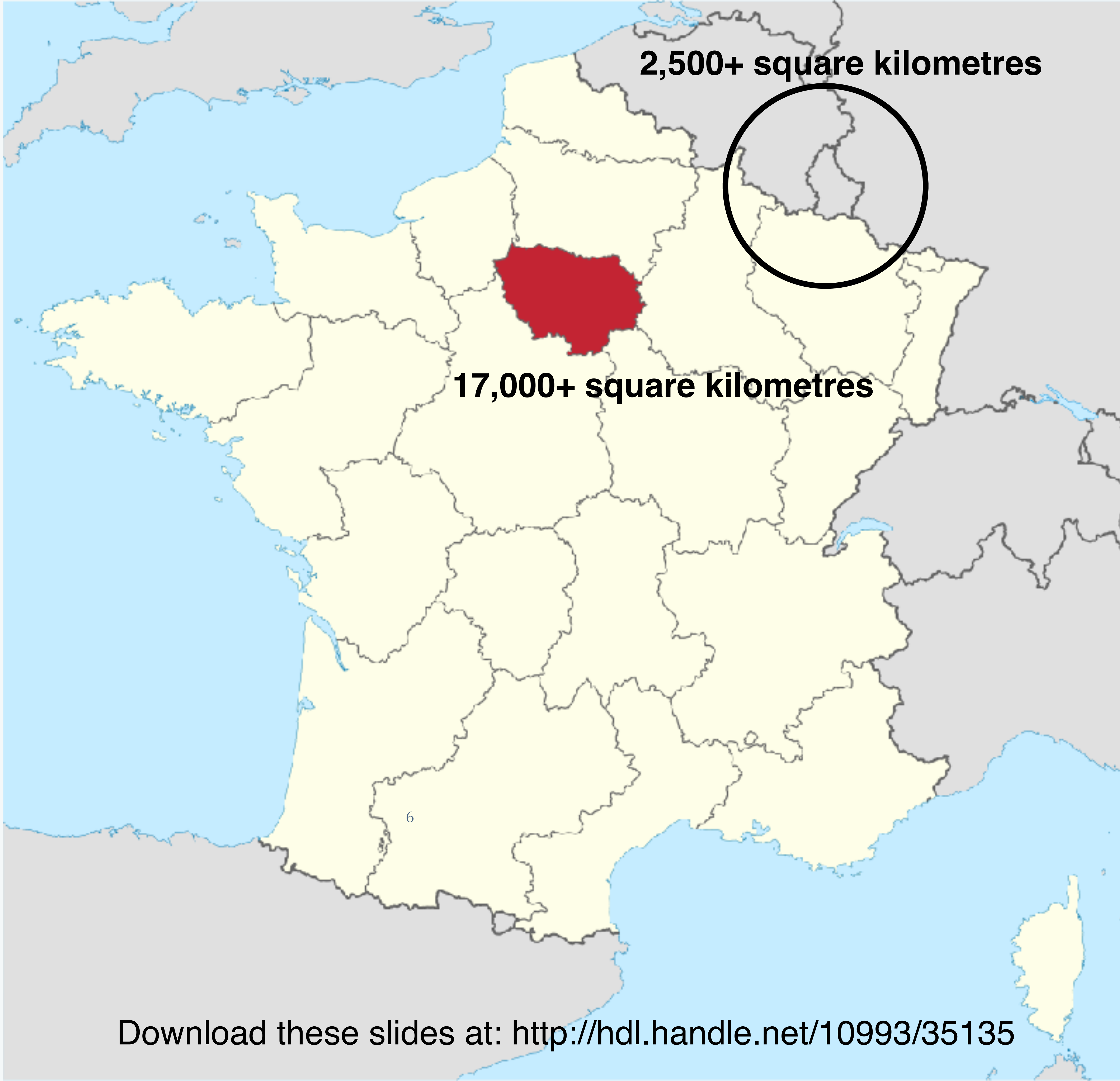

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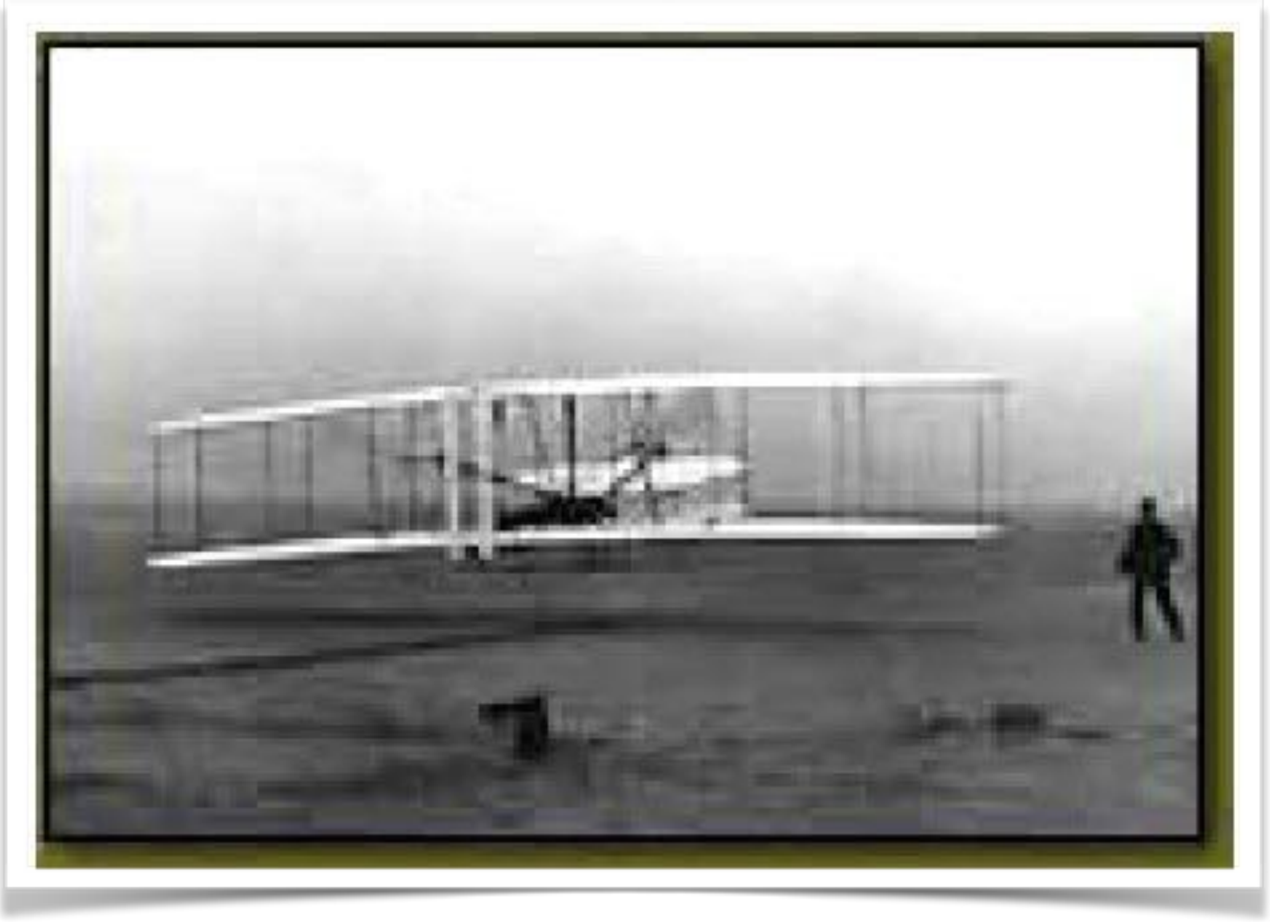
Wilbur and Orville Wright

Wright Flyer

10:35am Dec 17, 1903

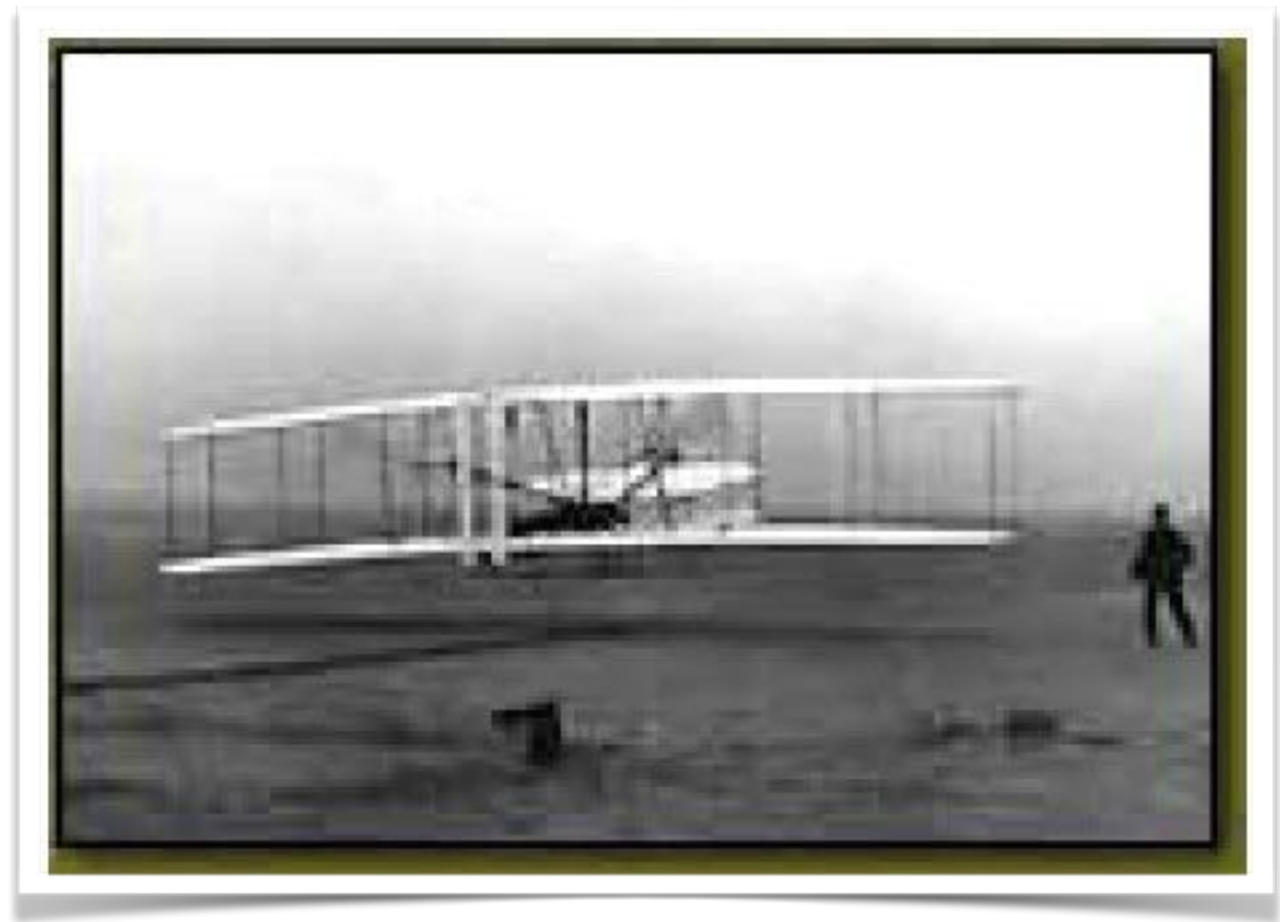


Wilbur and Orville Wright

On Dec 14 Wilbur won the coin toss, made the first attempt and stalled

Orville made the first flight on Dec. 17

12 seconds & 120 ft

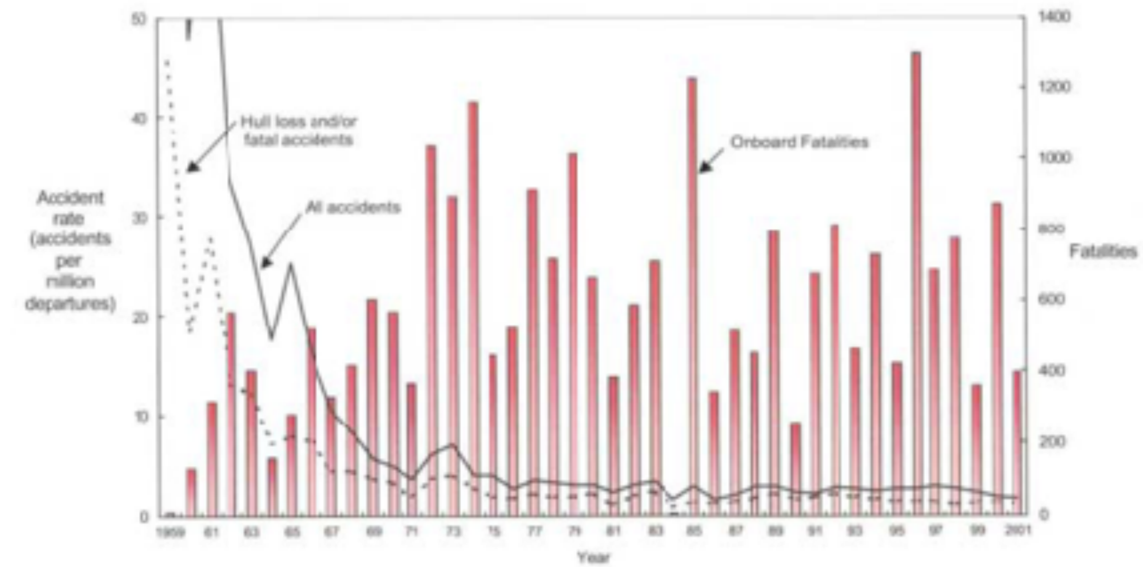


Aircraft safety

20,000 years

Worldwide statistics

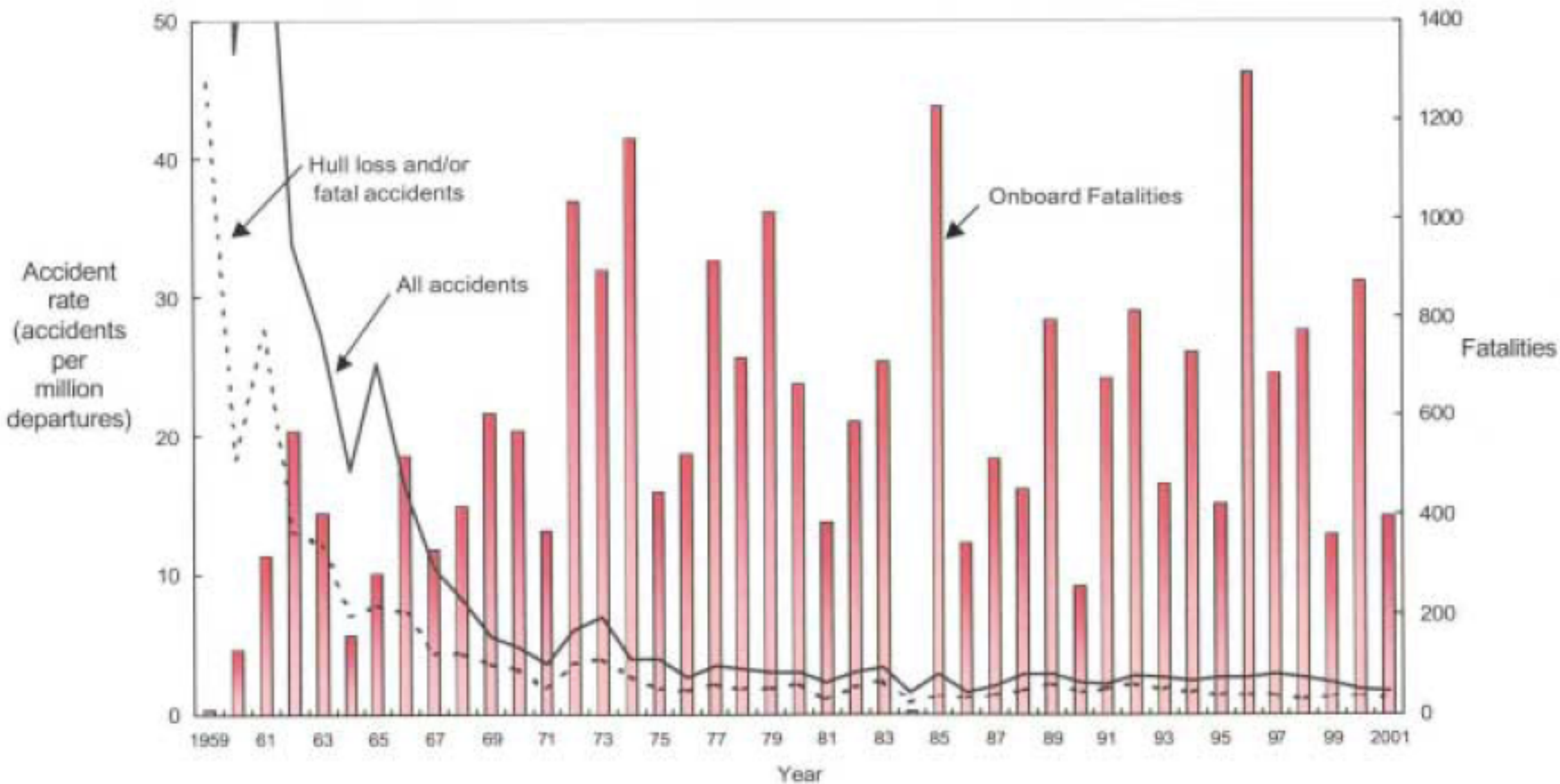
[1959-2001] 1,307 commercial jet aircraft losses



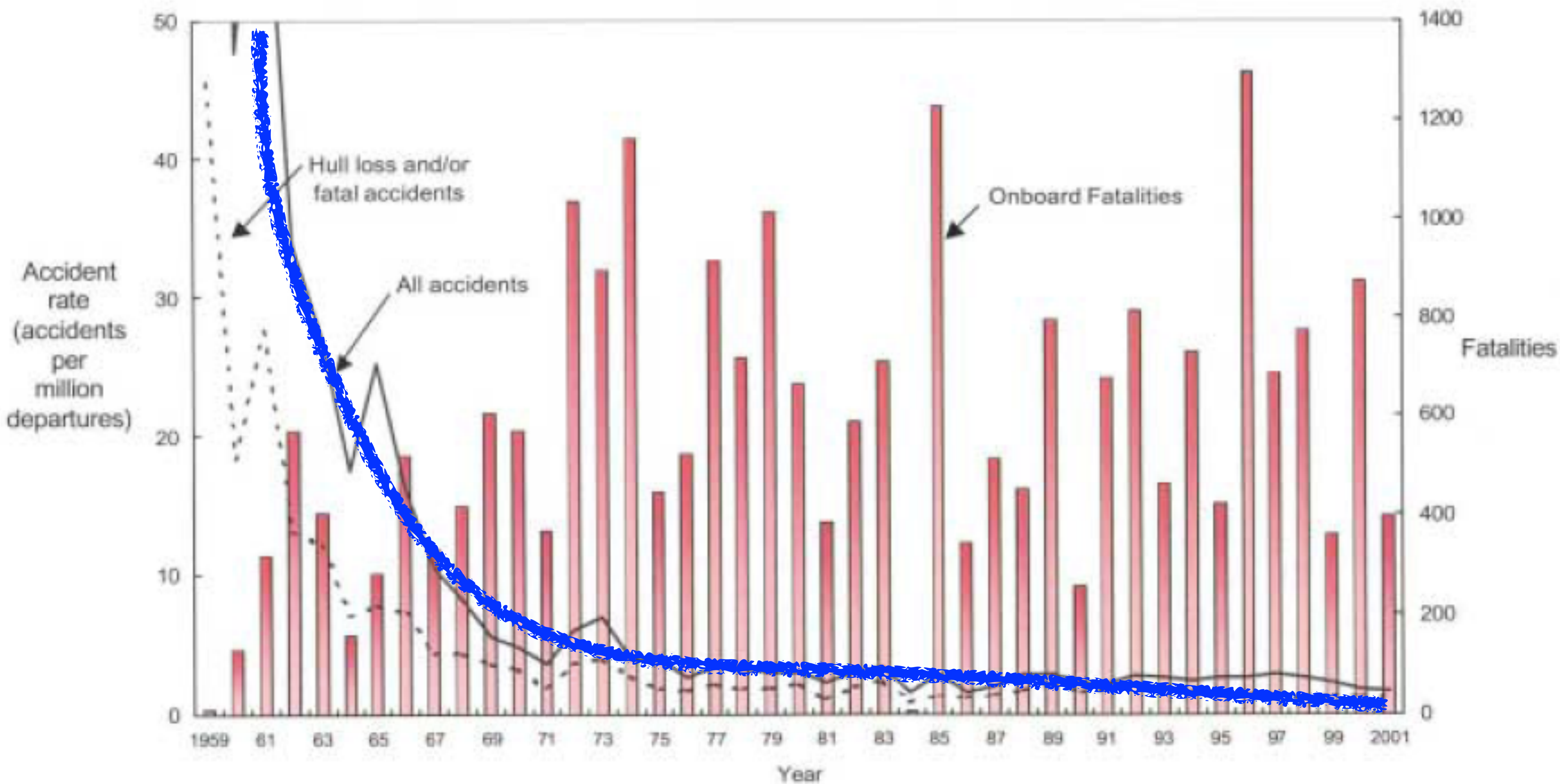
Today:

1 accident per 1,000,000 departures

Accident rates and fatalities/year

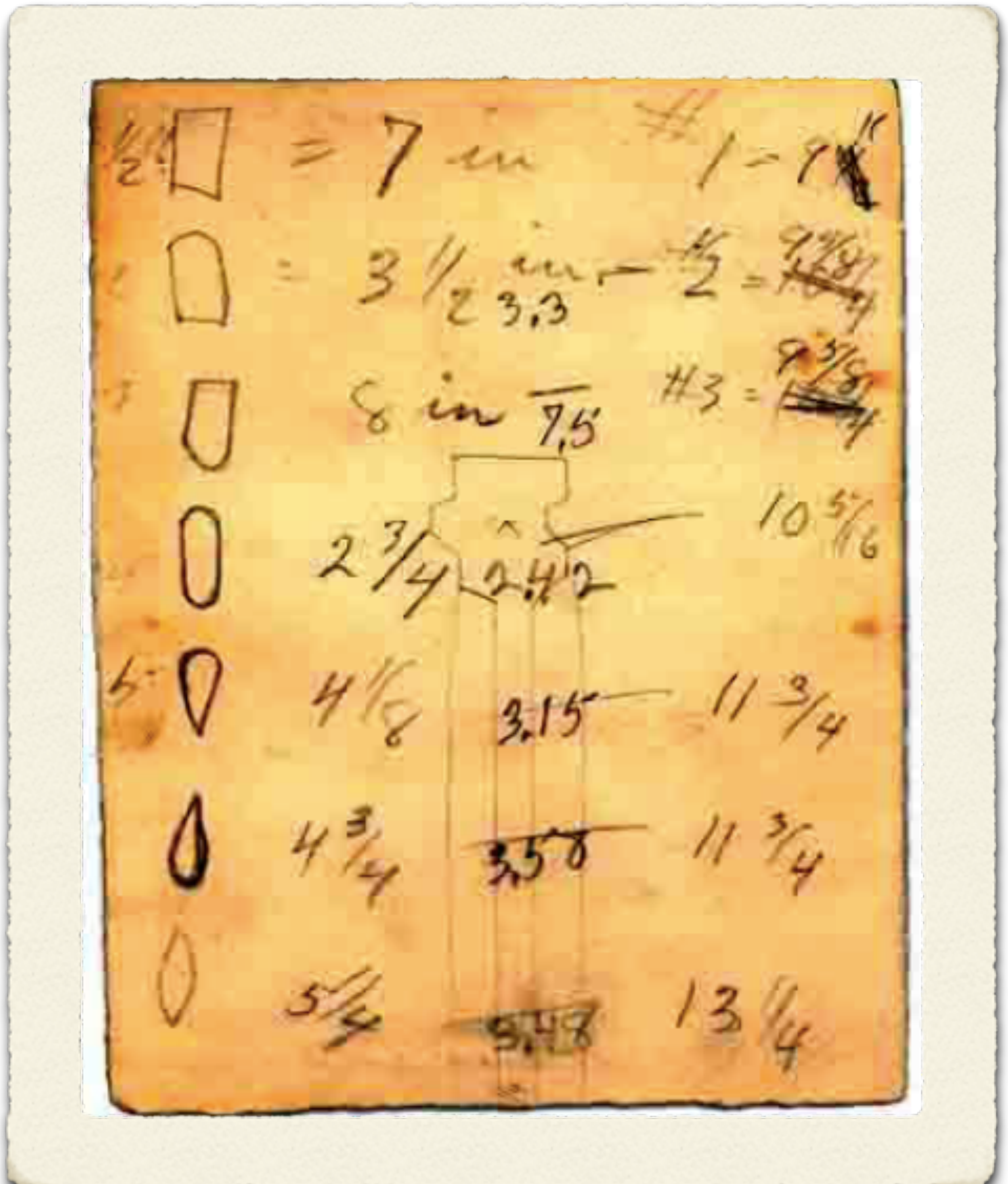


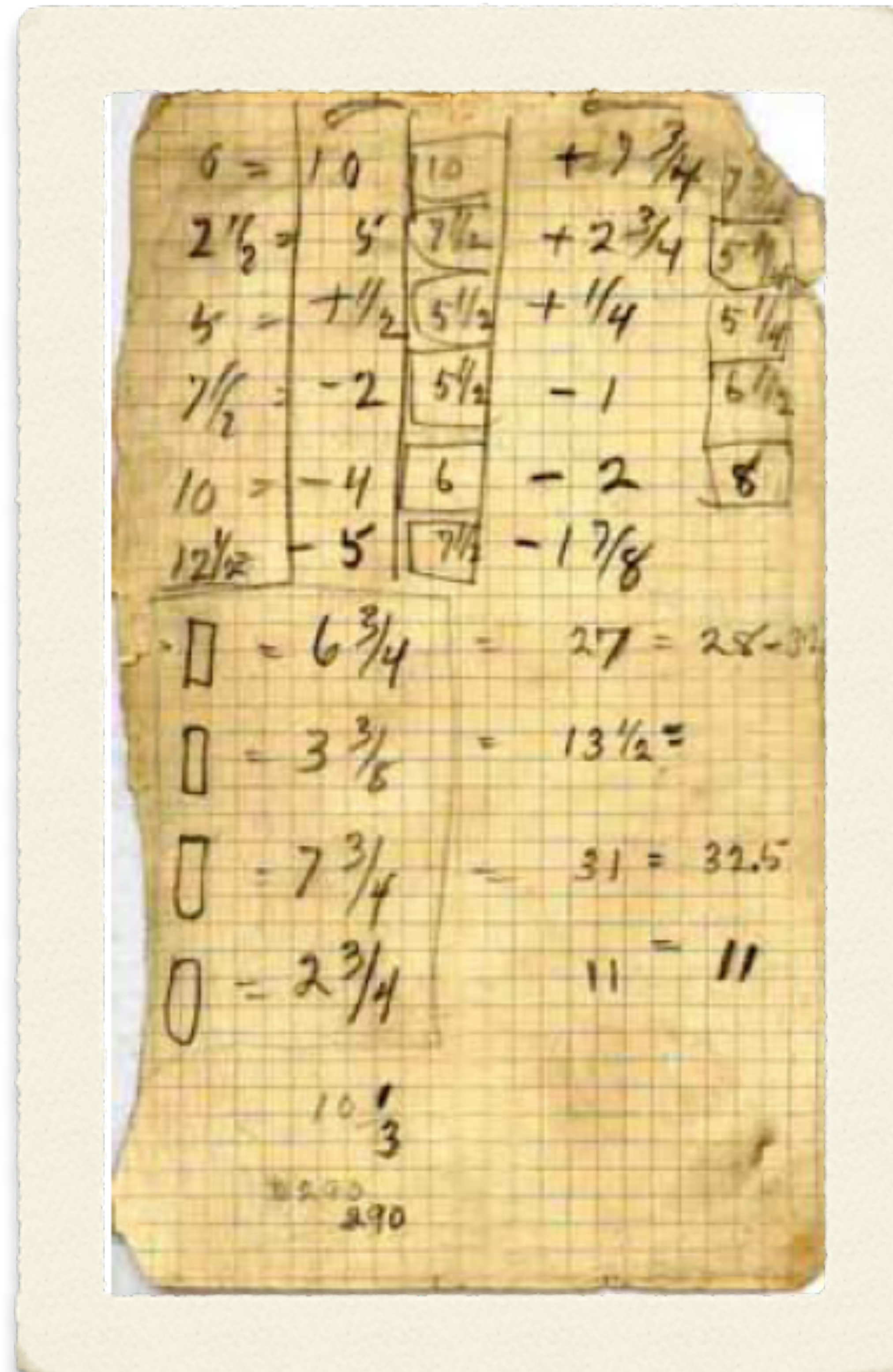
Accident rates and fatalities/year



Source: Flight Safety Foundation/Boeing Commercial Airplane Group

Learning from intuition & theory





Franklin Institute Science Museum. Wilbur Wright's handwriting

Learning from experience

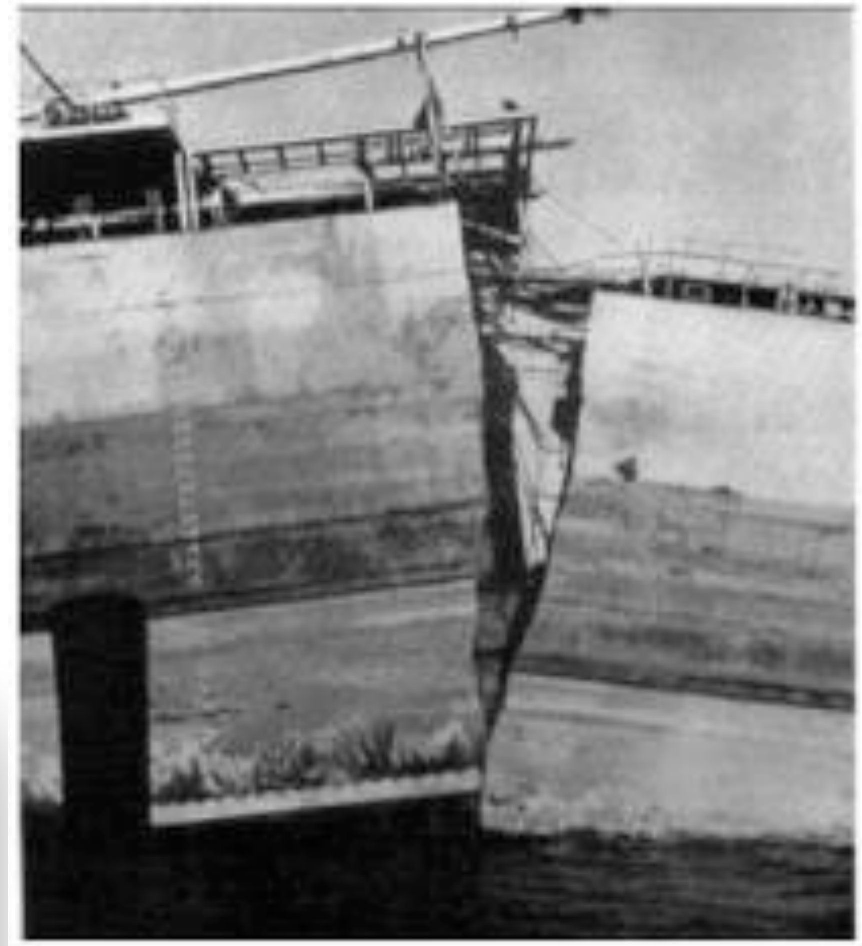
Increased practical understanding of mechanics — in particular fracture and fatigue

Aloha airlines accident - fatigue cracks at corners

Novel convertible aircraft

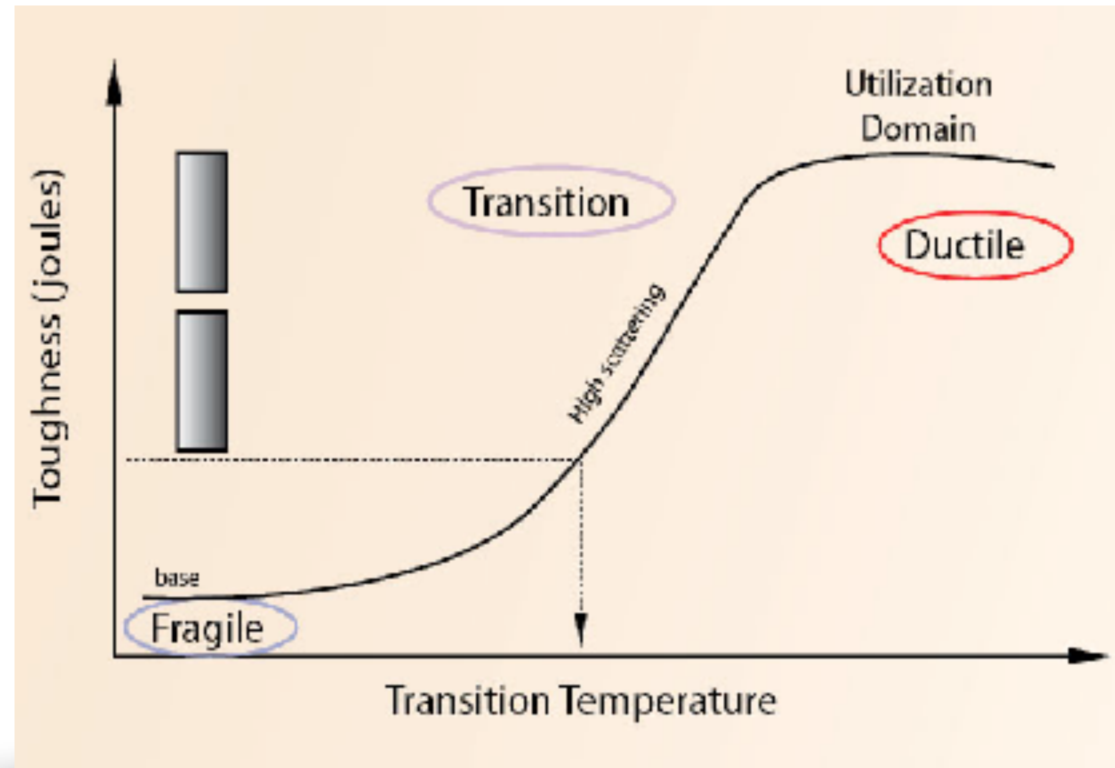
Learning from experience

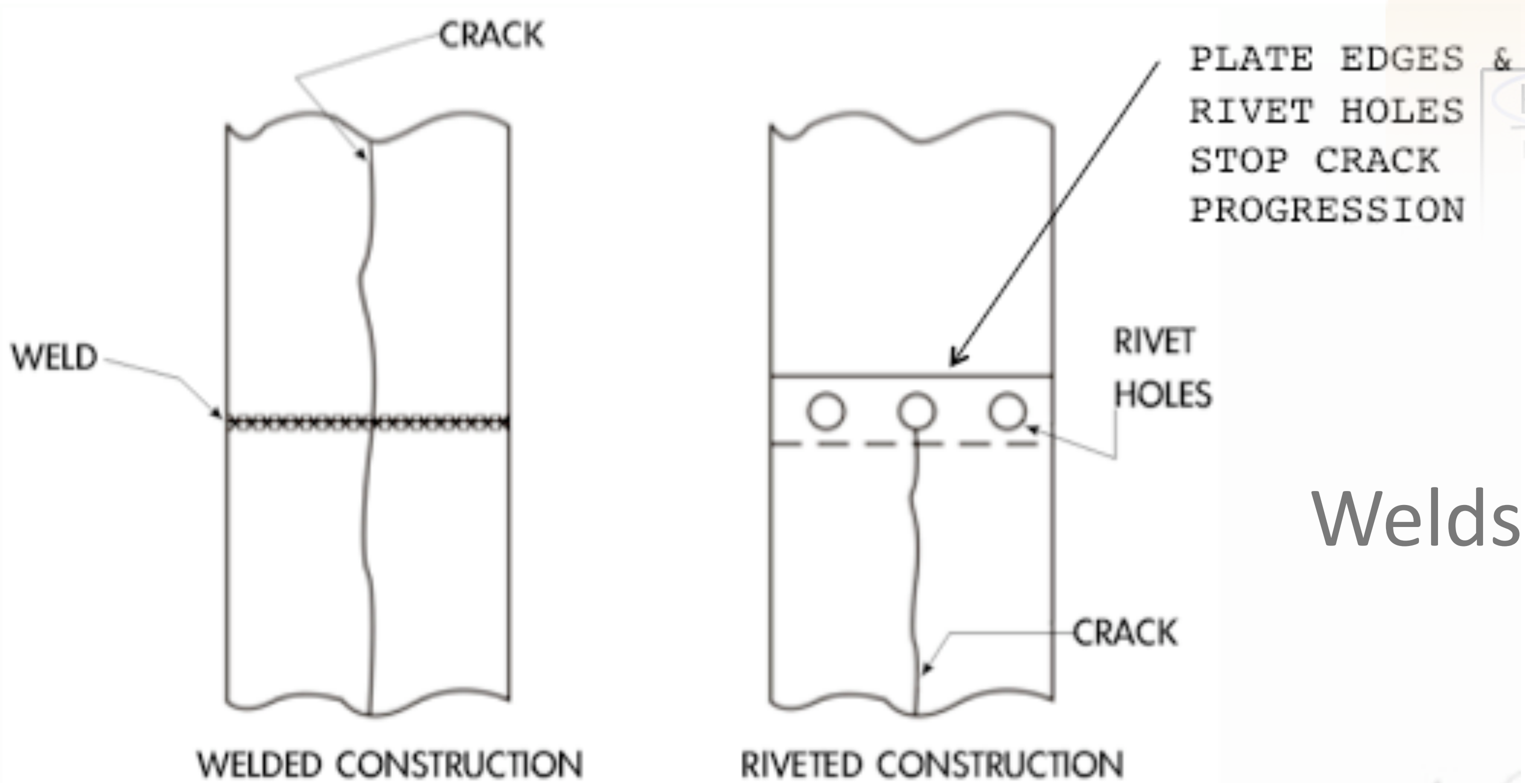
The Liberty Ships



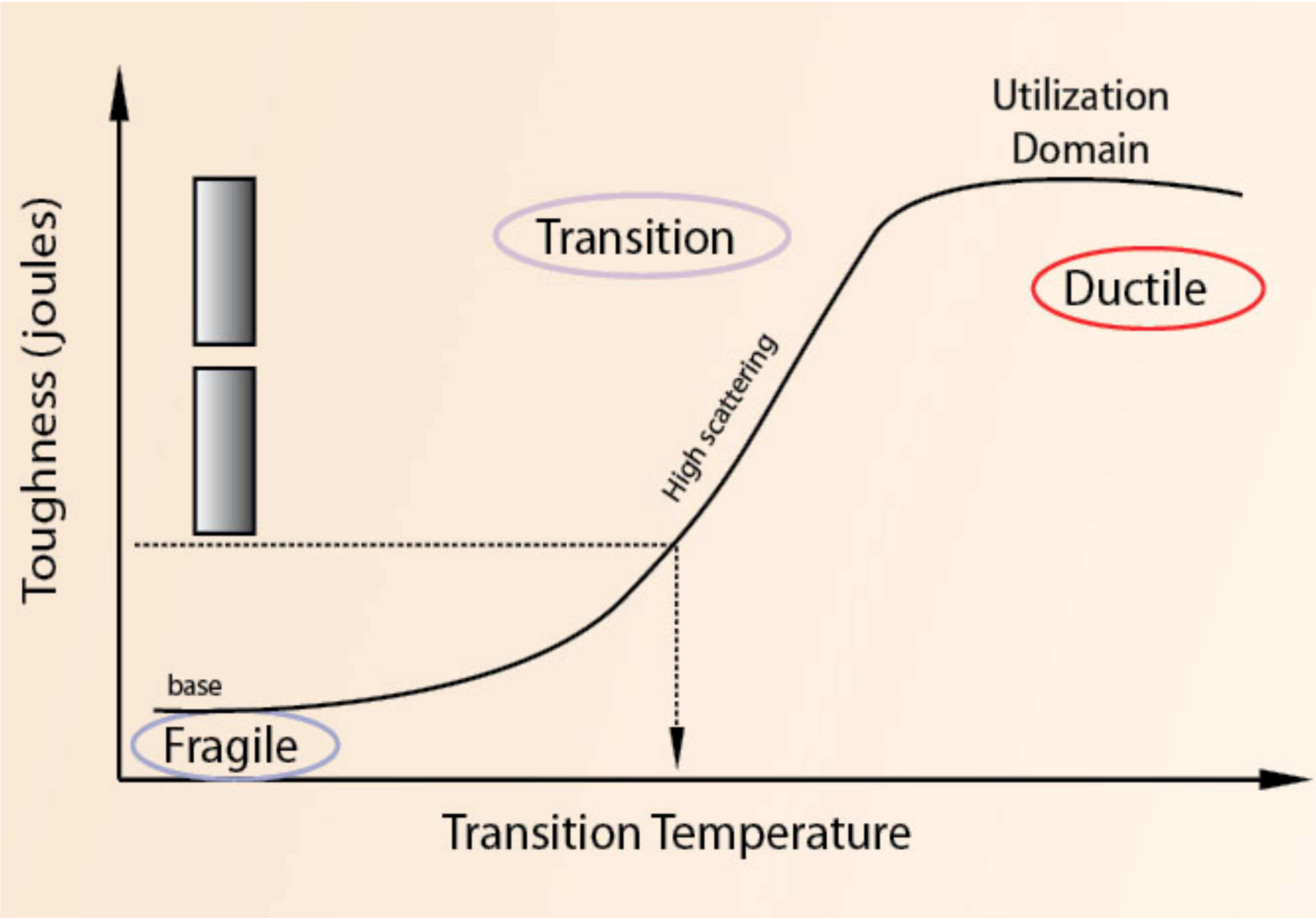
Learning from experience

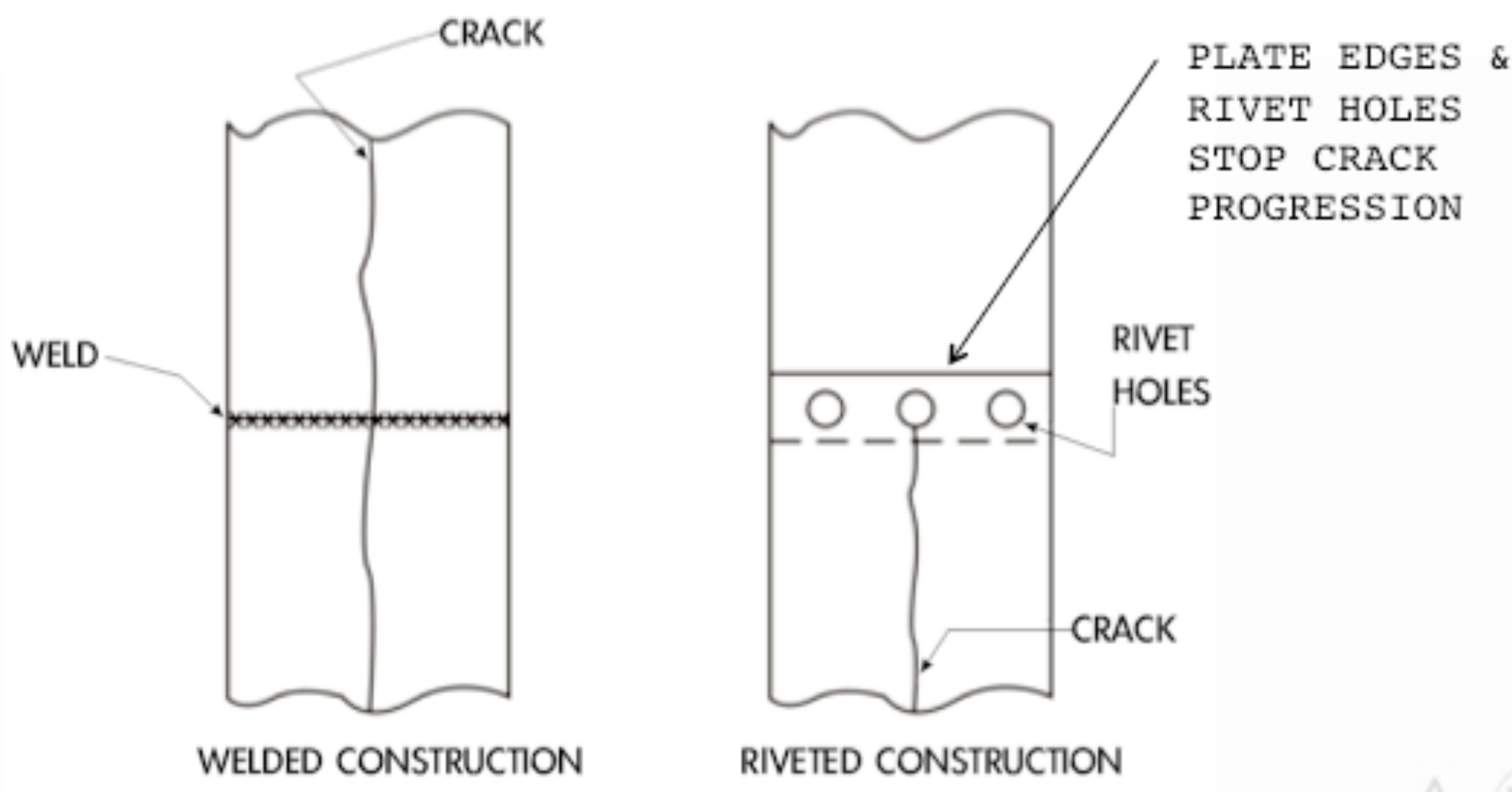
At low temperatures, steel becomes more brittle



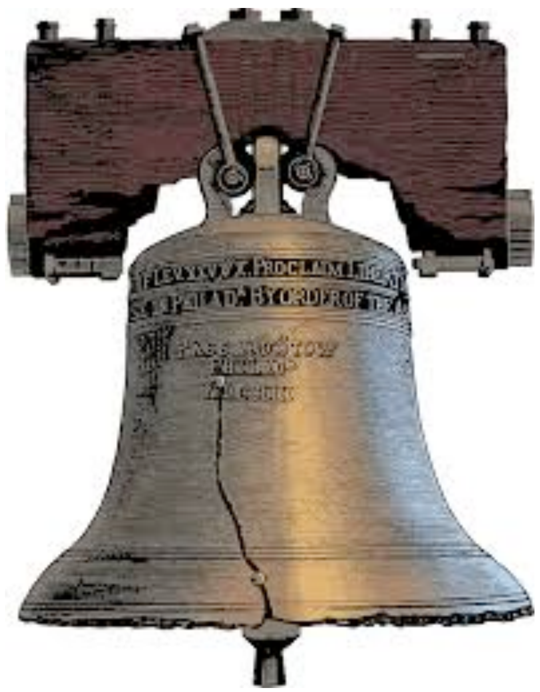


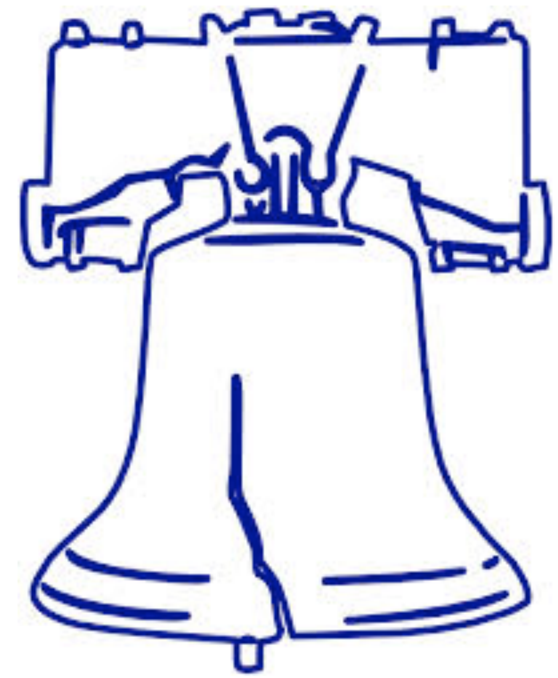
Weds are not good crack arrestors


Utilization
Domain
Transition
Ductile
High scattering
Toughness (joules)
base
Fragile
Transition Temperature


CRACK
WELD
WELDED CONSTRUCTION
PLATE EDGES & RIVET HOLES STOP CRACK PROGRESSION
RIVET HOLES
CRACK
RIVETED CONSTRUCTION

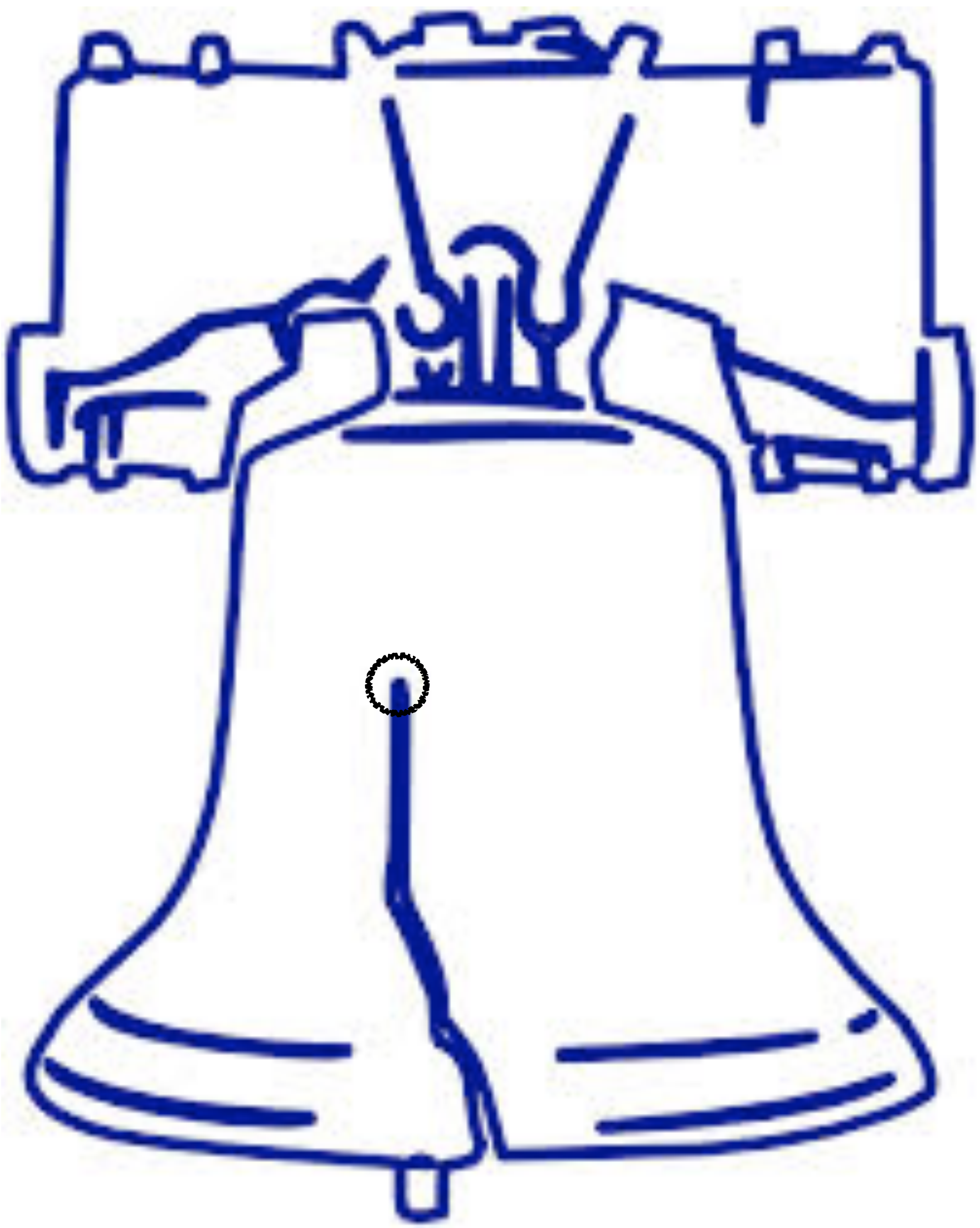
Learning from experience





The liberty bell
(Philadelphia)

Learning from experience



The liberty bell
(Philadelphia)

Learning from experi**ments**

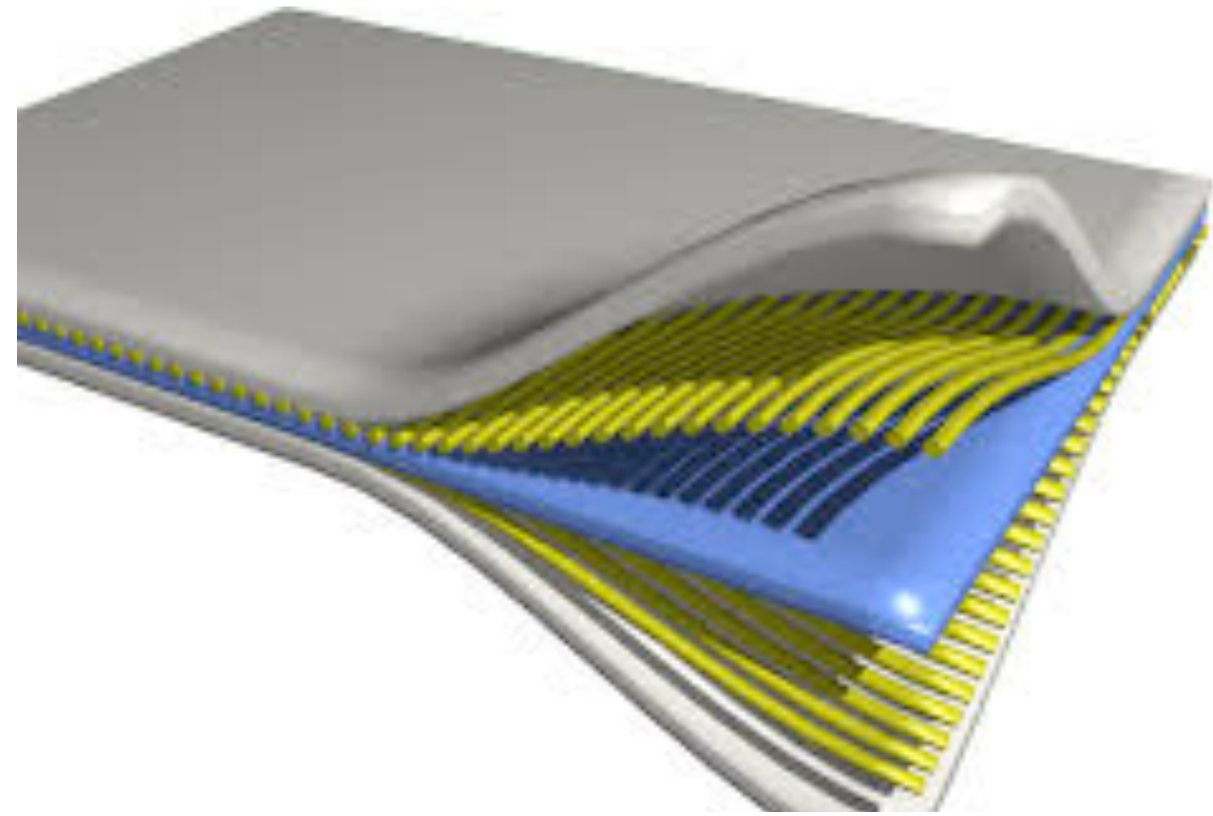
World's largest wind tunnel (2014)

Replica of the 1901 Wright Wind Tunnel (constructed with assistance from Orville Wright)

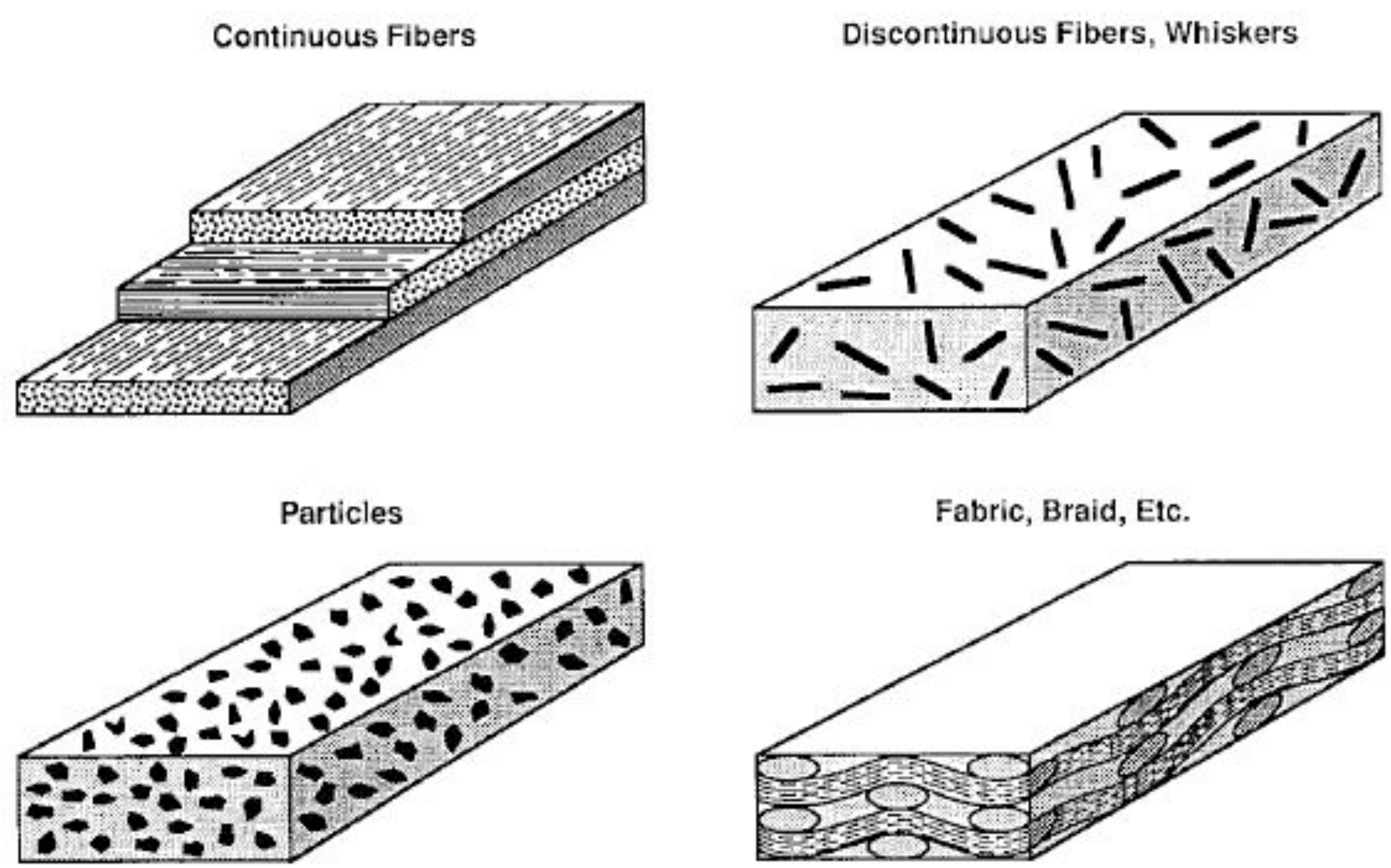
teaching...

New materials for more payload

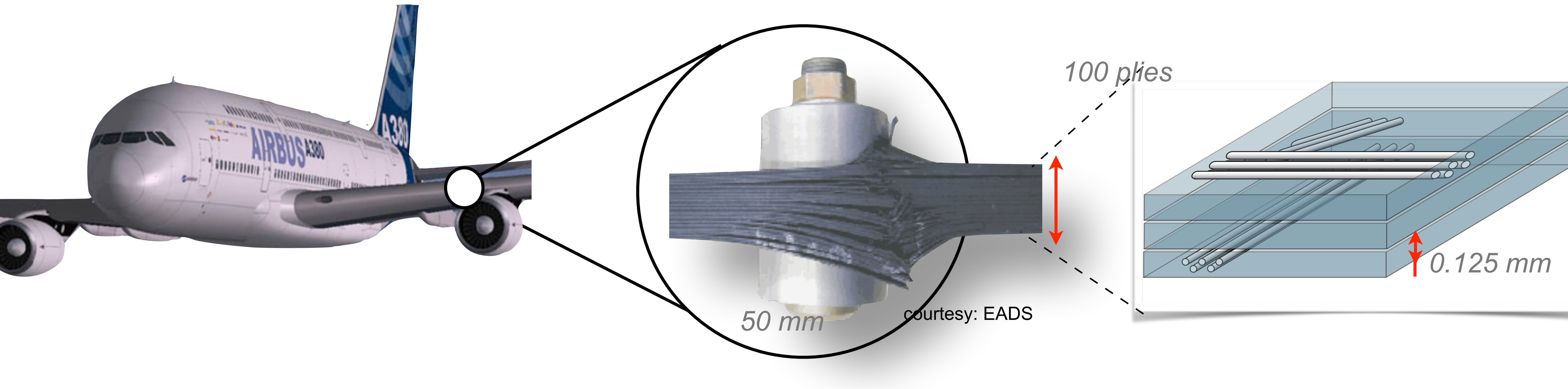
Introduction of composite materials have reduced the weight of structures by 20%



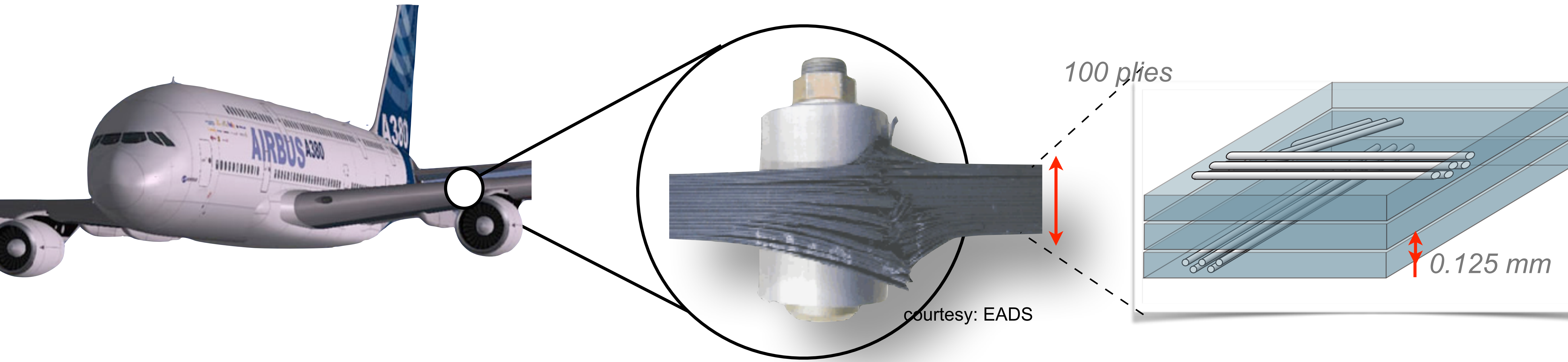
Over 1,000km saving of 8,660kg of fuel [A340-300]



Material complexity

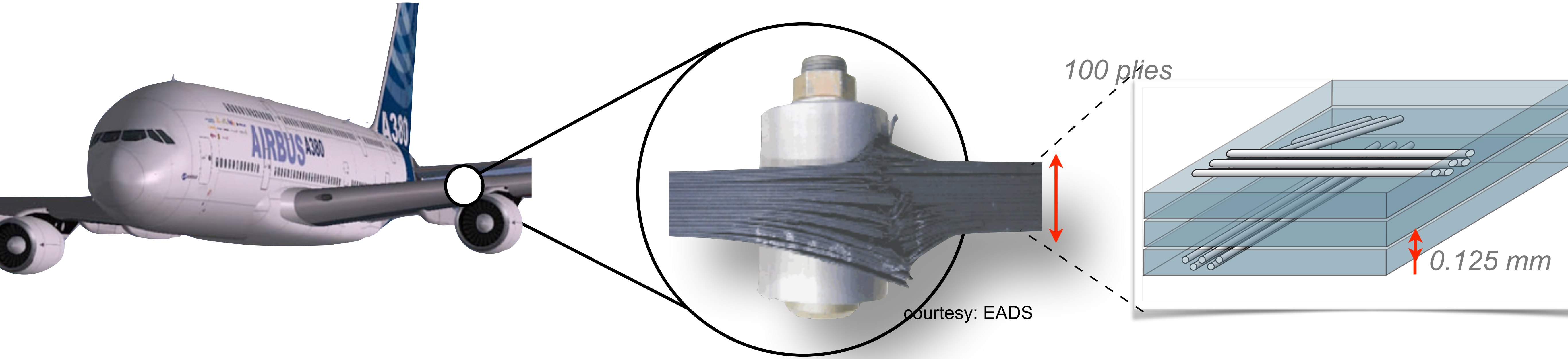


Material complexity



- Heterogeneous & multi-functional
- Experiments required to attain sufficient confidence in their behavior are increasingly costly

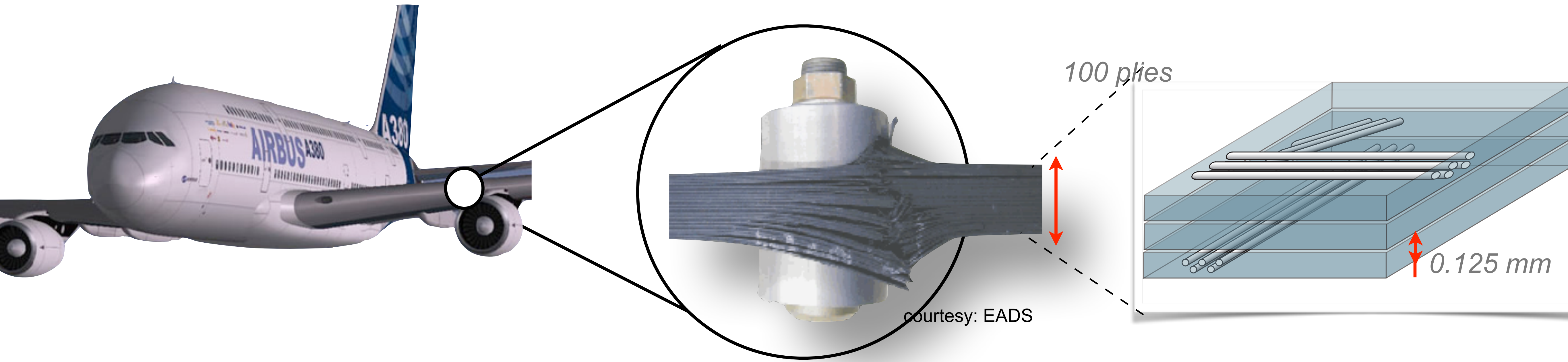
Material complexity



- Heterogeneous & multi-functional
- Experiments required to attain sufficient confidence in their behavior are increasingly costly
- Factor-of-Safety or probabilistic based methods cannot handle unknown unknowns

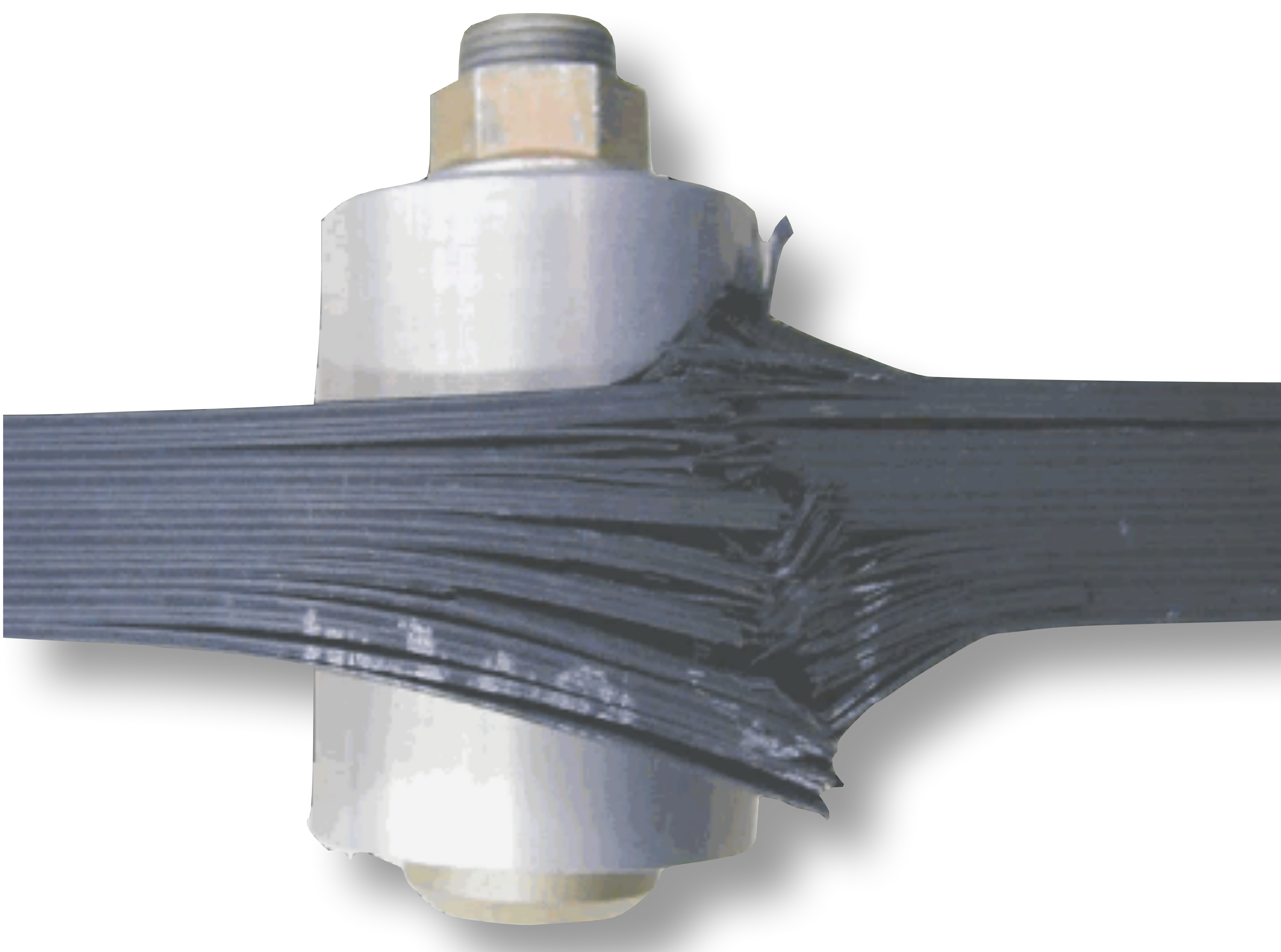
- Lack of similitude between testing (experimental) and operating conditions — also encountered in geophysics...

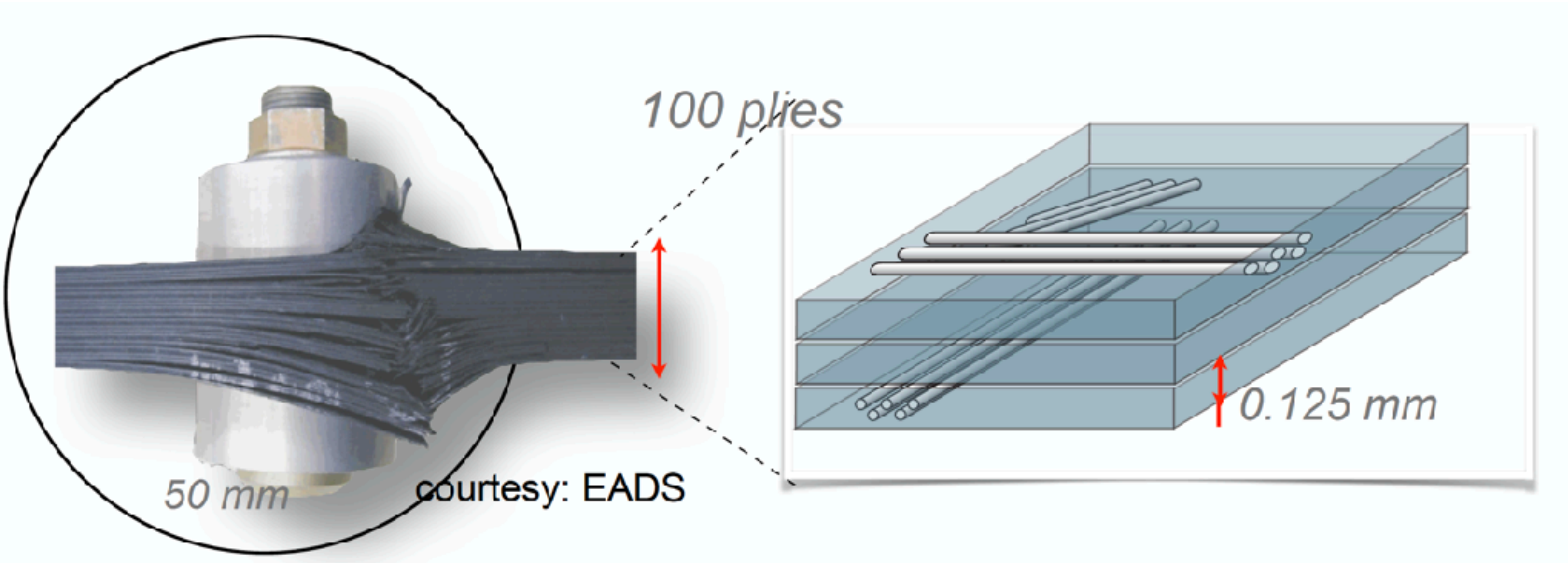
Material complexity

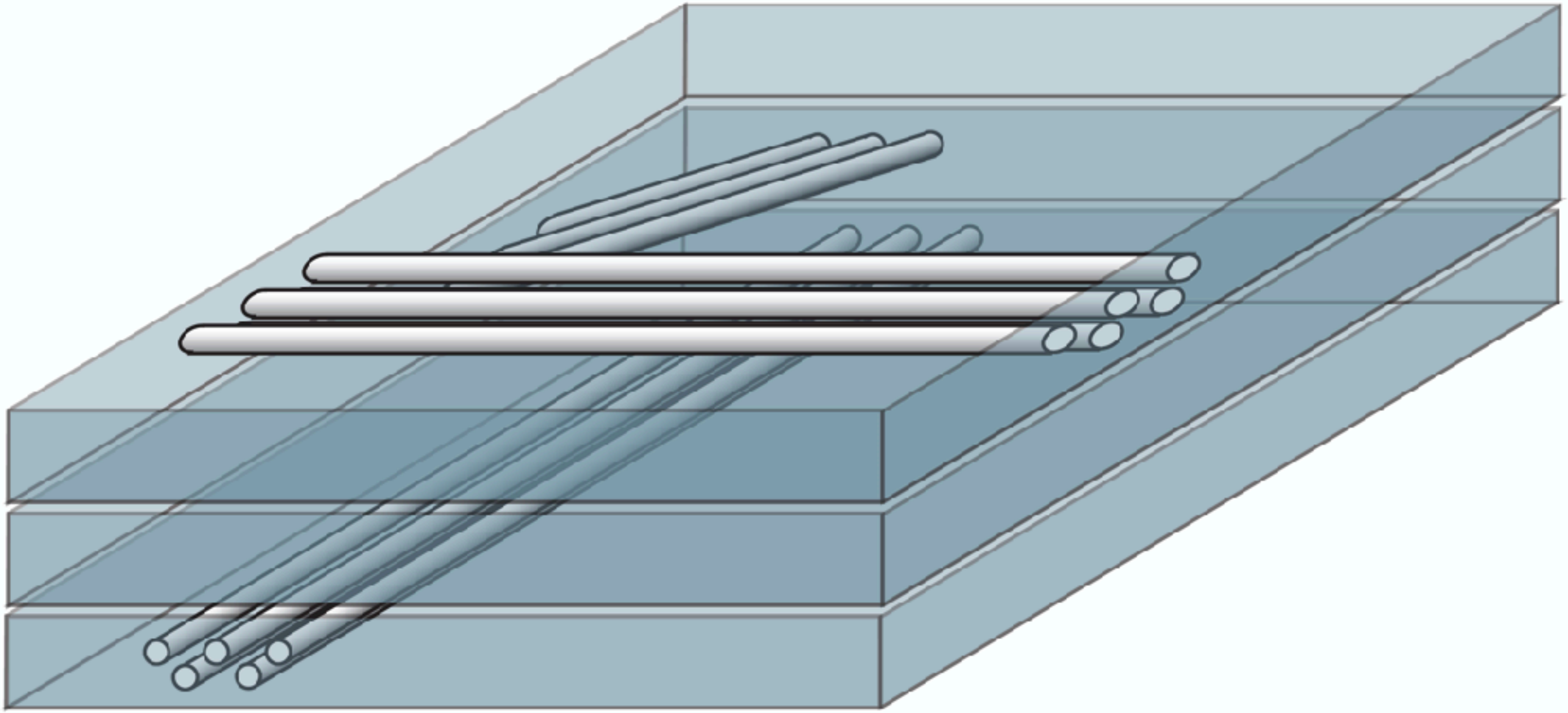


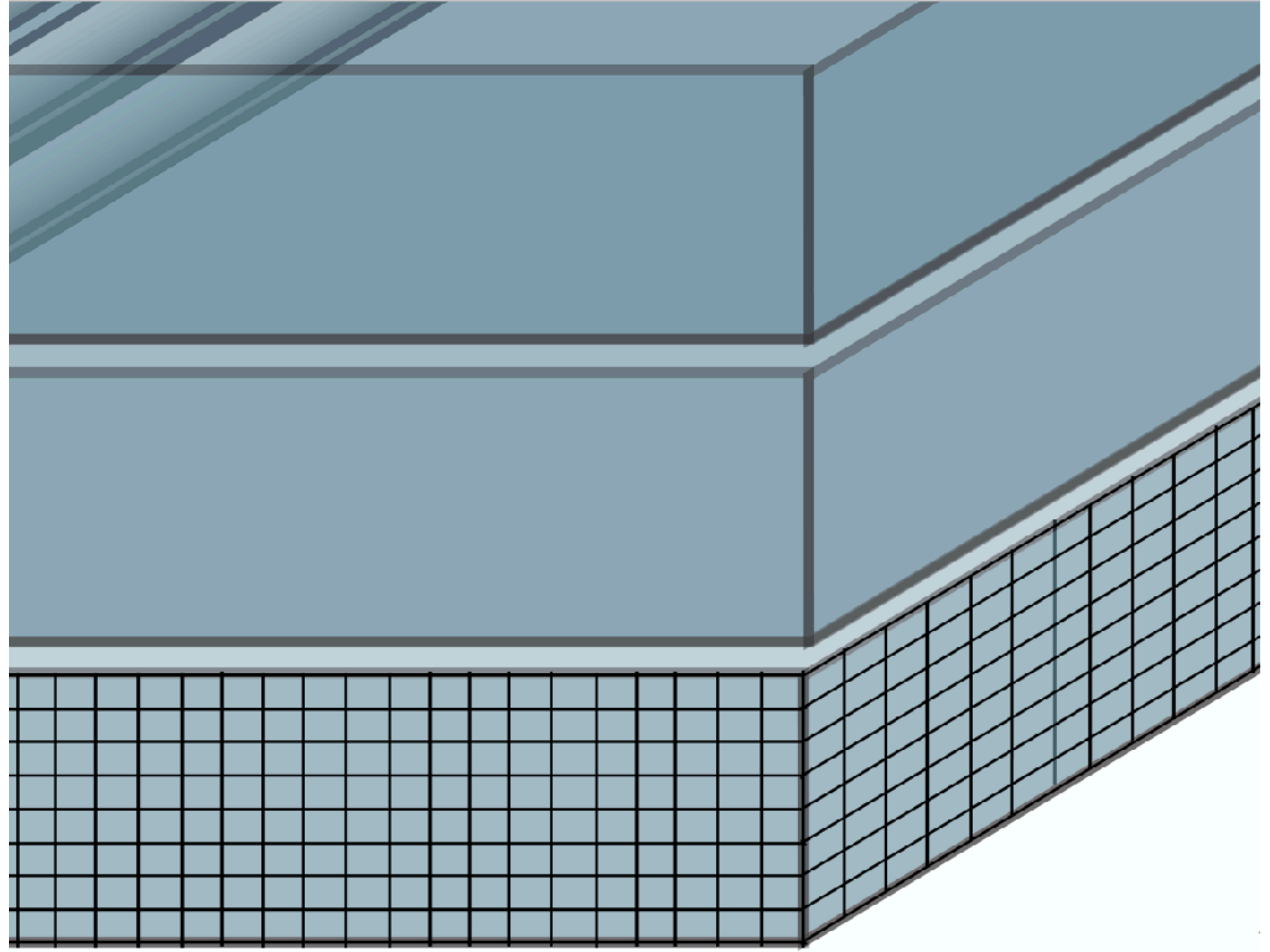
- Heterogeneous & multi-functional
- Experiments required to attain sufficient confidence in their behavior are increasingly costly
- Factor-of-Safety or probabilistic based methods cannot handle unknown unknowns - lack of similitude
- Move **away from heuristics** and experience-based engineering
- Develop **fundamental understanding** of physical processes (degradation, ...)
- Reduce weight

A bolted joint

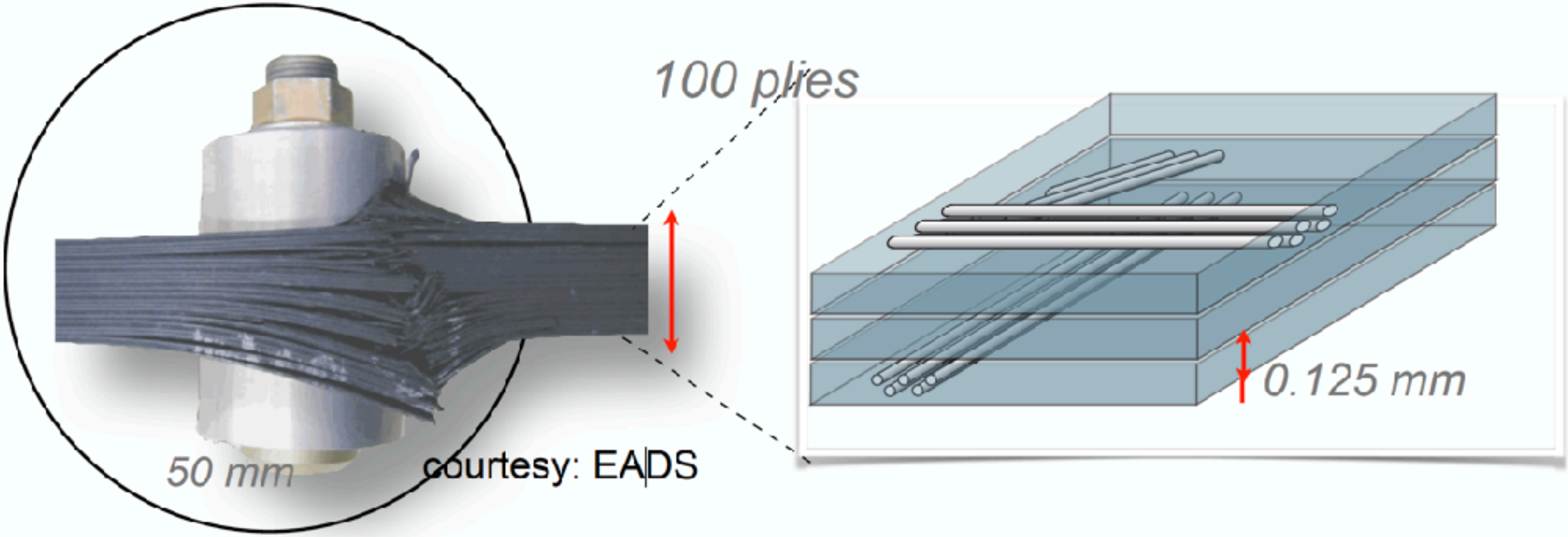



100 plies
0.125 mm
50 mm
courtesy: EADS



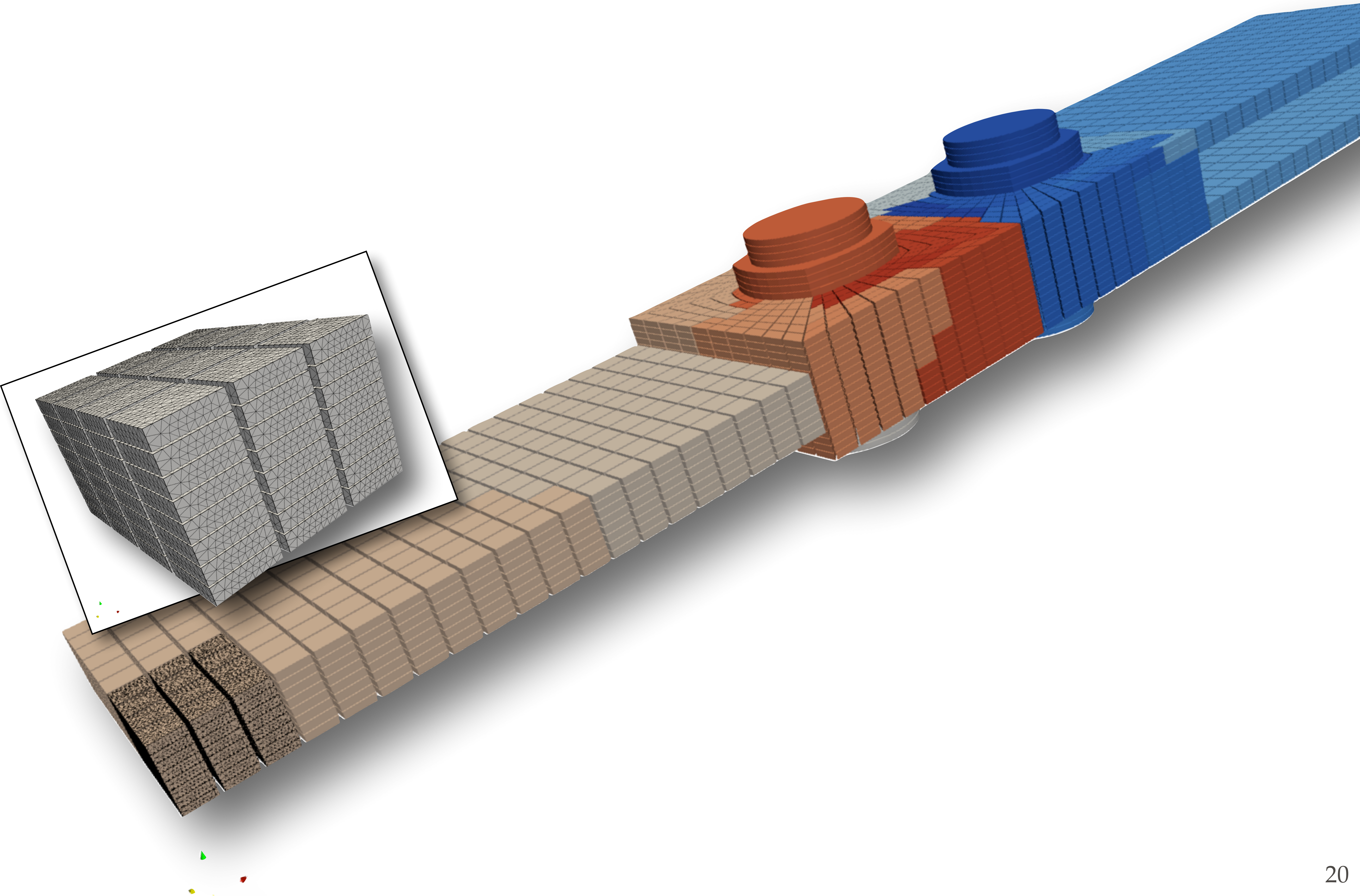


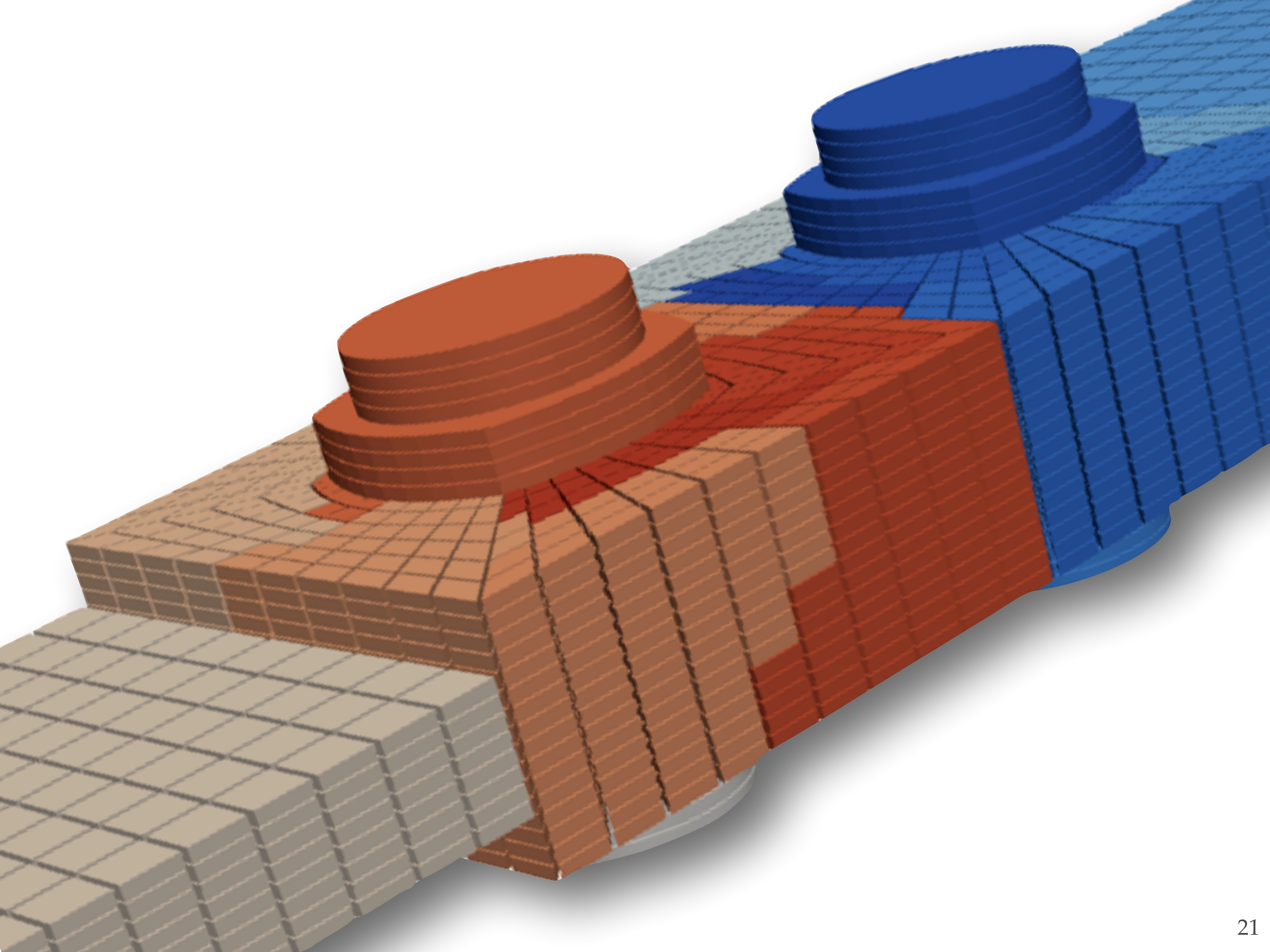
One single bolted joint

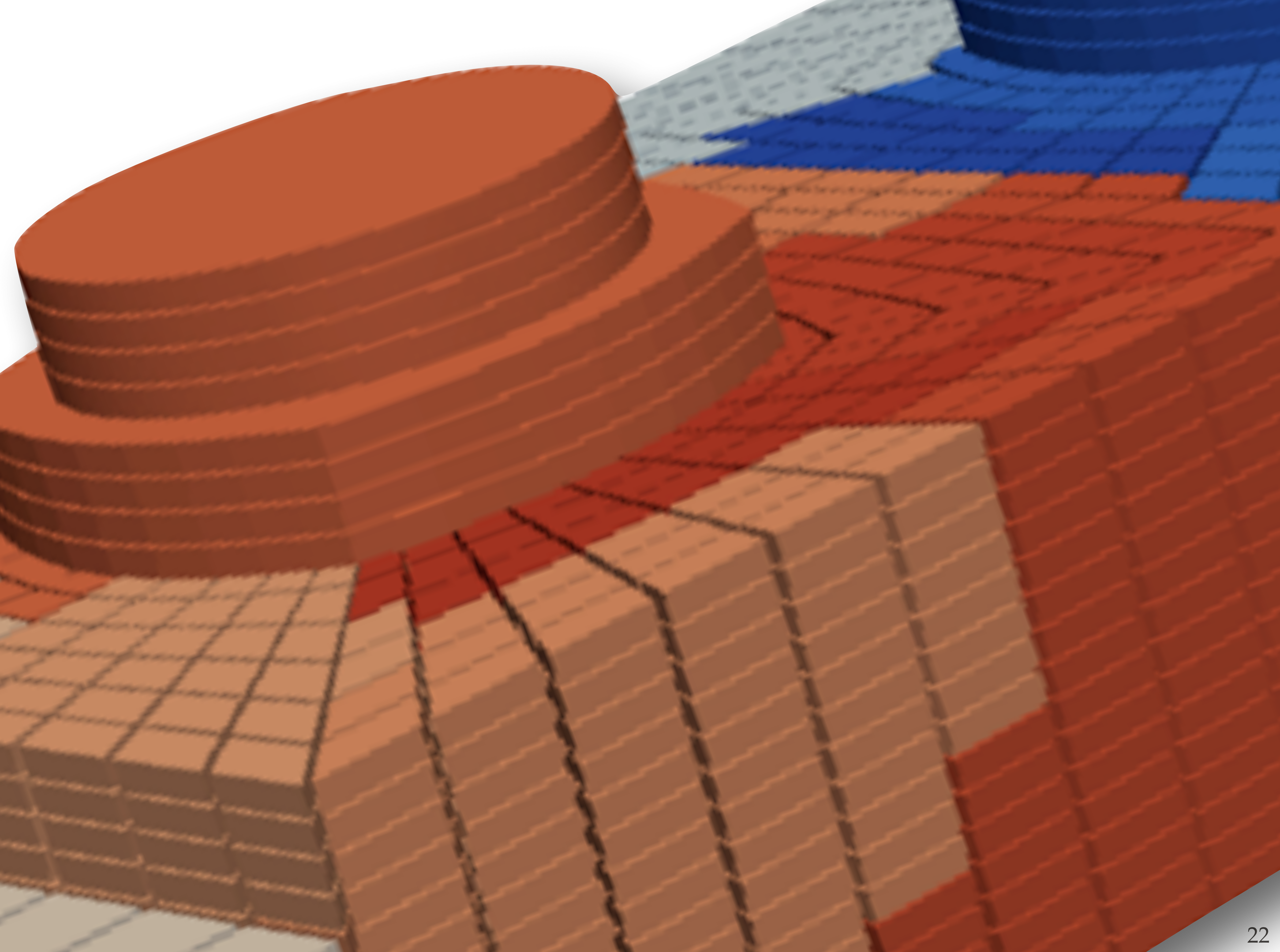


- 5 elements through the thickness of a ply => 0.025mm/element
- 50mm bolted joint area => 2,000 elements
- 50mm x 50mm x 100 plies => 2,000 x 2,000 x (100 x 5)

=> **2 billion elements**

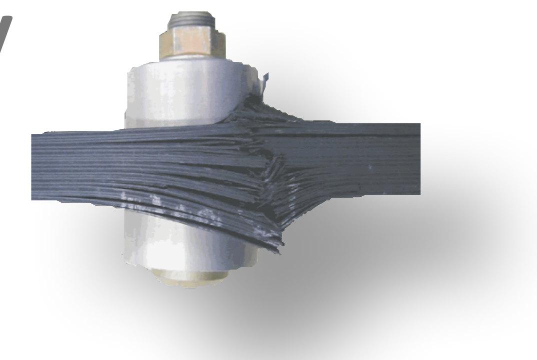




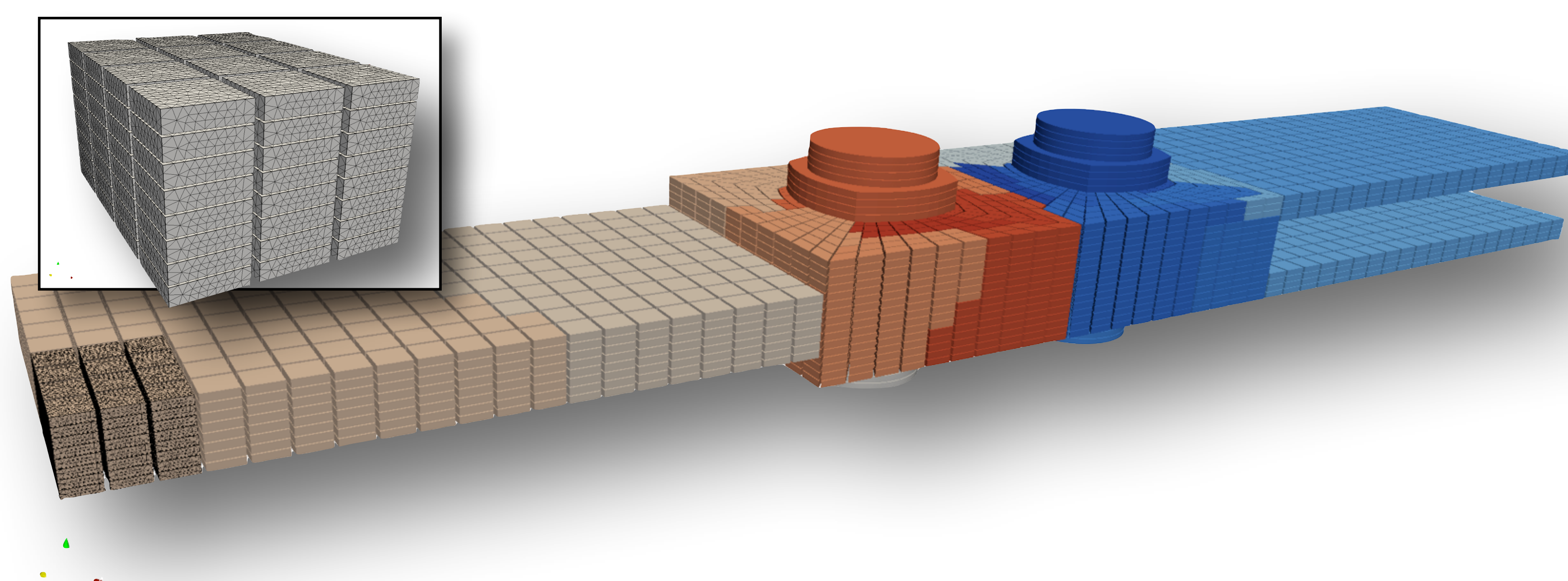


Large structures

whose behaviour is governed by small-scale effects



=> **intractable problem size**



How can the problem size be reduced but the accuracy controlled?

Challenge

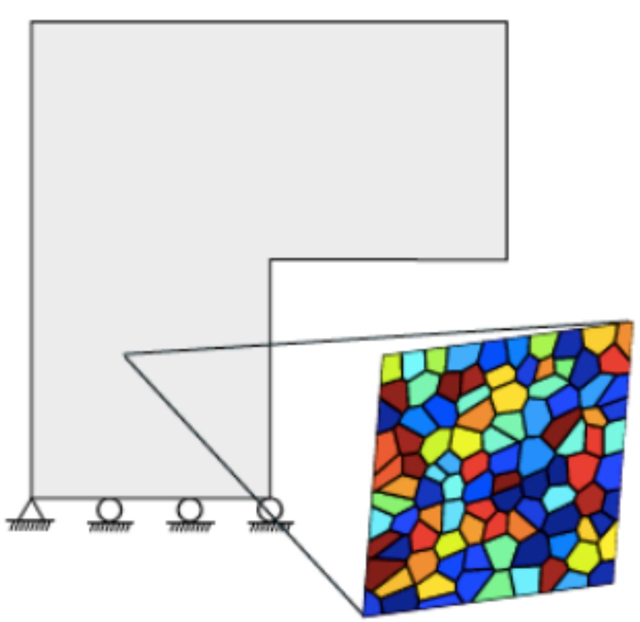
- Reduce the problem size
- Preserve essential features

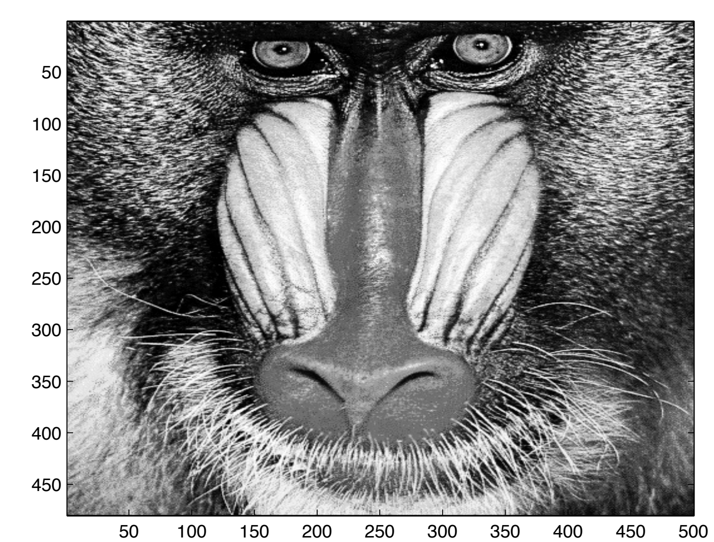
Reduce computational expense

Control the error

Physics based model reduction a.k.a**. Multiscale Methods**

Algebraic based model reduction a.k.a**. Machine Learning**





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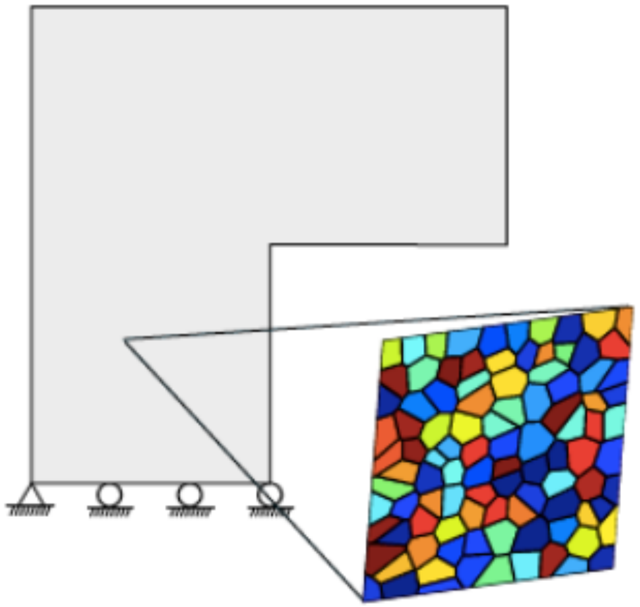
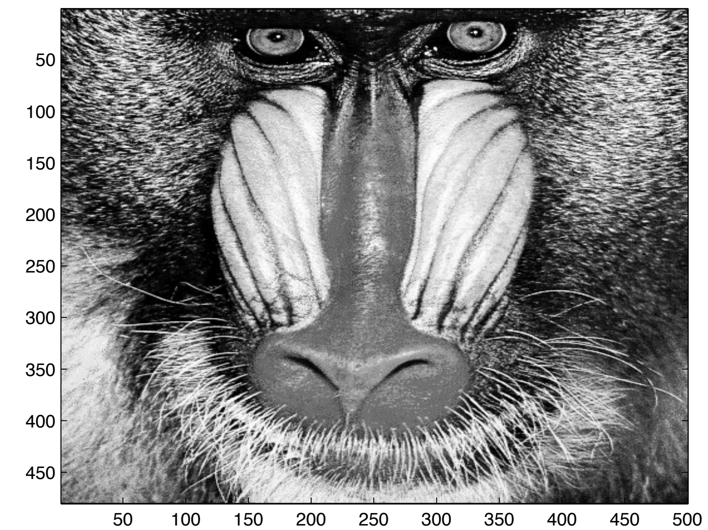
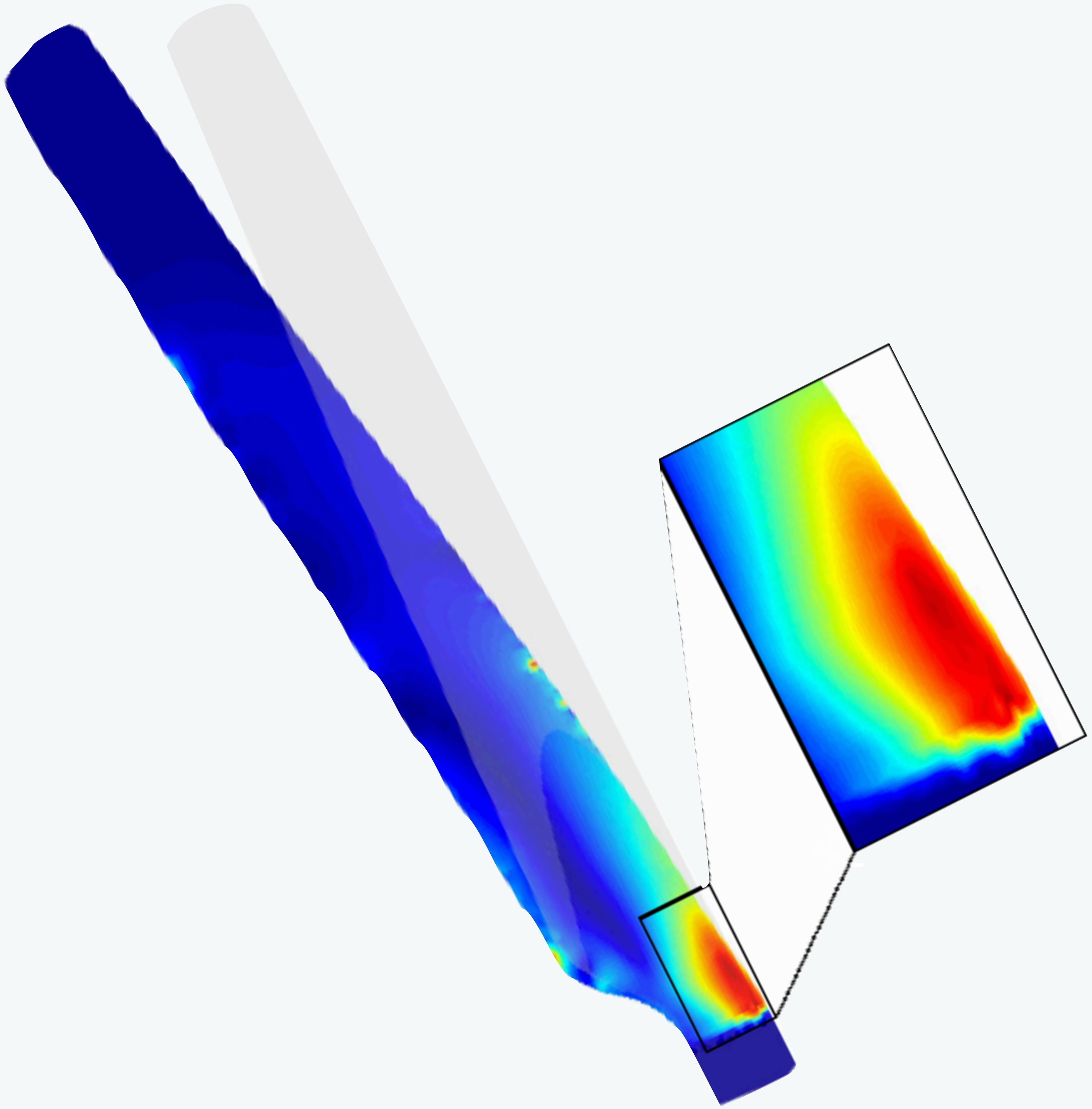
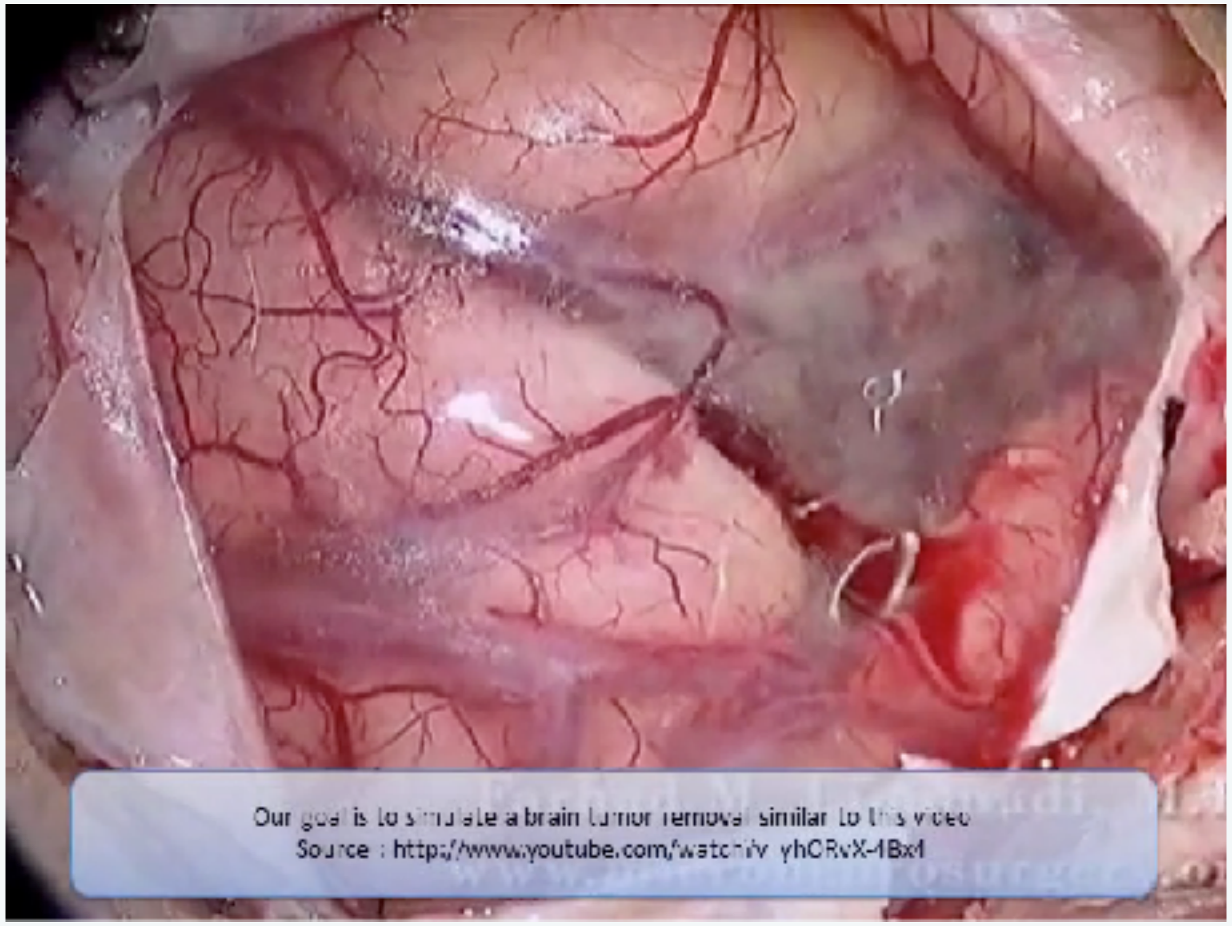




Lack of scale separation

A view from reduced order modelling and homogenisation





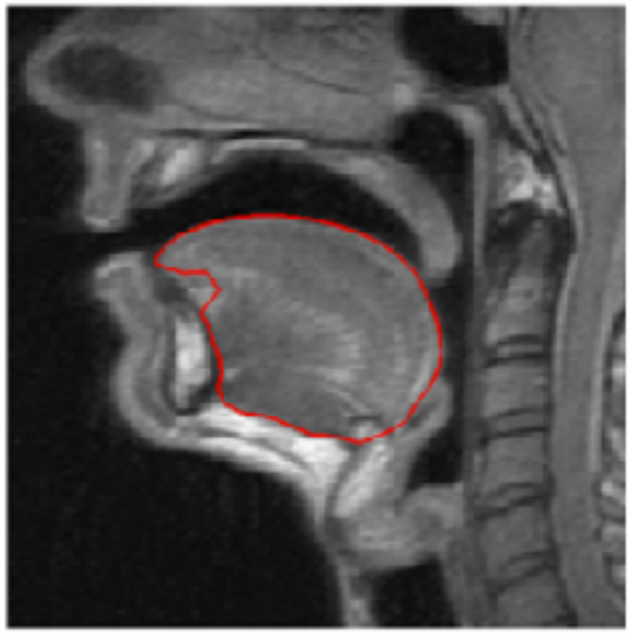
Mathematical Modelling

Continuous Problem

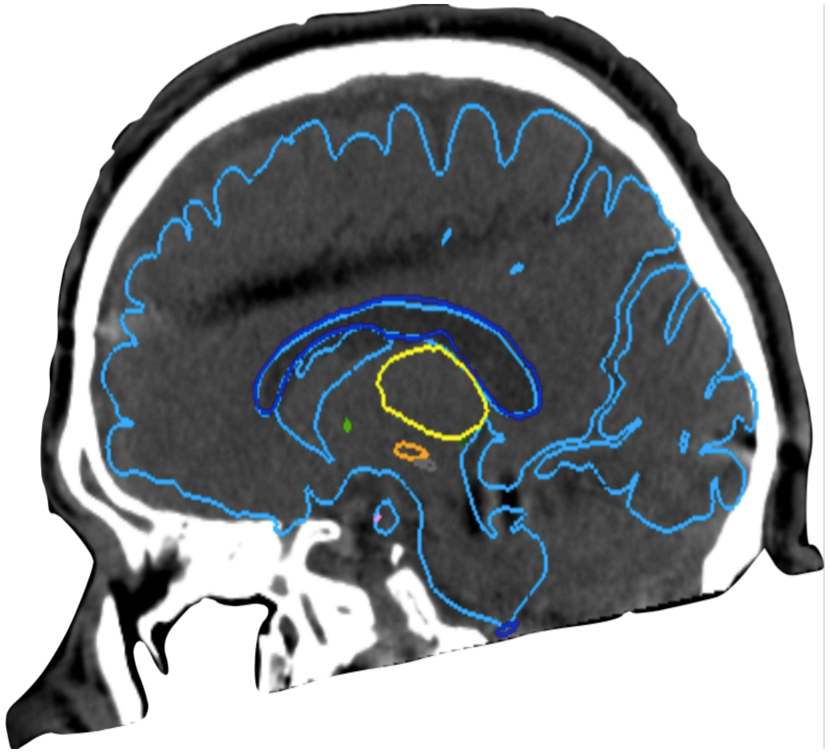
Stéphane Pierre Alain BORDAS, Department of Computational Engineering & Sciences University of Luxembourg and Cardiff University

Mathematical Modelling

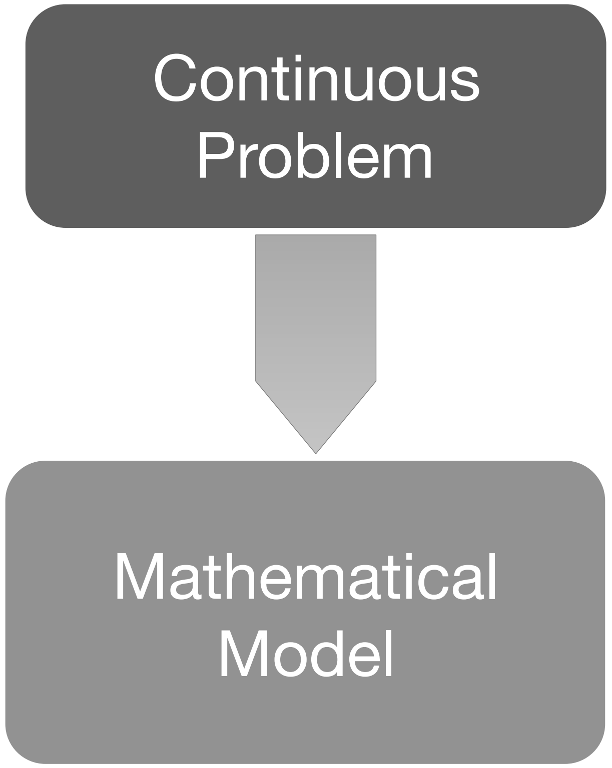
Continuous Problem



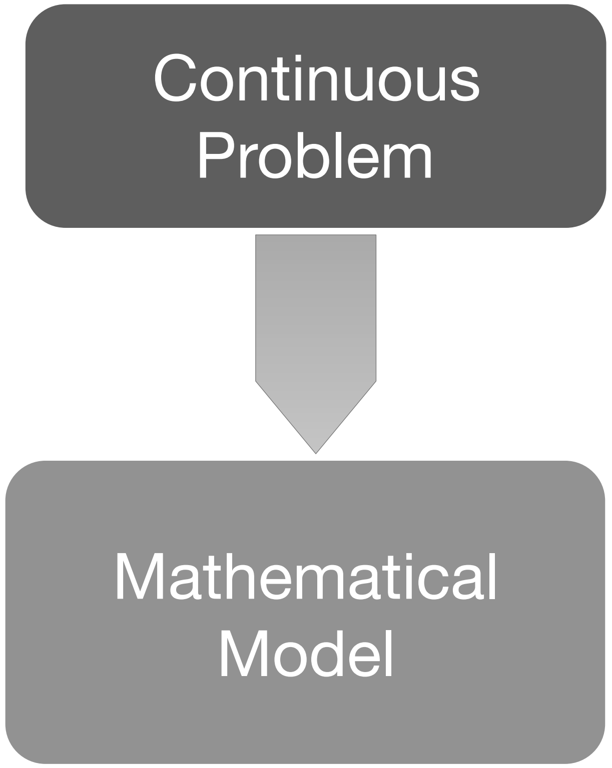
Bijar, Rohan, Perrier & Payan 2015



Mathematical Modelling



Mathematical Modelling



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

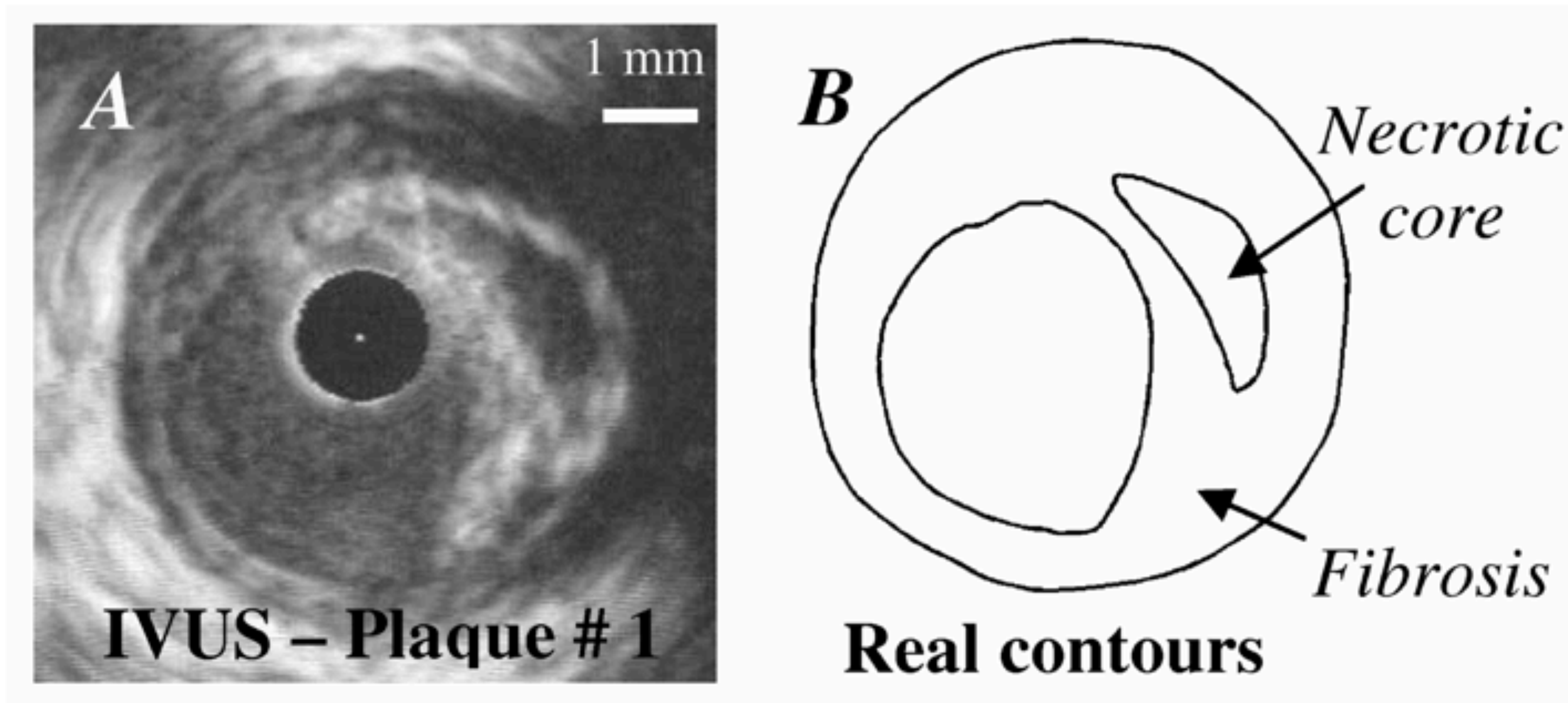
with $\quad \boldsymbol{\sigma}(\mathbf{u},\beta) = \underbrace{\boldsymbol{\sigma}_P(\mathbf{u})}_{\text{passive material}} + \underbrace{\boldsymbol{\sigma}_A(\beta)}_{\text{muscular activation}} \quad \begin{cases} \boldsymbol{\sigma}_A(\beta) = \beta T e_A \otimes e_A \\ e_A : \text{ fiber direction}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

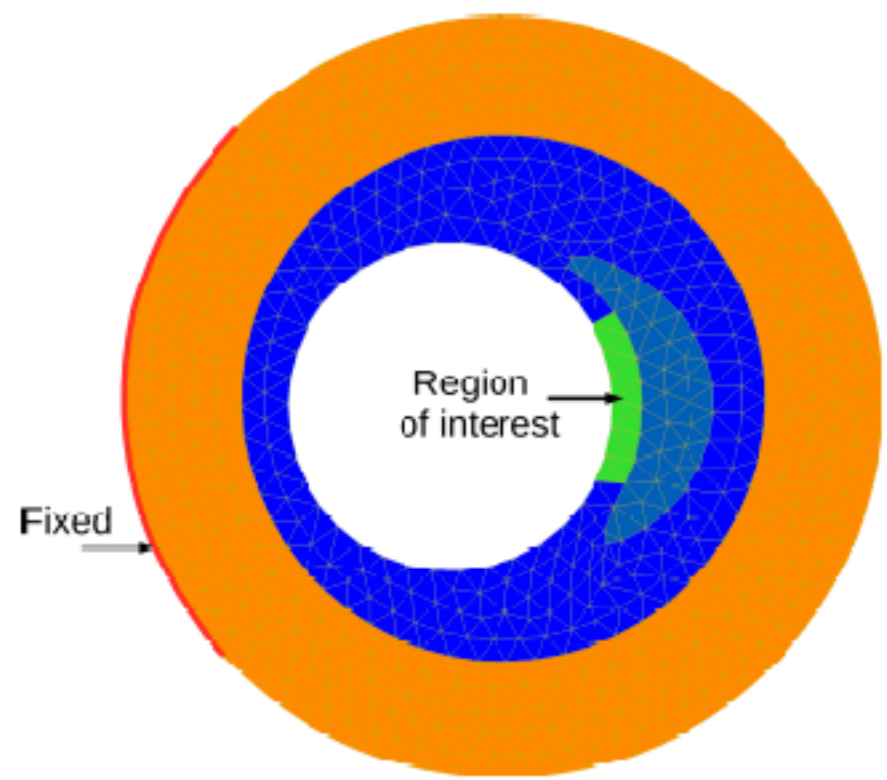
Mathematical Modelling

Continuous Problem

↓

Mathematical Model





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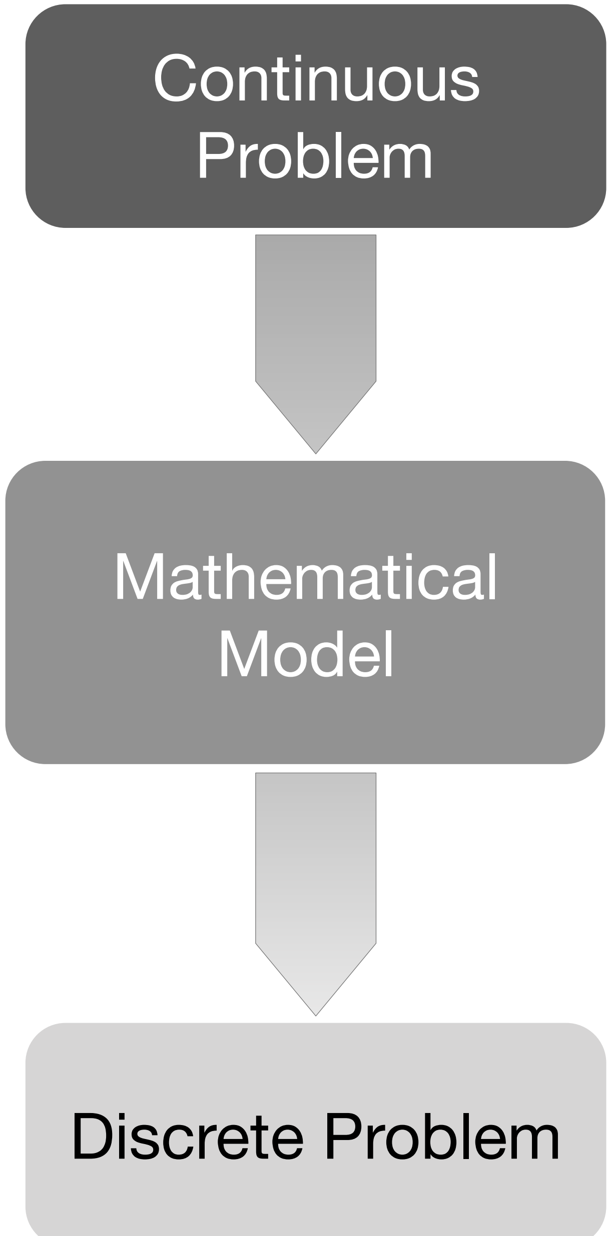
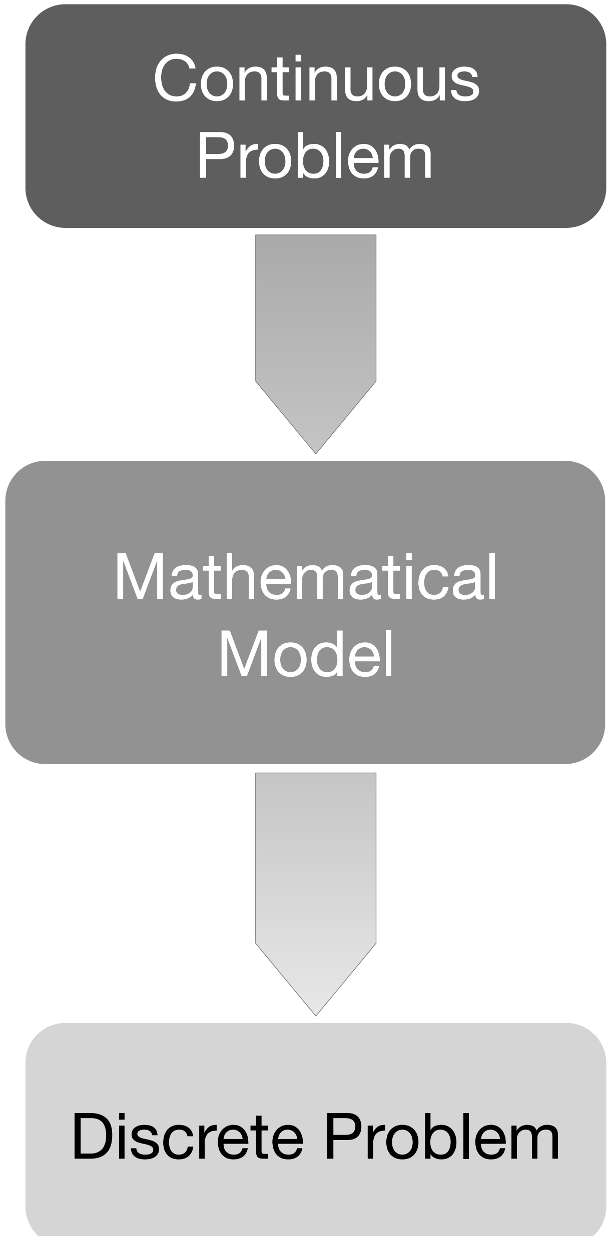
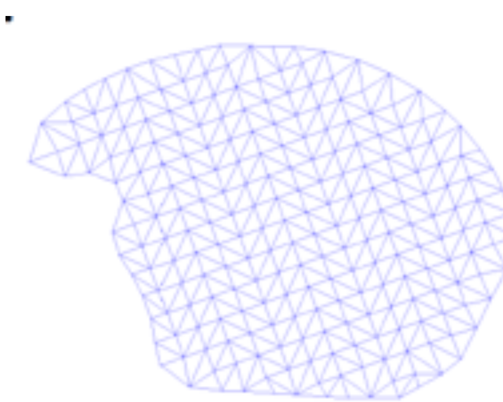
Mathematical Modelling



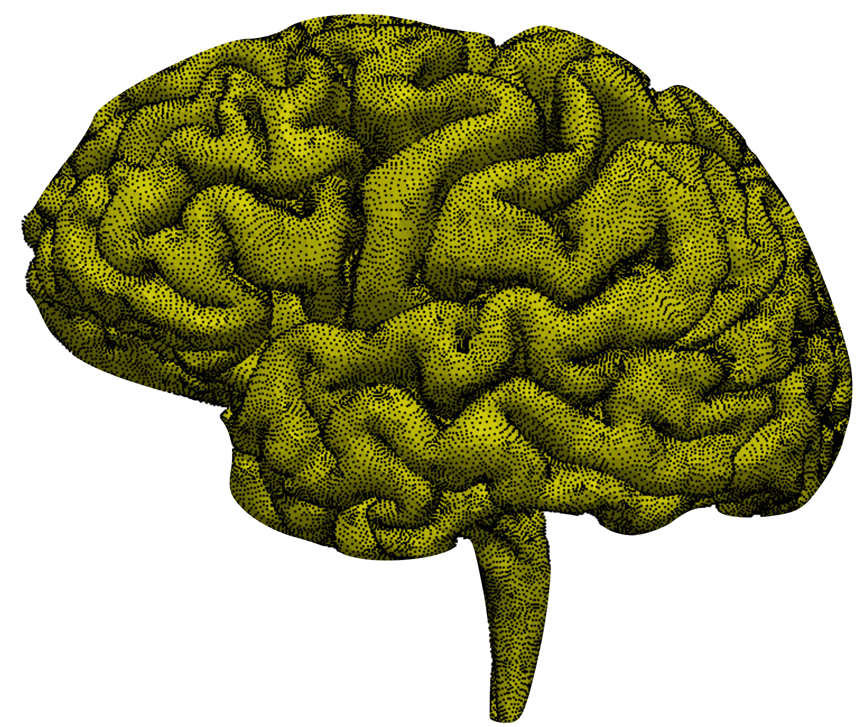
Mathematical Modelling





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

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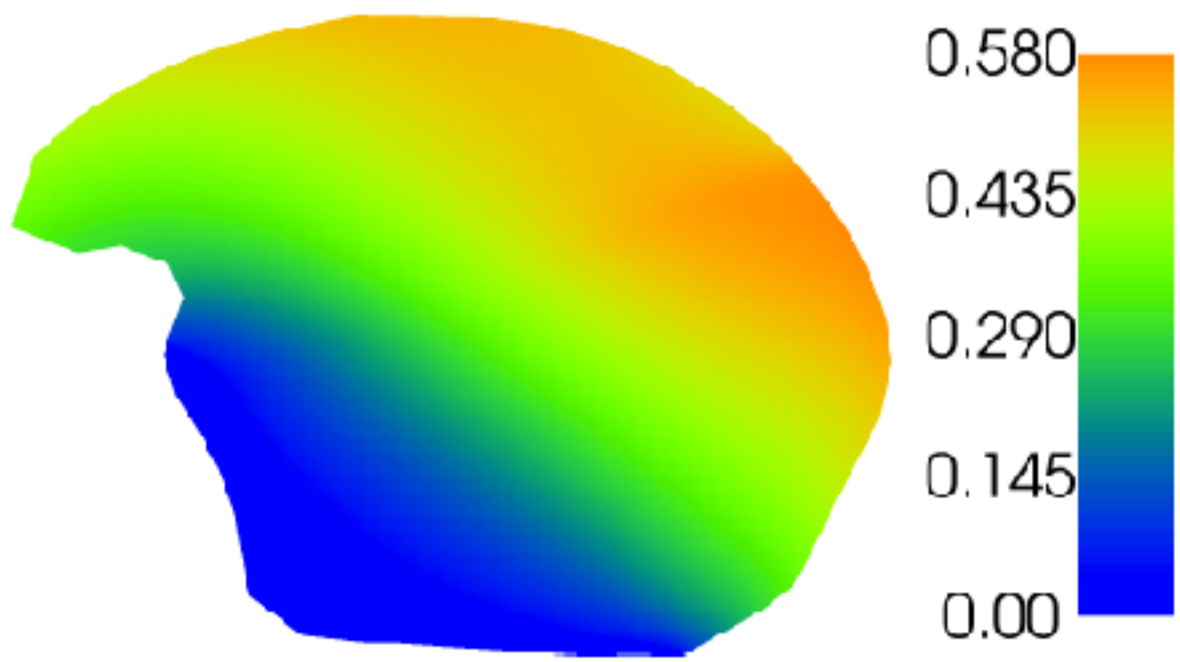
Mathematical Model

↓

Discrete Problem

↓

Numerical Solution



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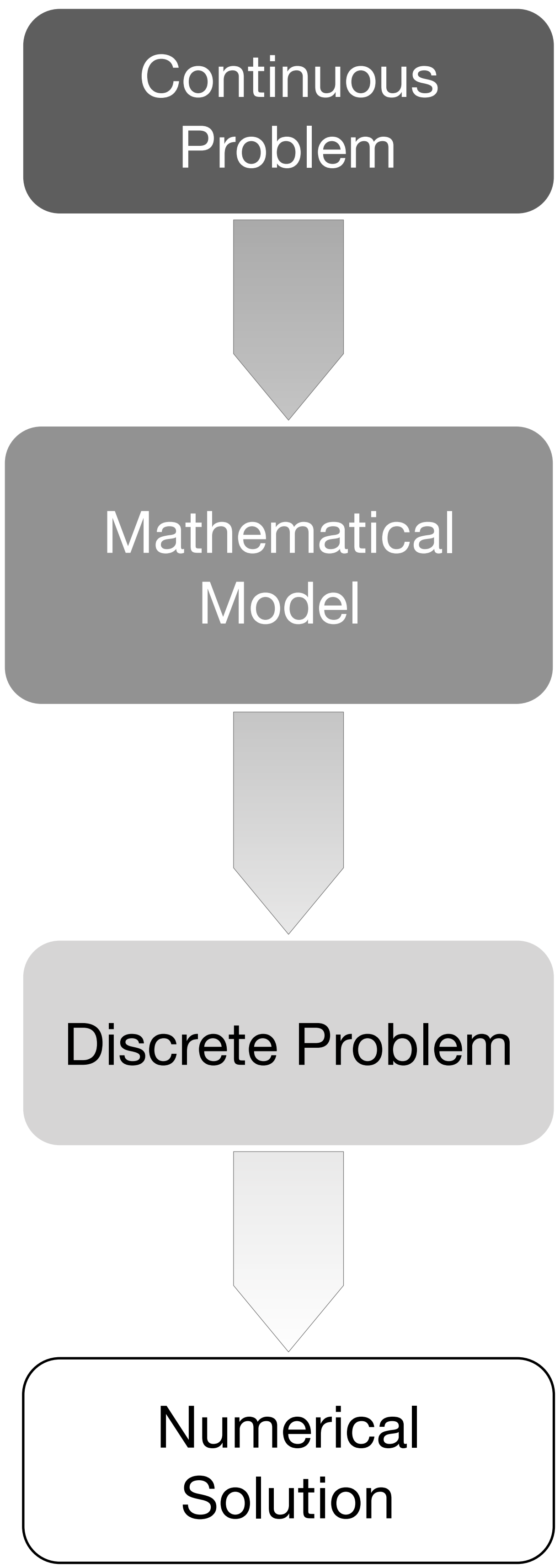
Mathematical Modelling



Mathematical Modelling

Continuous Problem

↓

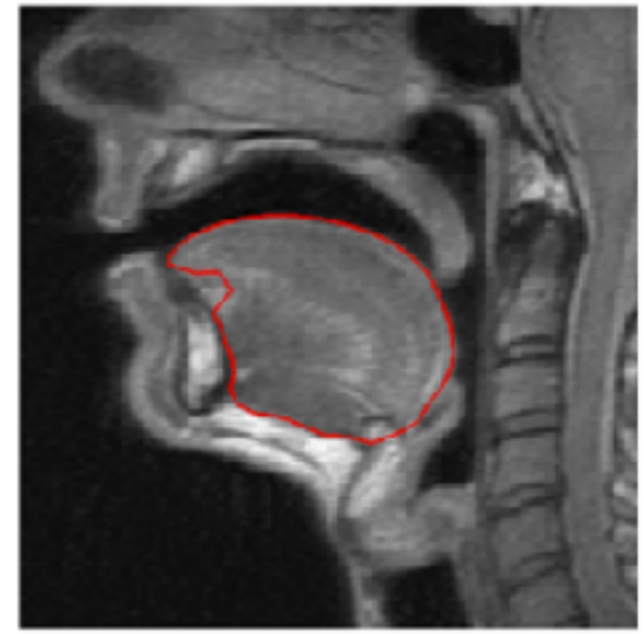
Mathematical Model

↓

Discrete Problem

↓

Numerical Solution



Bijar, Rohan, Perrier & Payan 2015

$$\neq$$

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

Mathematical Modelling

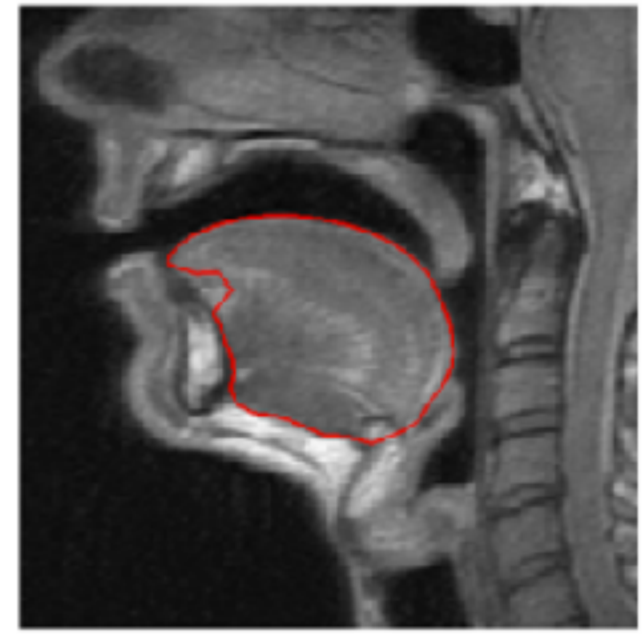
Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error



Bijar, Rohan, Perrier & Payan 2015

$$\neq$$

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

Physical Problem
Constitutive Model
Material Parameters

Mathematical Modelling

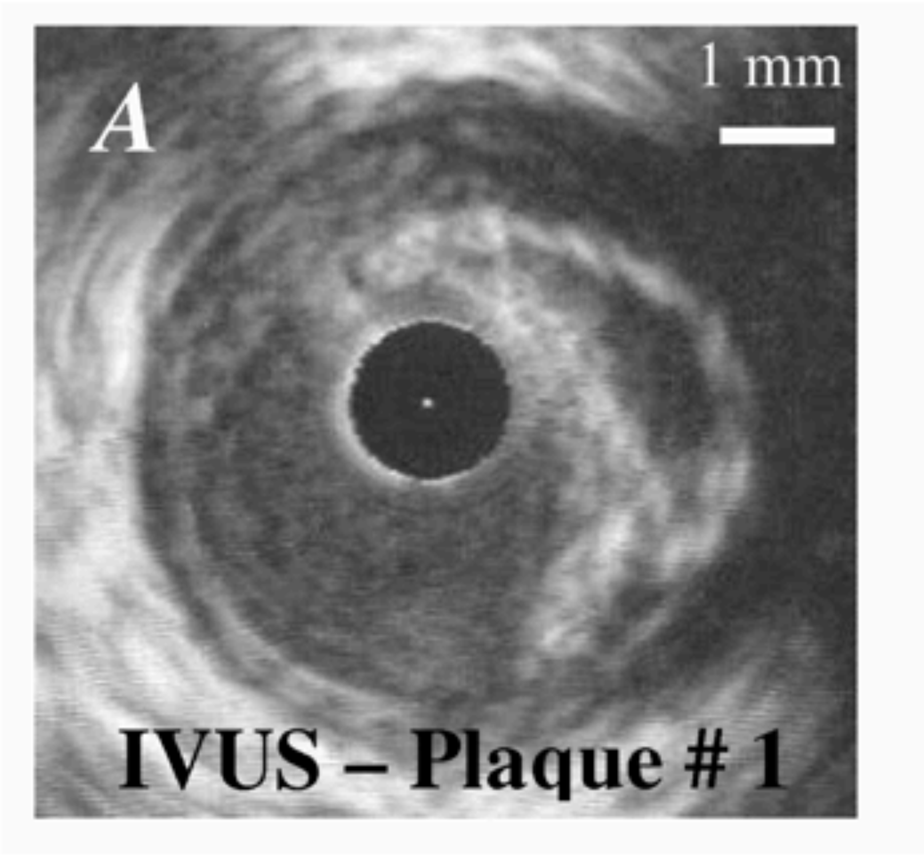
Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error



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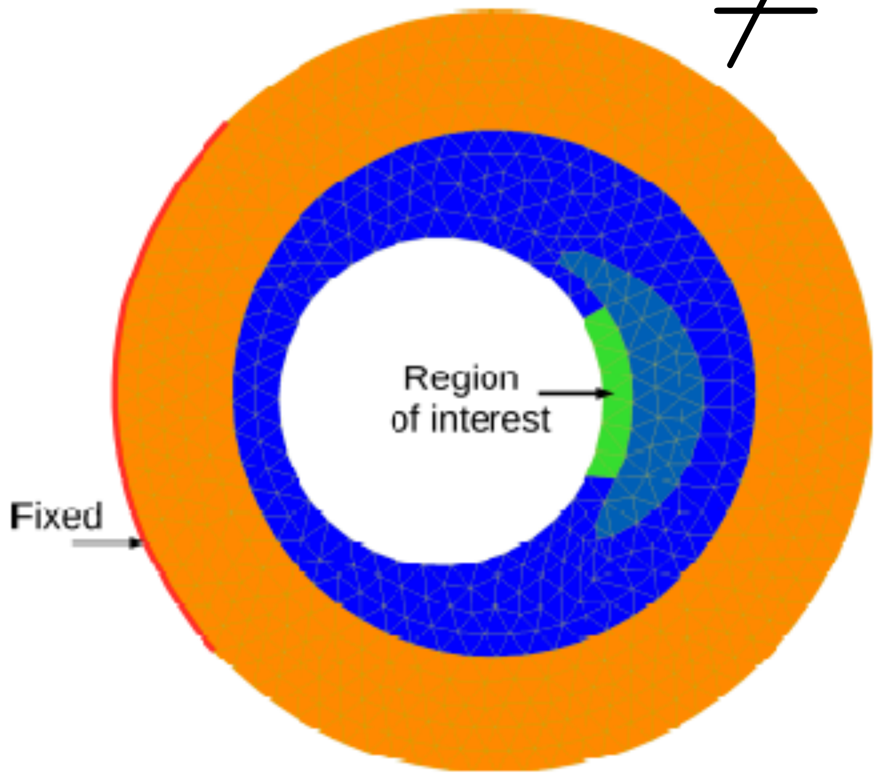


Geometry
Boundary conditions

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

Mathematical Modelling

Continuous Problem

↓

Mathematical Model

↓

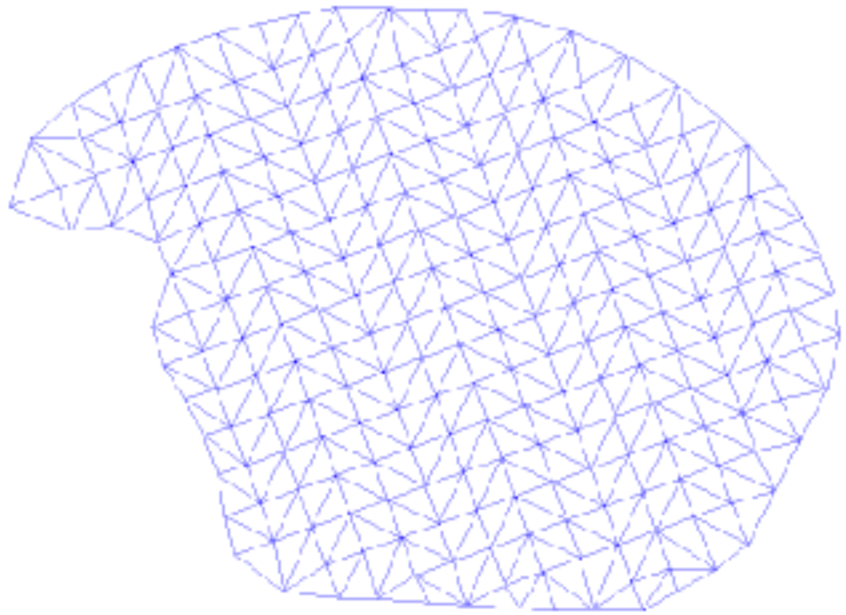
Discrete Problem

↓

Numerical Solution

Model Error

Discretization Error



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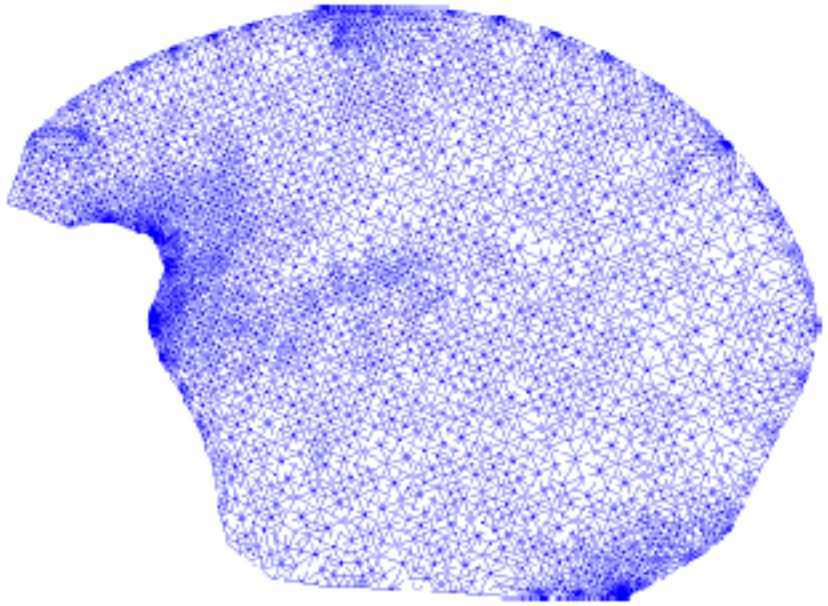

Mathematical Modelling

Continuous Problem

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Mathematical Model

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Discrete Problem

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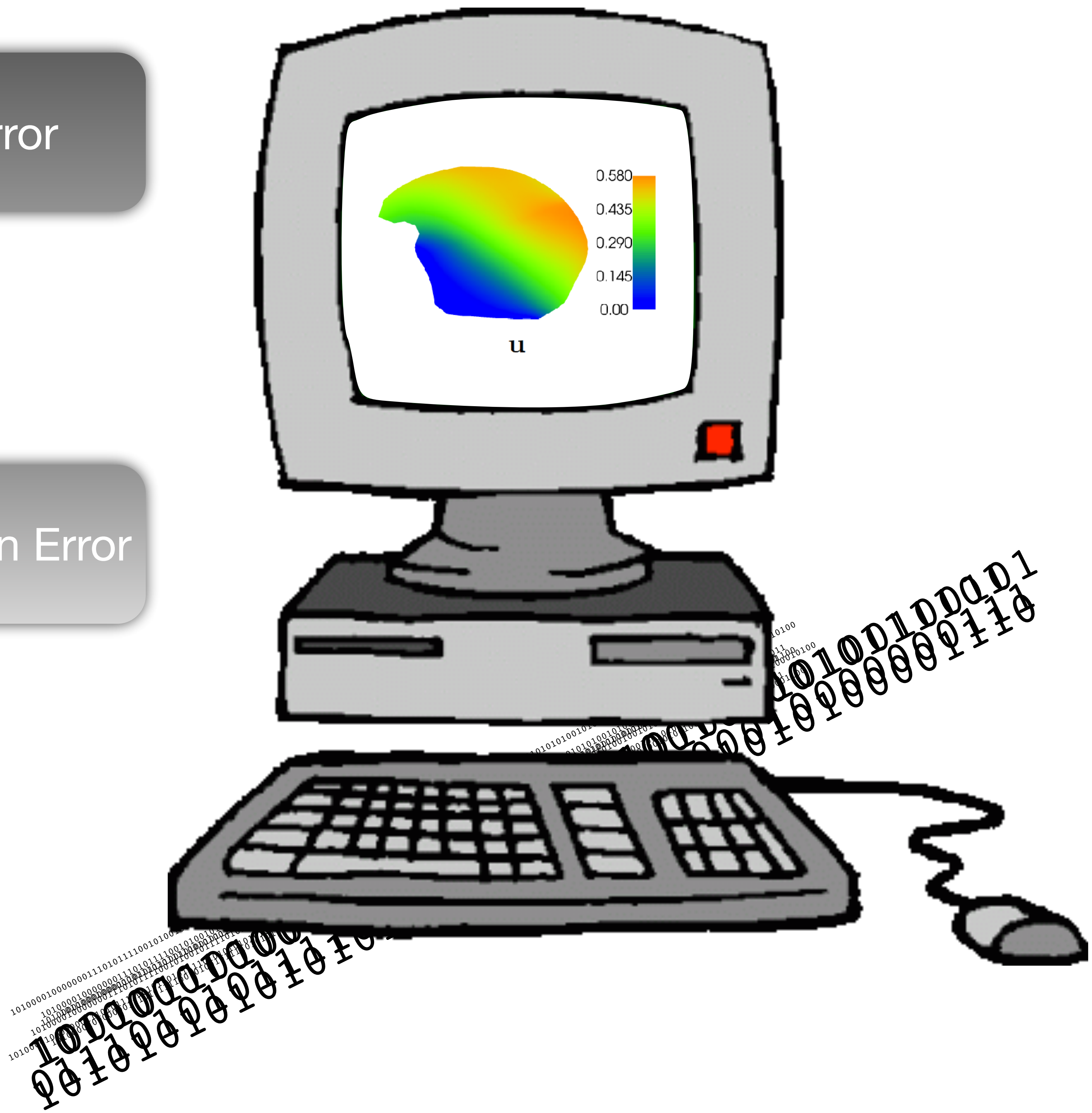
Model Error

Discretization Error



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

Mathematical Modelling

32 bit?

64 bit?

Continuous Problem

Mathematical Model

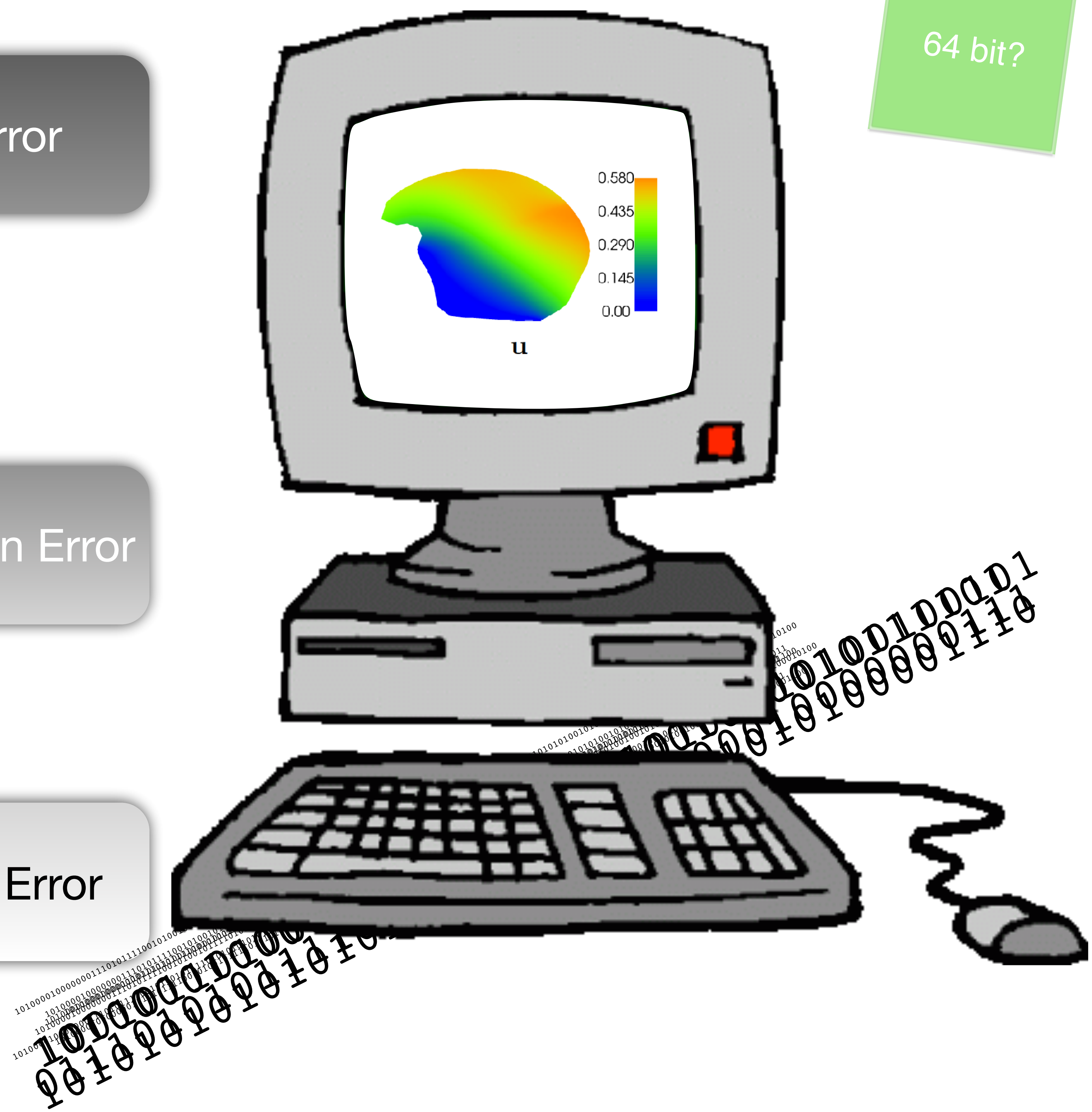
Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error



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

Mathematical Modelling

Continuous Problem

↓

Mathematical Model

↓

Discrete Problem

↓

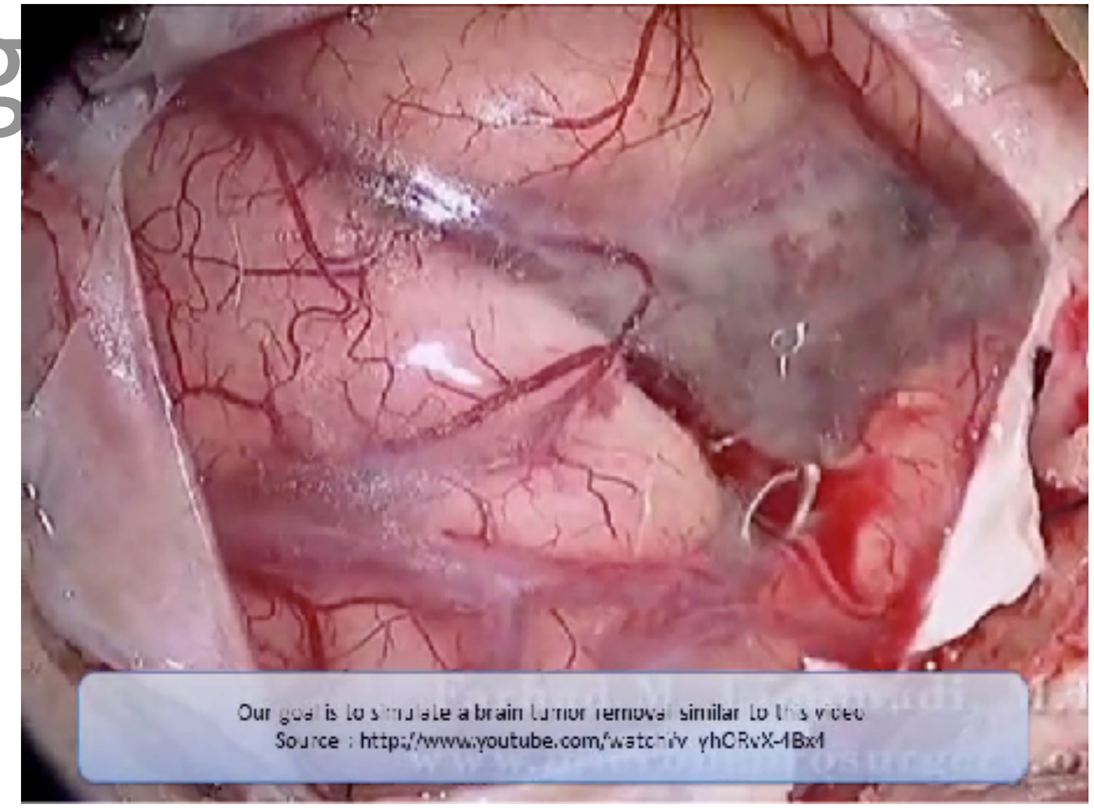
Numerical Solution

Model Error

Discretization Error

Numerical Error

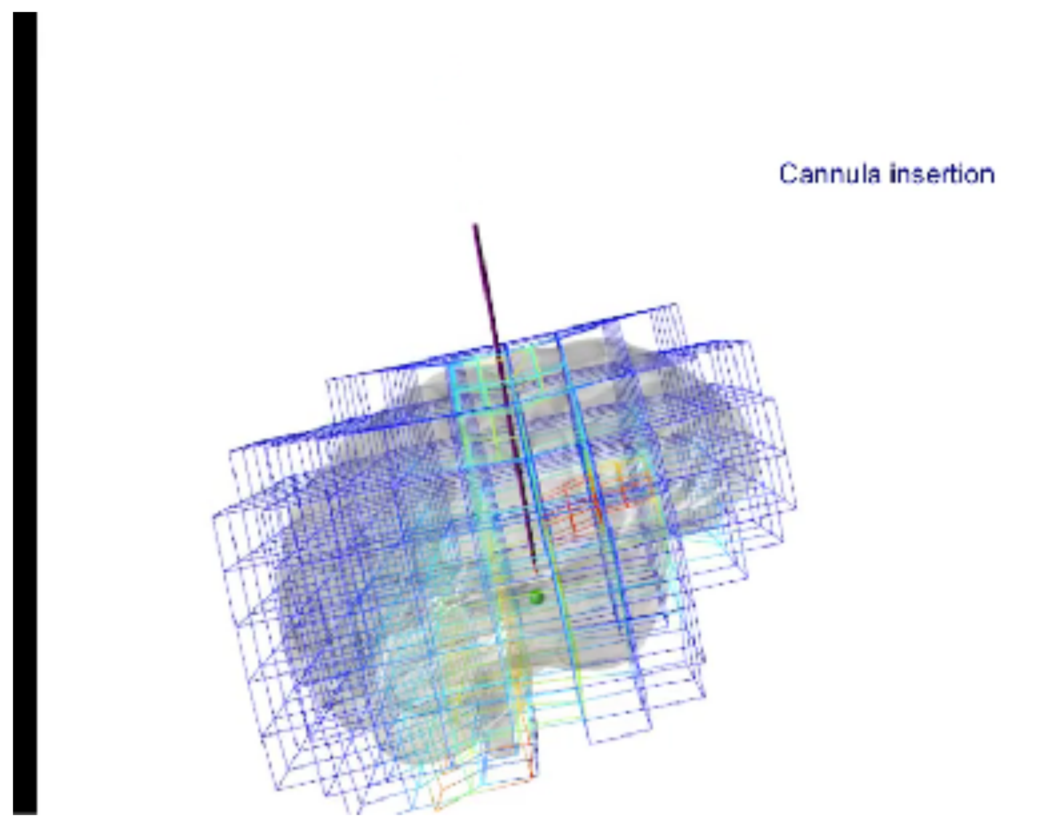
Total Error



Reality

vs.

Simulation



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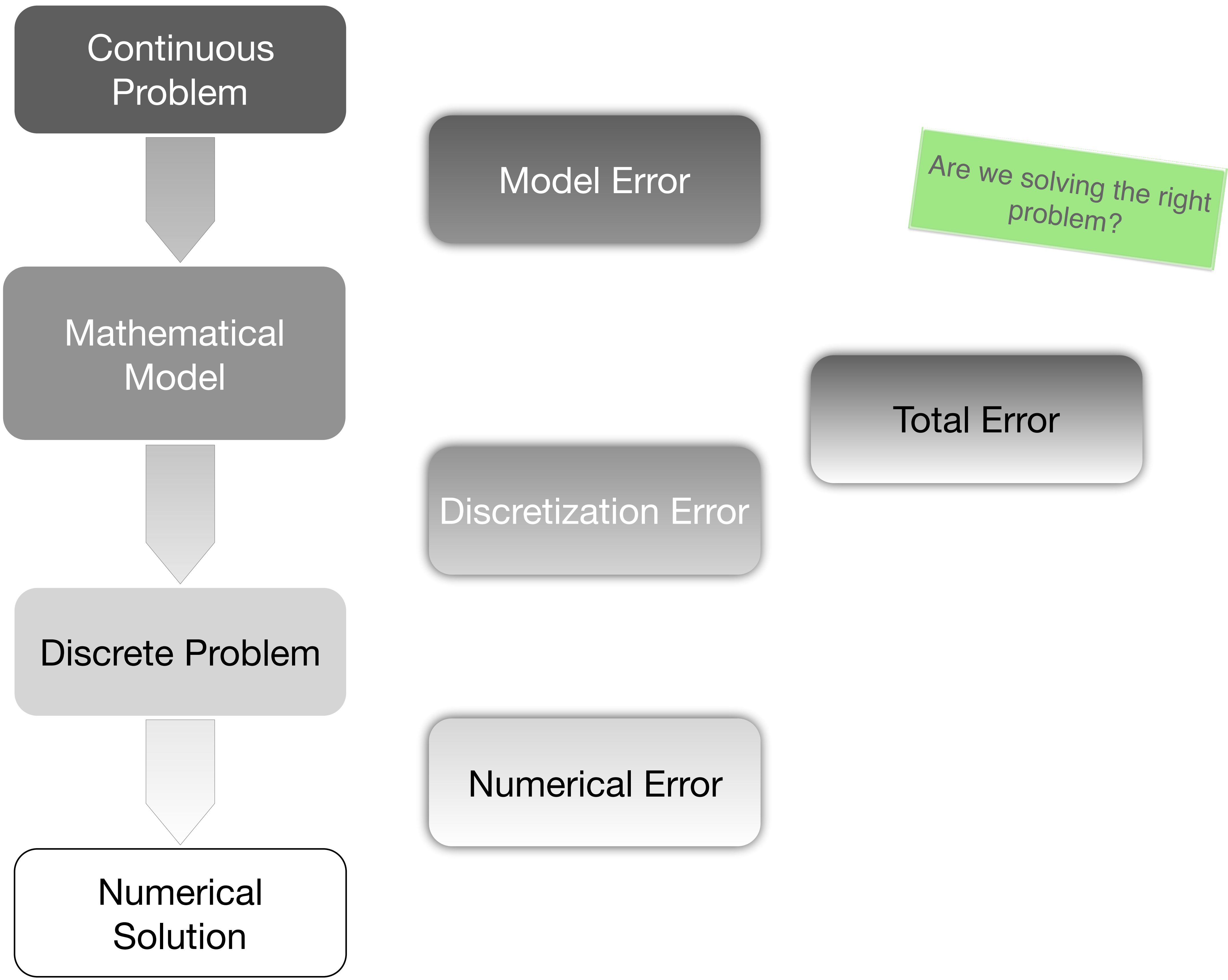
Mathematical Modelling



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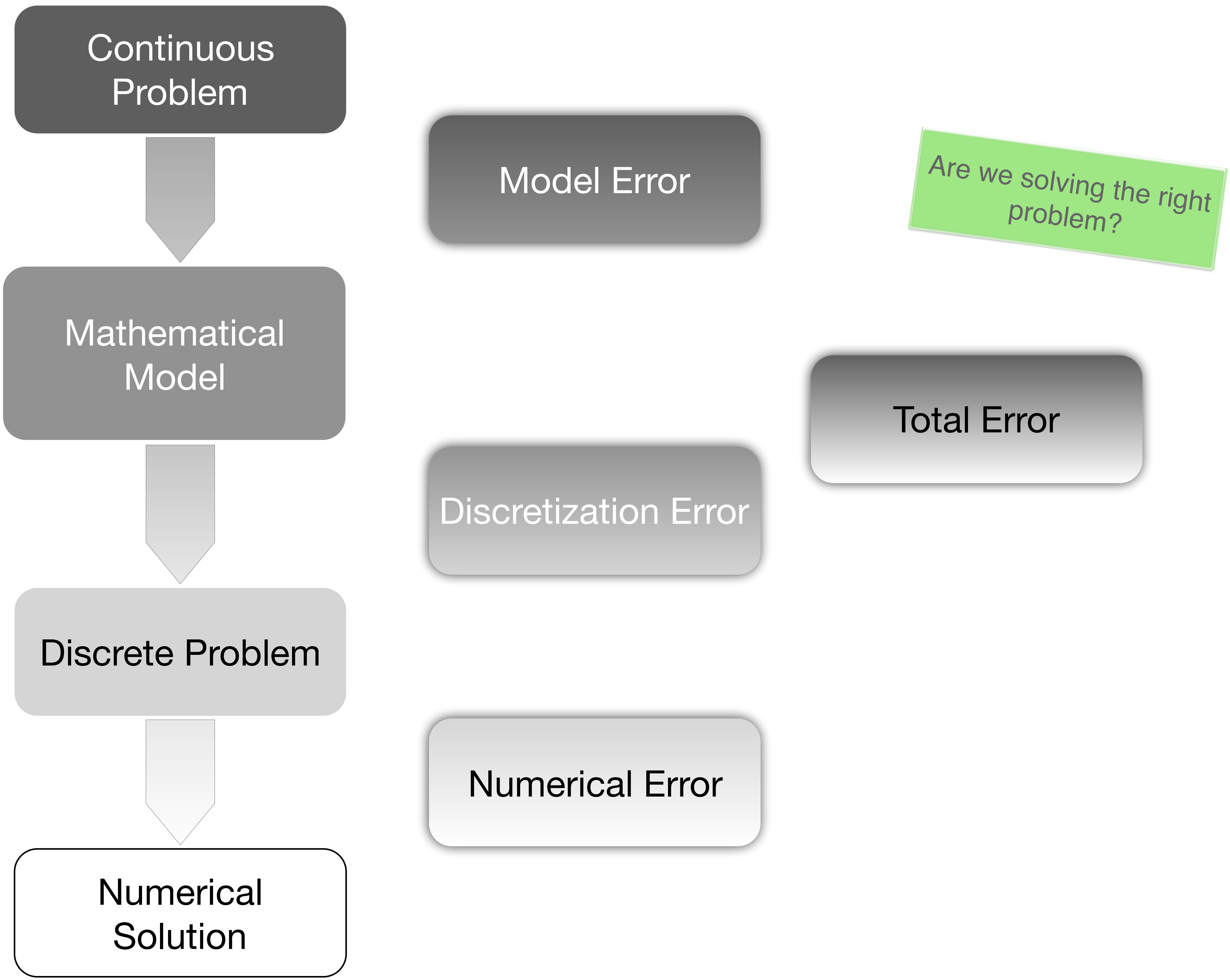
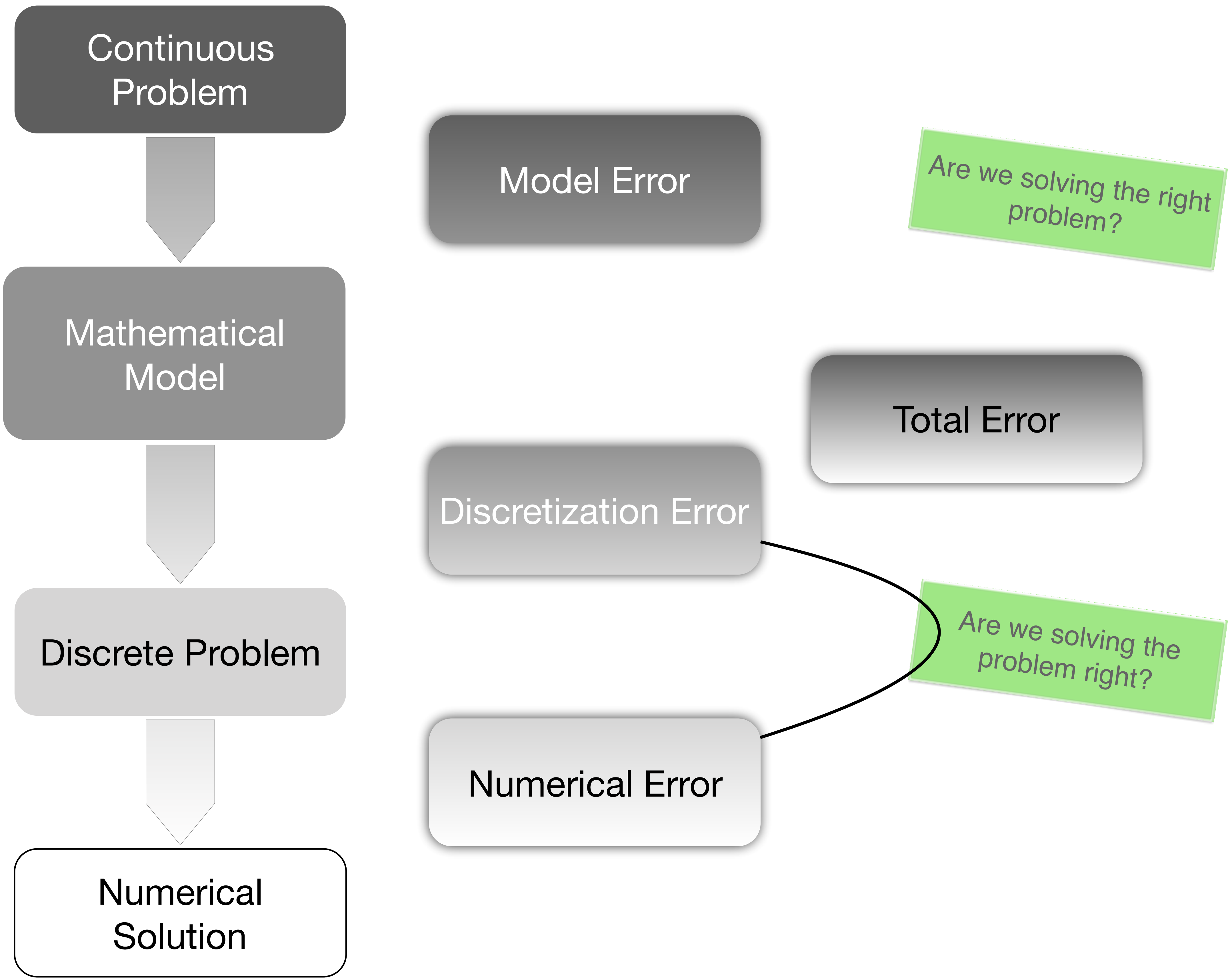
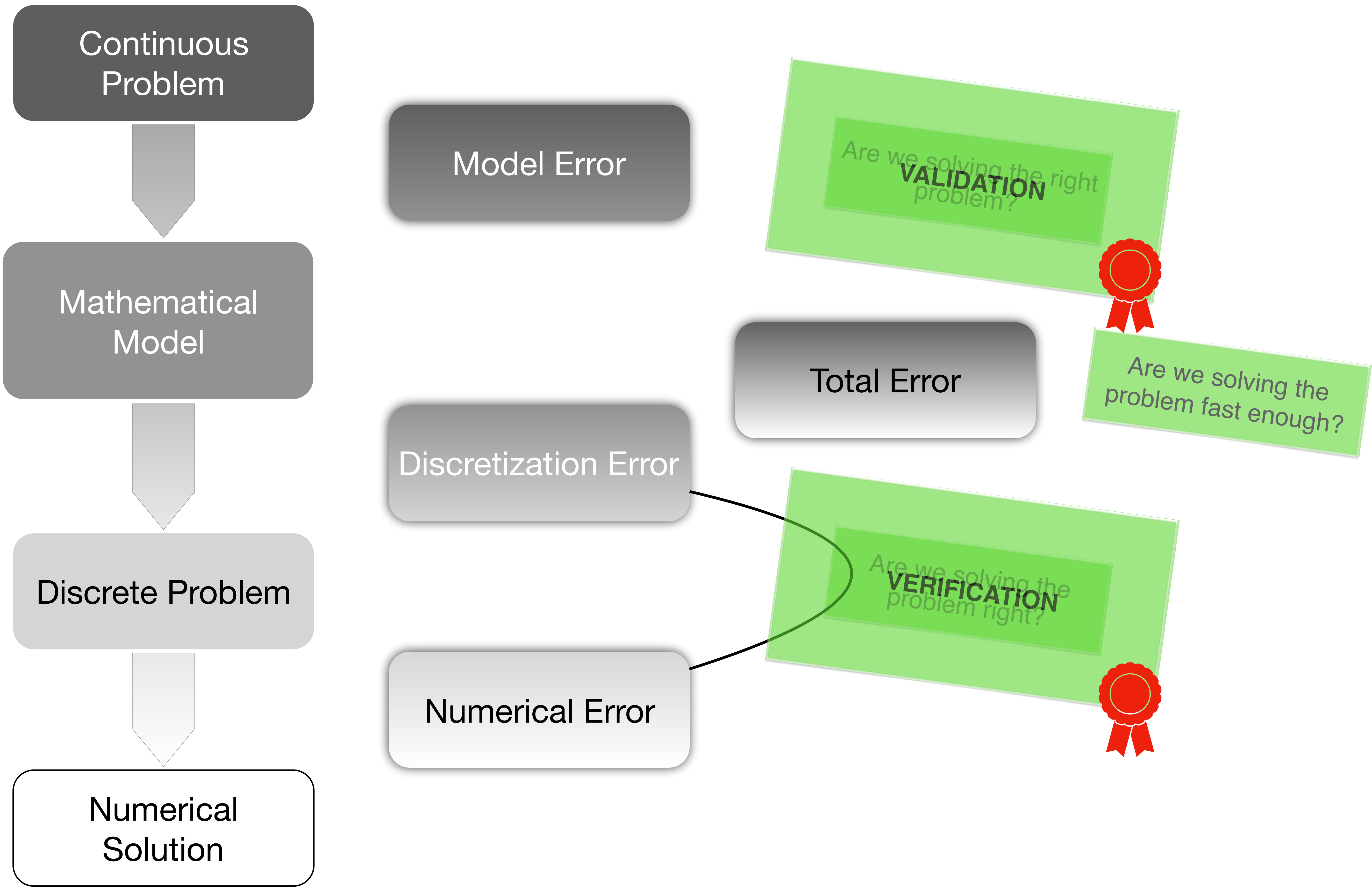
Mathematical Modelling



Mathematical Modelling

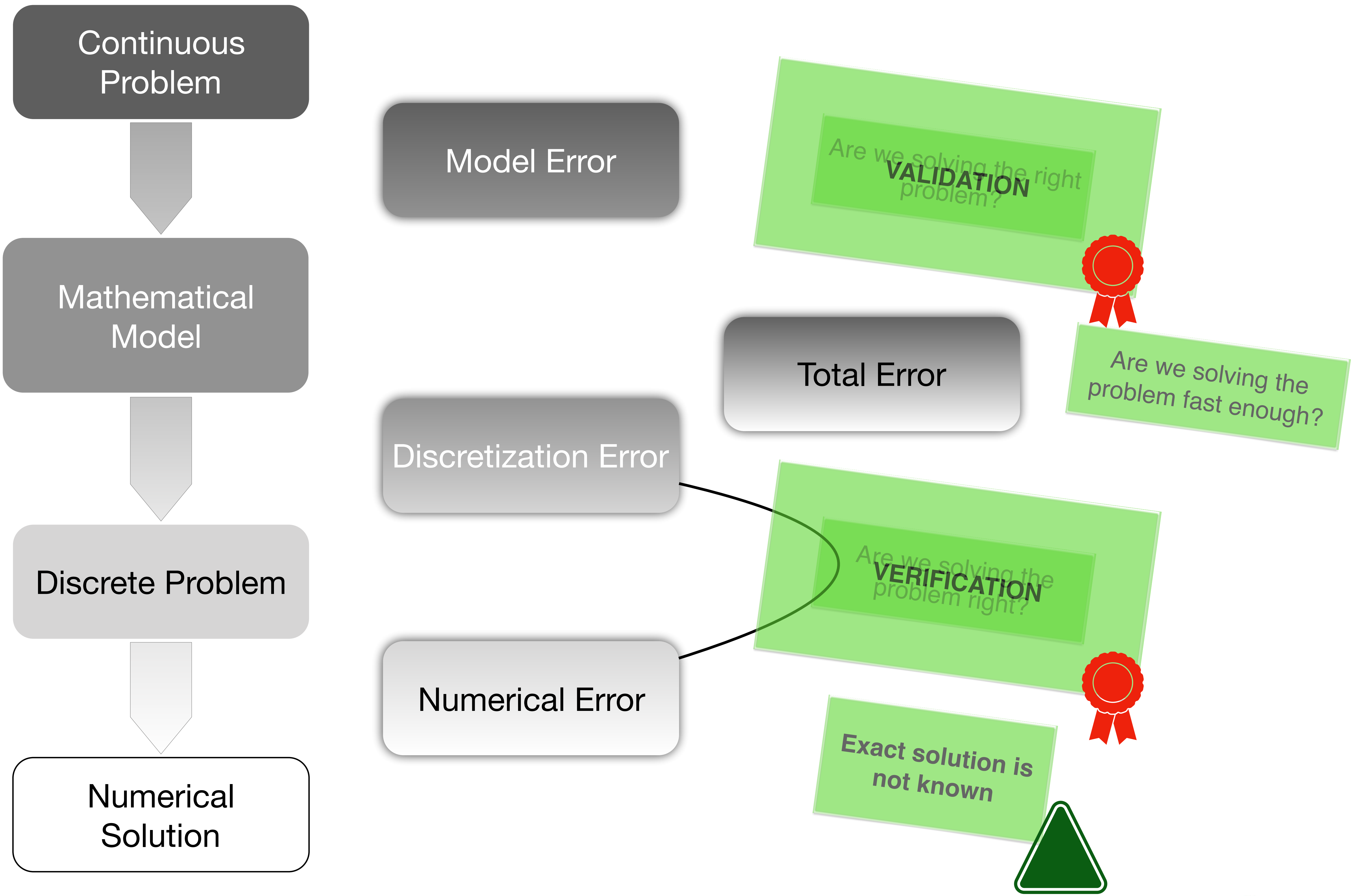


Mathematical Modelling



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

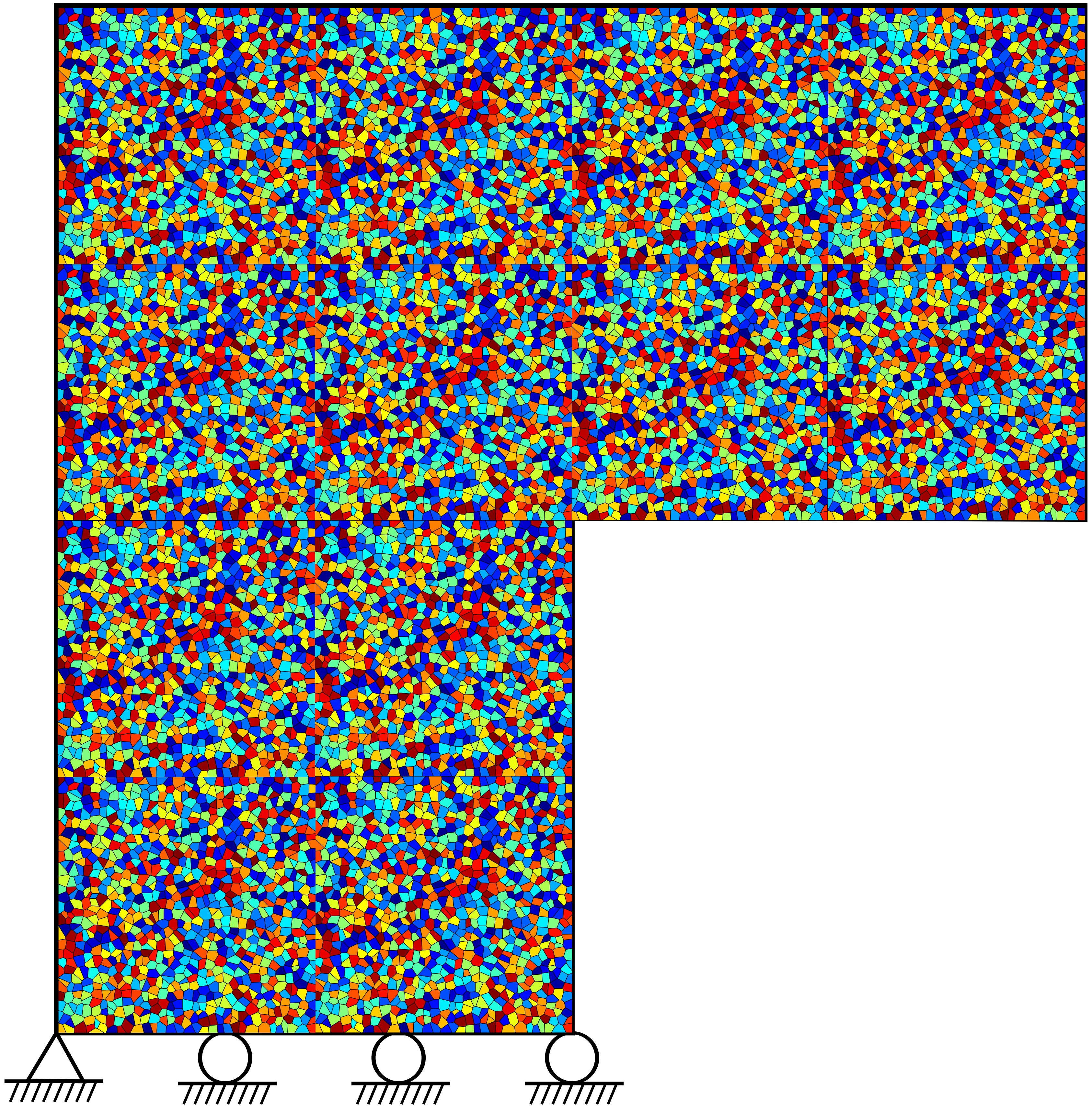
Mathematical Modelling

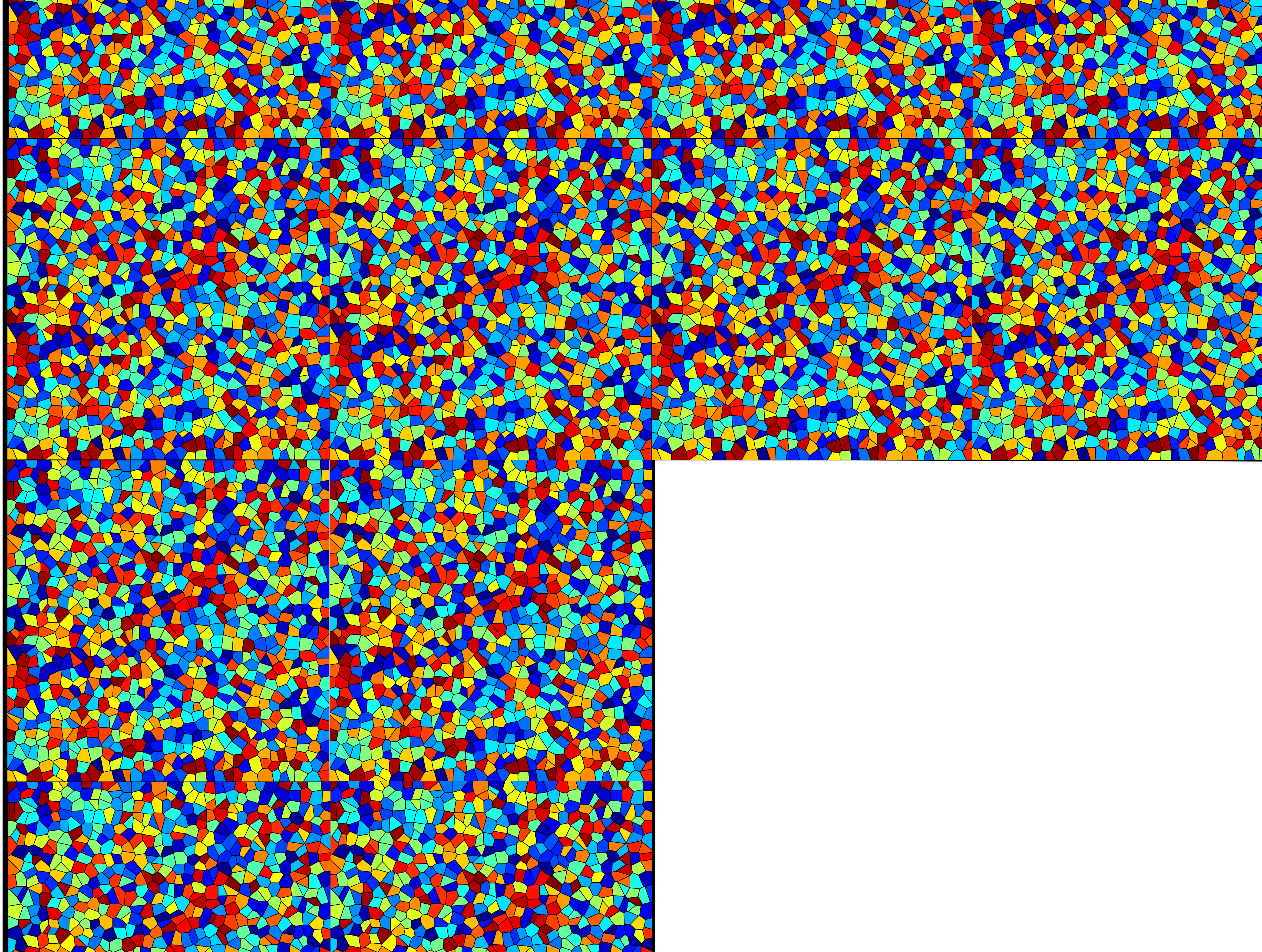


Physics-based model reduction methods

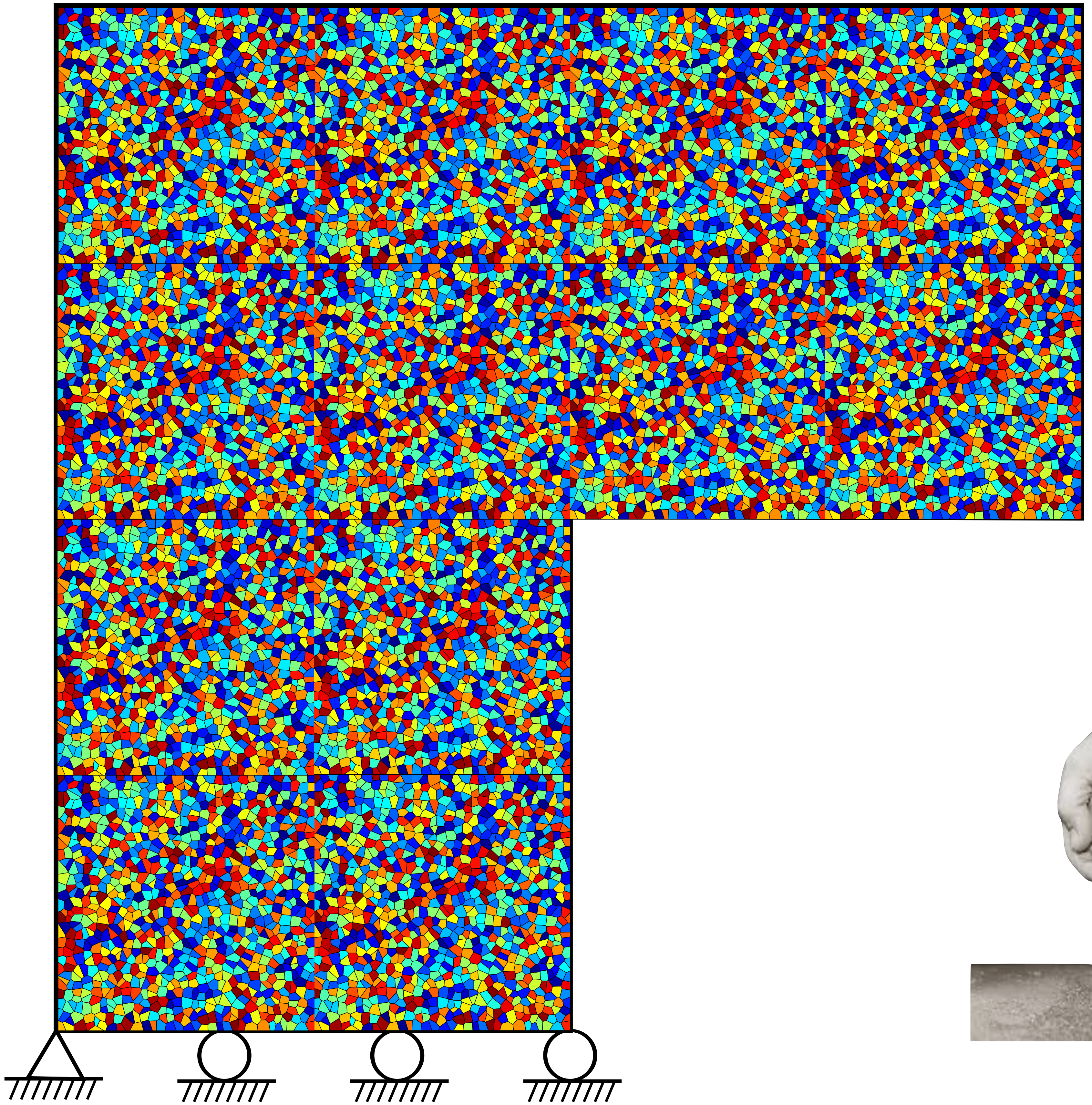
multi-scale methods

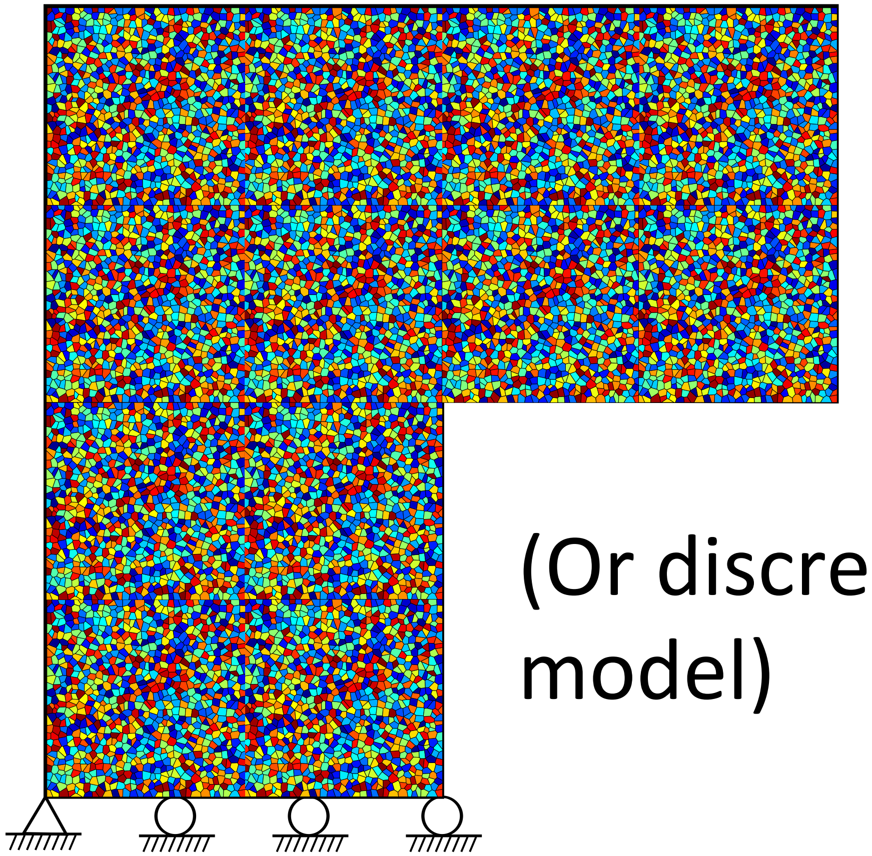
Full-scale





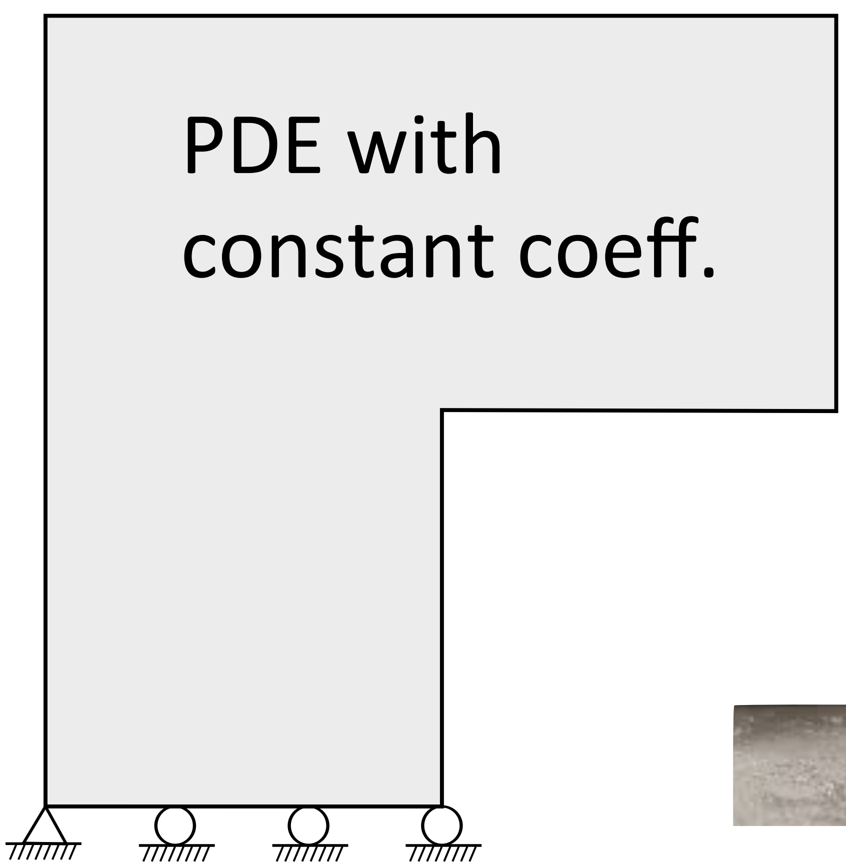
Full-scale





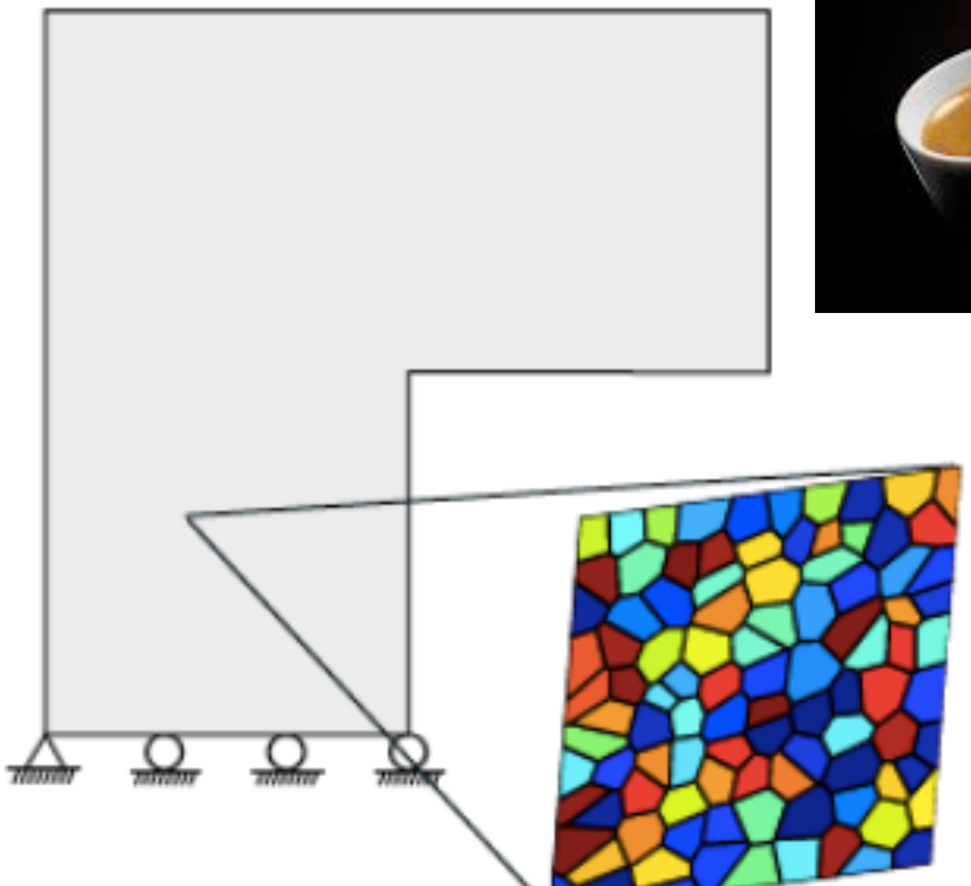
(Or discrete model)

↓ Homogenisation

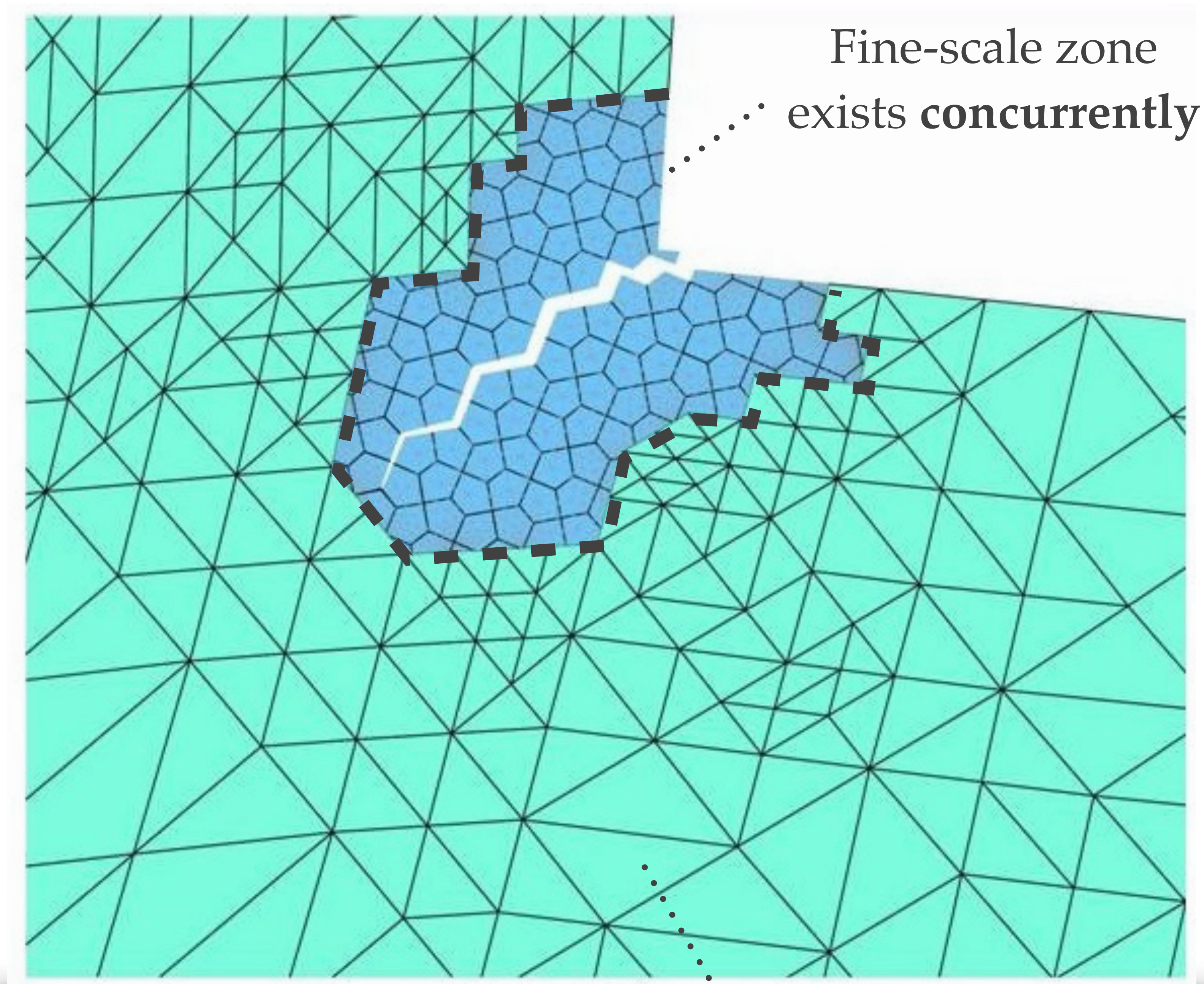


Multi-scale methods

Replace the heterogeneous fine-scale model by an equivalent smoother model at the scale where the predictions are required



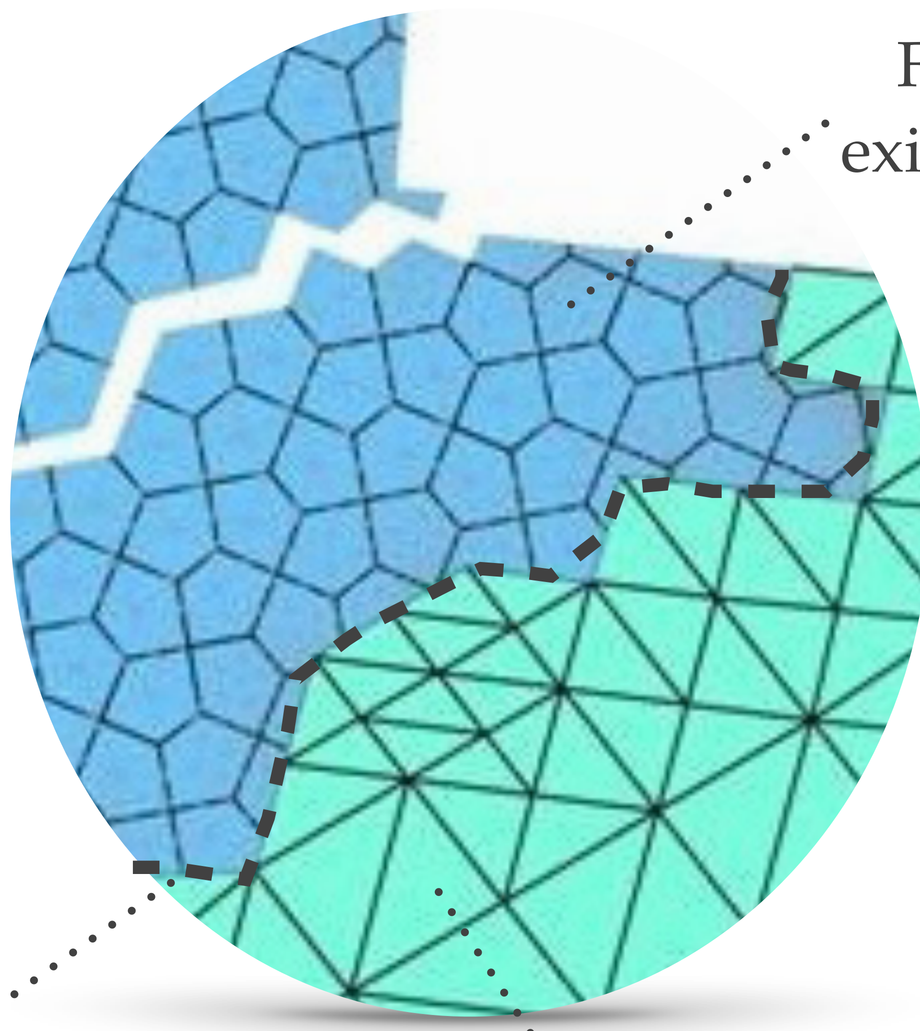
Concurrent methods



to the **coarse scale zone**

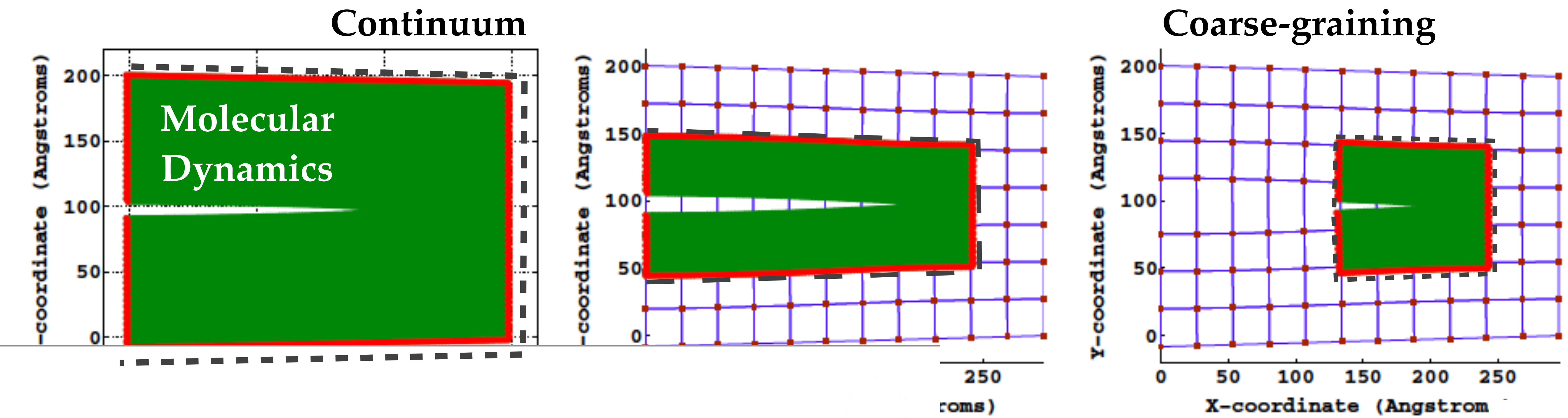
Akbari, Kerfriden, Bordas, 2014

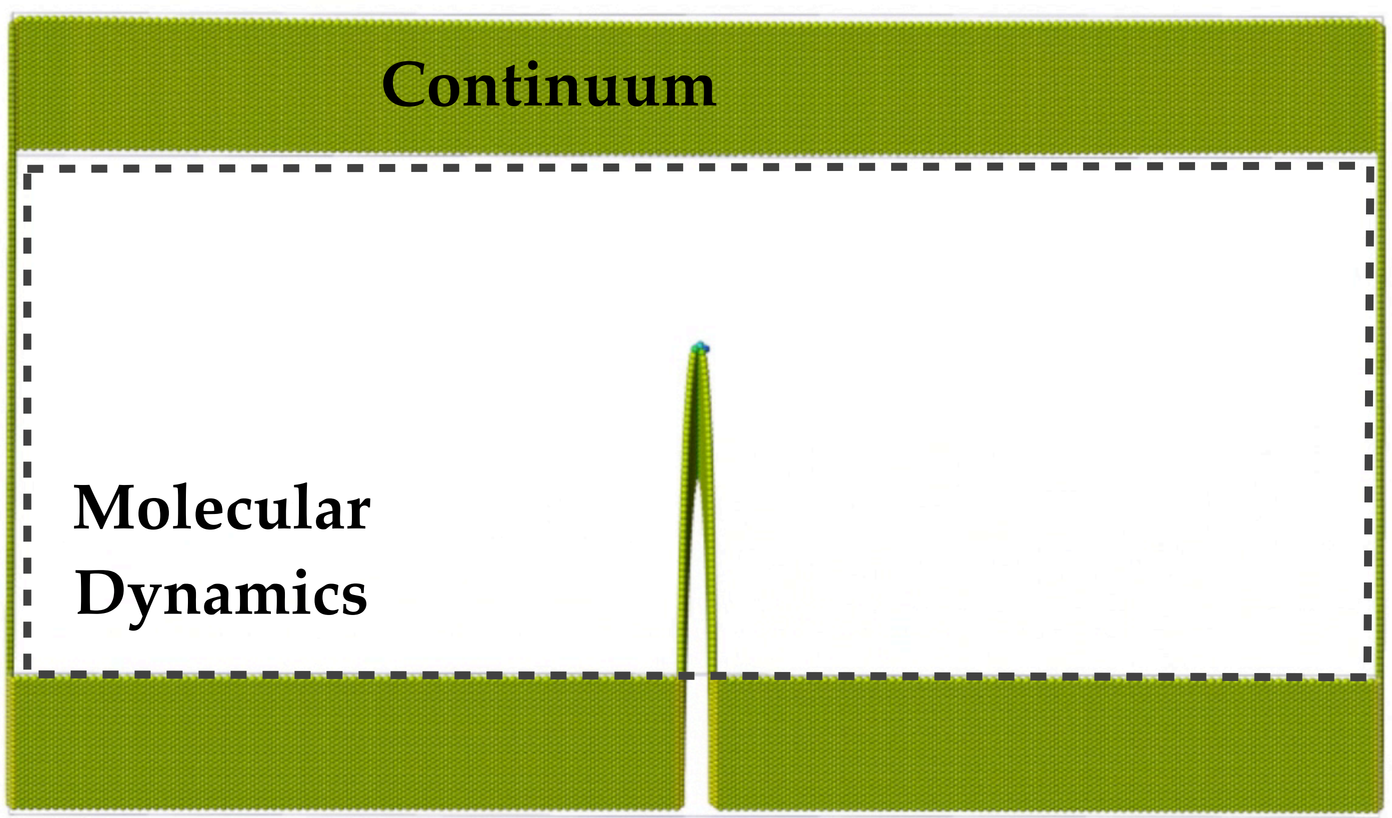
Concurrent methods

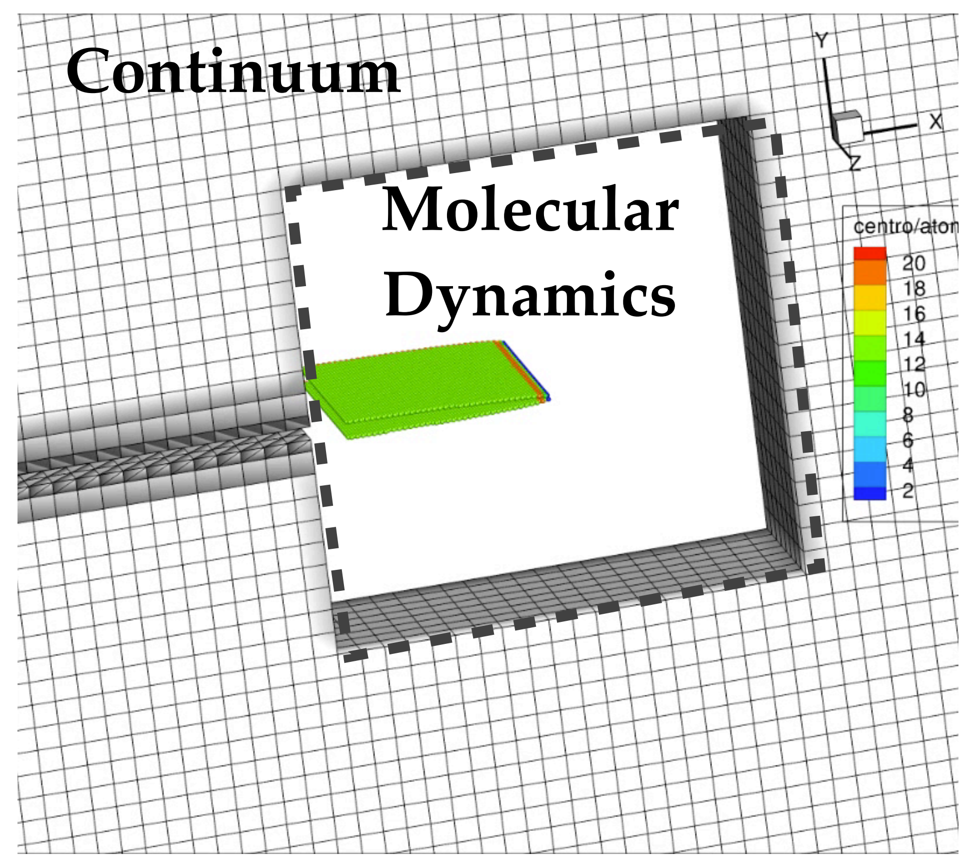


Akbari, Kerfriden, Bordas, 2014

Concurrent methods

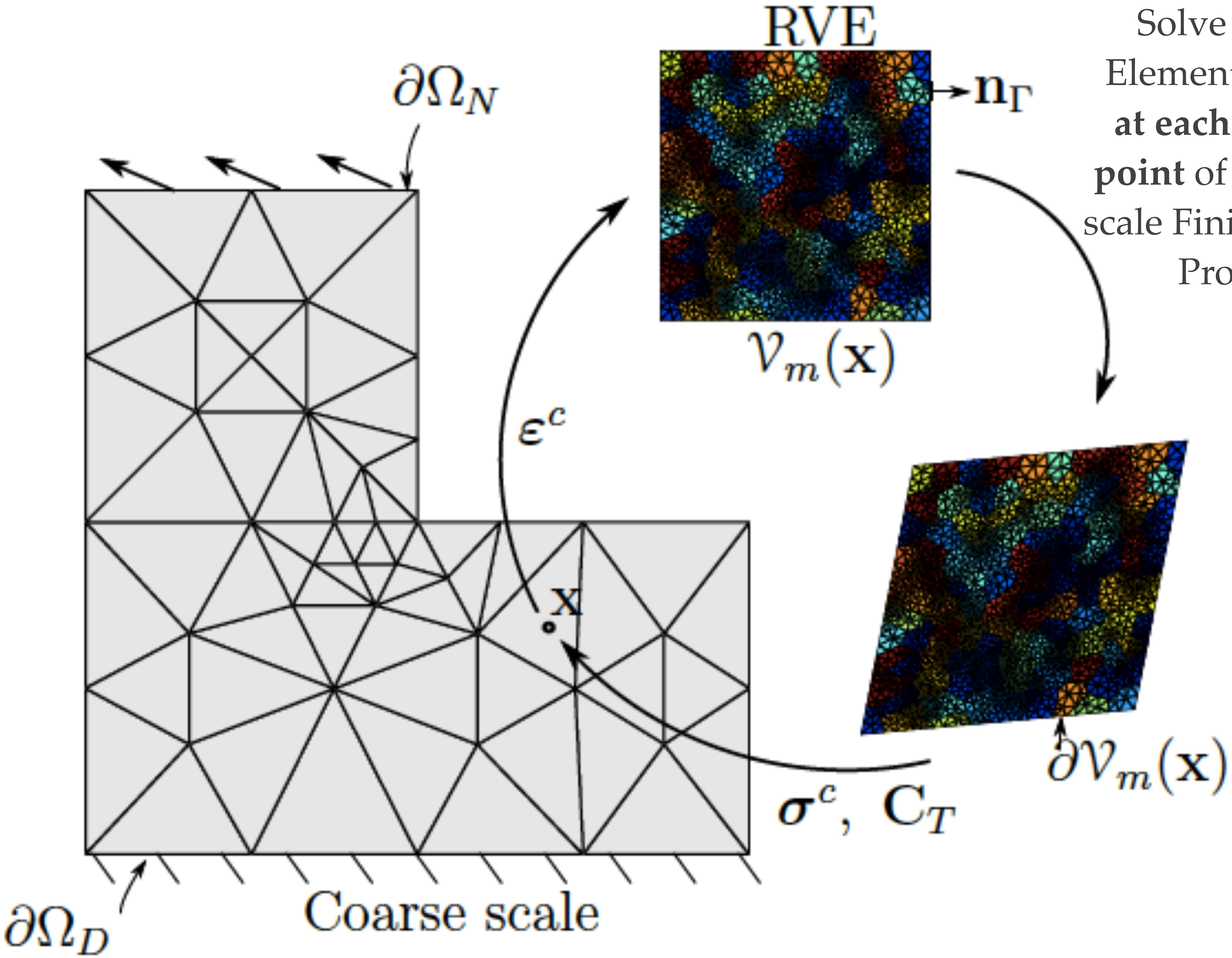






Talebi, Ramaia, Rabczuk, Bordas, Kerfriden, 2014

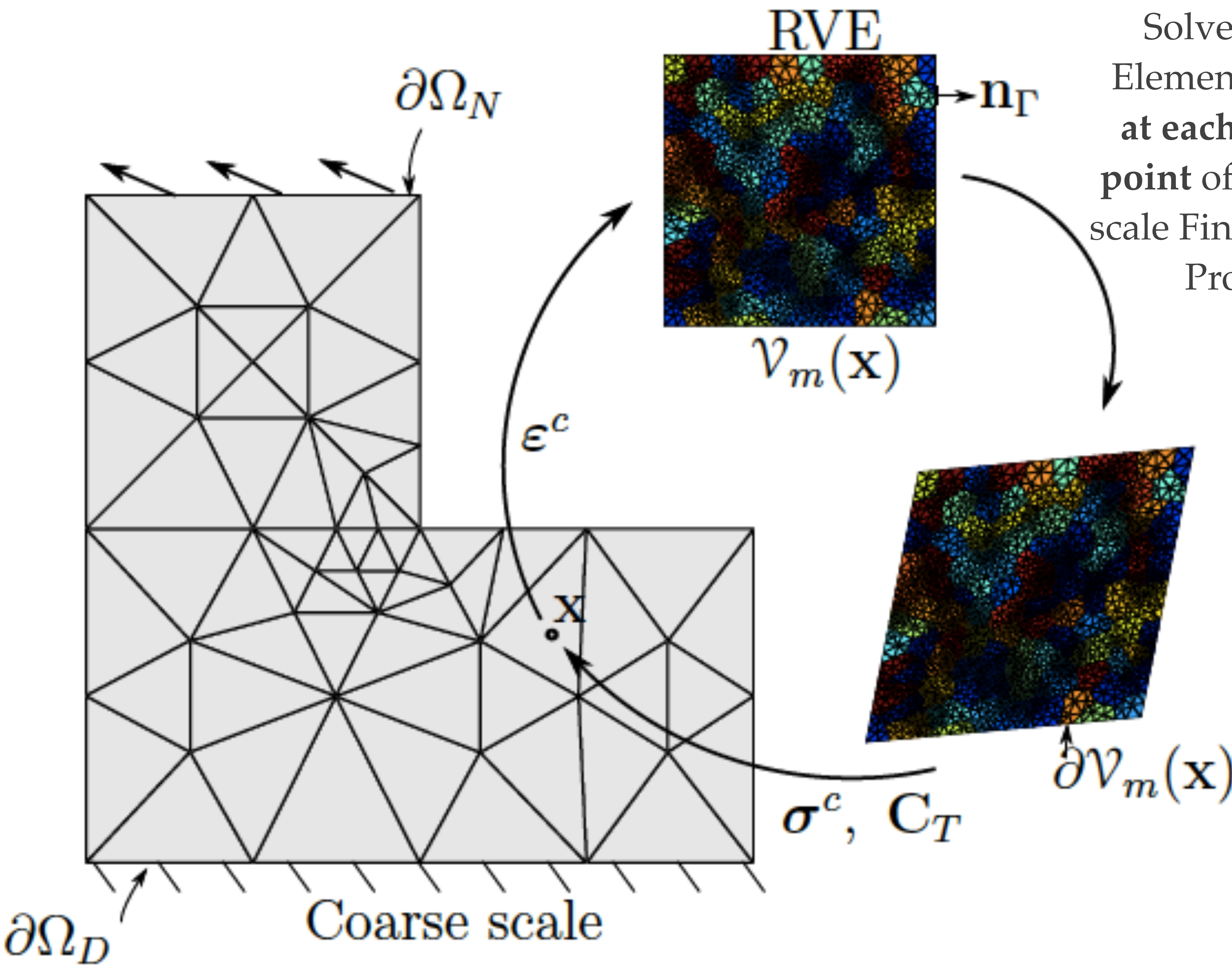
Hierarchical methods FE^2



Solve a Finite Element Problem **at each material point** of the coarse scale Finite Element Problem

Akbari, Kerfriden, Bordas, 2014

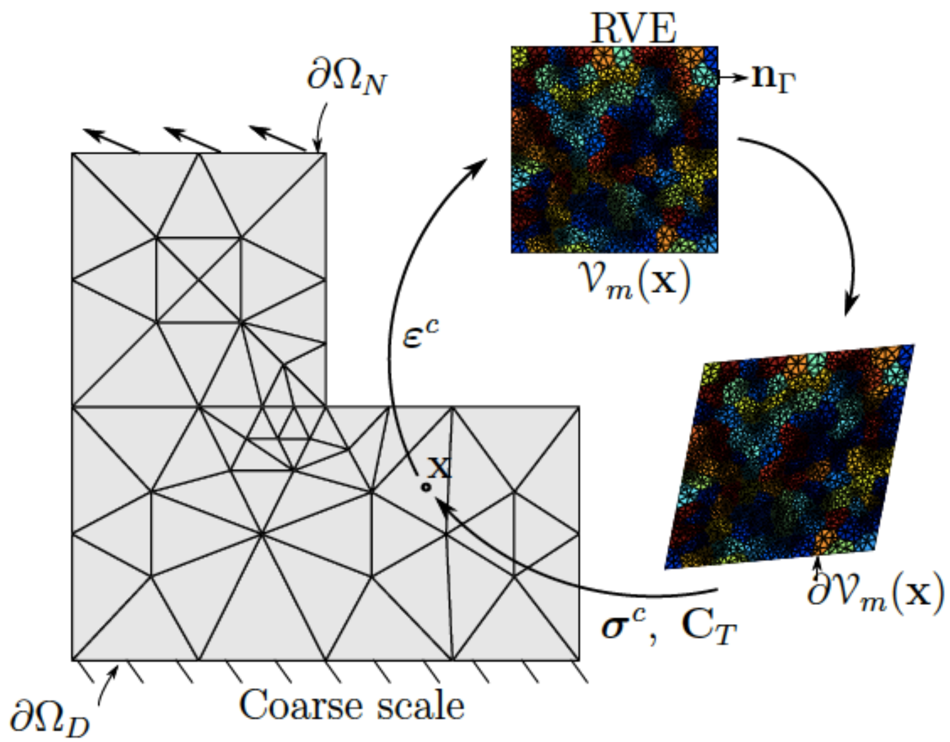
Hierarchical methods FE^2

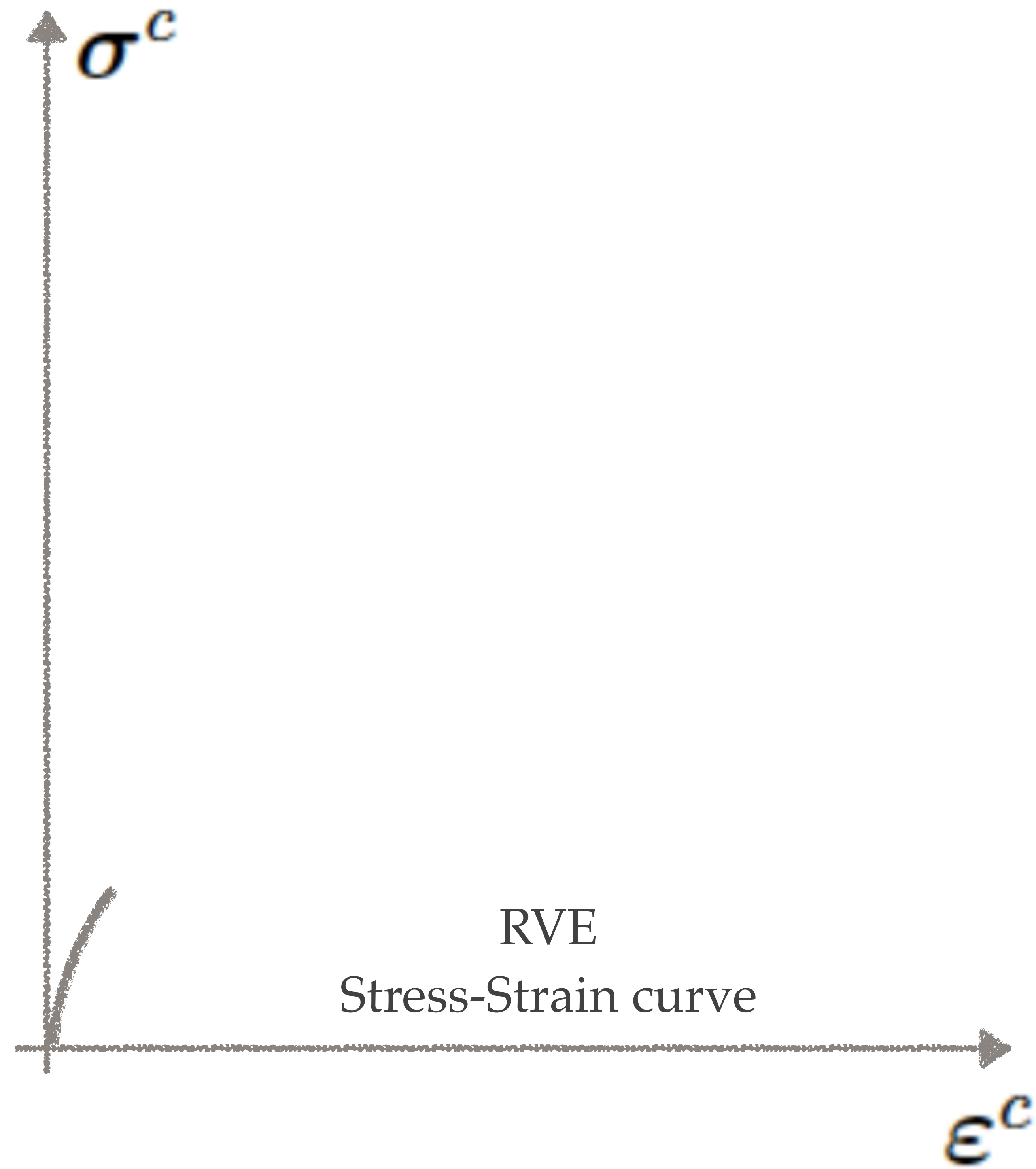


Solve a Finite Element Problem **at each material point** of the coarse scale Finite Element Problem

Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2

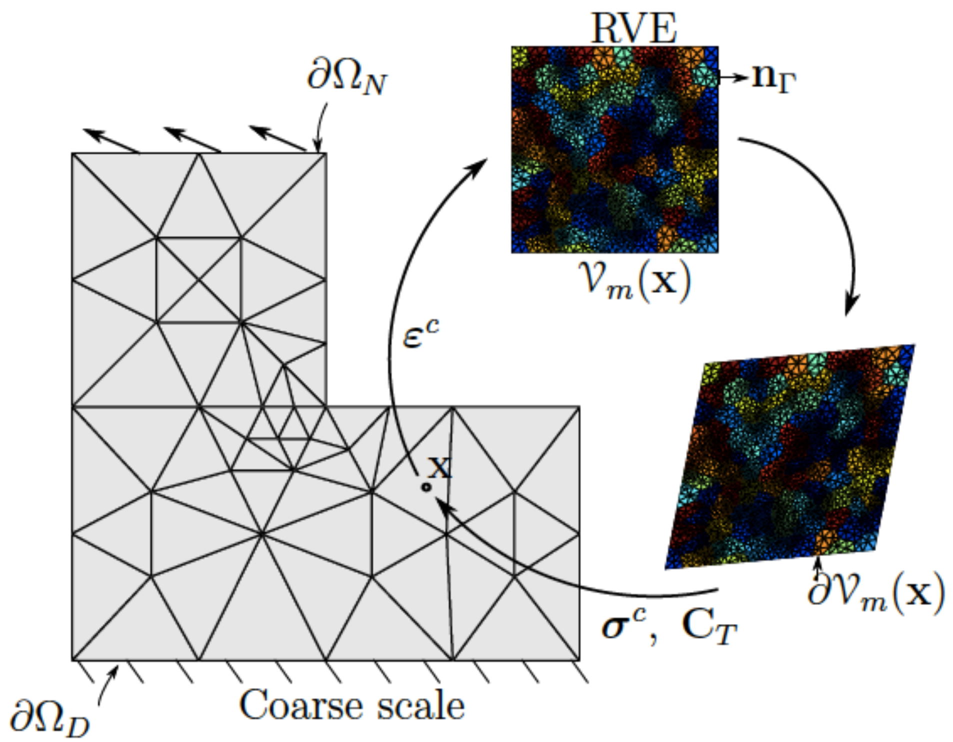


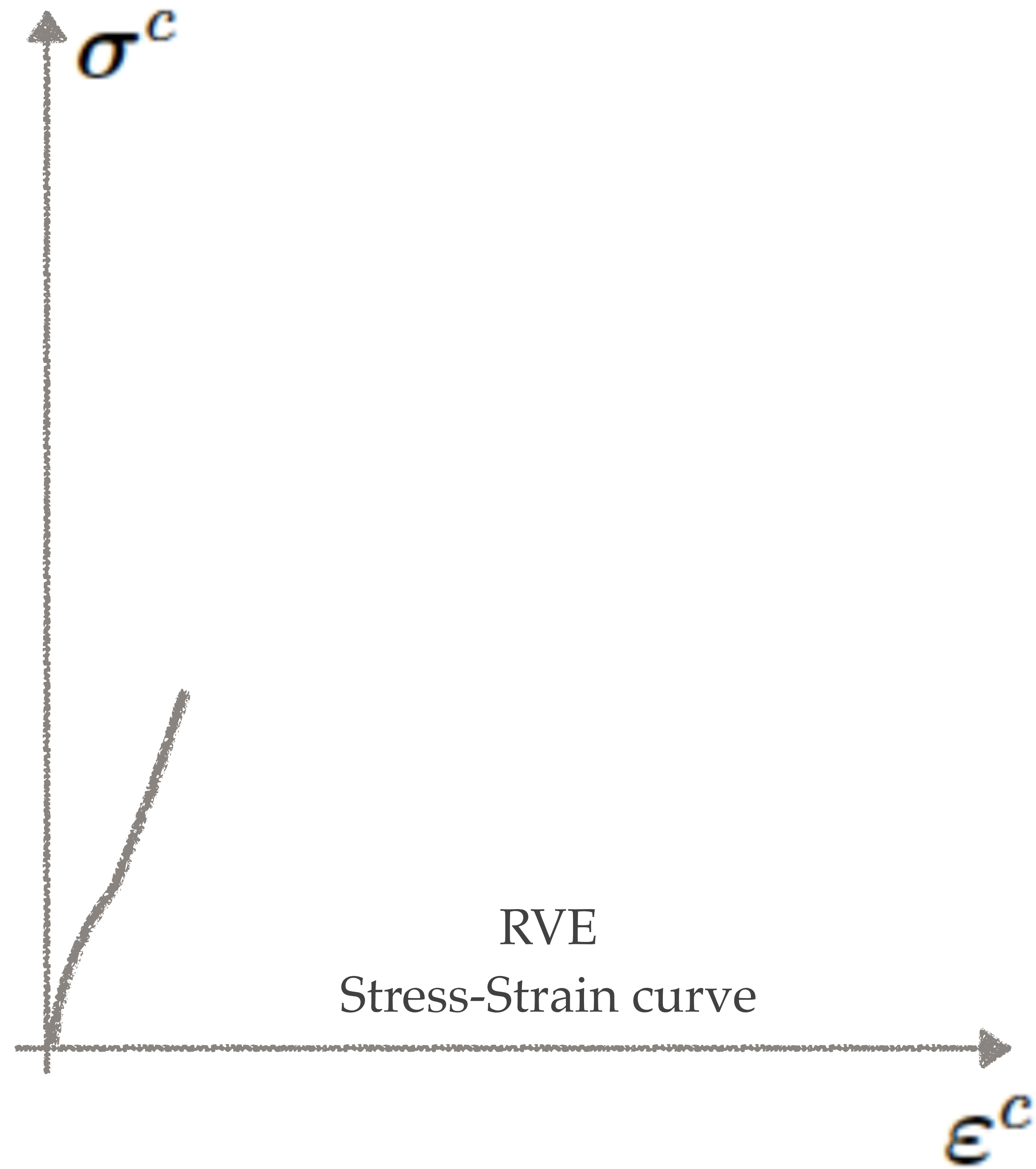


Loading

Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2

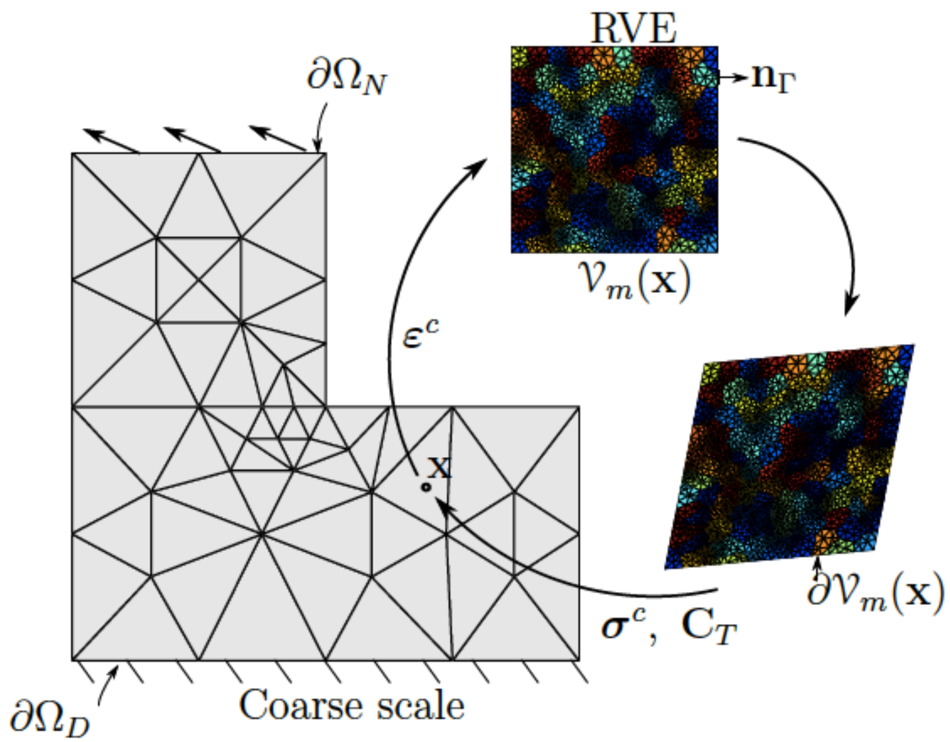




Loading

Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2



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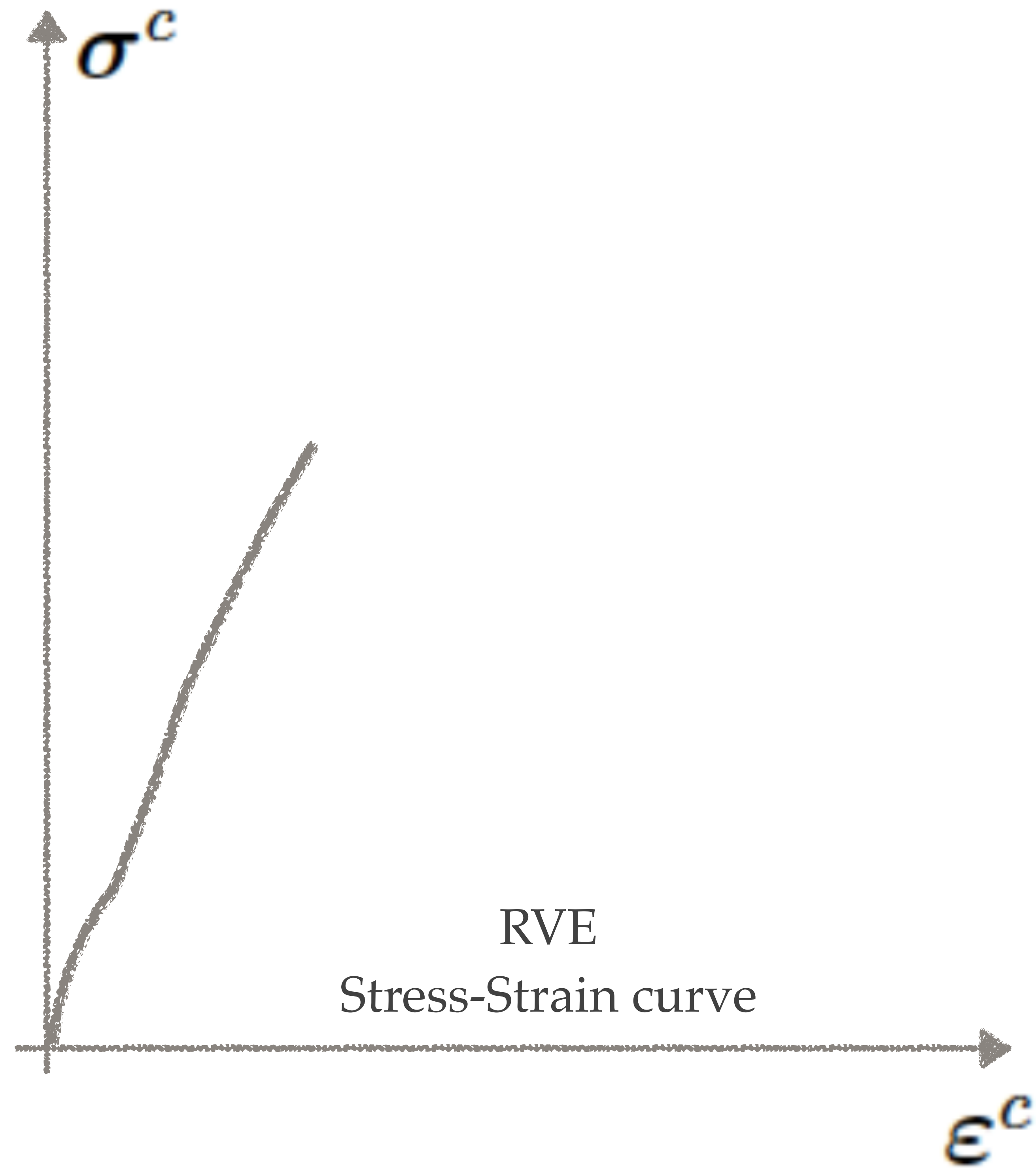
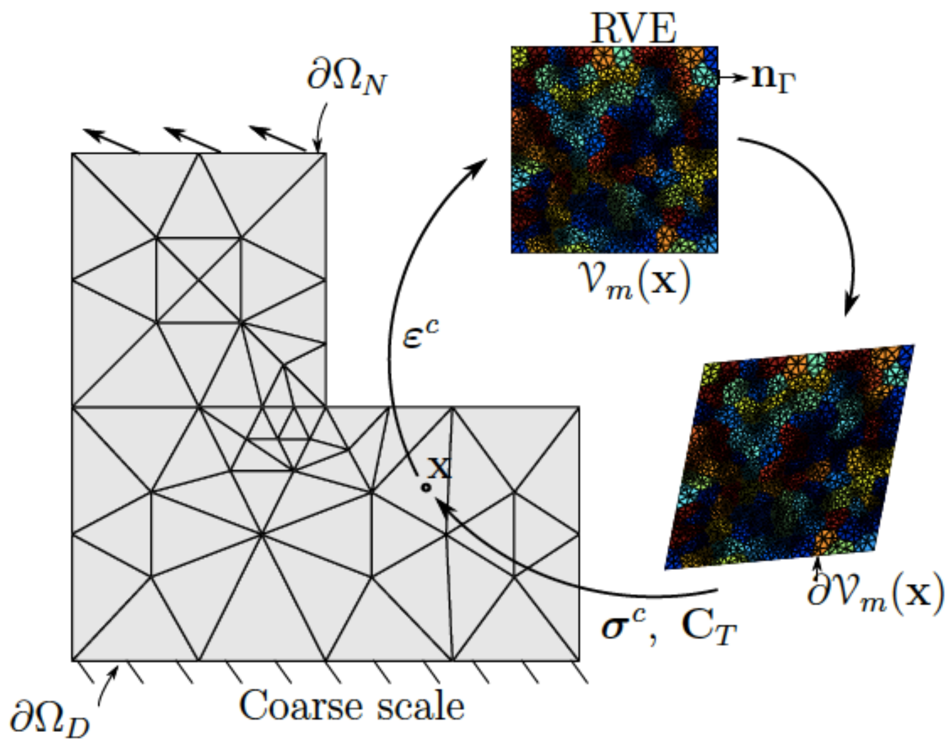
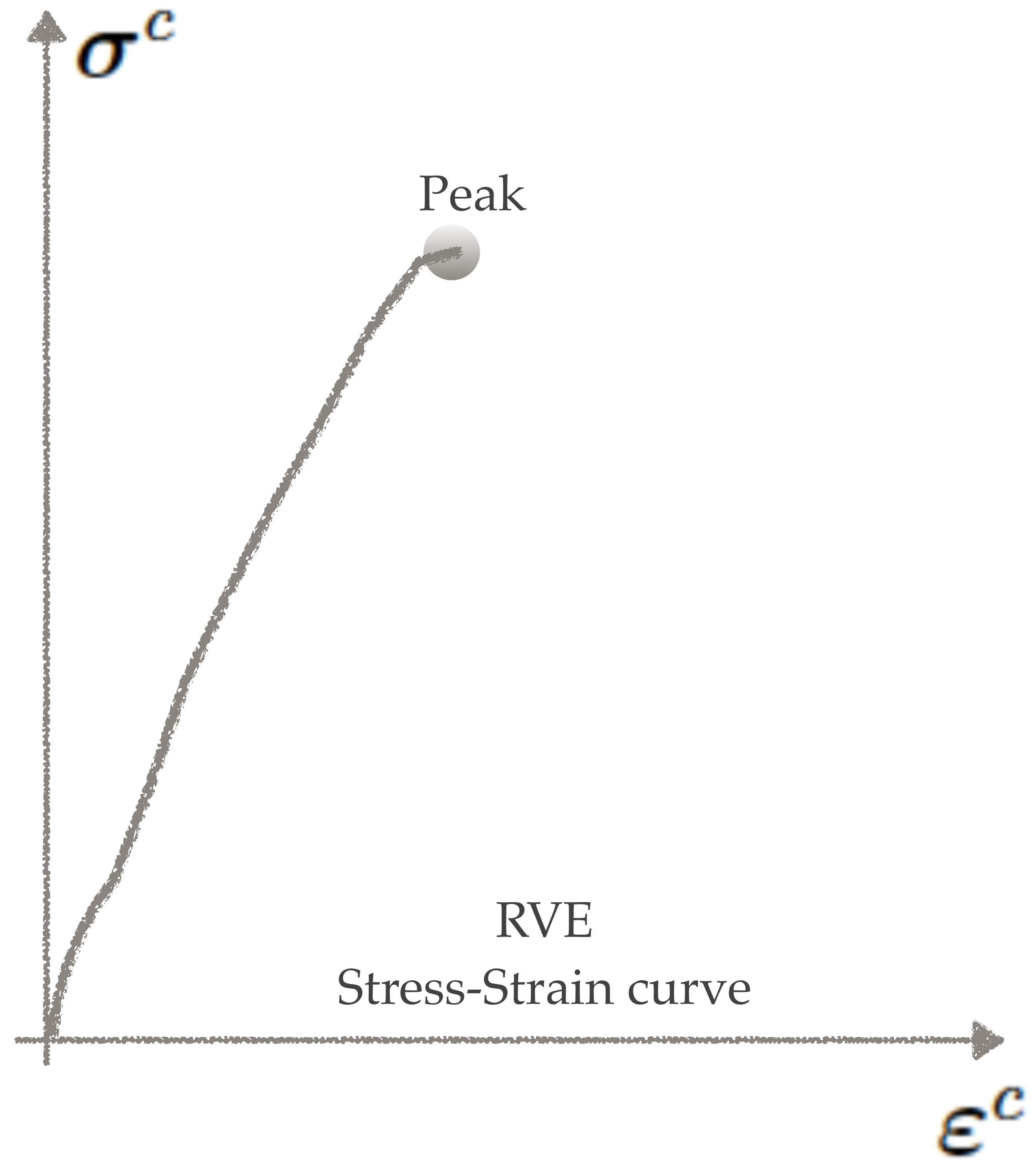


Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2

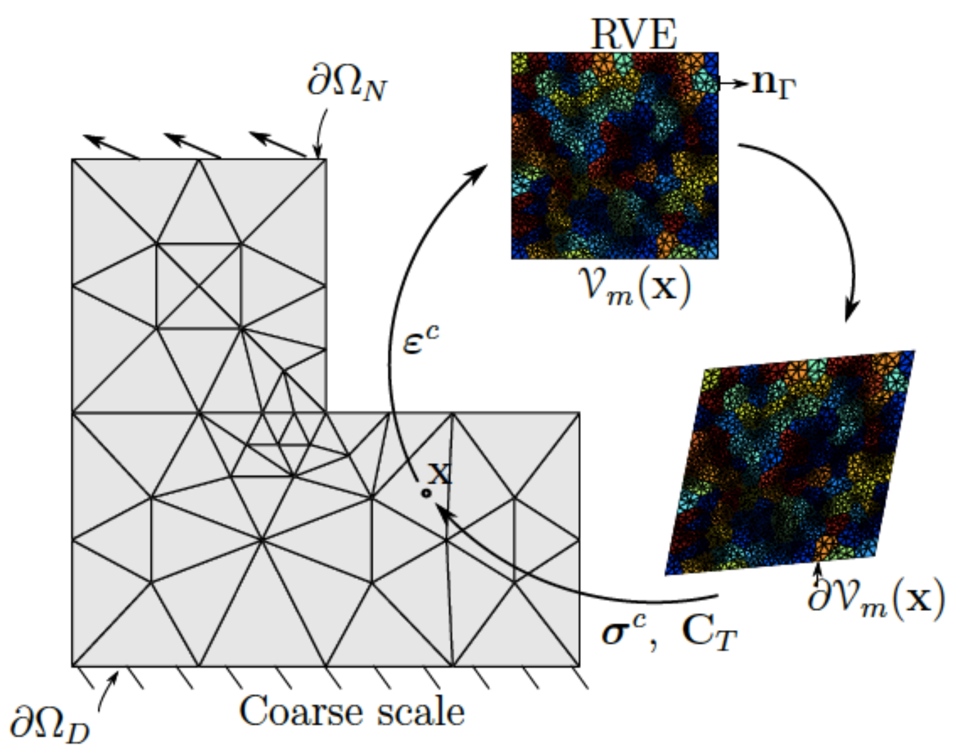




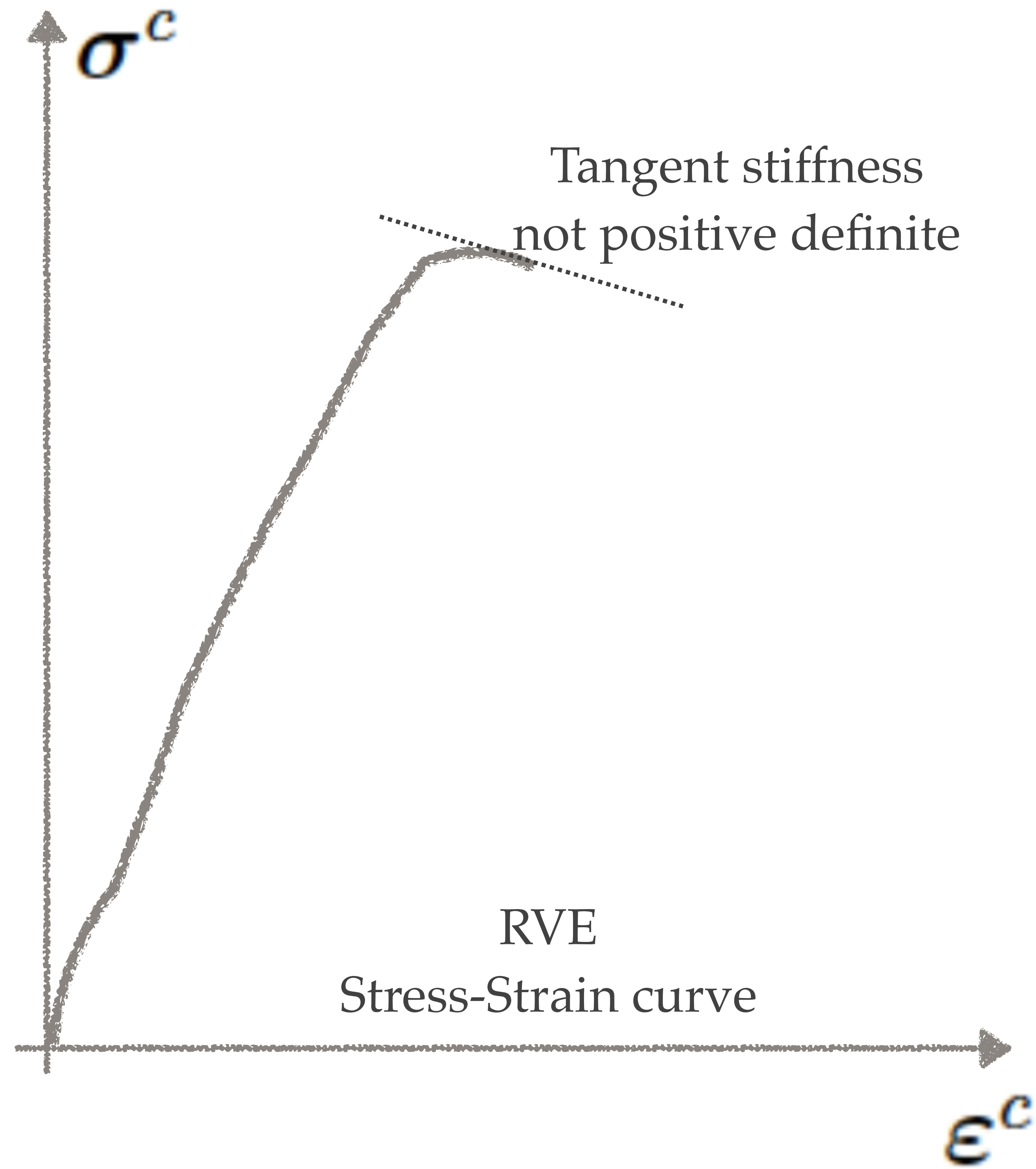
Peak

Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

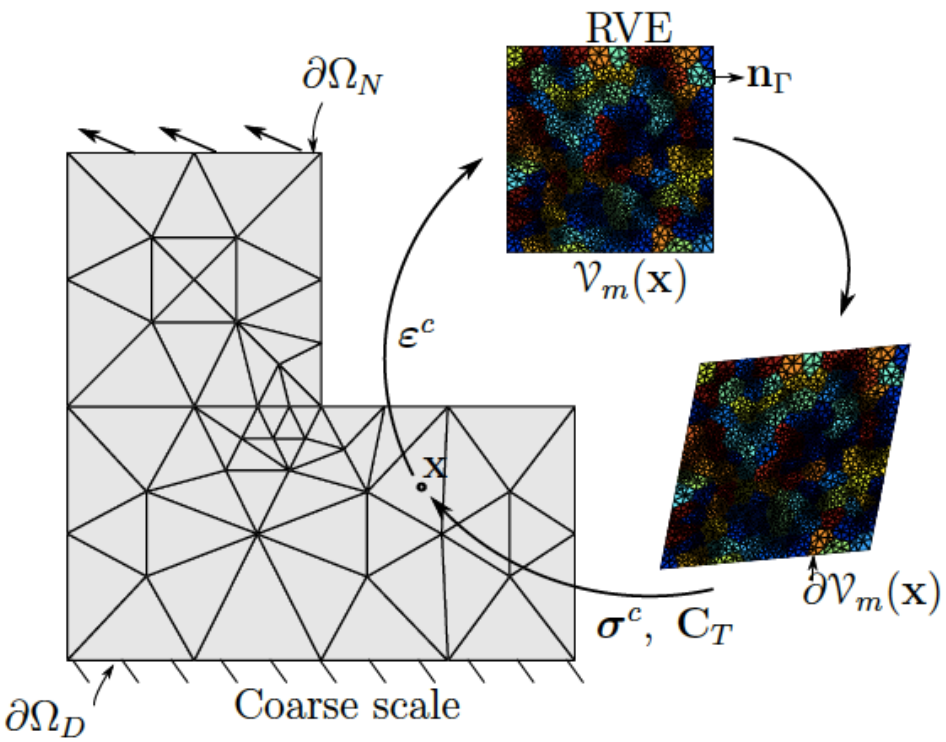
Hierarchical methods FE^2



Unloading

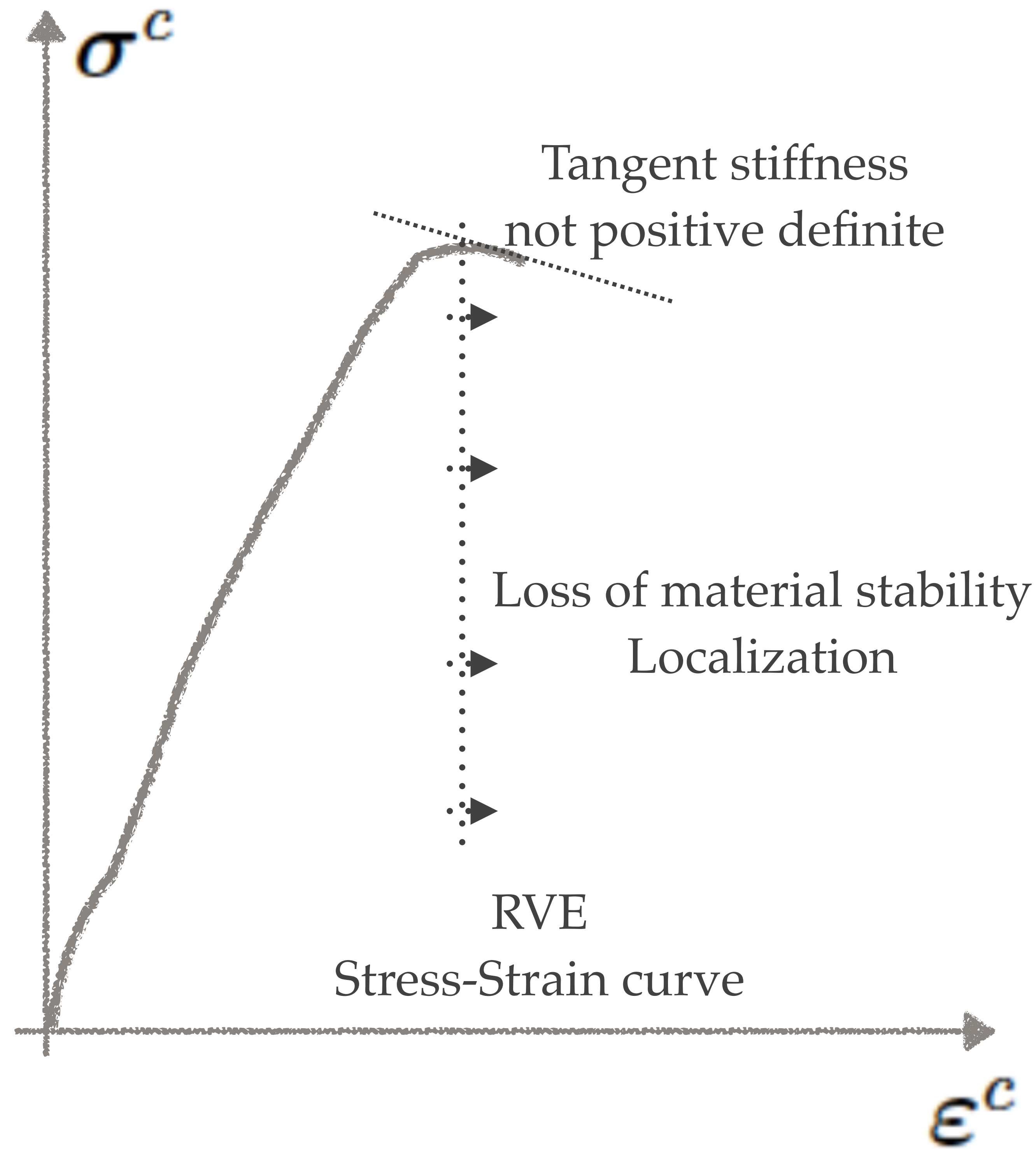


Hierarchical methods FE^2



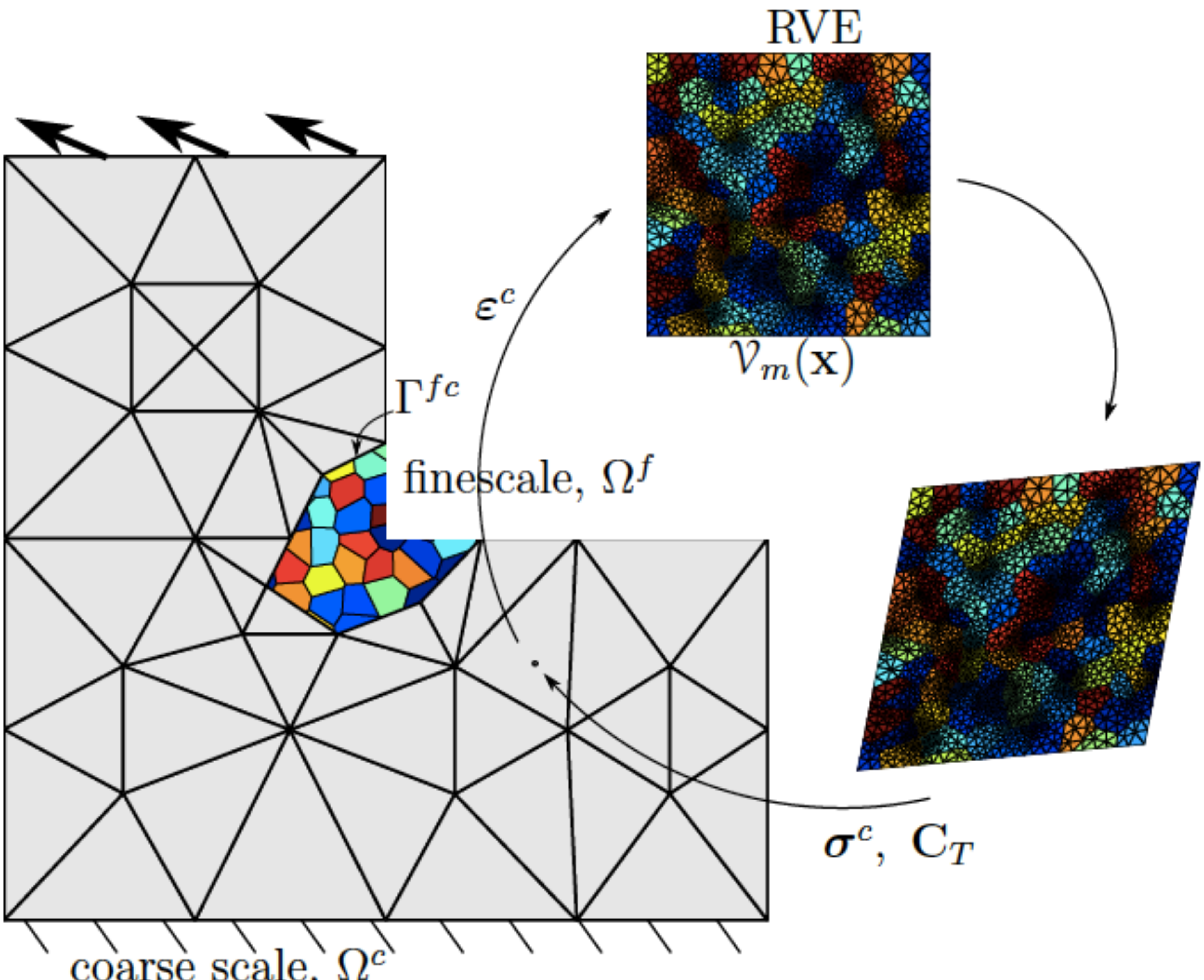
Unloading

RVE does not exist



Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

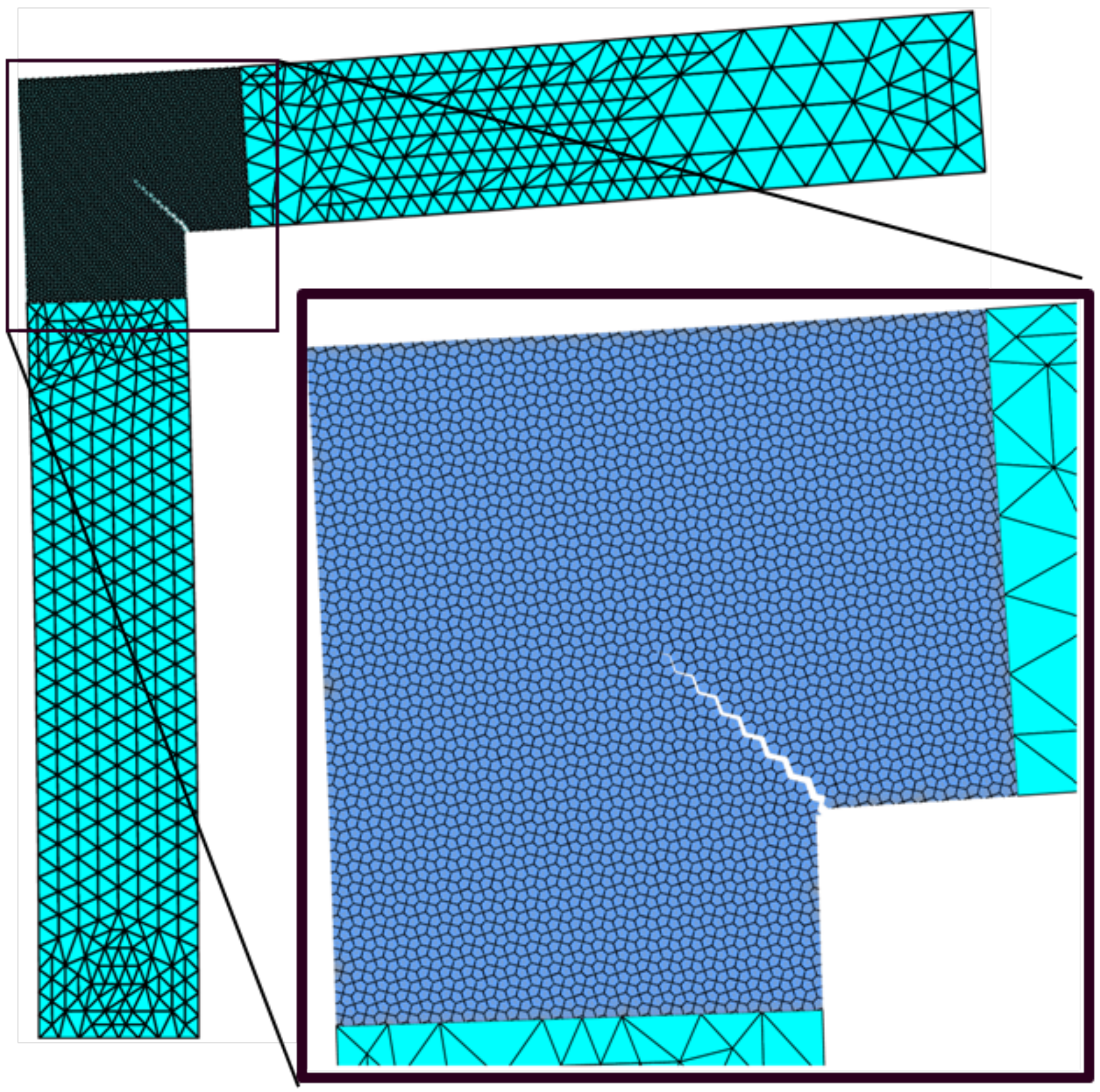
Hybrid methods



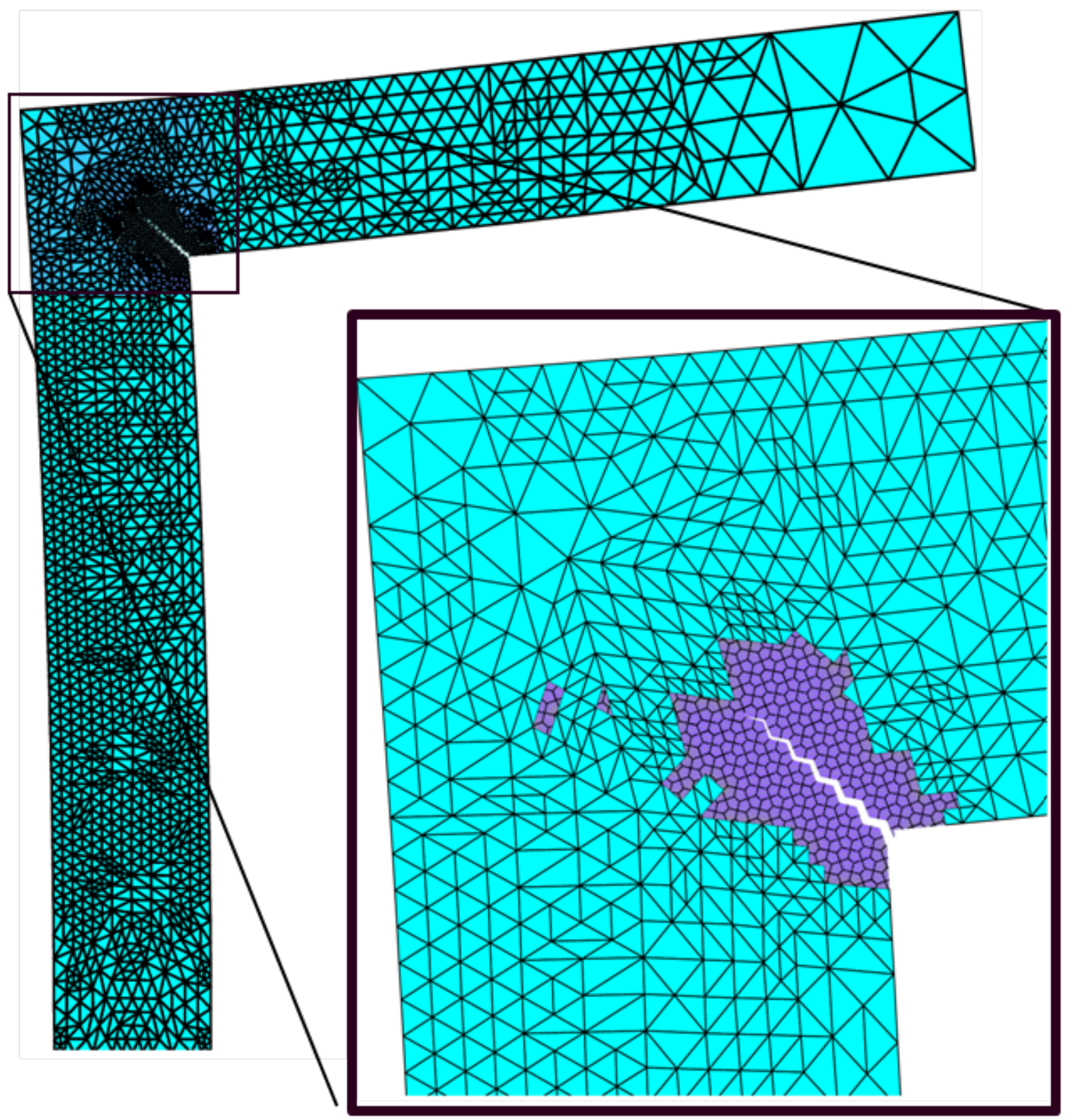
Akbari, Kerfriden, Bordas, 2014

Example

Direct Numerical Solution



Adaptive Multiscale method

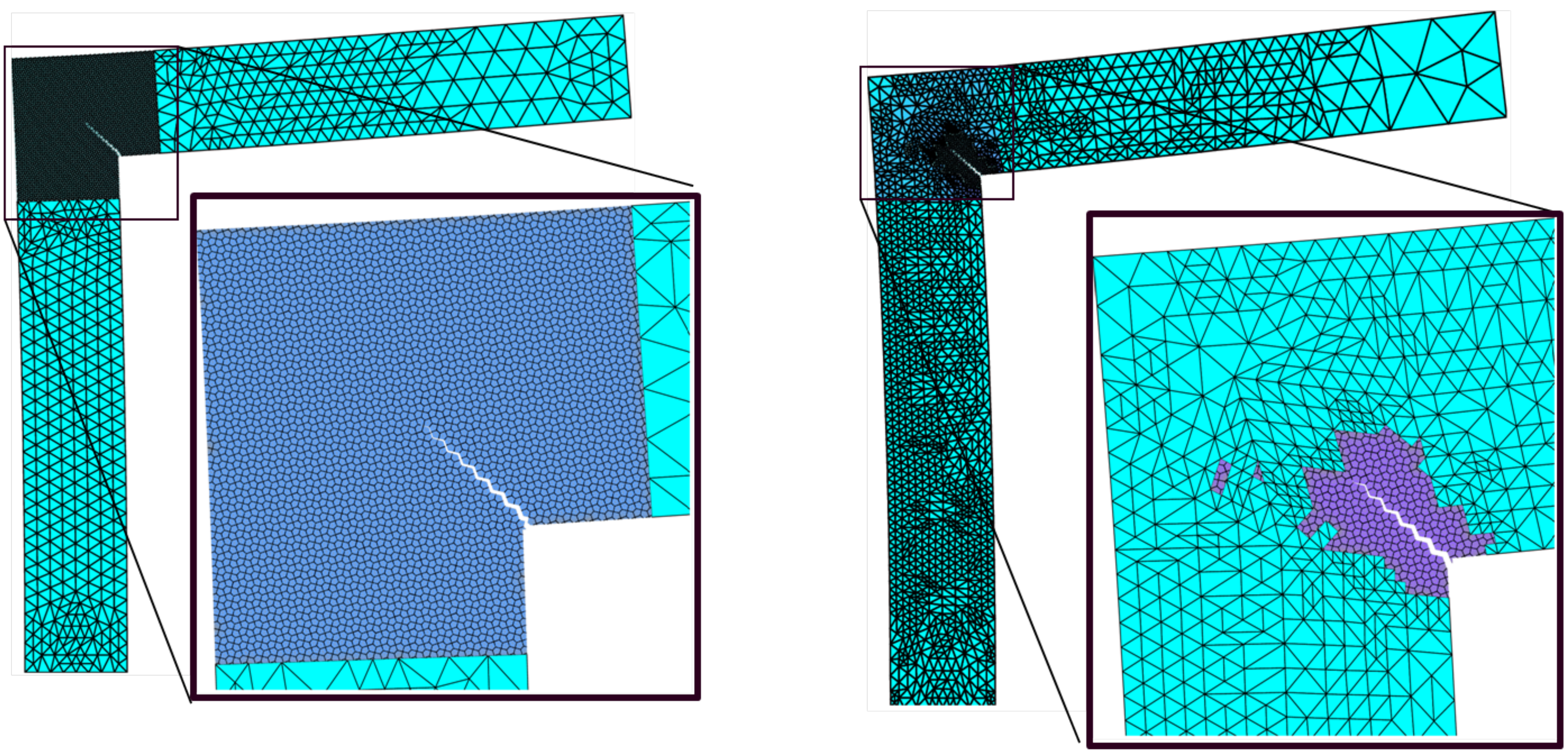


Example

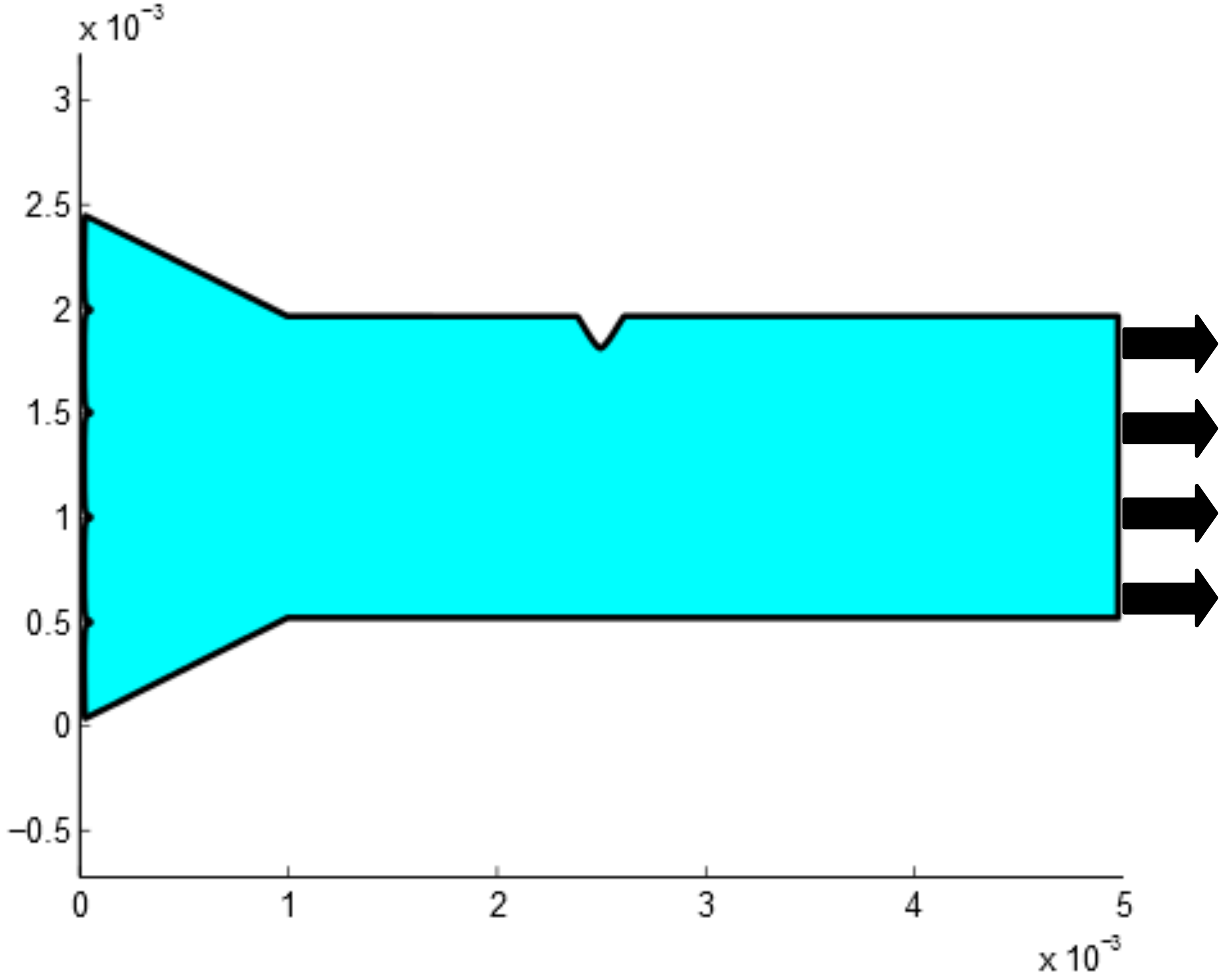
20-100 times fewer unknowns in 2D ~ 1000 times fewer in 3D

Direct Numerical Solution

Adaptive Multiscale method



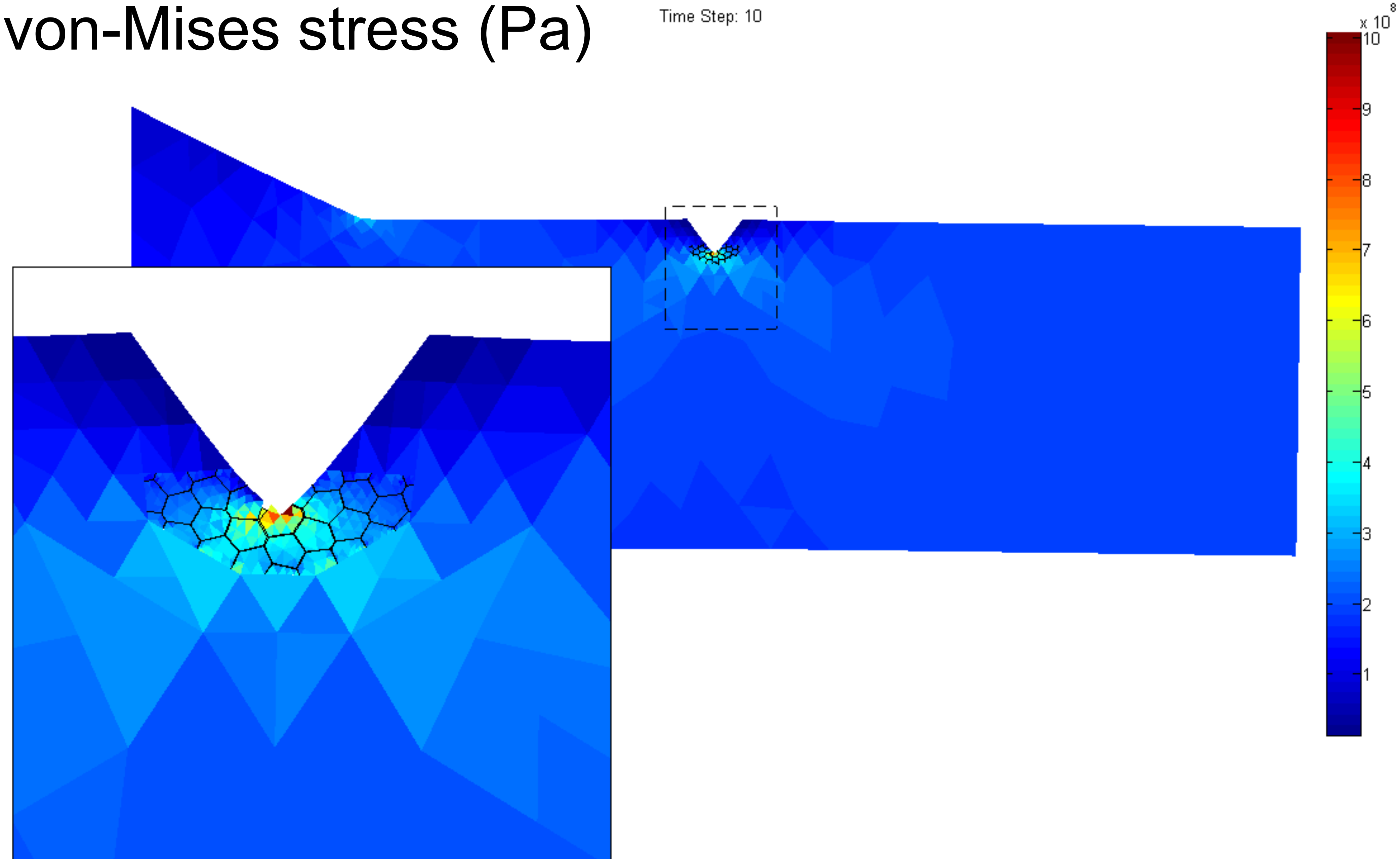
Results: uni-axial tension



❖ Sizes are in mm

Results: uni-axial tension

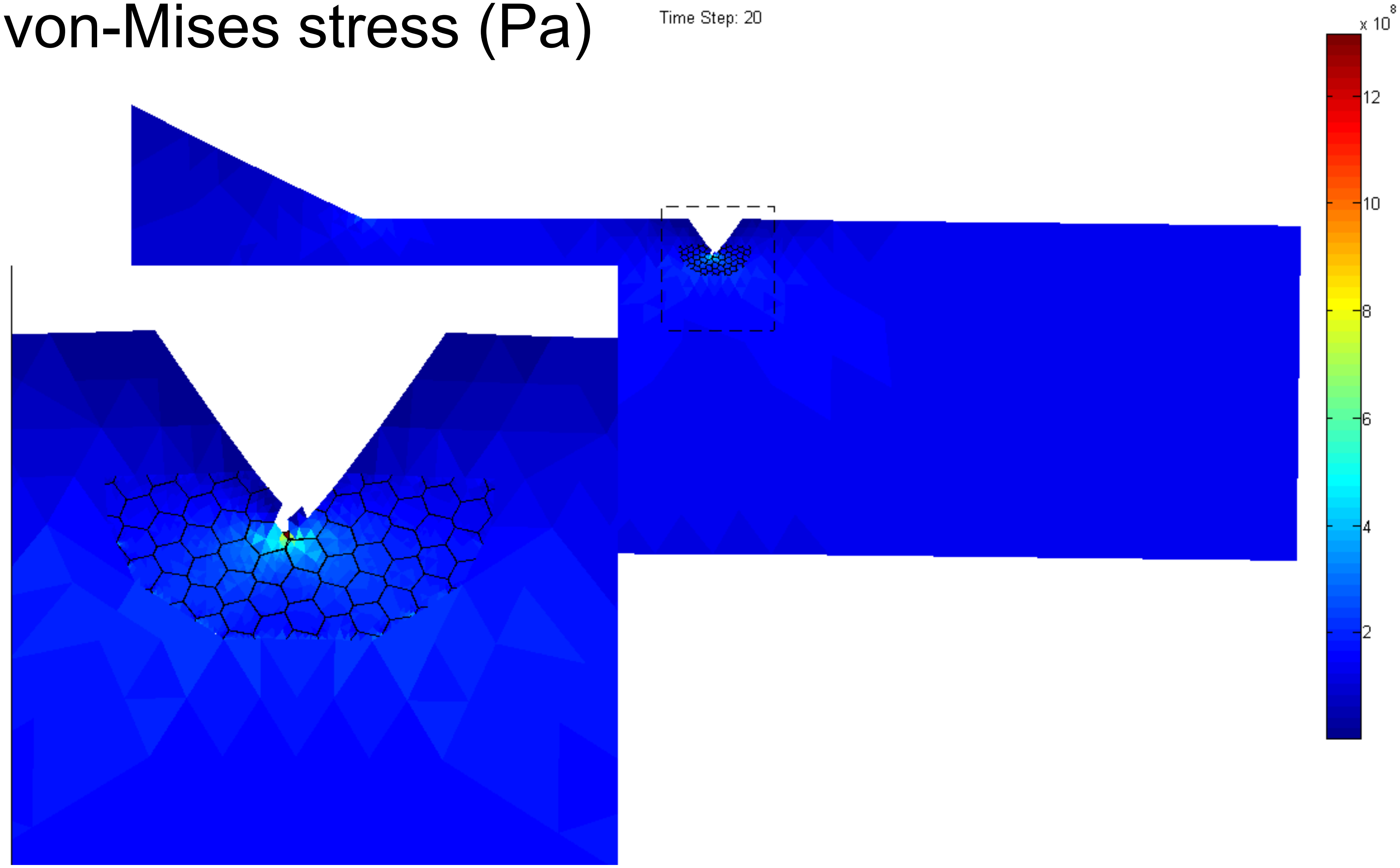
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

Results: uni-axial tension

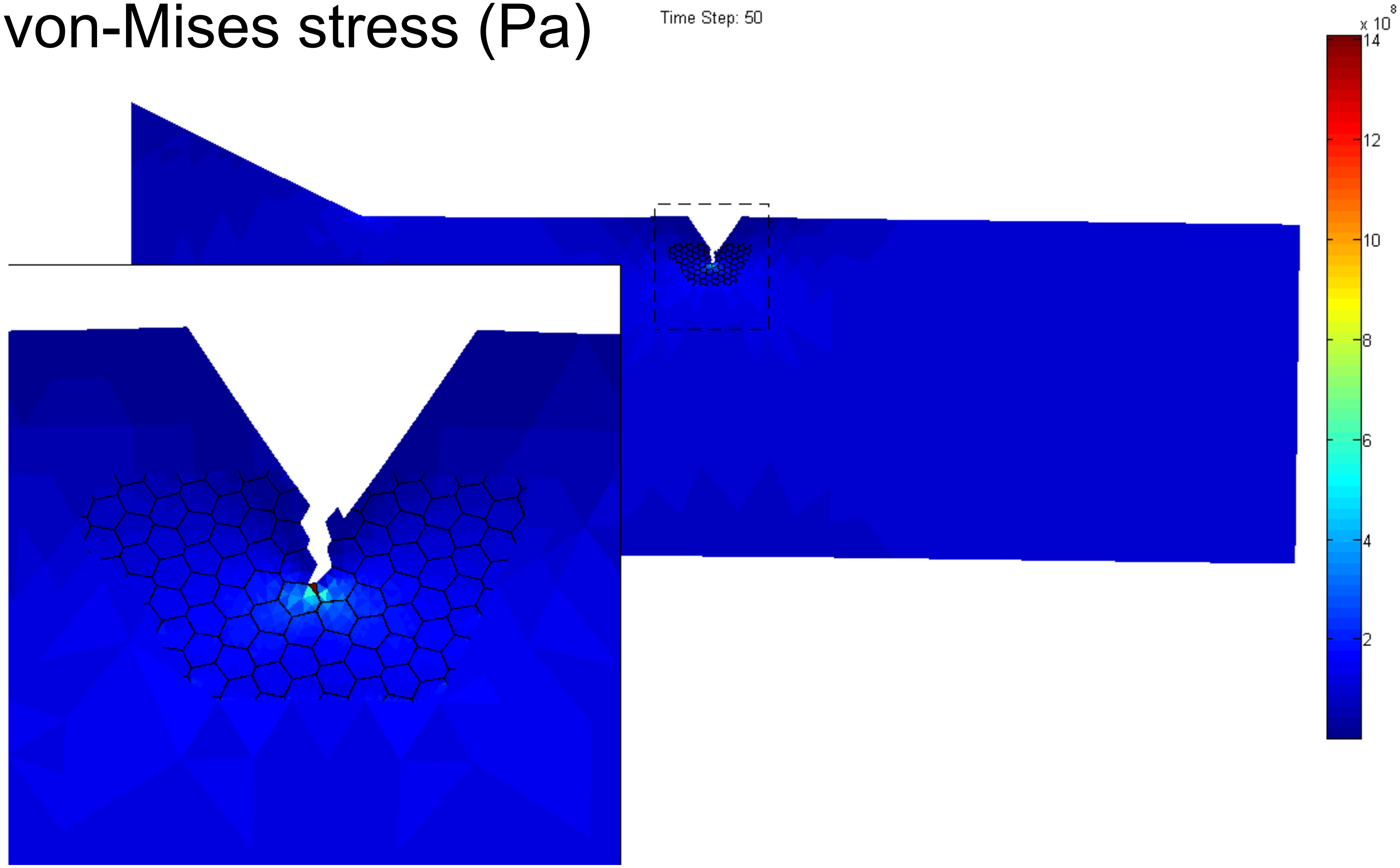
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

Results: uni-axial tension

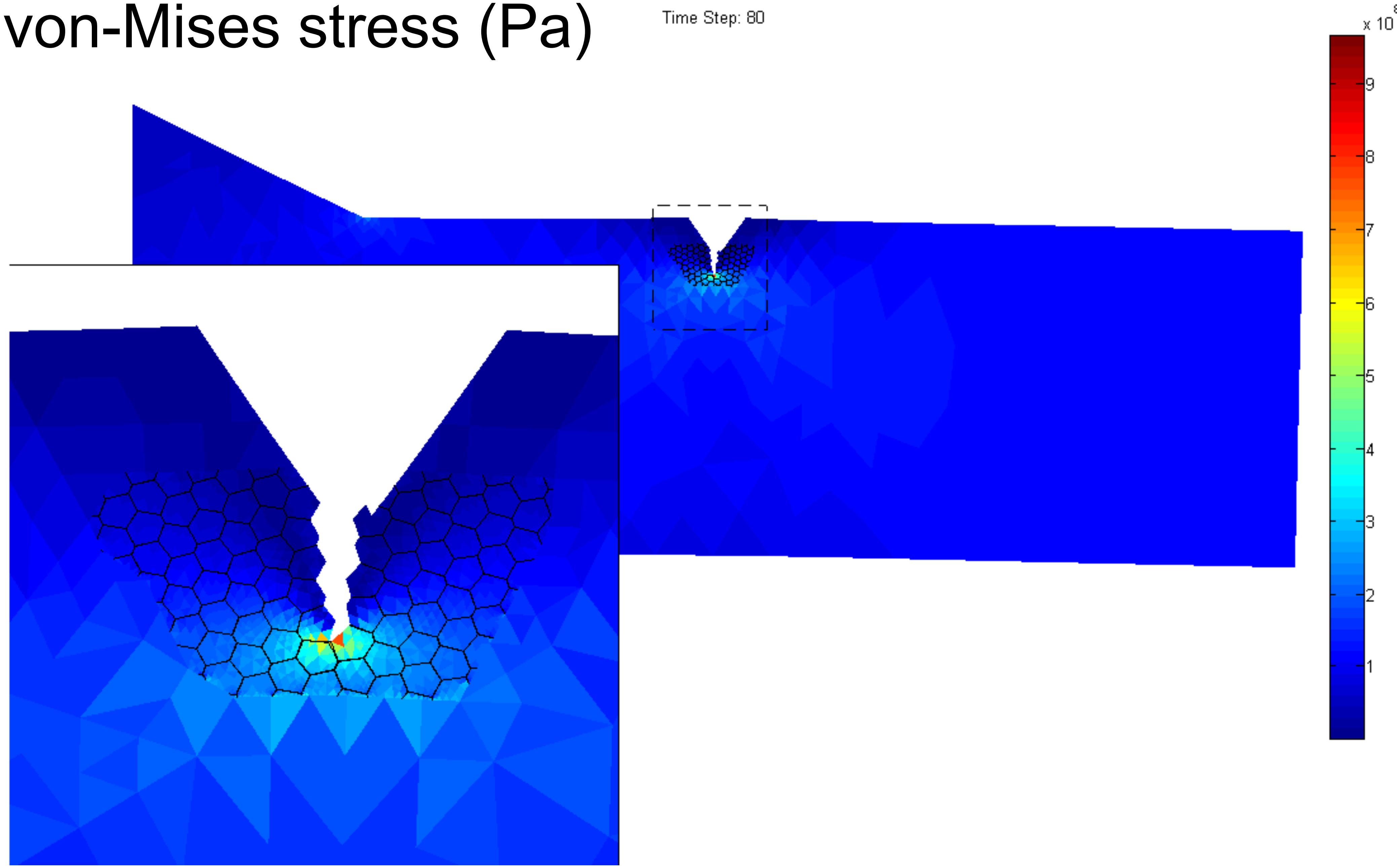
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

Results: uni-axial tension

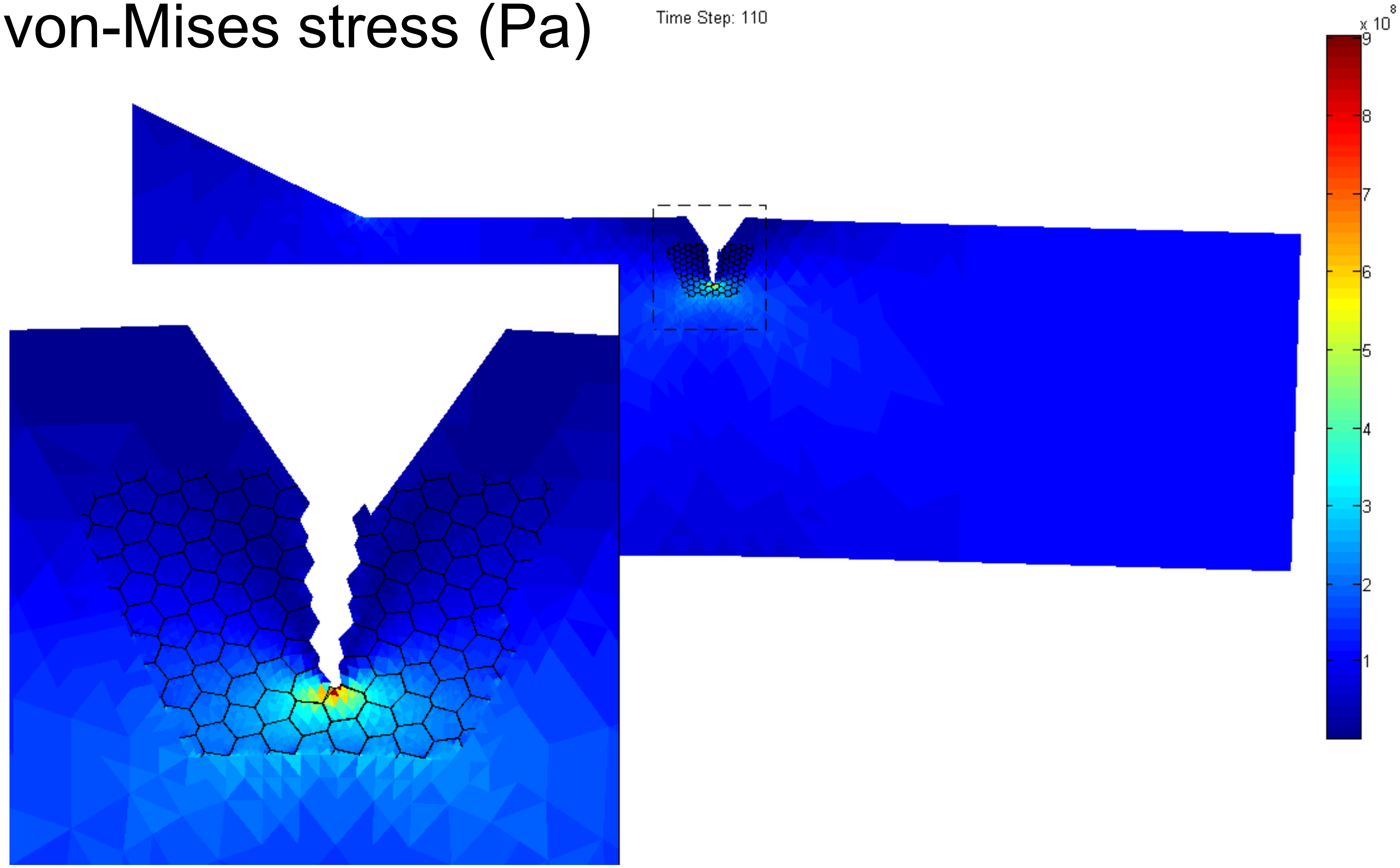
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

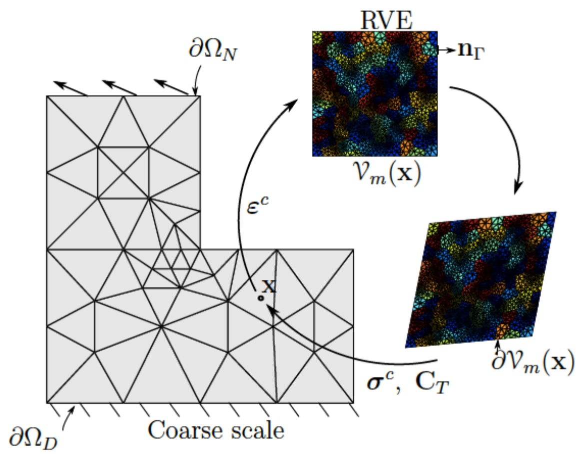
Results: uni-axial tension

von-Mises stress (Pa)

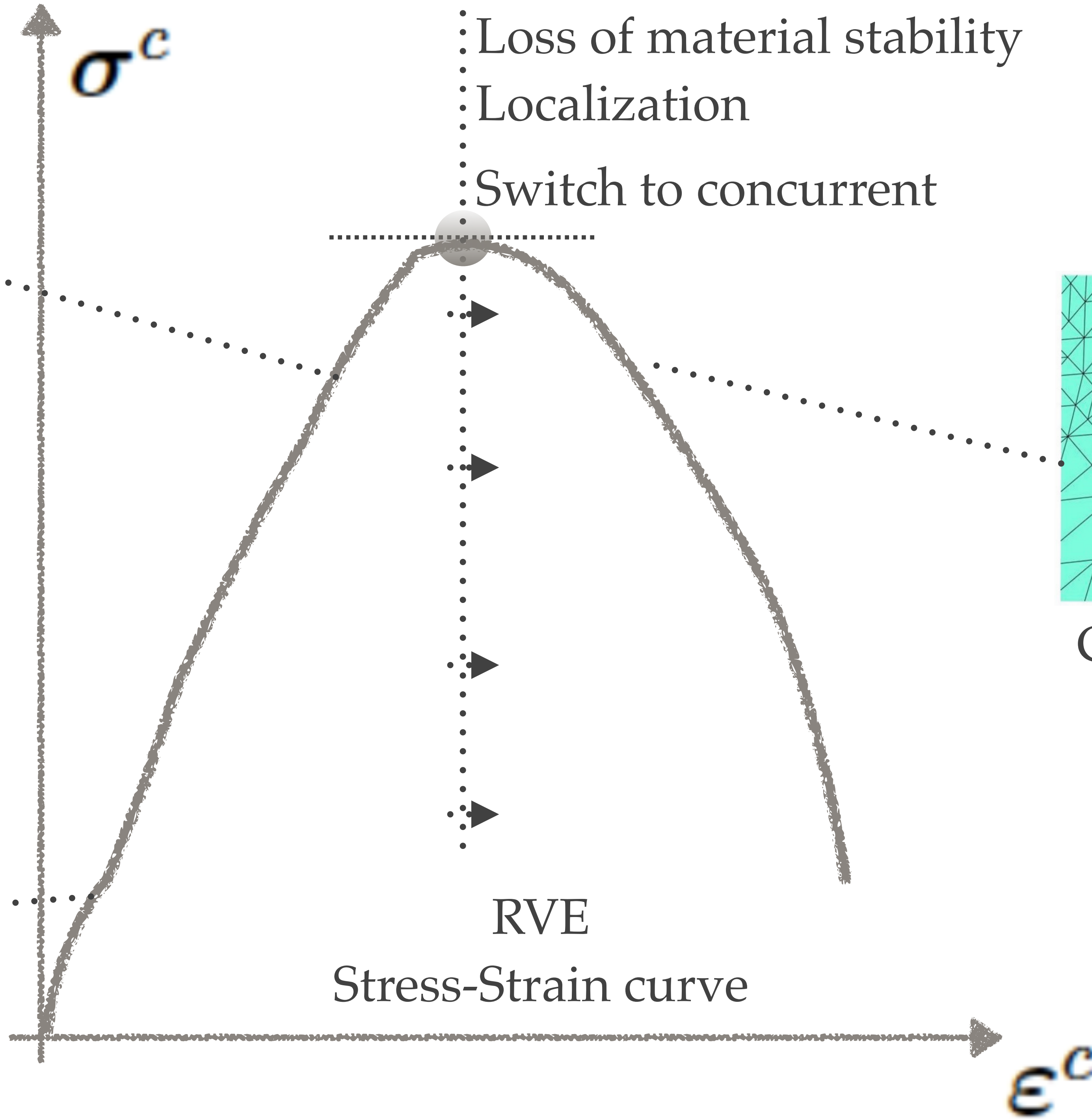


❖ 100X (magnification of displacement)

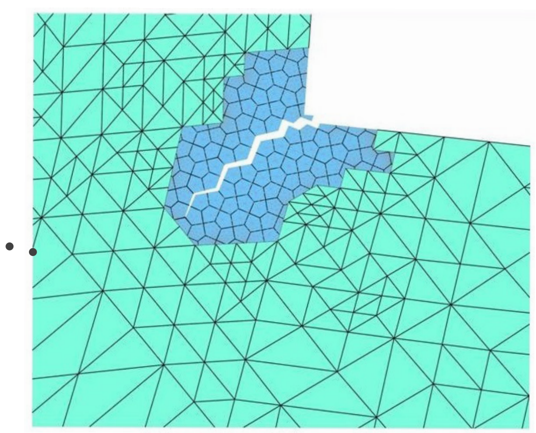
Adaptive multi-scale



Semi-concurrent
FE^2



Loss of material stability
Localization
Switch to concurrent



Concurrent

Analytical
homogenisation

RVE
Stress-Strain curve

Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Open problem

- model selection and error control

Possible approach

- machine learning and statistical inference, e.g. Bayesian statistics

Open problem

- statistical variability at the fine scale (geometry, material parameter)

Possible approach

- identification through small-scale experiments (costly, difficult to characterize interfaces)
- Monte Carlo

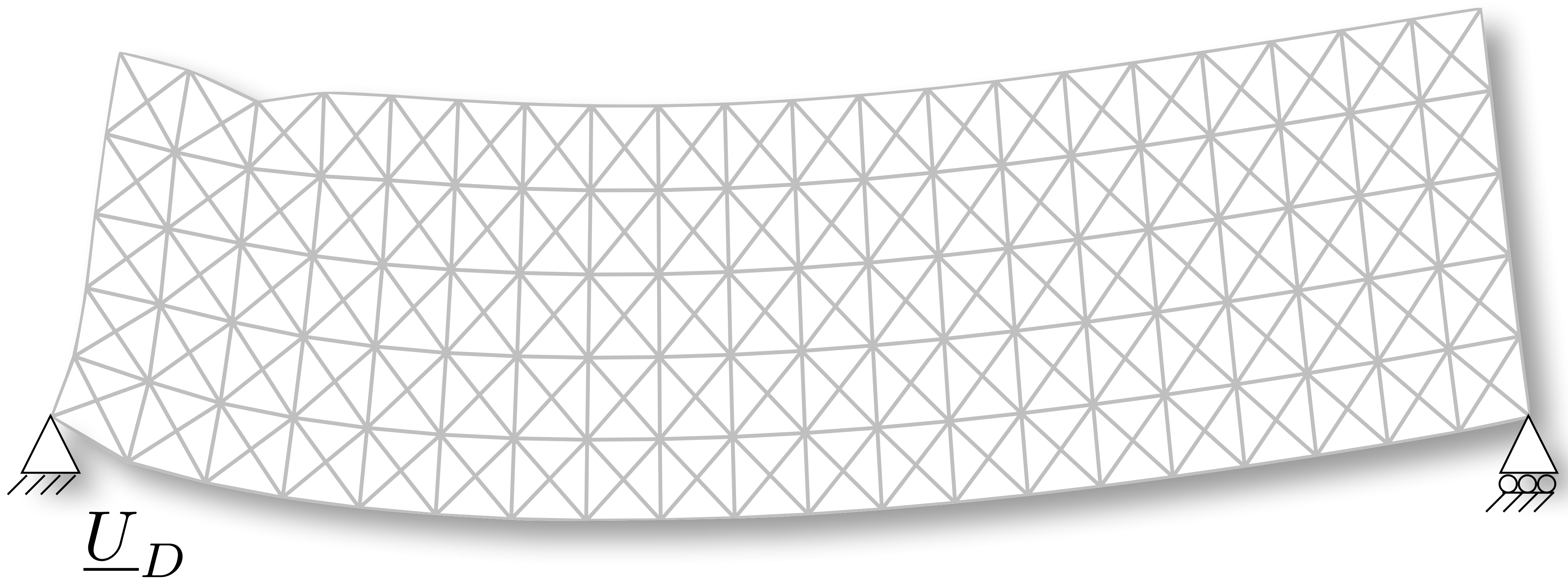
Algebraic model reduction methods

Use precomputed solutions to accelerate online simulations

Example - parametric problems

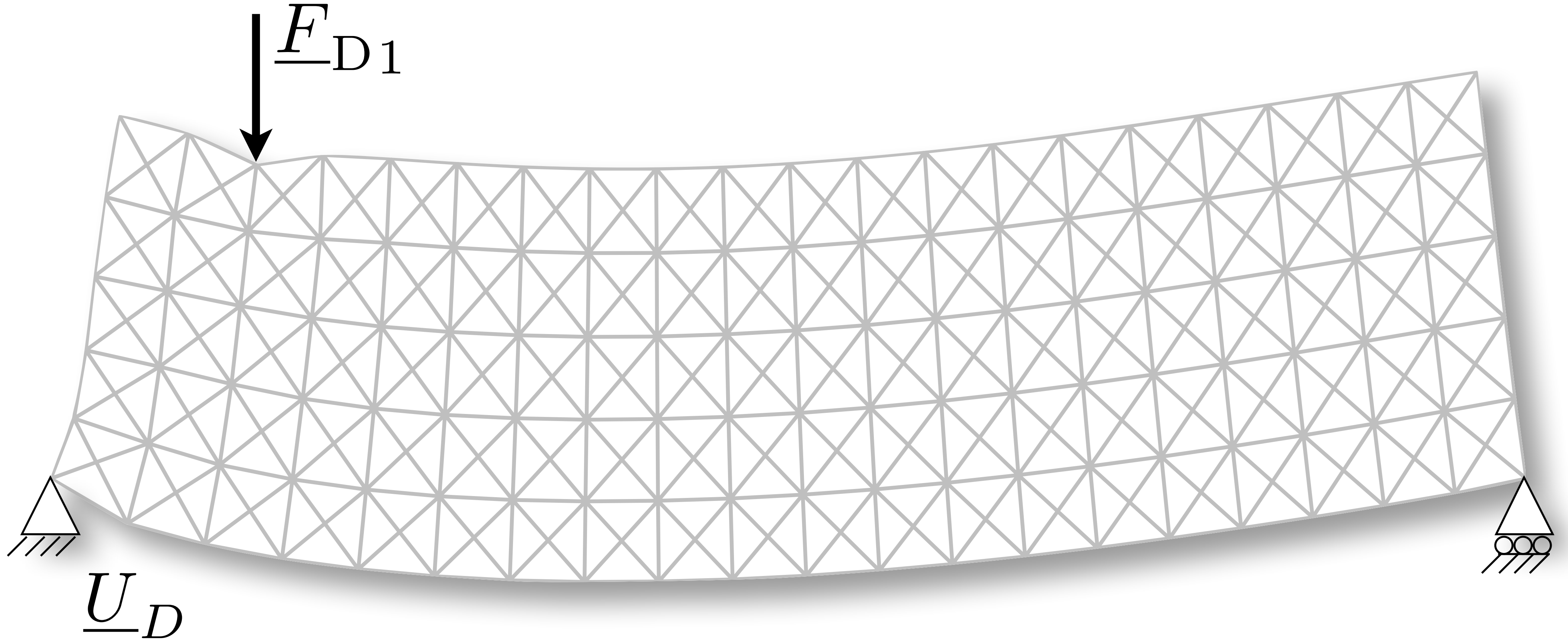
Method of separated representation

Lattice beam problem



Aim: accelerate the simulation using pre-computations

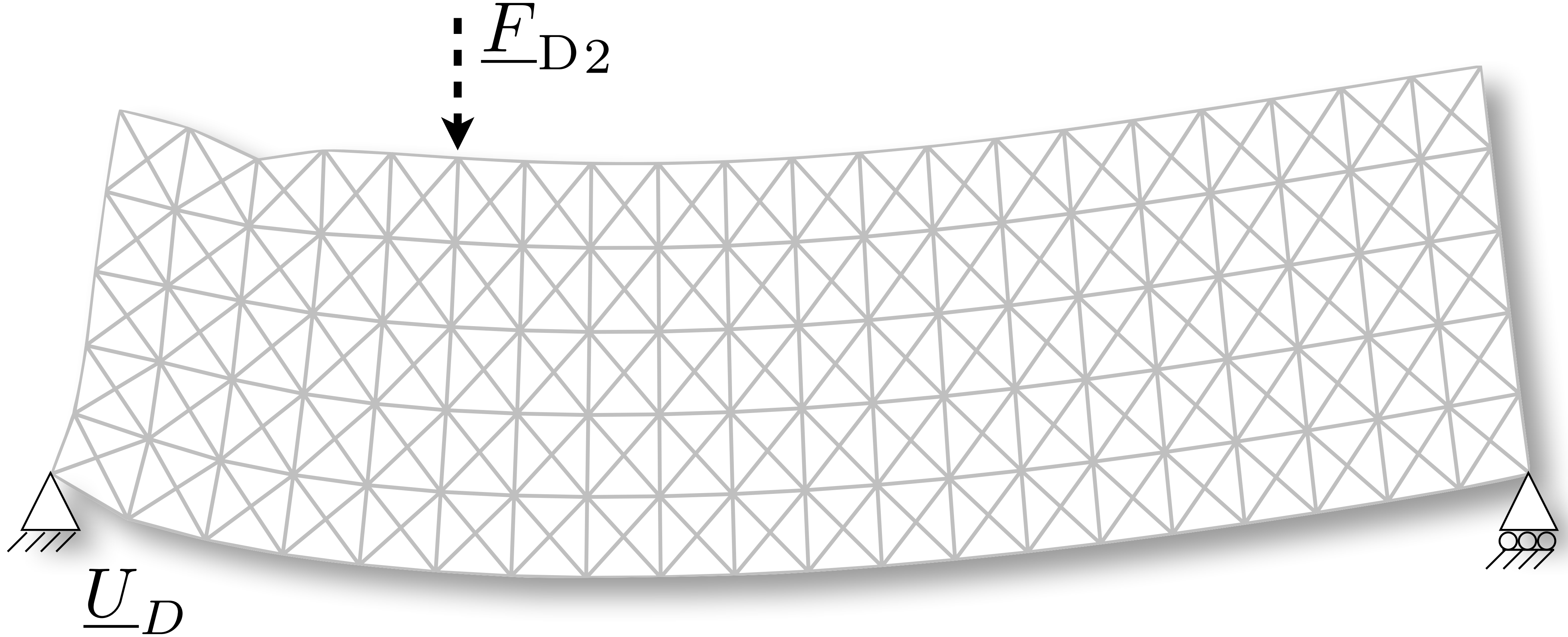
Lattice beam problem



$$\underline{\underline{\mathbf{S}}} = (\; \underline{\mathbf{S}}^1$$

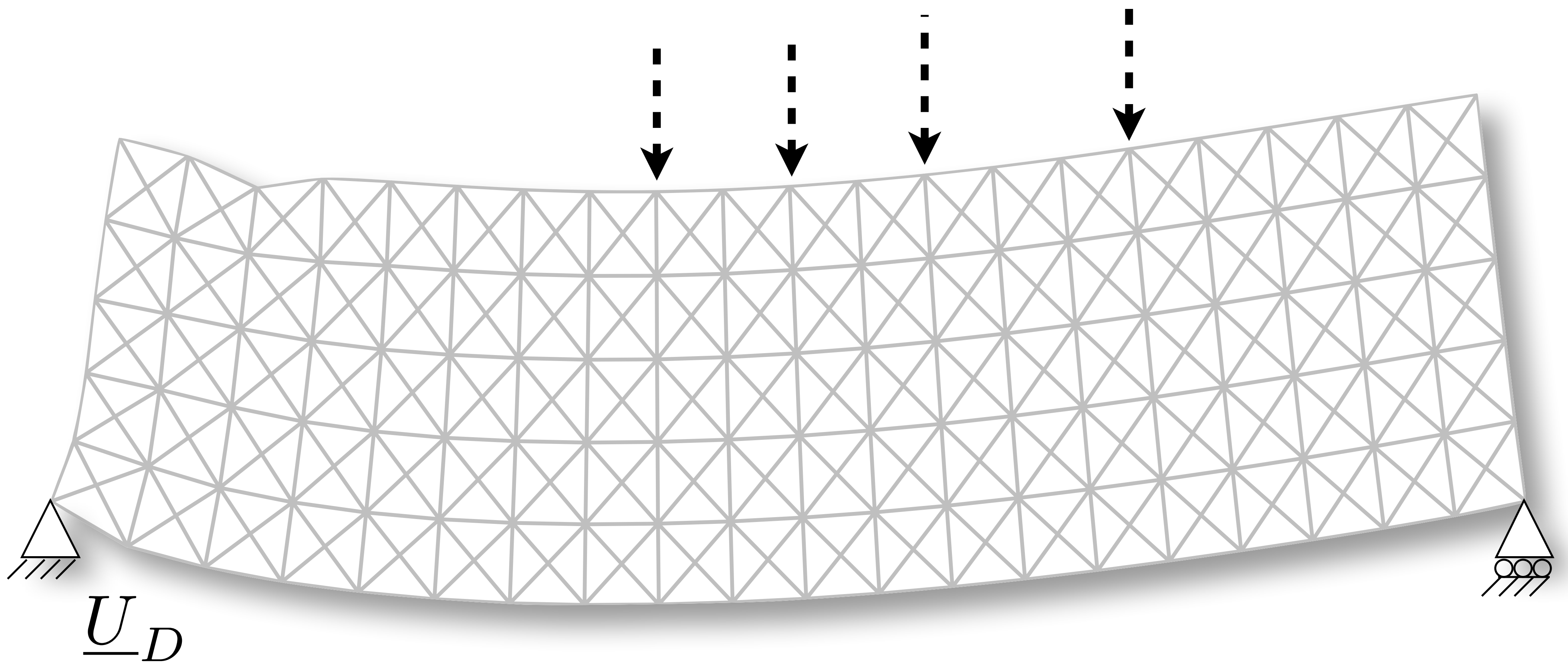
Compute solutions for several loading conditions

Lattice beam problem



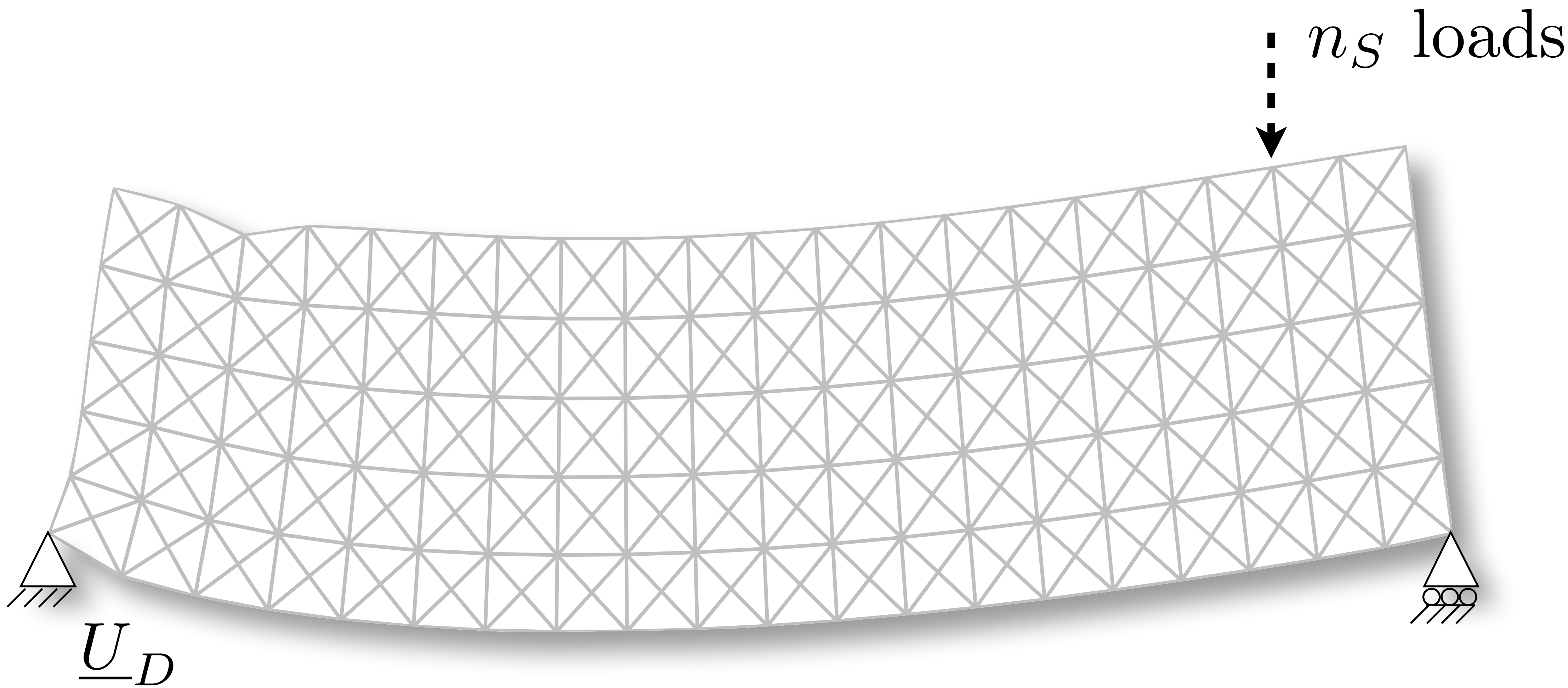
$$\underline{\underline{\mathbf{S}}} = \left(\ \underline{\mathbf{S}}^1 \quad \underline{\mathbf{S}}^2 \right.$$

Lattice beam problem



$$\underline{\underline{\mathbf{S}}} = \big(\ \underline{\mathbf{S}}^1 \quad \underline{\mathbf{S}}^2 \quad \ldots$$

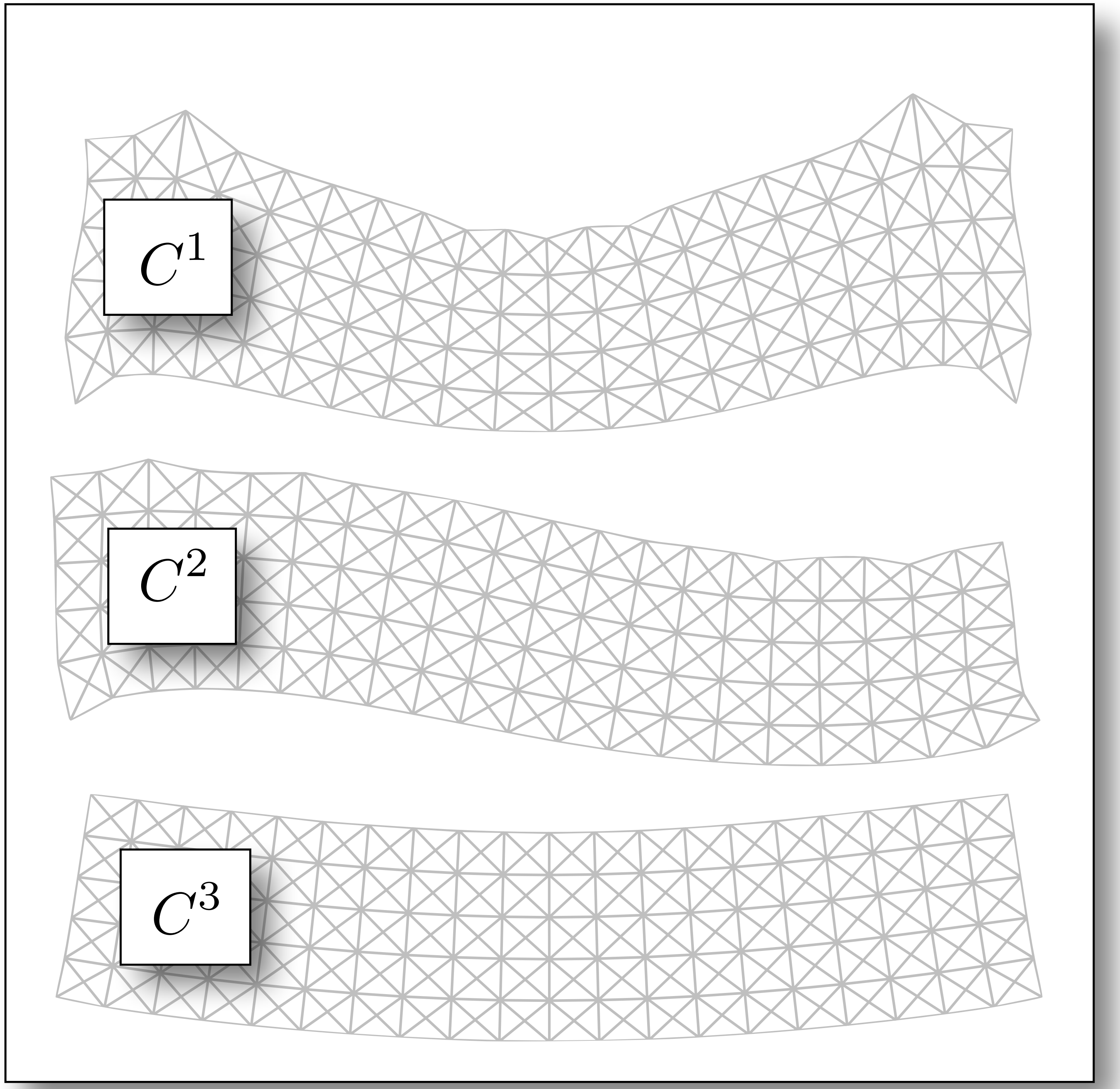
Lattice beam problem



$$\underline{\underline{\mathbf{S}}} = \left(\; \underline{\mathbf{S}}^1 \quad \underline{\mathbf{S}}^2 \quad \dots \quad \underline{\mathbf{S}}^{n_S} \; \right)$$

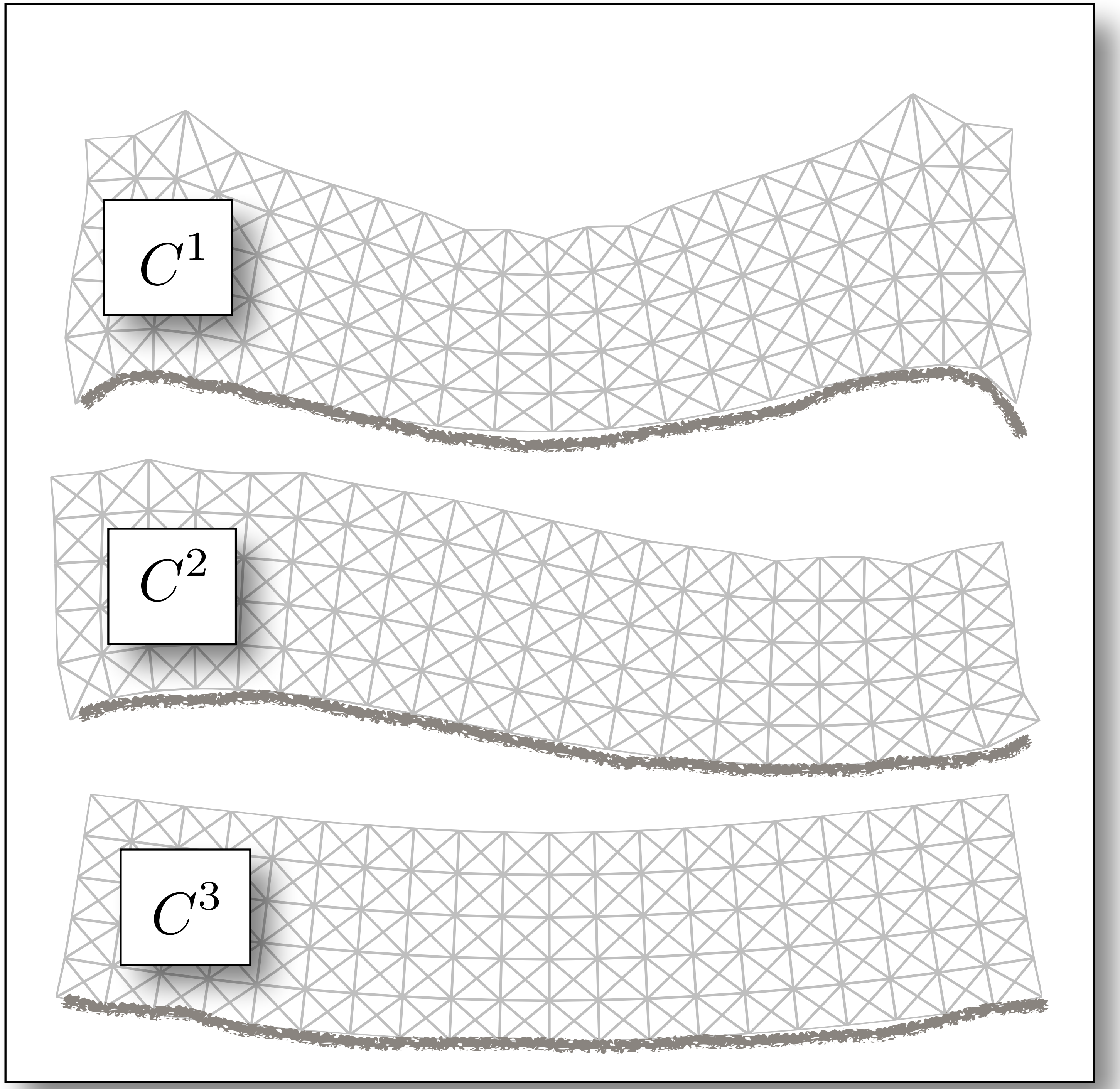
Perform singular value decomposition - POD to obtain "most energetic modes"

Reduced basis



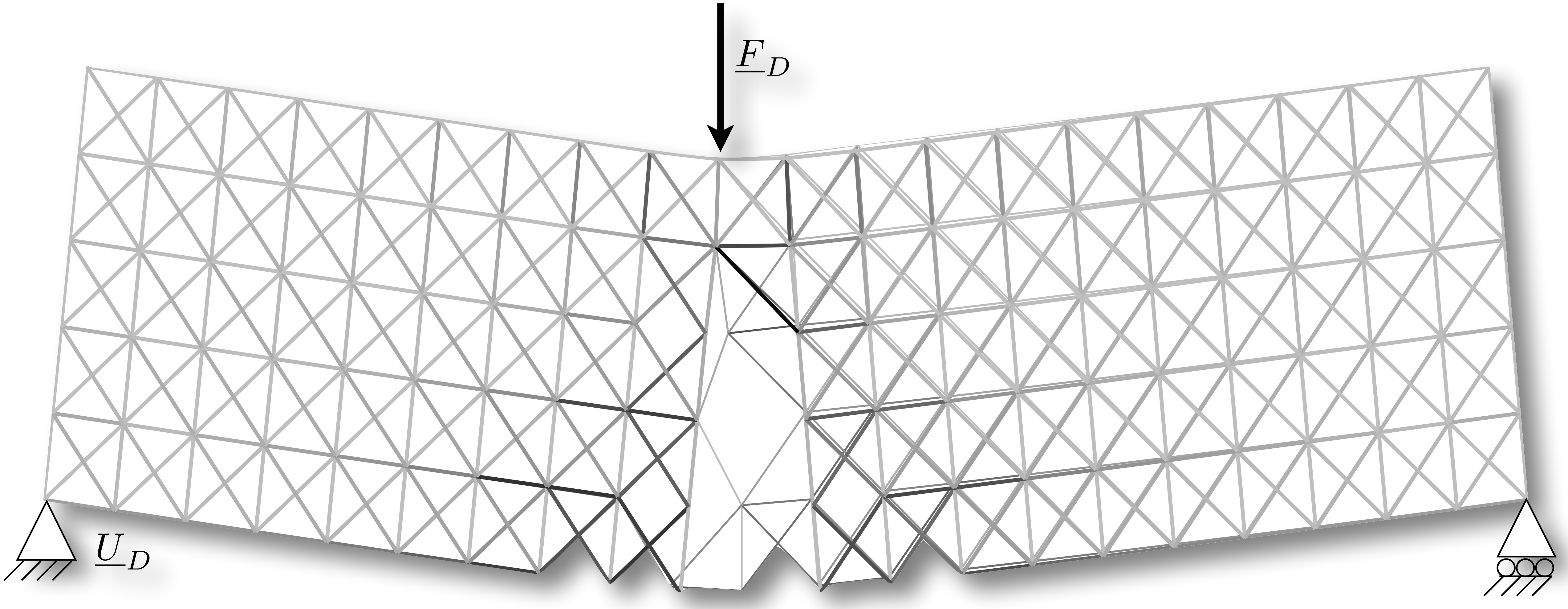
P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. *Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems*. Computer Methods in Applied Mechanics and Engineering, 200(5-8):850-866, 2011.

Reduced basis



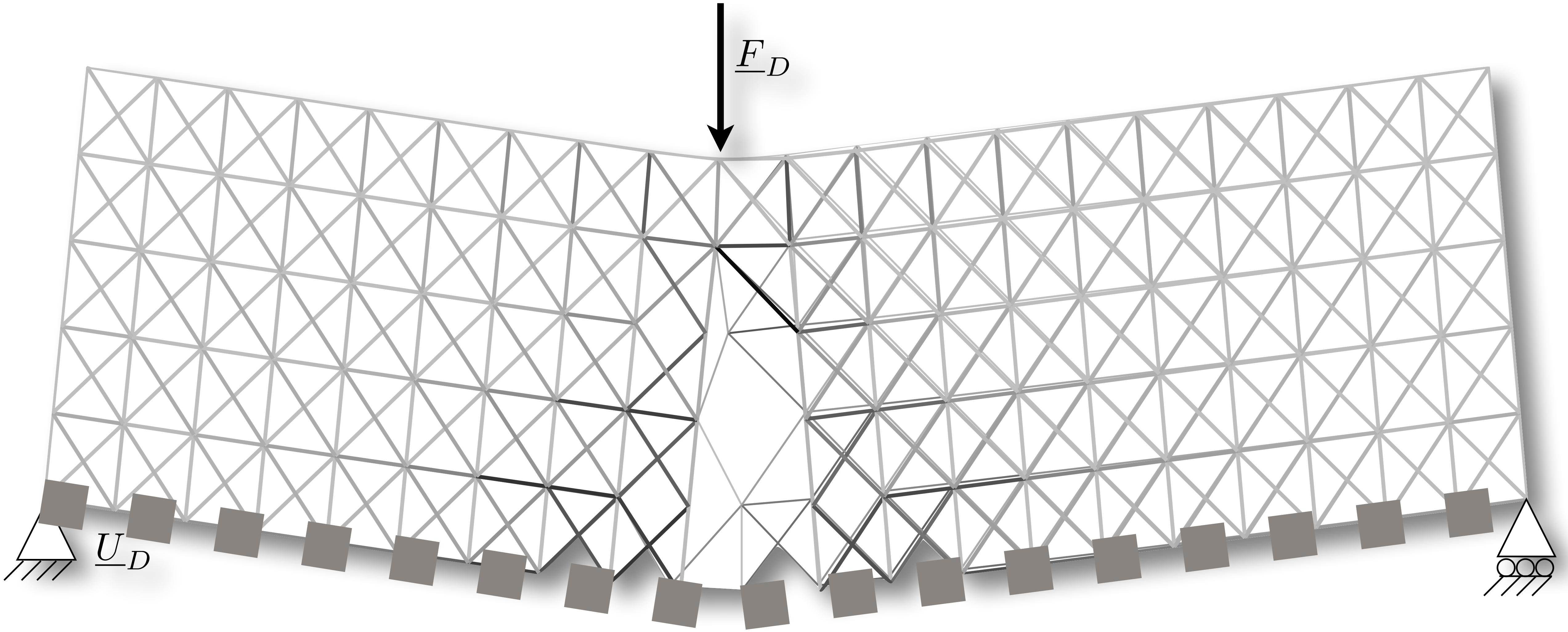
P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. *Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems*. Computer Methods in Applied Mechanics and Engineering, 200(5-8):850-866, 2011.

Beyond the elastic limit

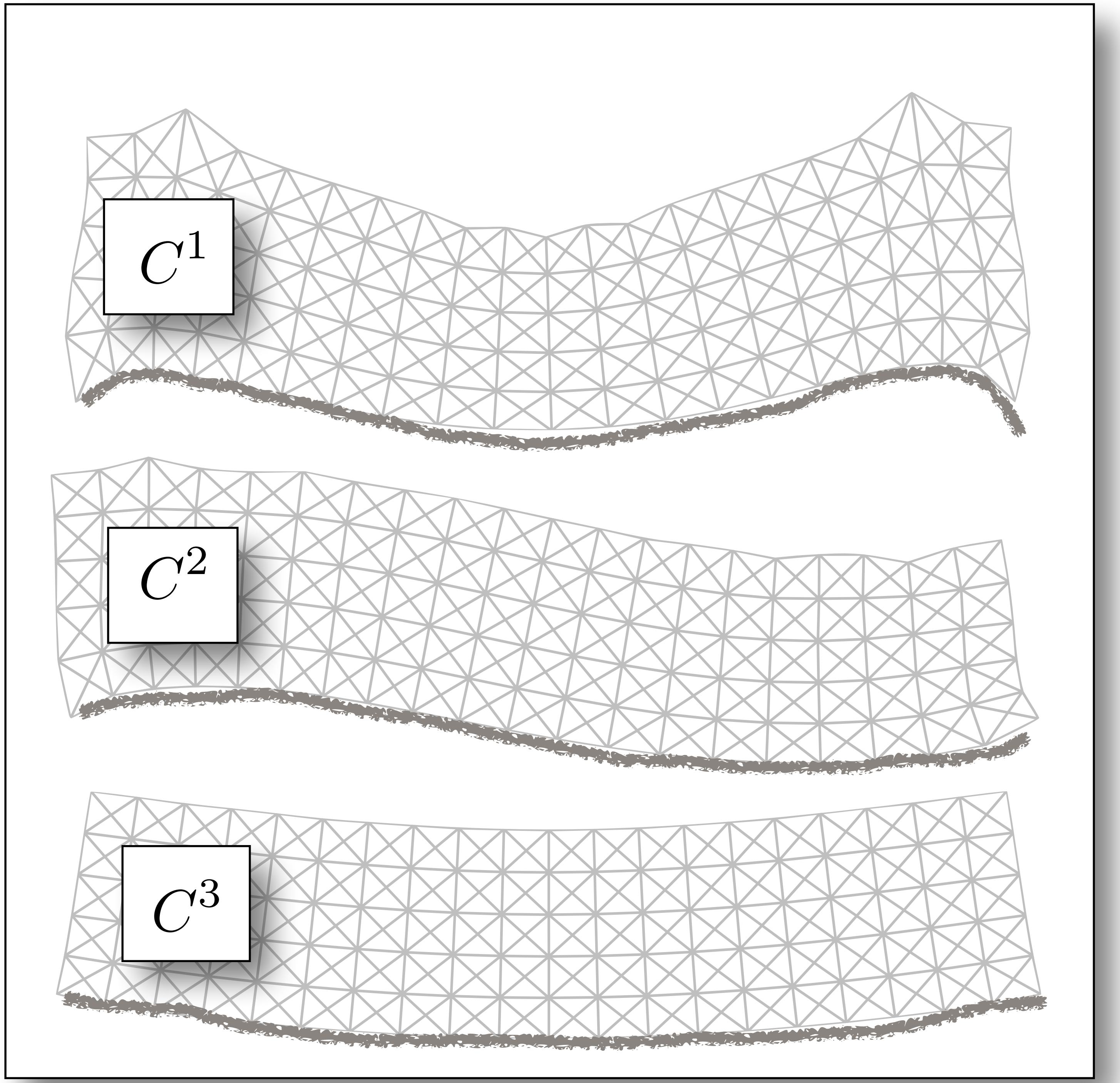


P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. *Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems*. Computer Methods in Applied Mechanics and Engineering, 200(5-8):850-866, 2011.

Beyond the elastic limit

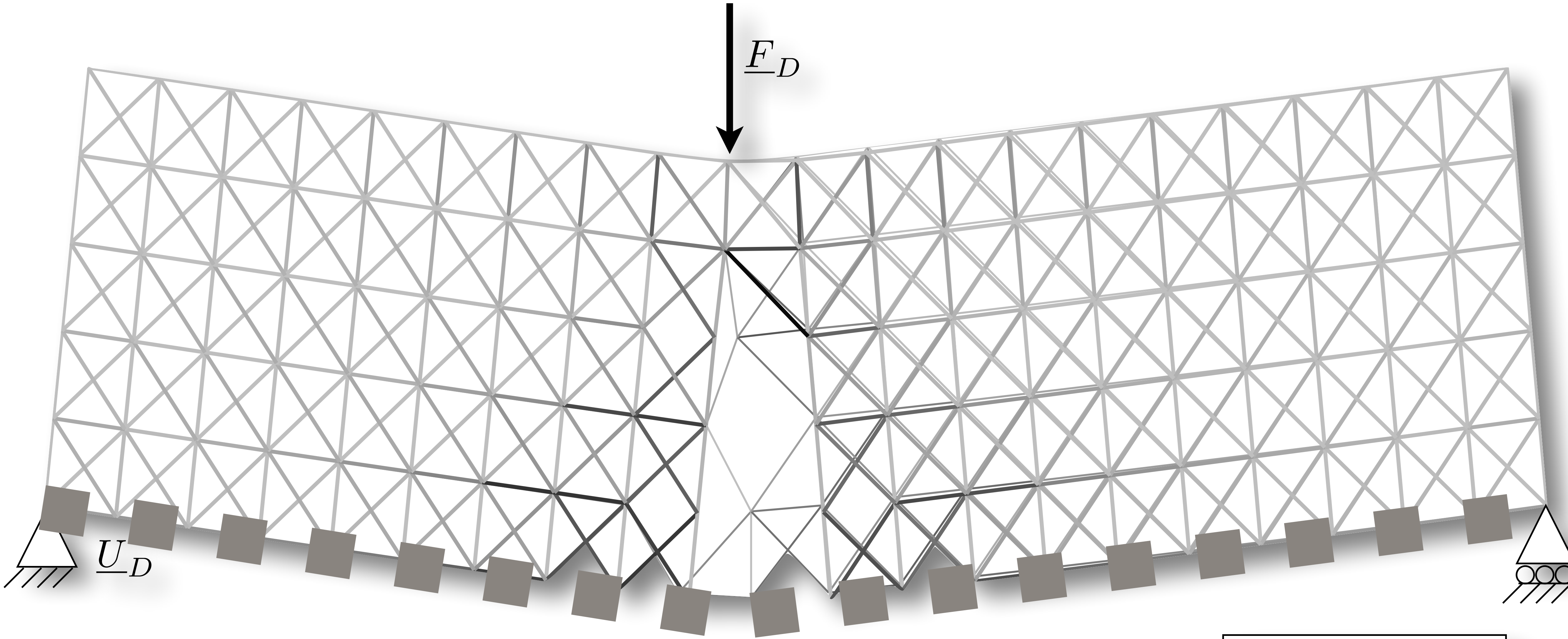


P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. *Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems*. Computer Methods in Applied Mechanics and Engineering, 200(5-8):850-866, 2011.

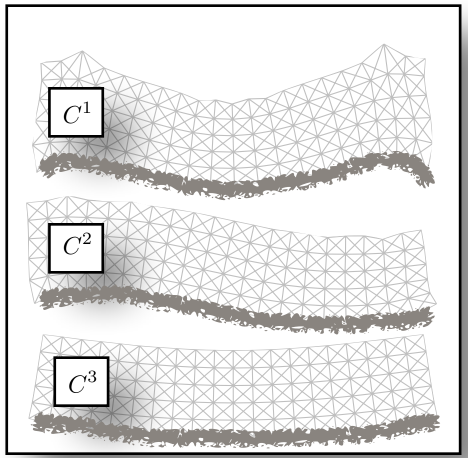


Smooth

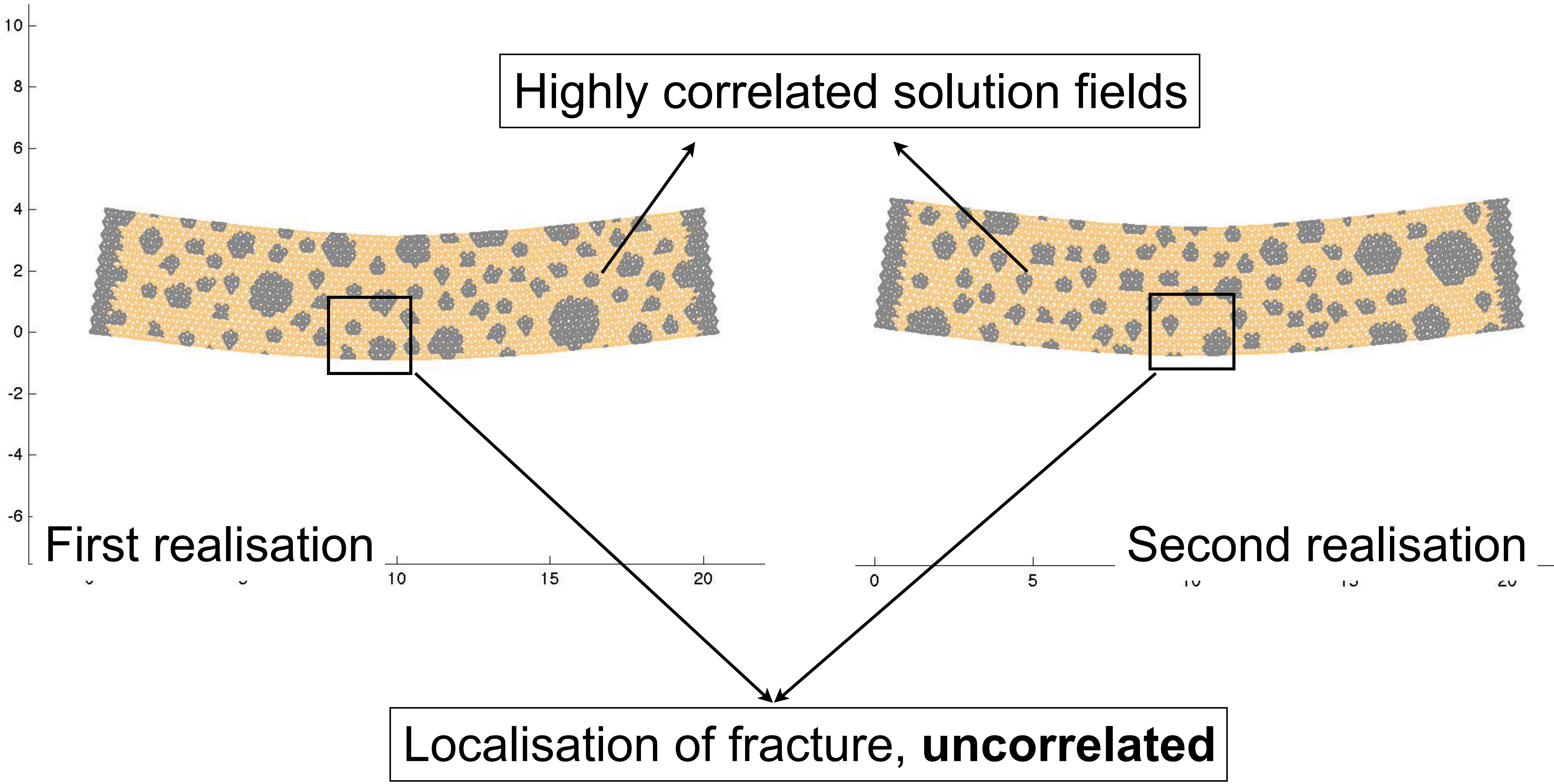
Kink



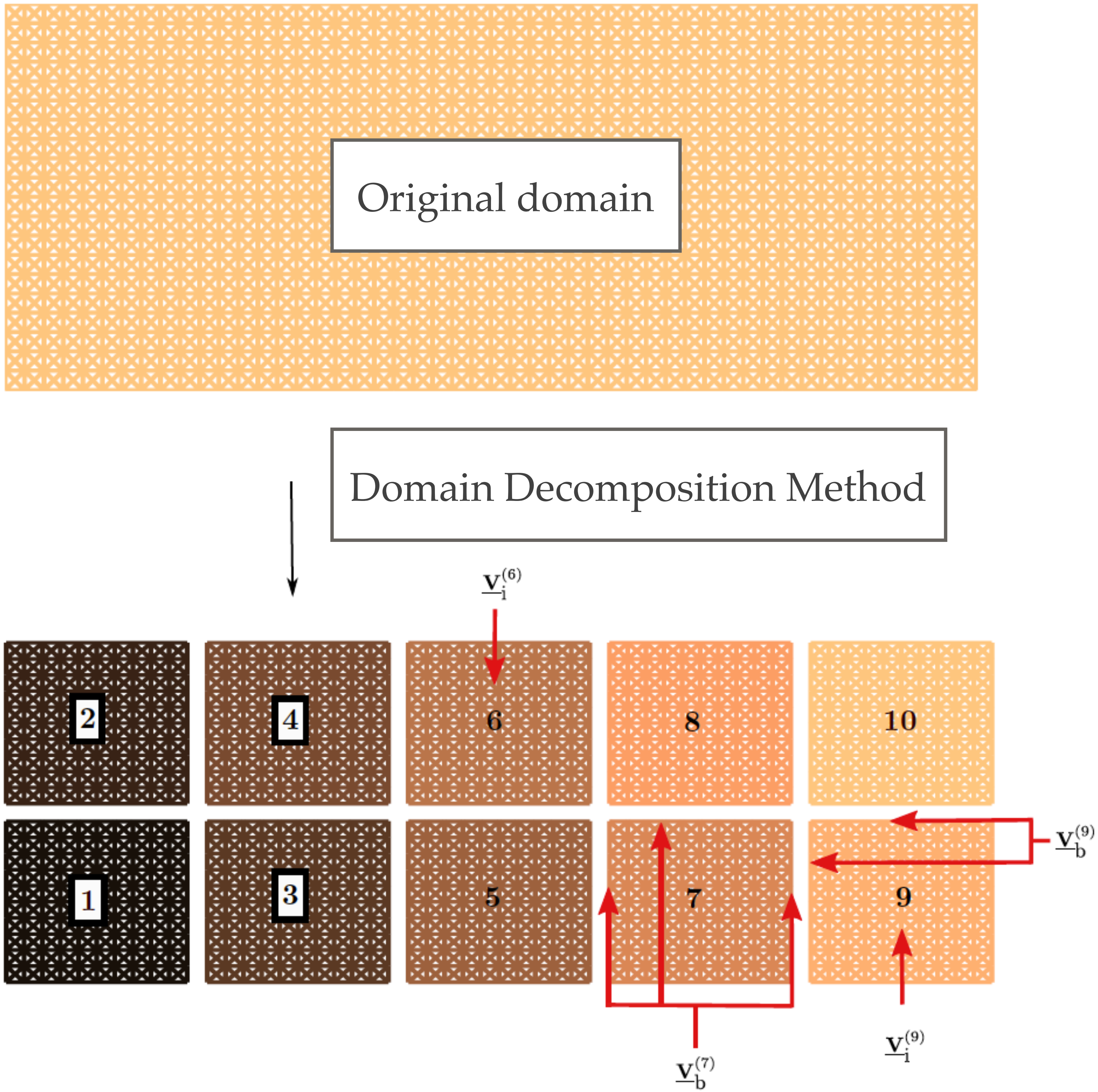
This solution is not in the snapshot !



Parametric / stochastic multiscale fracture mechanics



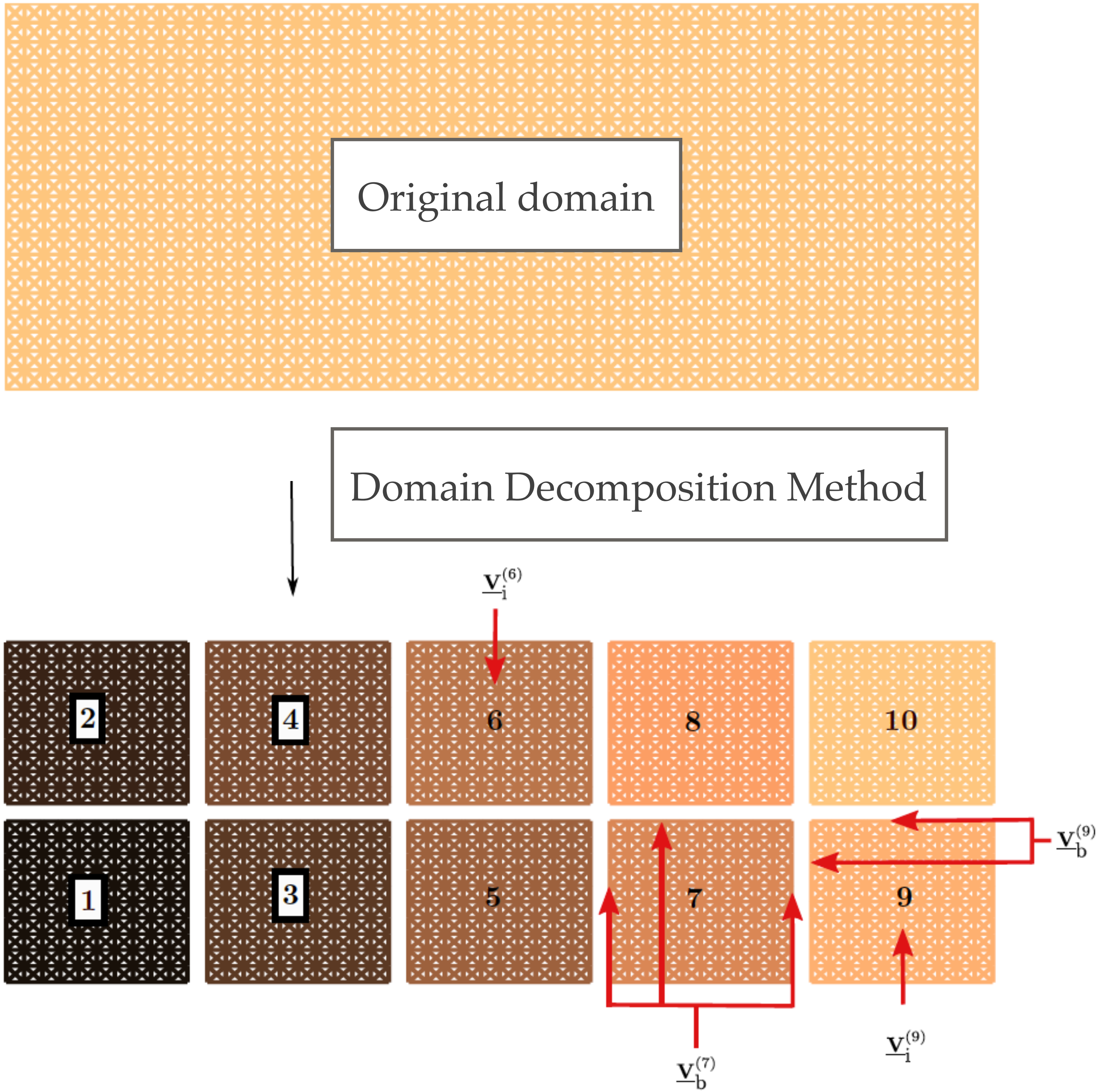
Partitioned POD/DDM

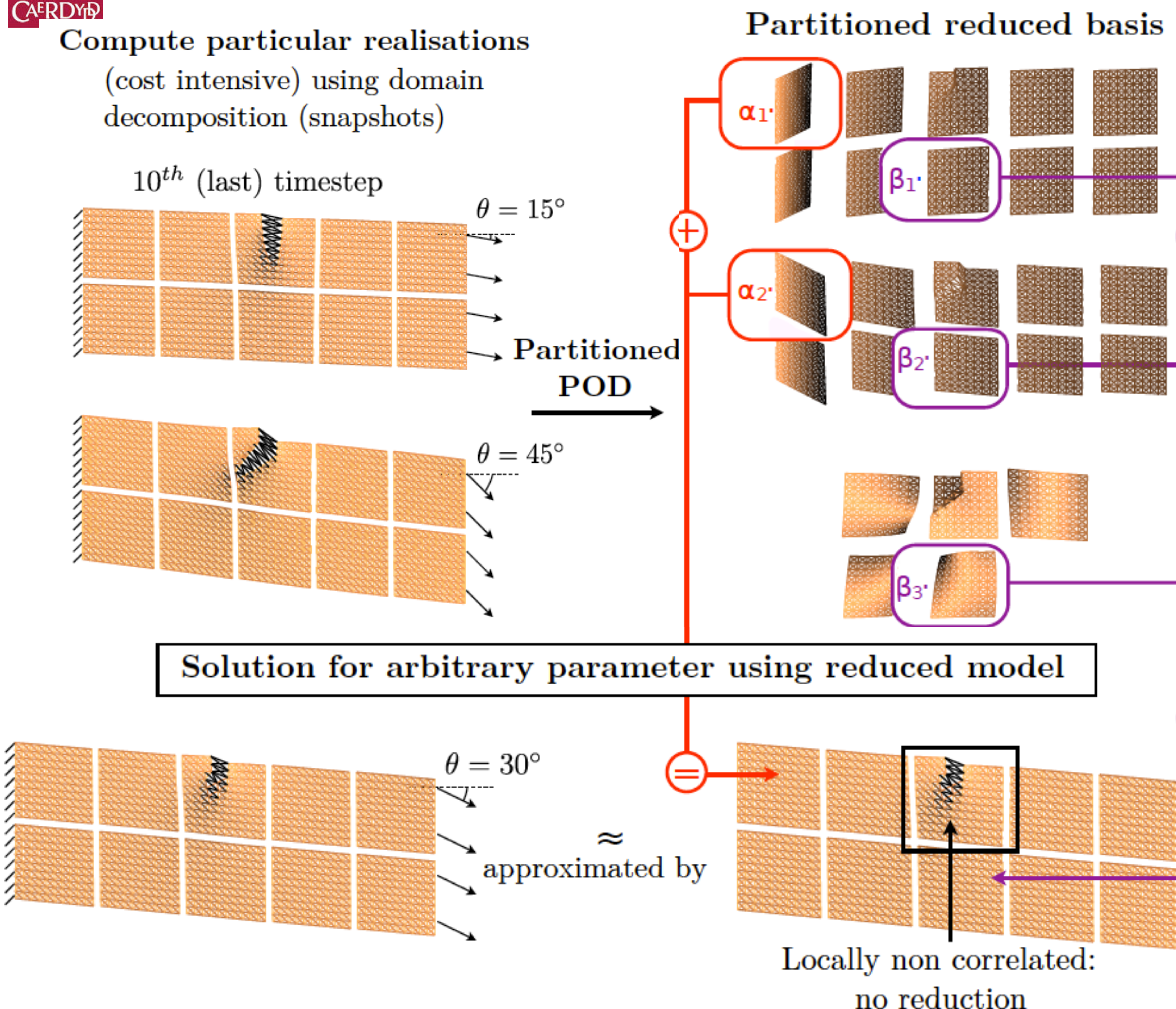


Partitioned POD/DDM

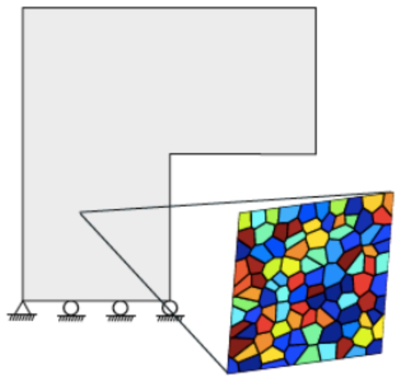
Domain Decomposition Method

Partitioned POD/DDM





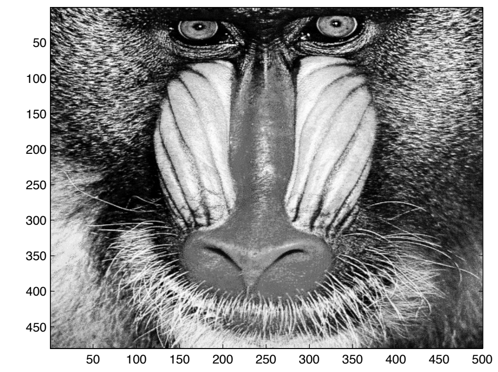
- Decompose the structure into subdomains
- Perform a reduction in the highly correlated region
- Couple the reduced to the non-reduced region by a primal Schur complement



Challenges

Reduce the problem size

Preserve essential features



Reduce computational expense - Control the error

Physics based model reduction a.k.a. **Multiscale Methods**	**Algebraic based model reduction** a.k.a. **Machine Learning**
Representative volume elements do not exist after the onset of fracture	**The problem is not reducible in the fracture process zone**
Adaptive Multi-scale Methods: hierarchical - semi-concurrent - concurrent	**Adaptive Domain Decomposition Proper Orthogonal Decomposition**

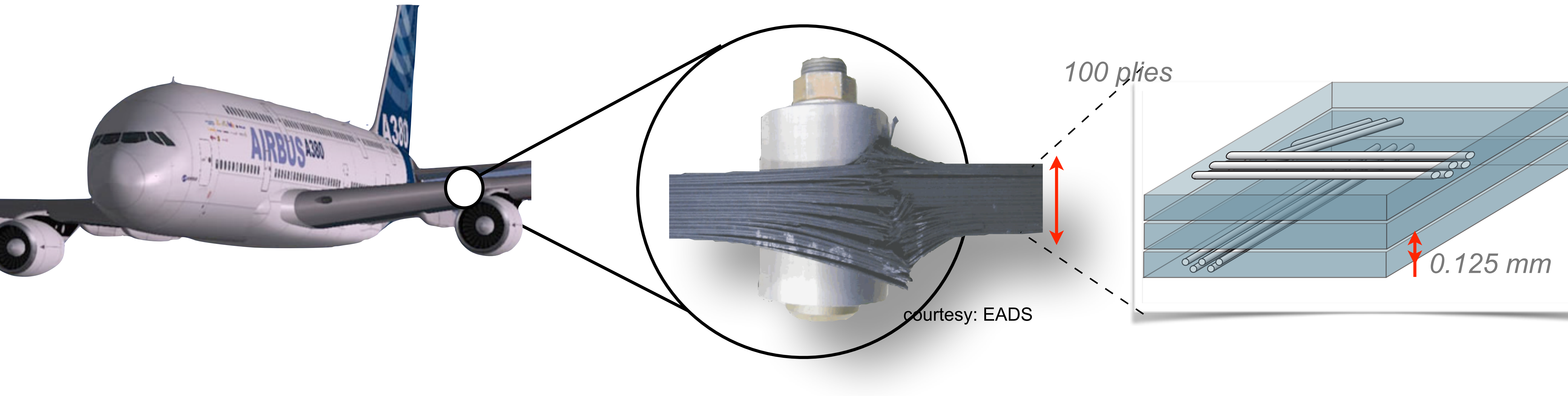
Open problems

- how to define the reduced area?

- precomputation time (offline)

Future?

Material complexity

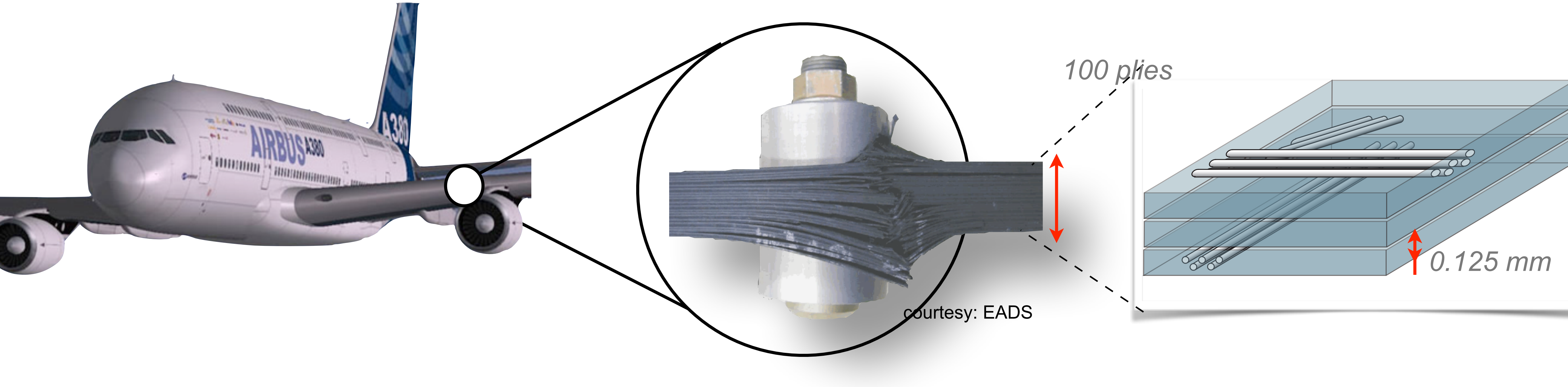


Heterogeneous & multi-functional materials

Can we optimise the material microstructure given macroscopic objective functions

Experiments required to attain sufficient confidence in their behavior are increasingly costly

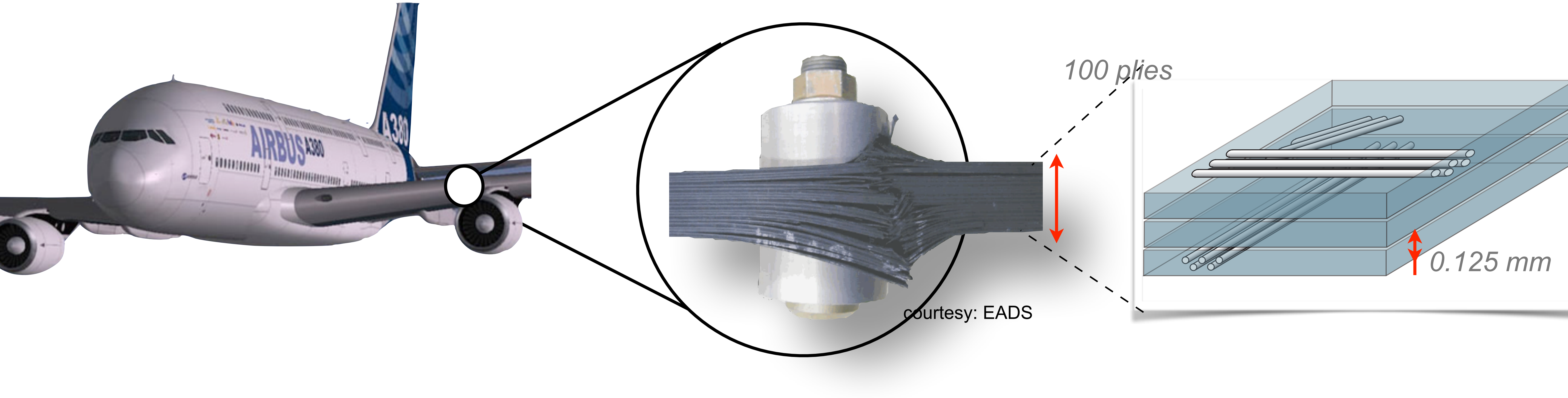
Material complexity



Factor-of-Safety or probabilistic based methods cannot handle unknown unknowns

Lack of similitude between testing (experimental) and operating conditions — also encountered in geophysics, medicine…

Challenges



- Move **away from heuristics** and experience-based engineering
- Develop **fundamental understanding** of physical processes (degradation, …)

Digital twin concept

Actual aircraft	**Digital aircraft model**
Life prediction and extension	Situation awareness
High fidelity modeling and simulation	Certification and design methods

Requires real-time data assimilation, and model update…

Parallel with medicine

Mechanics

Macro (wing) - Micro (carbon fibres)

Environmental effects (Temperature, irradiation…)

Experimental condition dissimilarities

Medicine

Macro (Body, Physiology) to micro (microbes, needle/ scalpel…)

Patient’s environment, living conditions, habits…

Organ properties depend strongly on age, gender, …

Medicine

The average drug developed by a major pharmaceutical company costs at least $4 billion, and it can be as much as $11 billion.

Mechanics

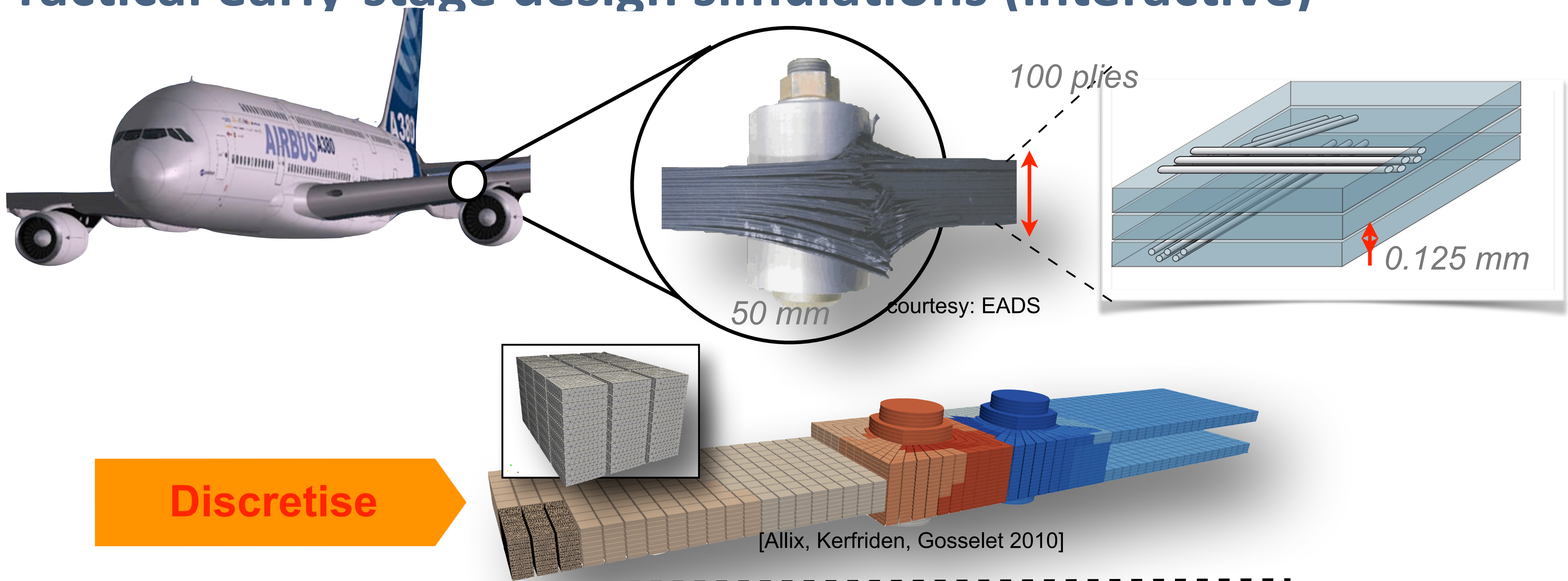
The development cost of the A380

11 billion euros…

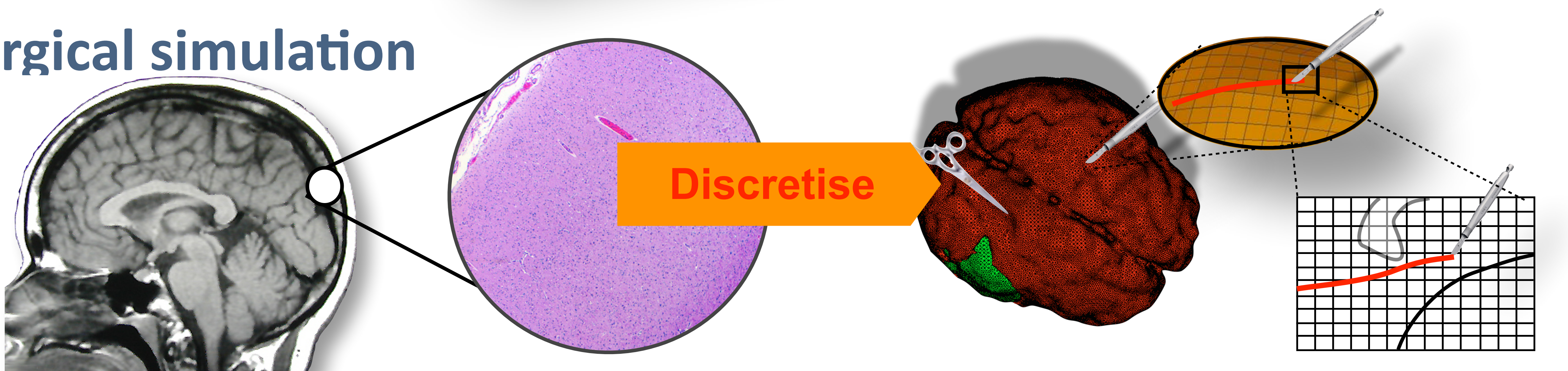
of the dreamliner… $32 billion

Patient/plane-specific simulation

Practical early-stage design simulations (interactive)



Surgical simulation



- Reduce the problem size while controlling the error (in QoI) when solving very large (multiscale) mechanics problems

CARDIFF UNIVERSITY
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thanks for your attention

Partners and Funding

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EPSRC
Pioneering research and skills

Fonds National de la Recherche Luxembourg

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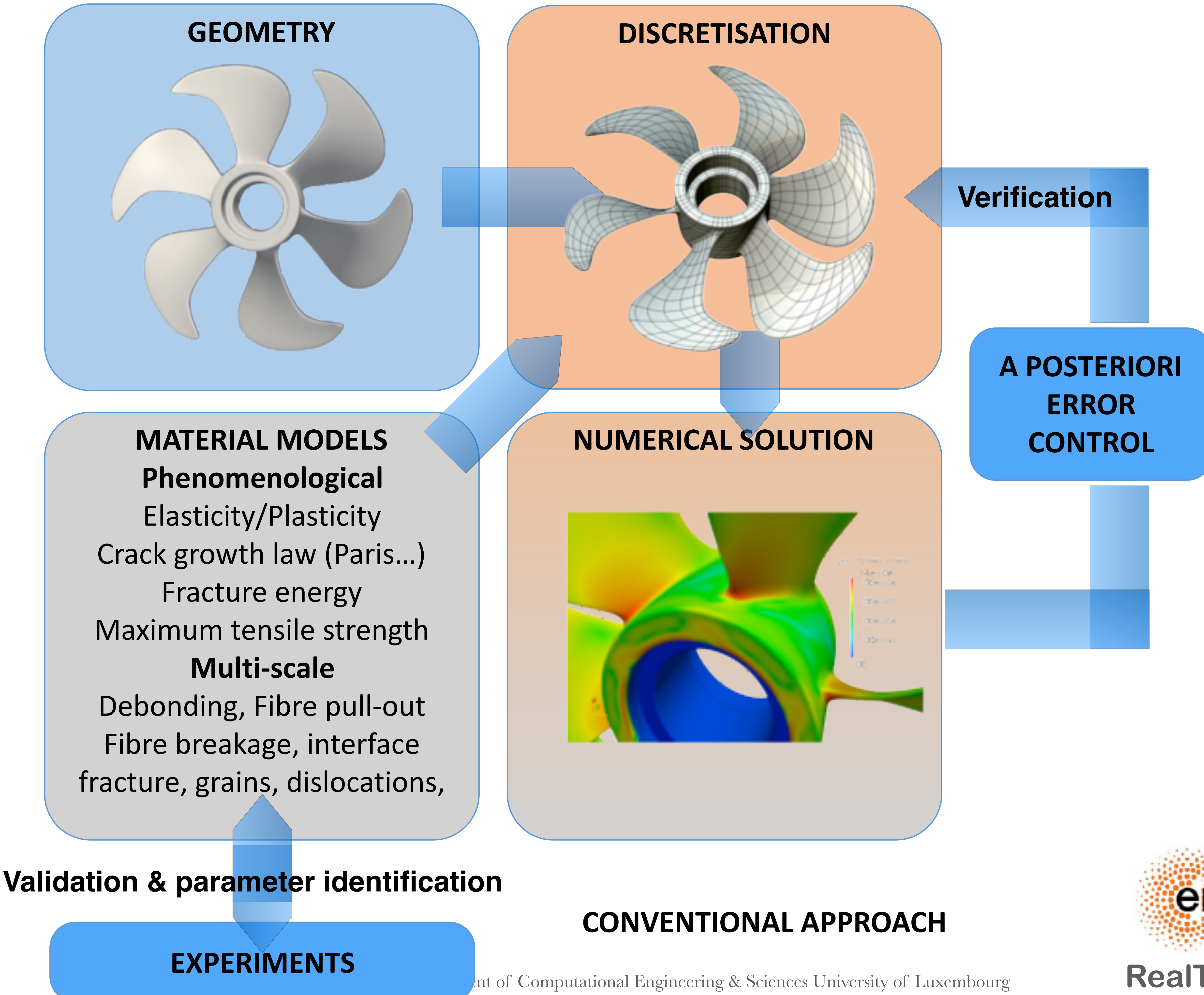
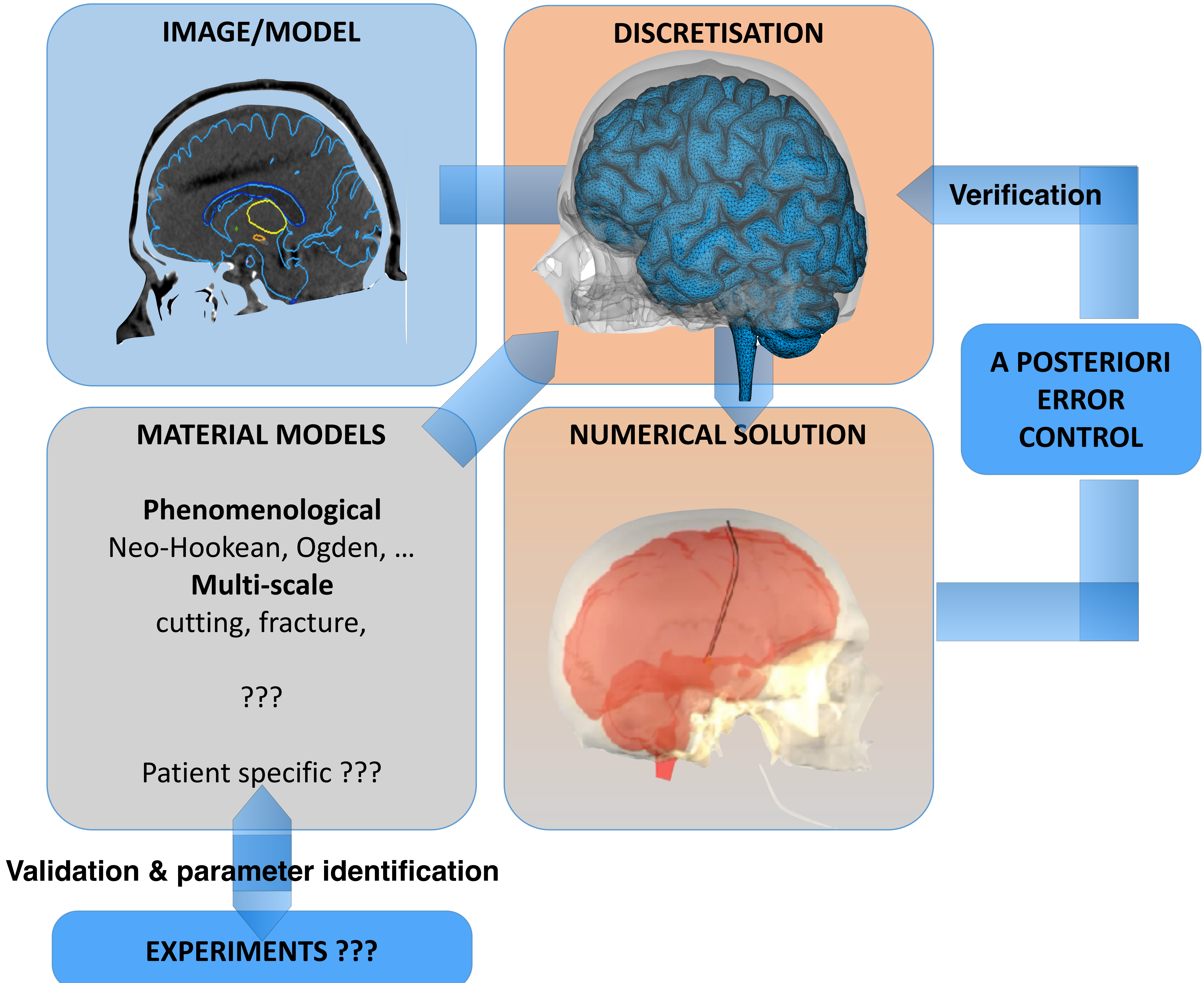
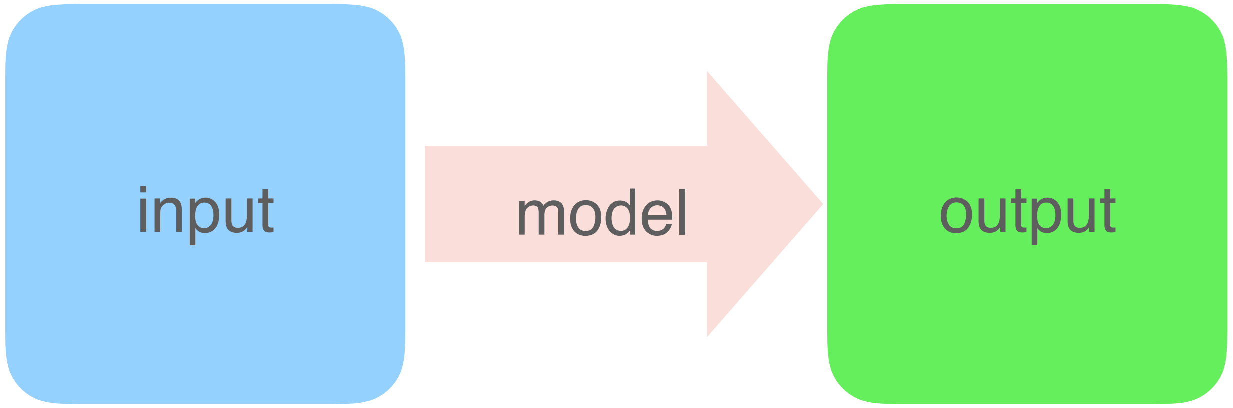

GEOMETRY
DISCRETISATION
Verification
A POSTERIORI ERROR CONTROL
MATERIAL MODELS
Phenomenological
Elasticity/Plasticity
Crack growth law (Paris…)
Fracture energy
Maximum tensile strength
Multi-scale
Debonding, Fibre pull-out
Fibre breakage, interface
fracture, grains, dislocations,
NUMERICAL SOLUTION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


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

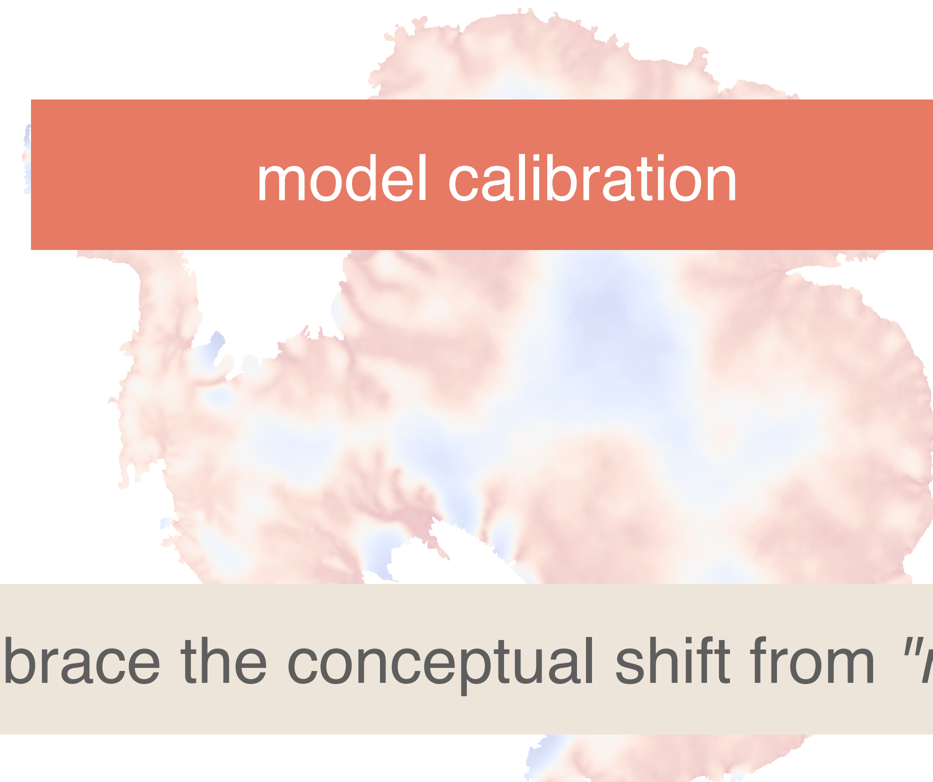
Data-driven Modelling



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

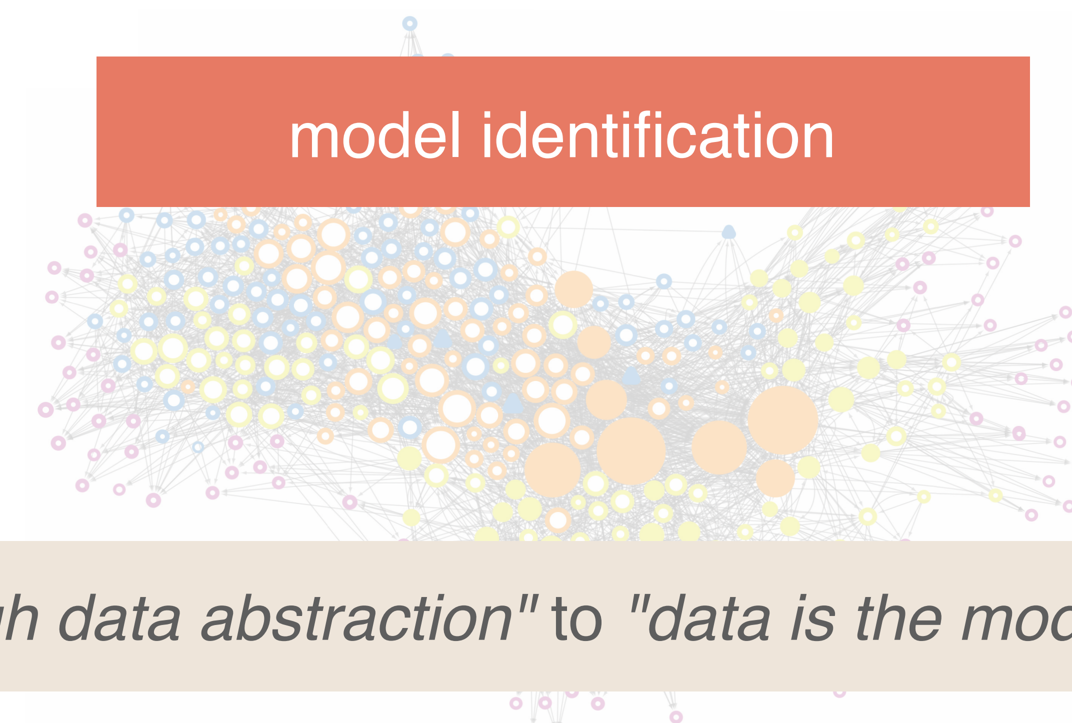
The structure of *f* is known but its parameters are not.

model calibration



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

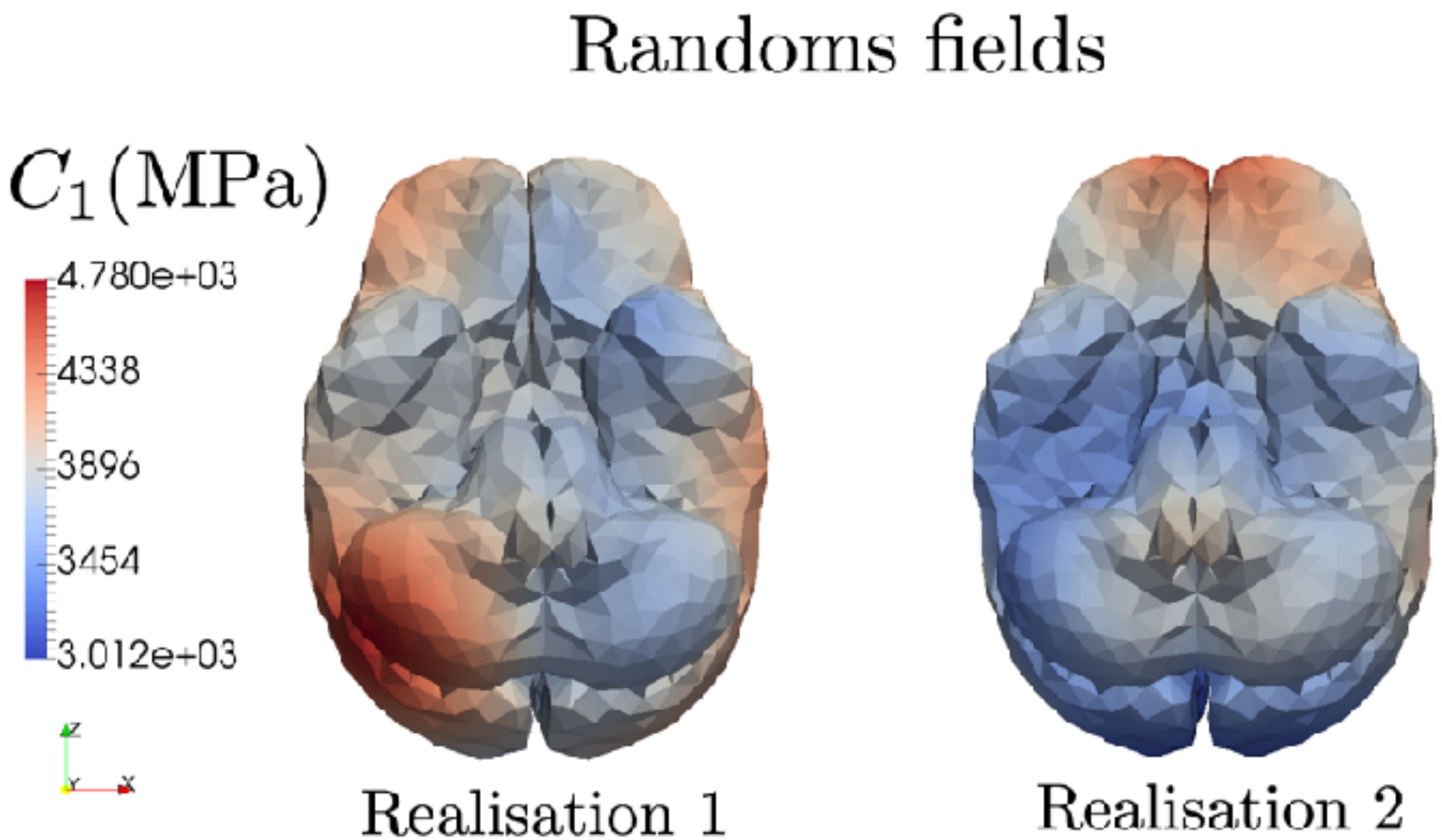
model identification



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

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

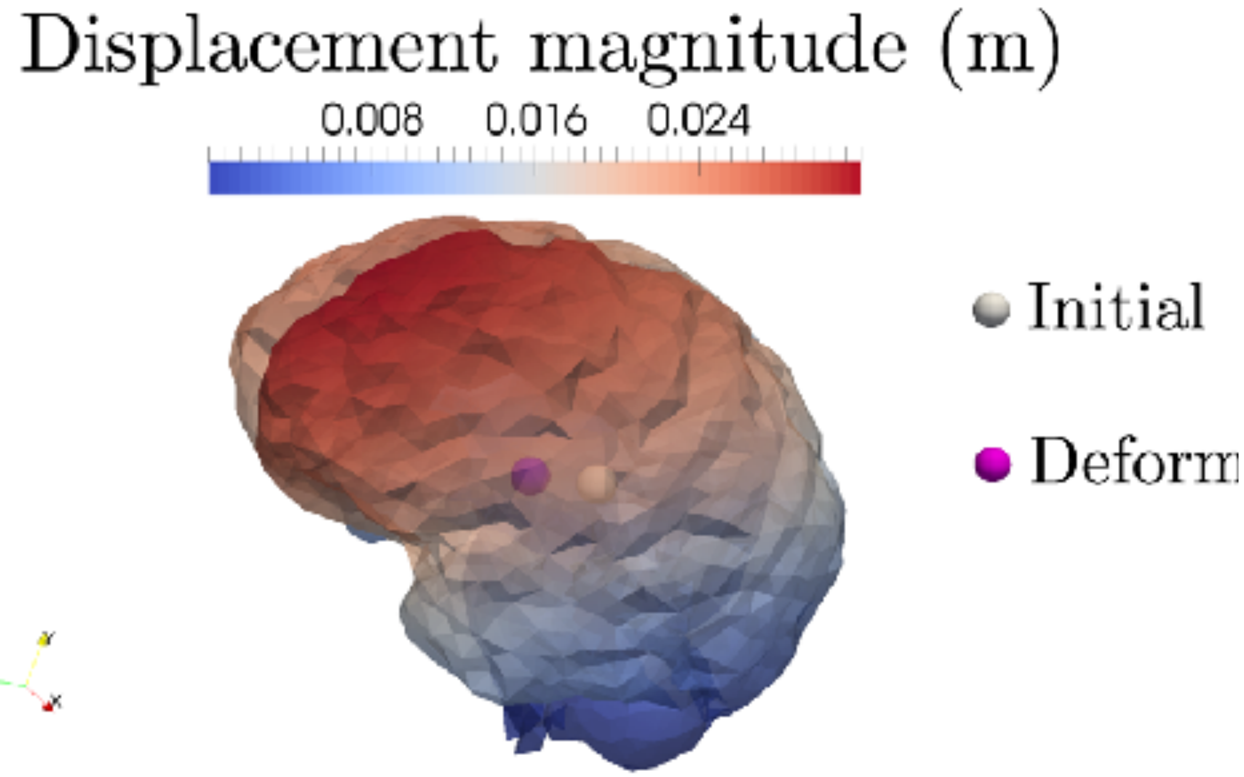
- Different methods: Karhunen–Loève expansion [Adler 2007], Fast Fourier transform [Nowak 2004].

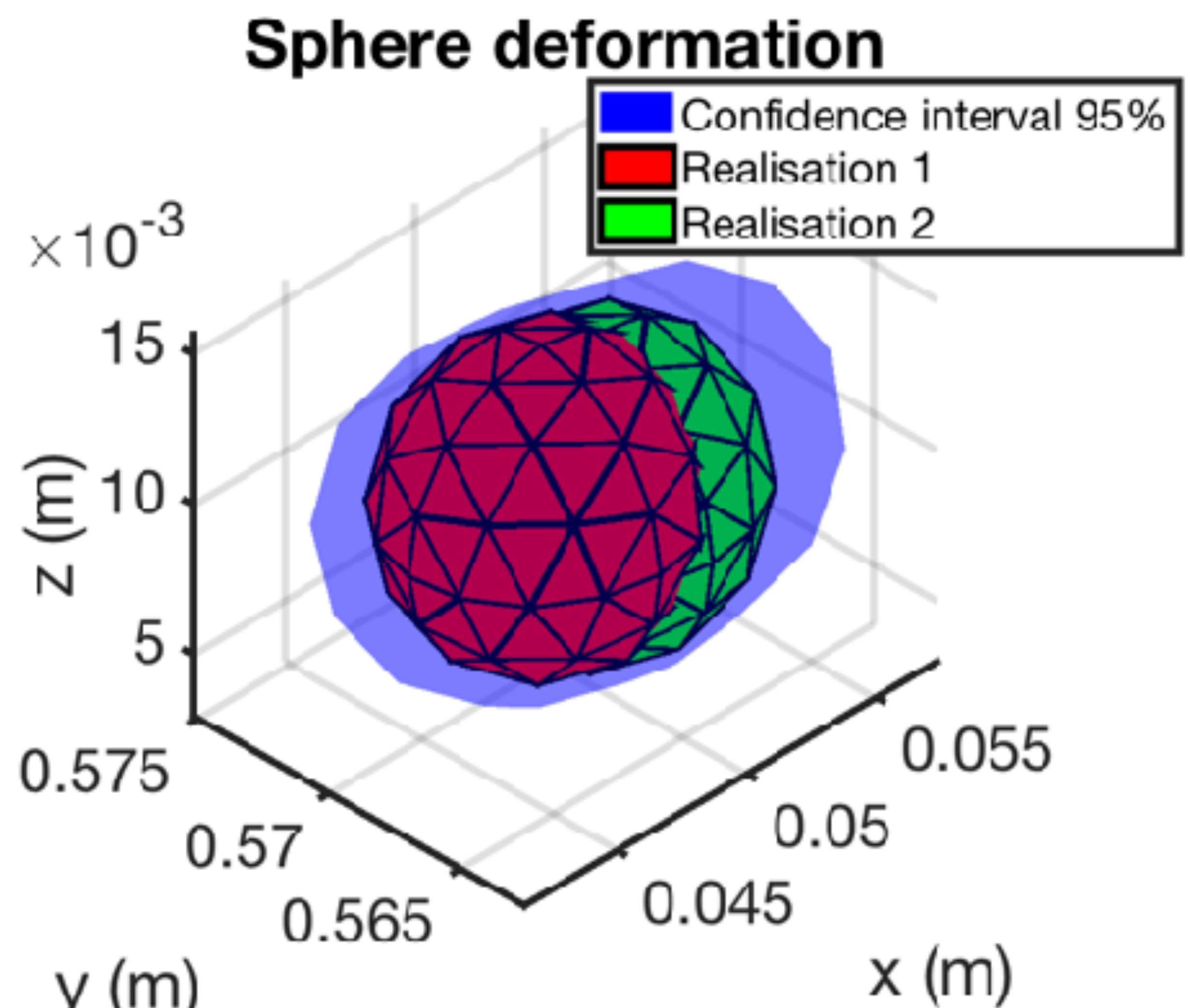


Two realisations of RF, with a log-normal distribution, for the parameter C_1 (in MPa).

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

Confidence level in predicting the target location

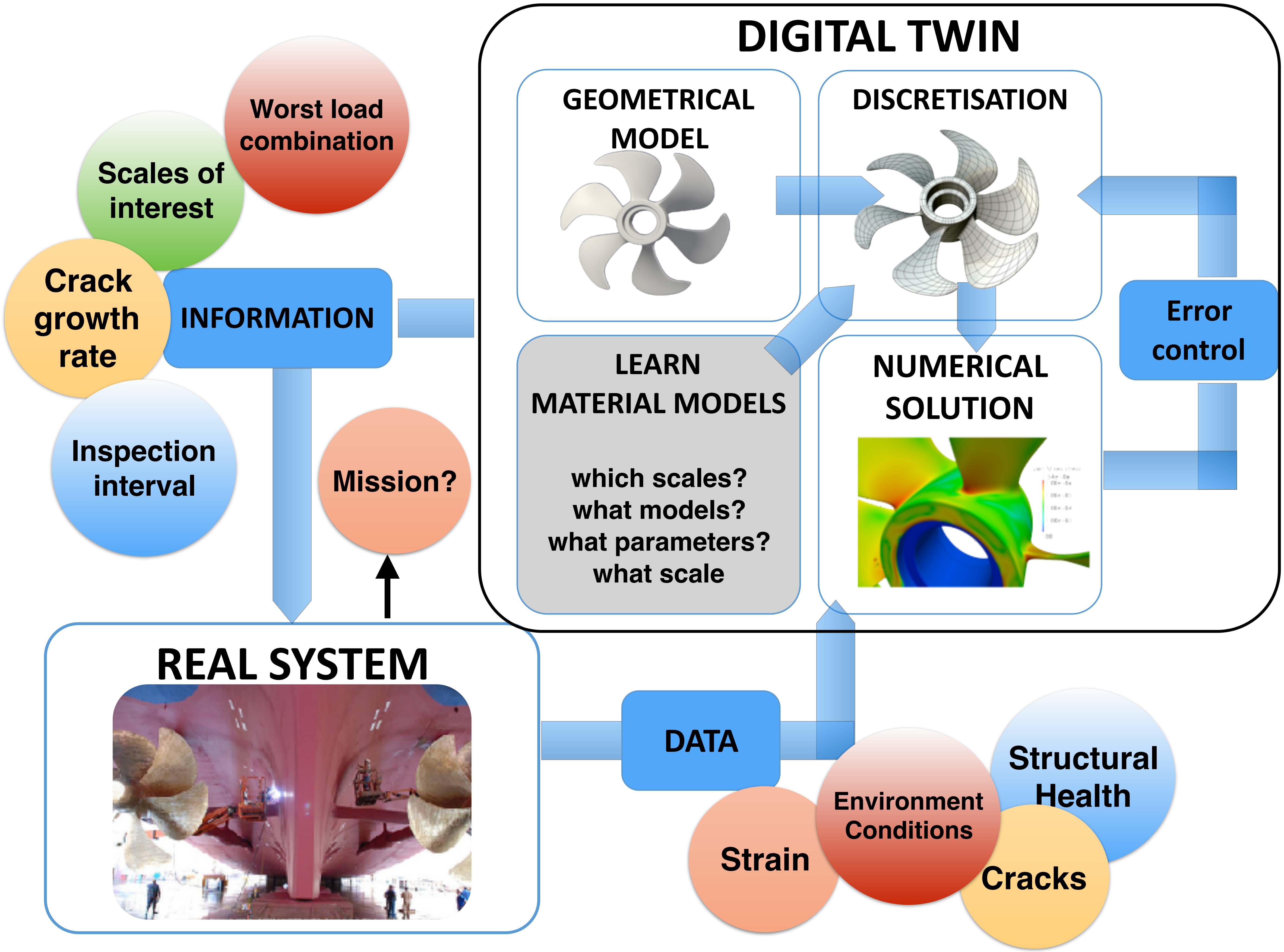


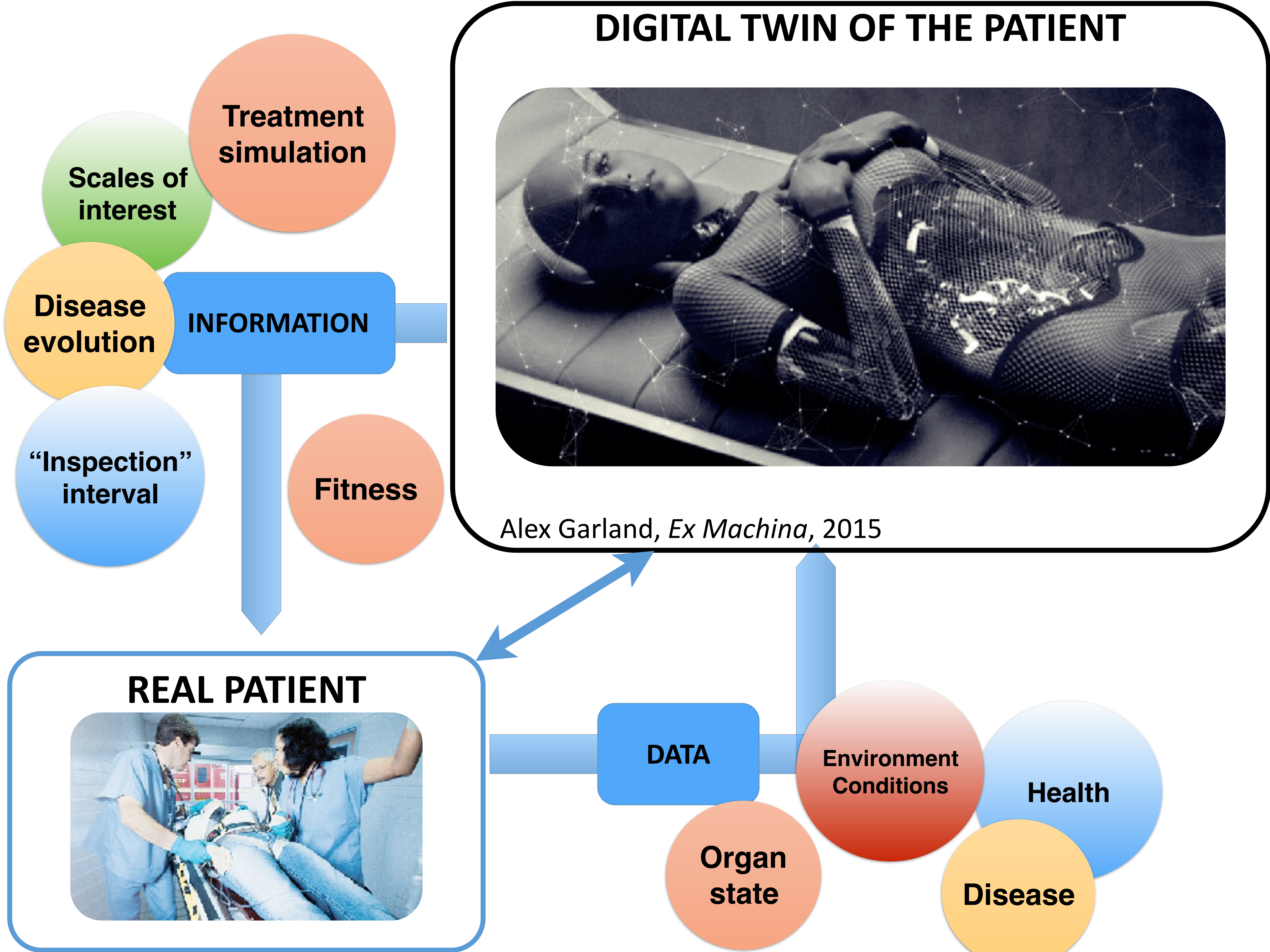


What is the influence of material parameters on computed quantities of interest?

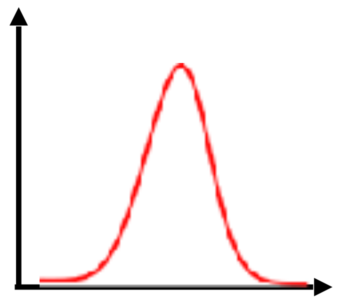
RealTCut

Possible approach

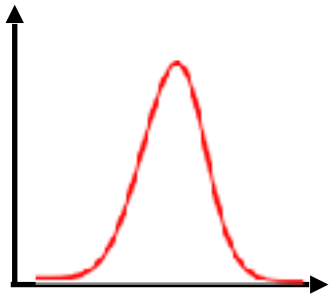



DIGITAL TWIN OF THE PATIENT
Alex Garland, Ex Machina, 2015
Treatment simulation
Scales of interest
Disease evolution
INFORMATION
"Inspection" interval
Fitness
REAL PATIENT
DATA
Environment Conditions
Health
Organ state
Disease

Prior Knowledge



Prior Knowledge



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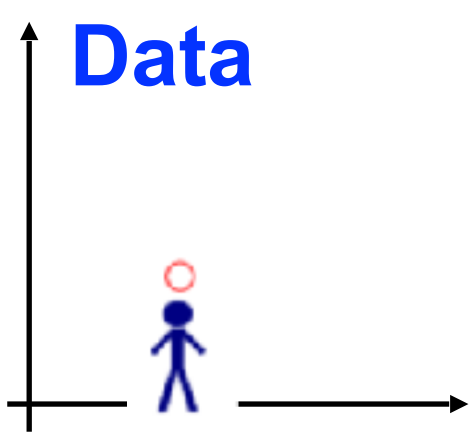
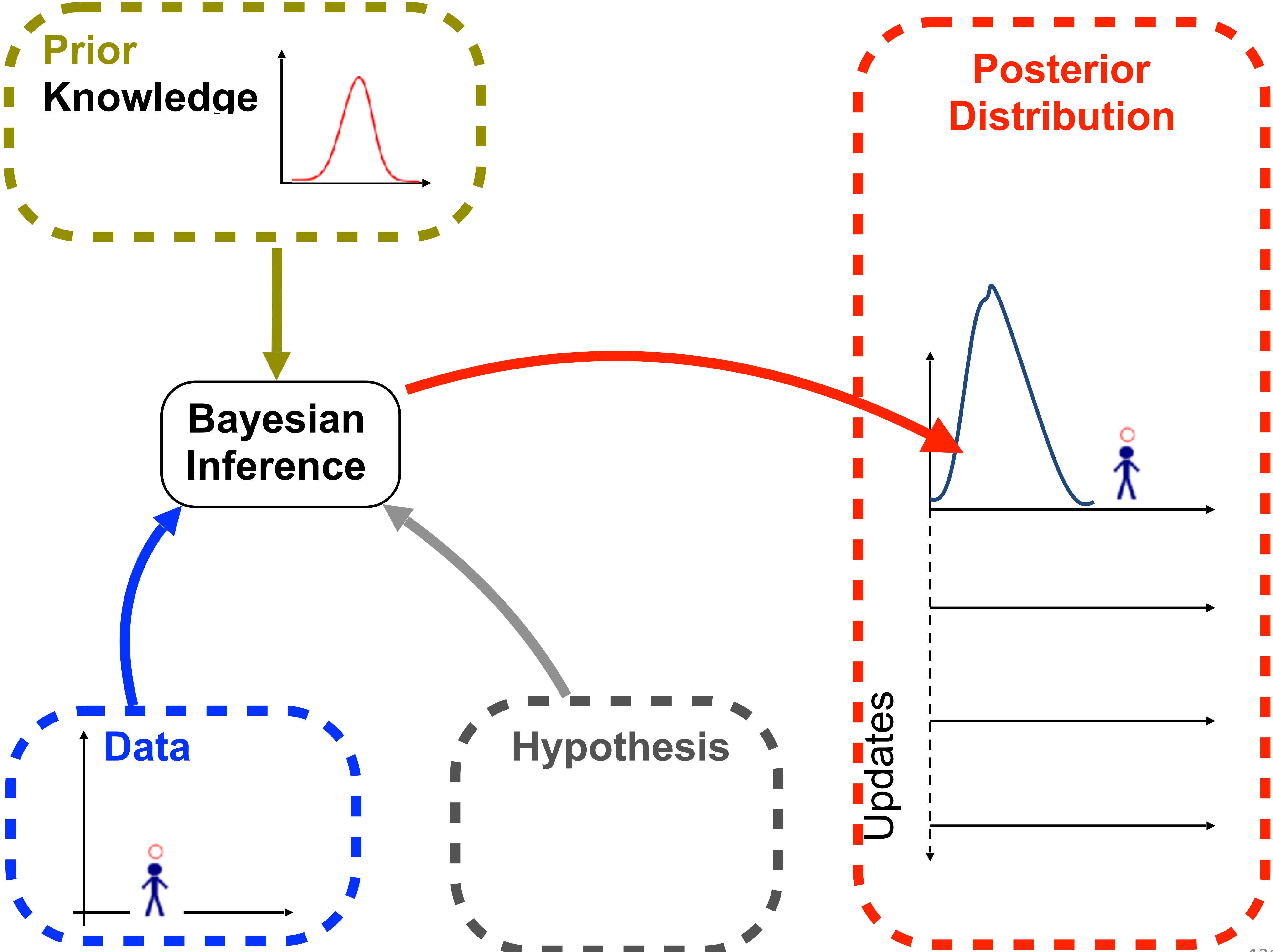


Hypothesis



Prior
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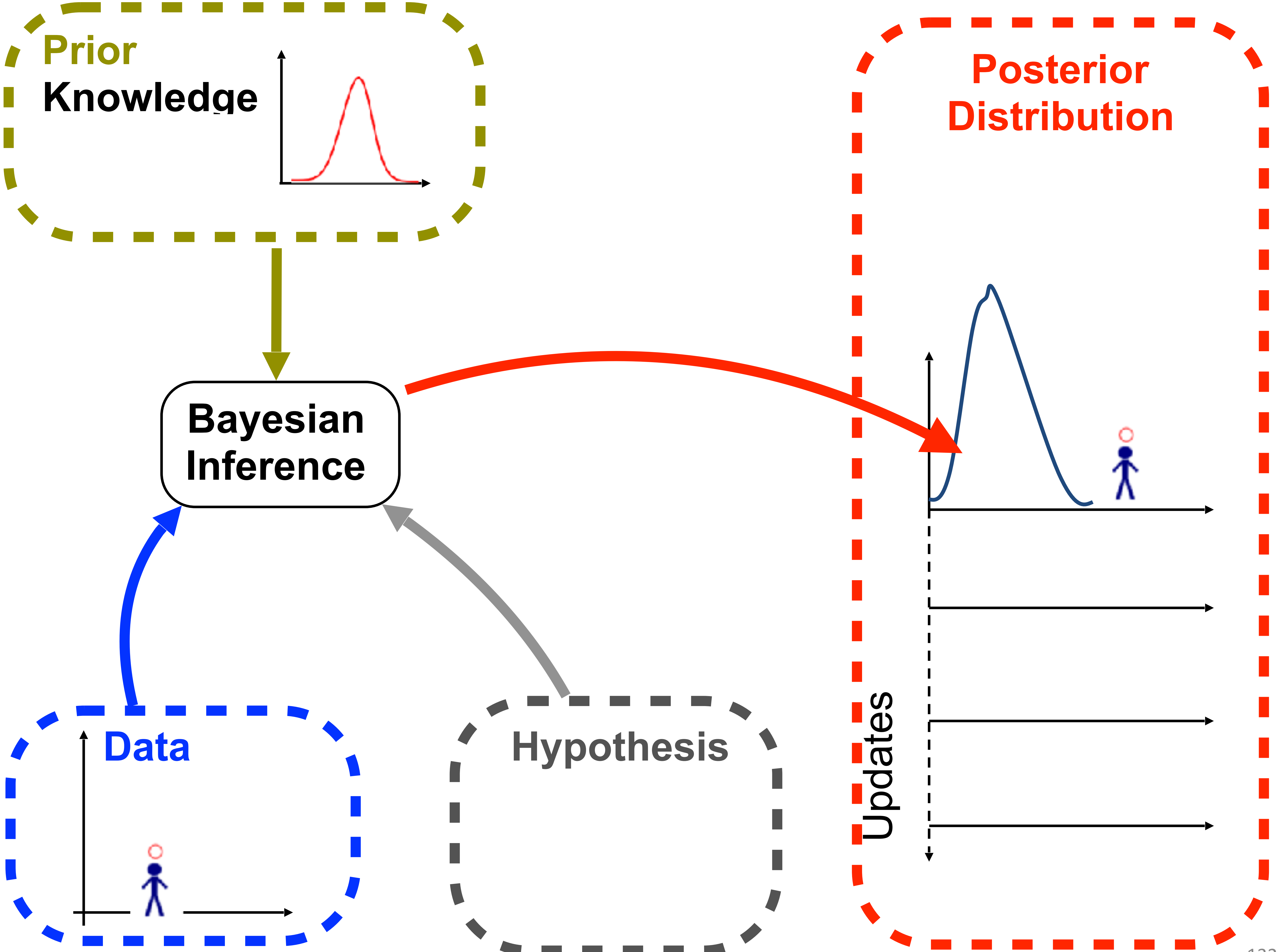
Bayesian
Inference
Posterior
Distribution
Updates
Data
Hypothesis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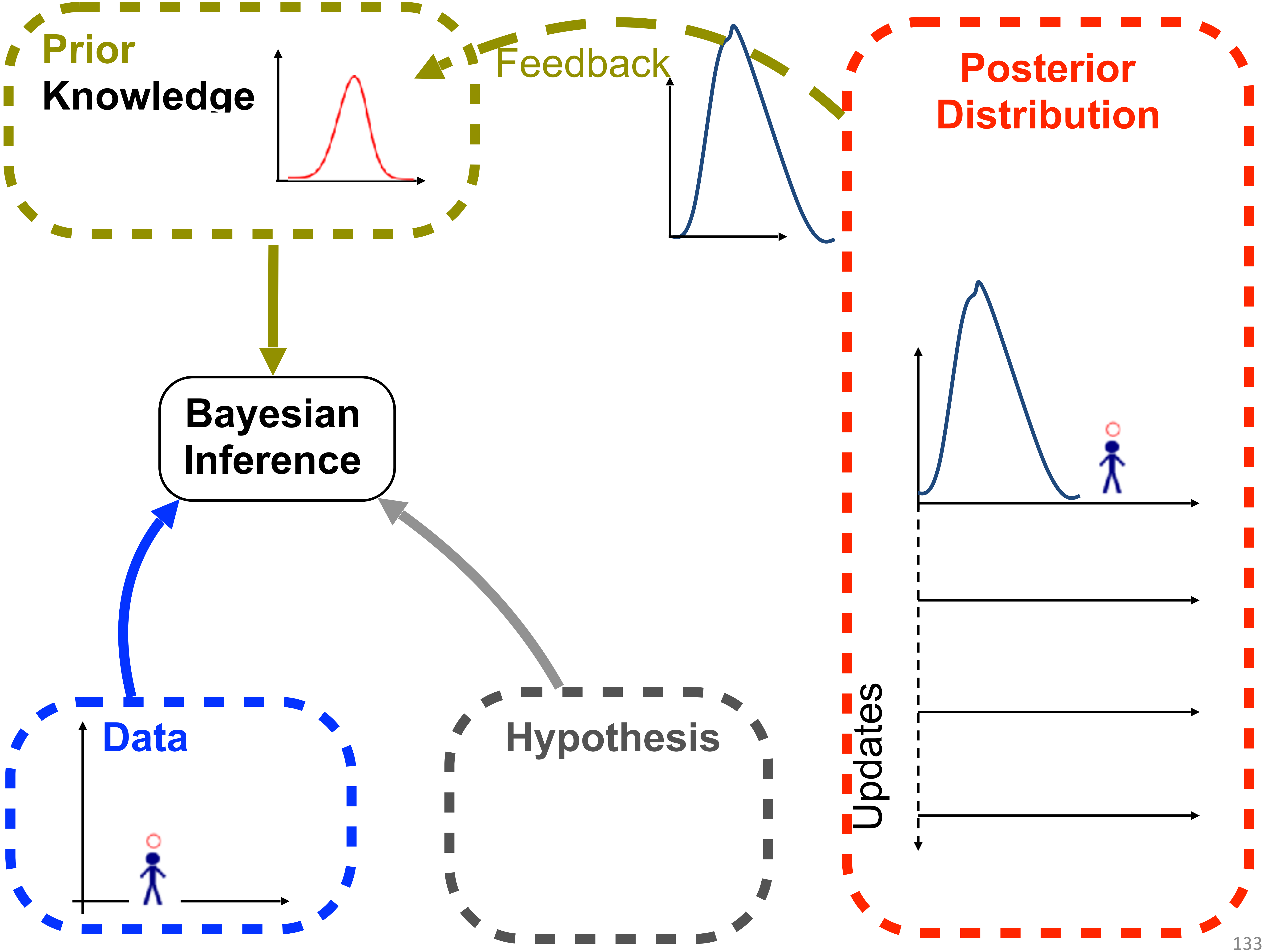
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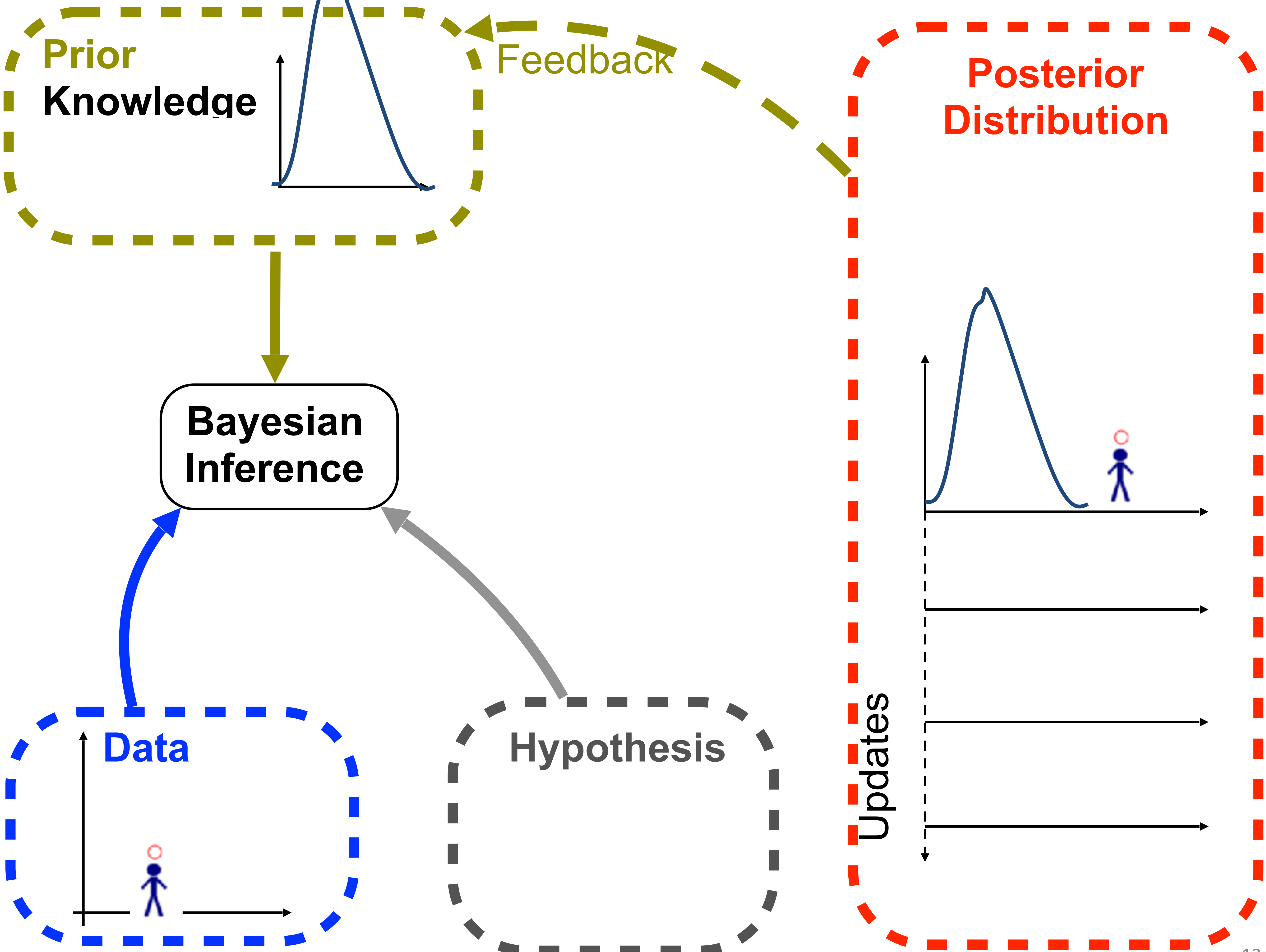

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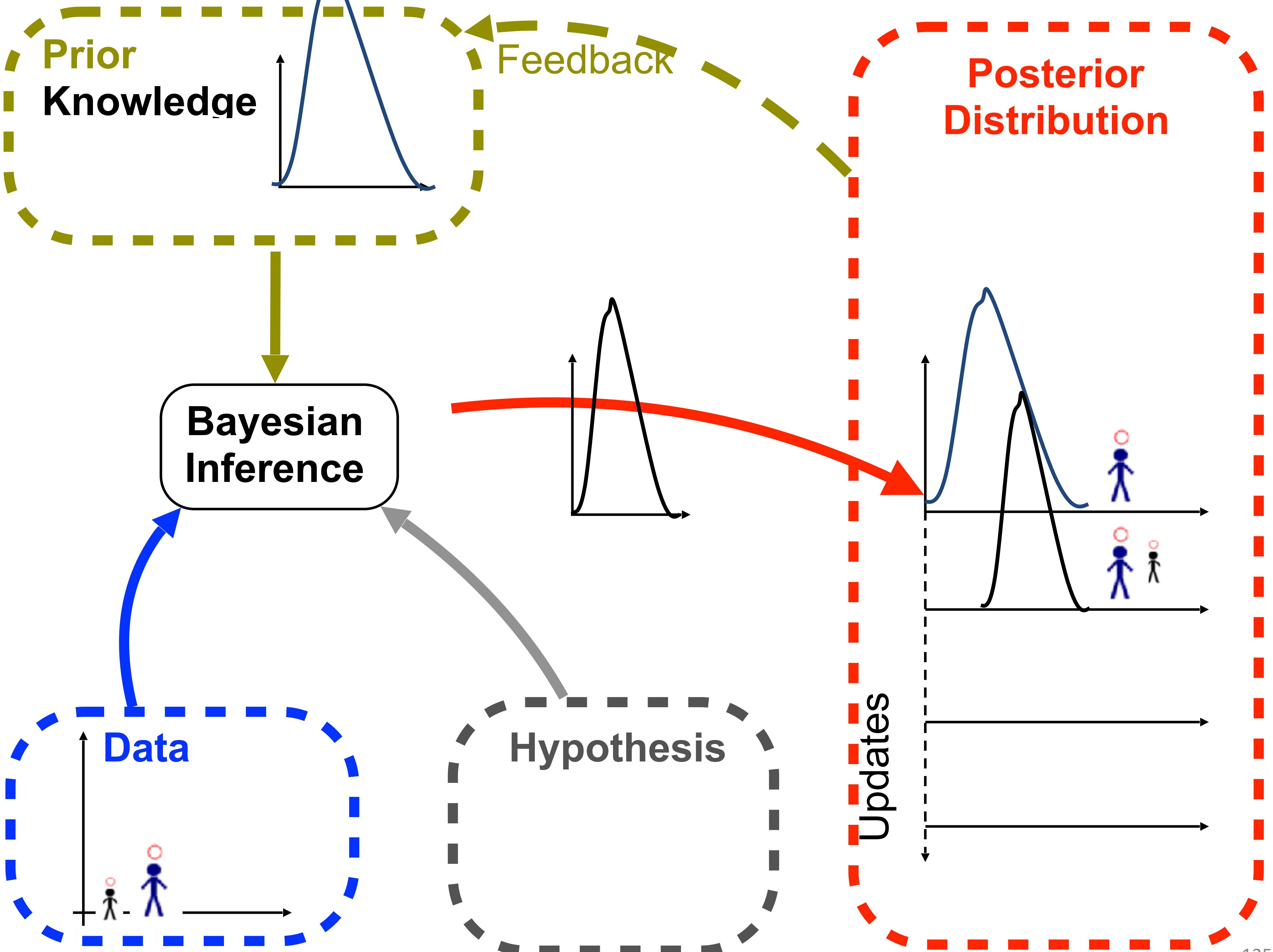

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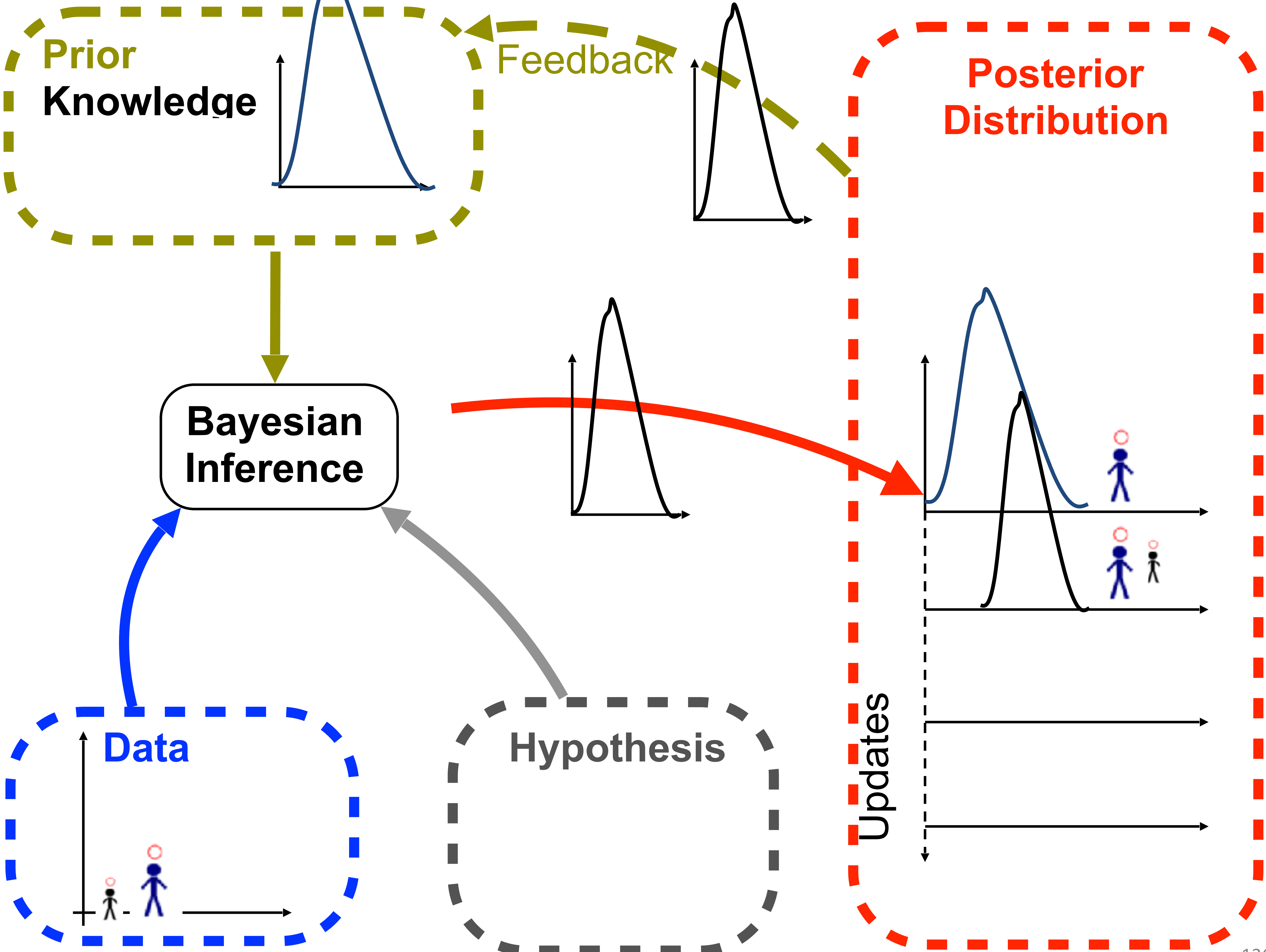

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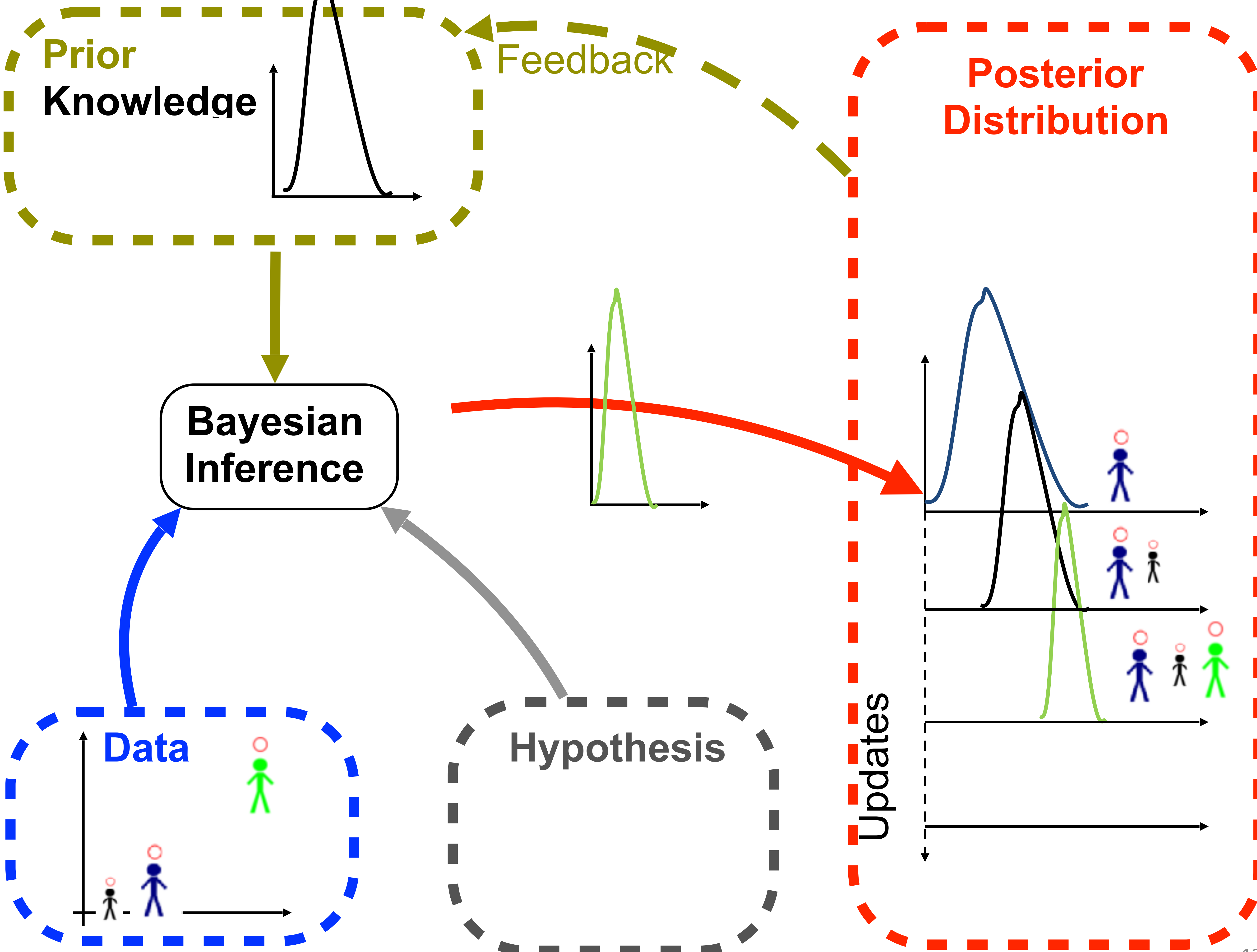

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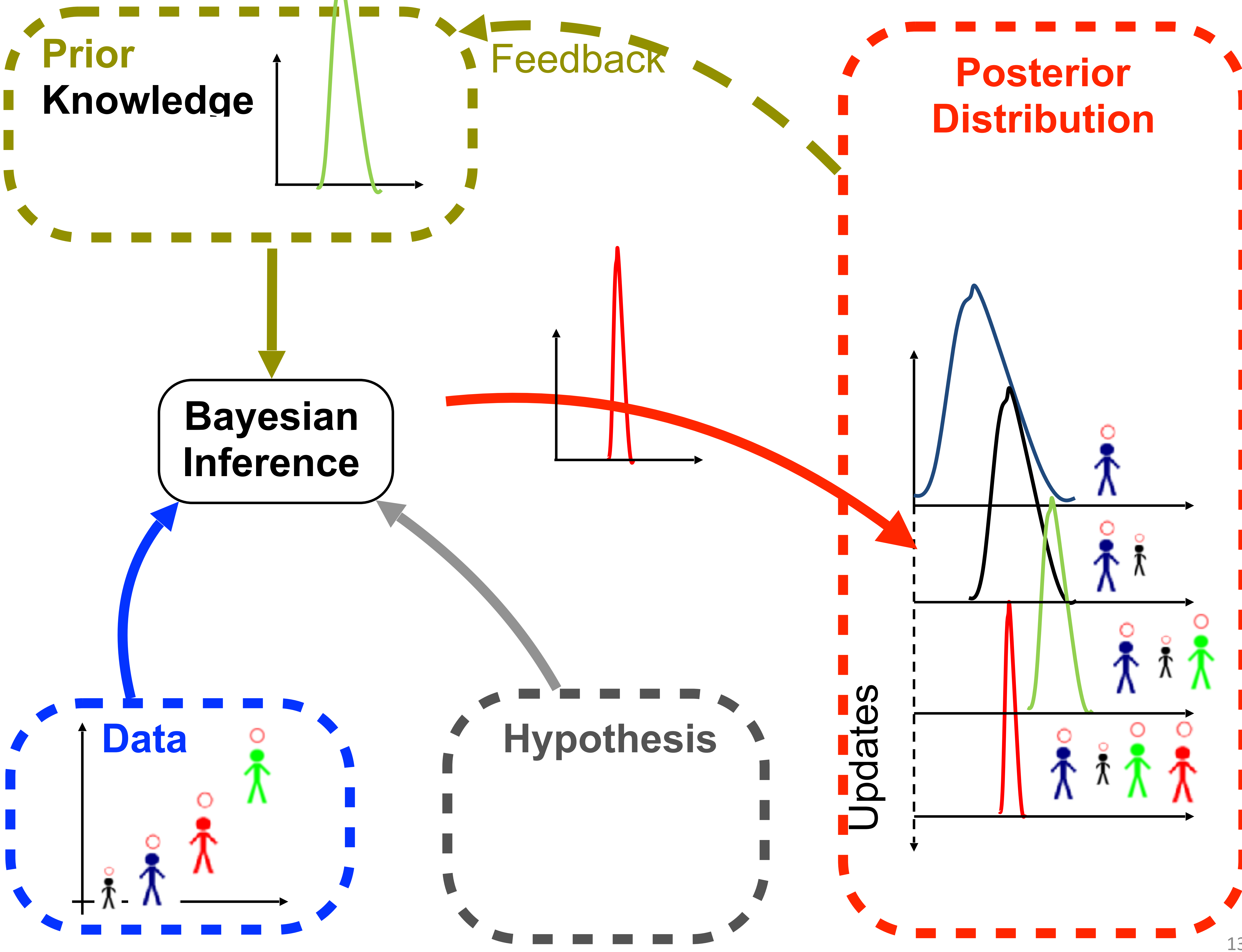
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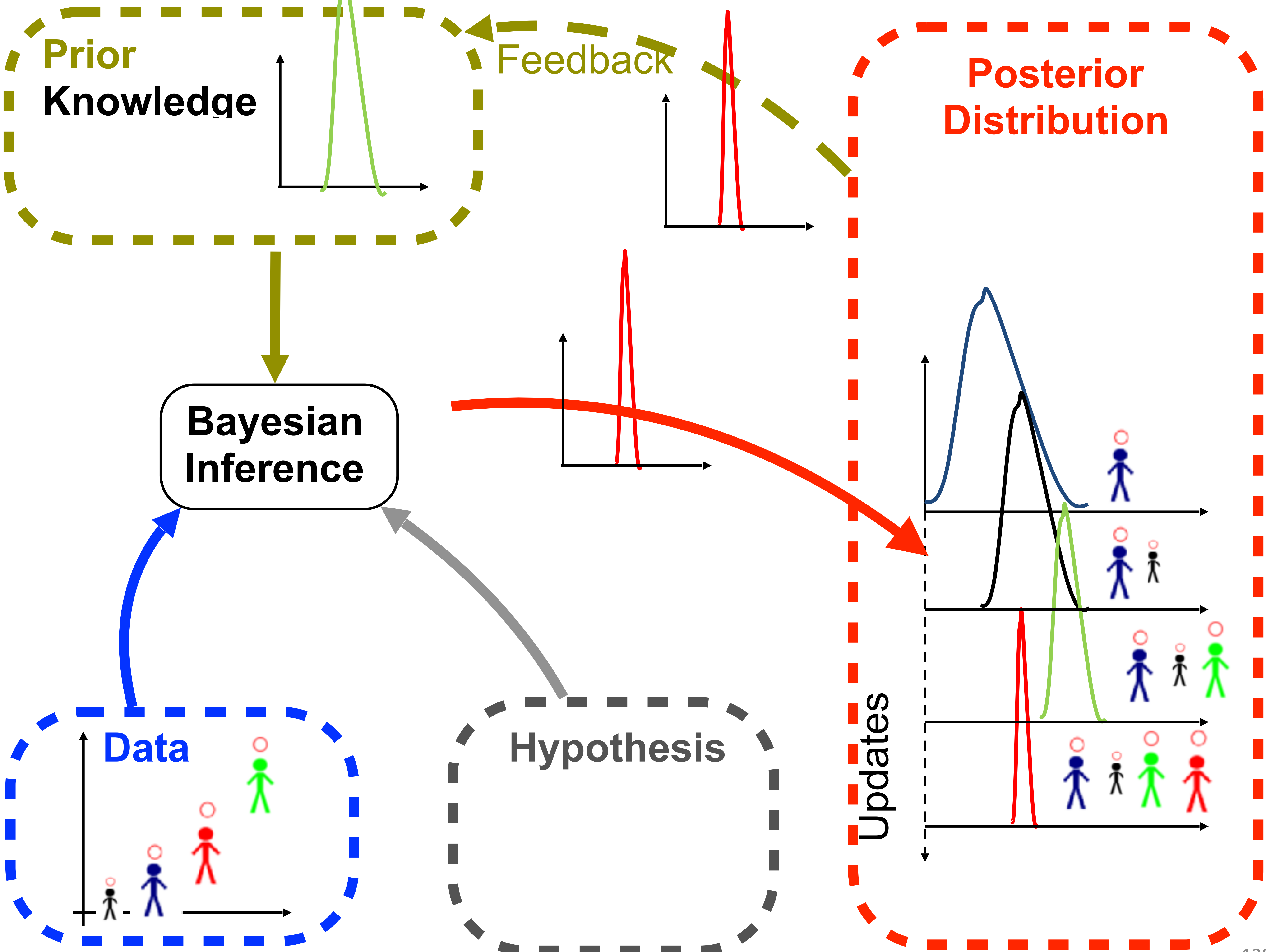
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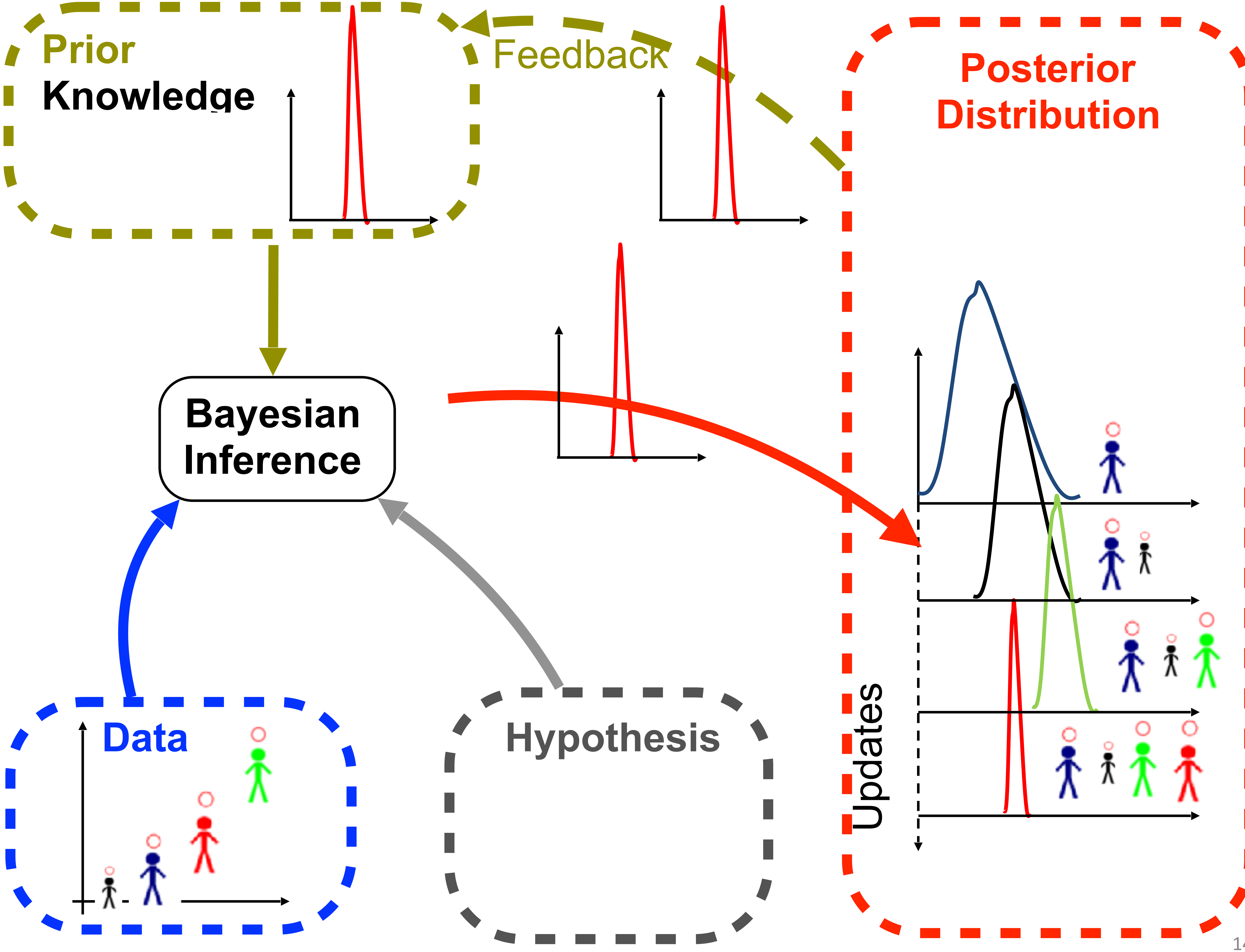
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