Faculty of Sciences,
Technology
and Communication

Multi-scale Computational Mechanics

industrial applications

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Motivation understand and optimise material durability

Multi-scale **Methods** - two approaches compared

Industrial and Clinical Applications

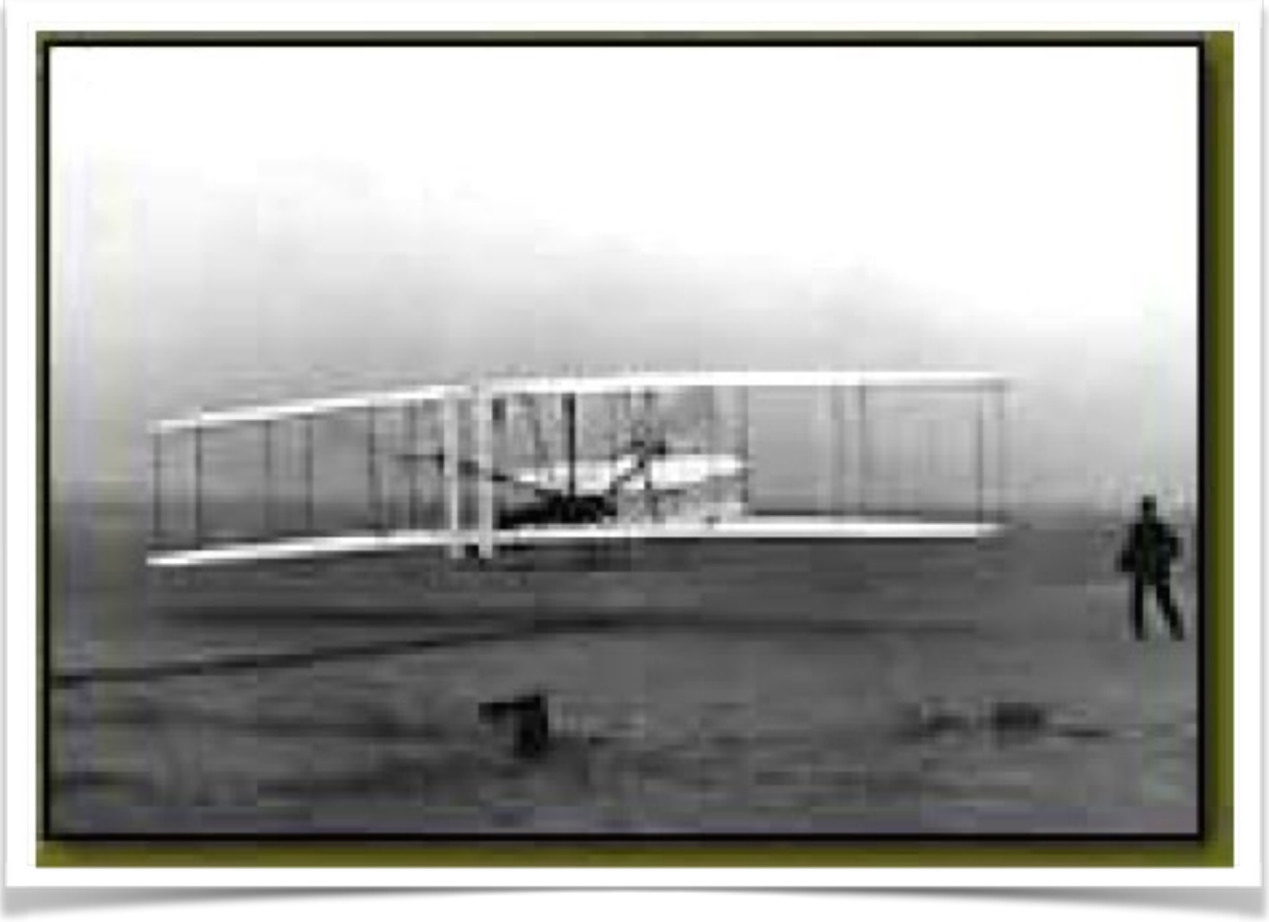
Outlook

Challenges

Wilbur and Orville Wright, 1903

Wright Flyer

10:35am Dec 17, 1903

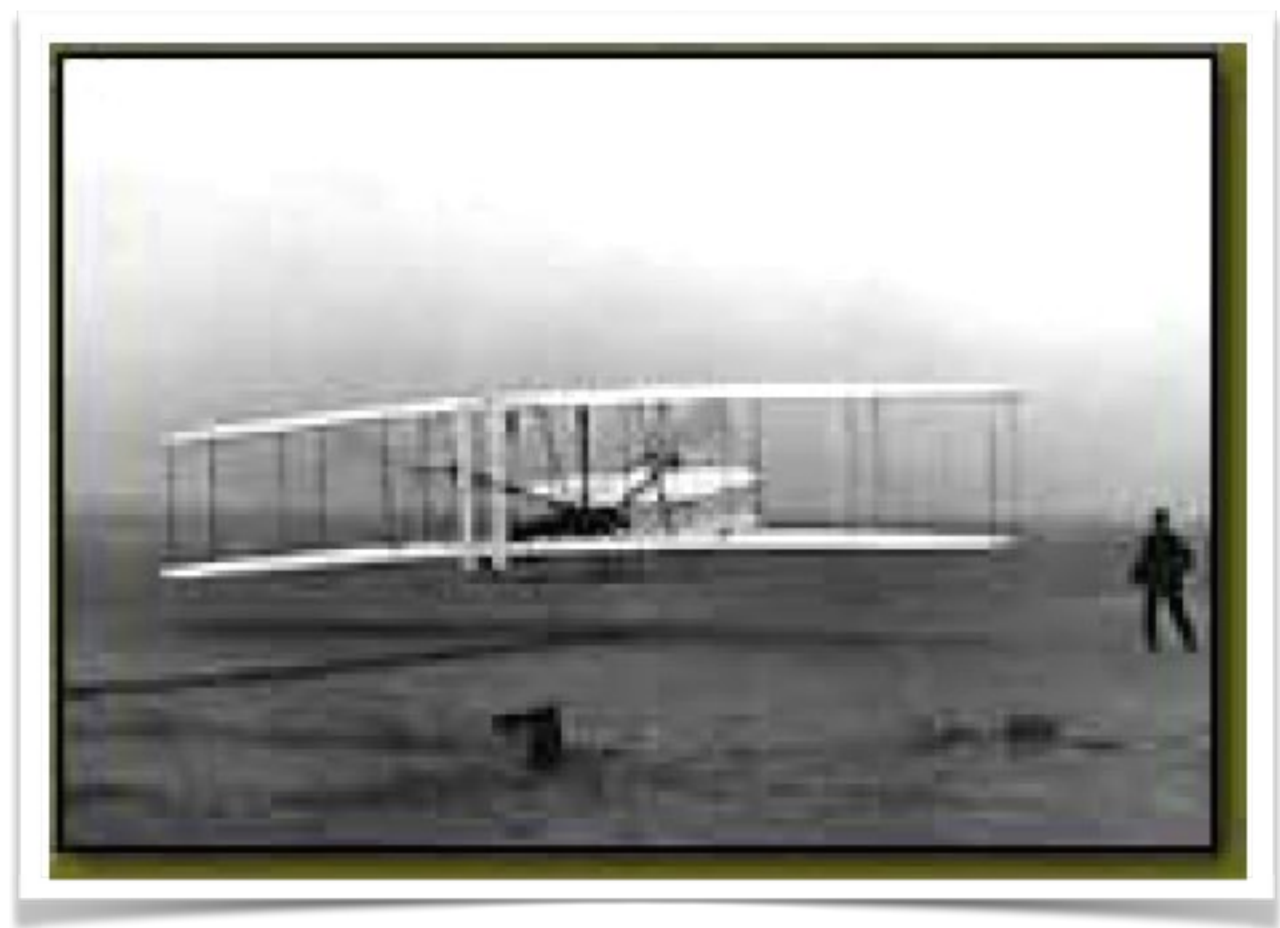


Wilbur and Orville Wright, 1903

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

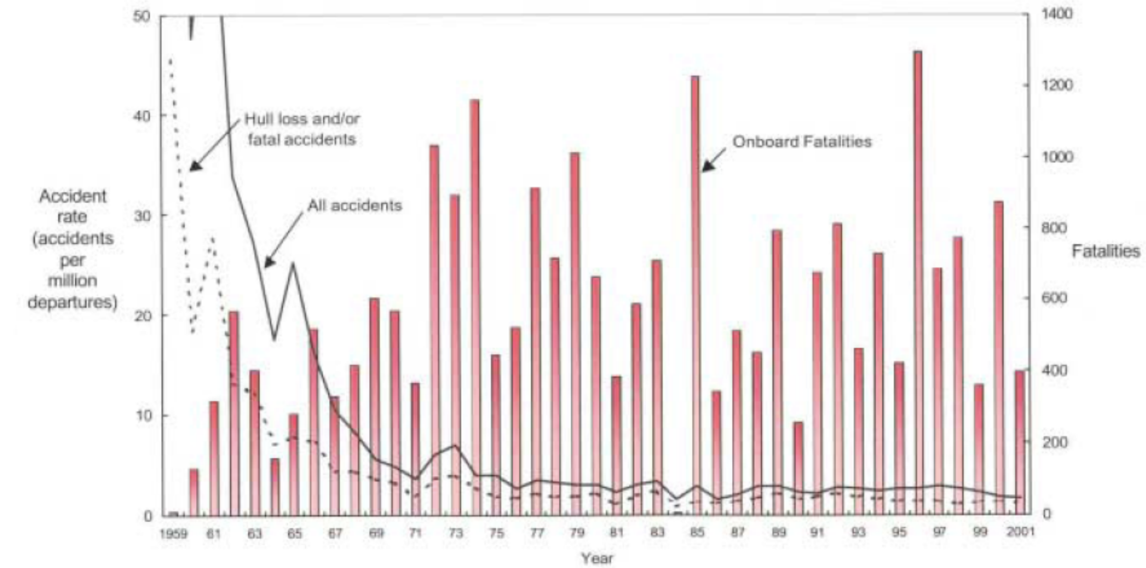


Aircraft safety

20,000 years

Worldwide statistics

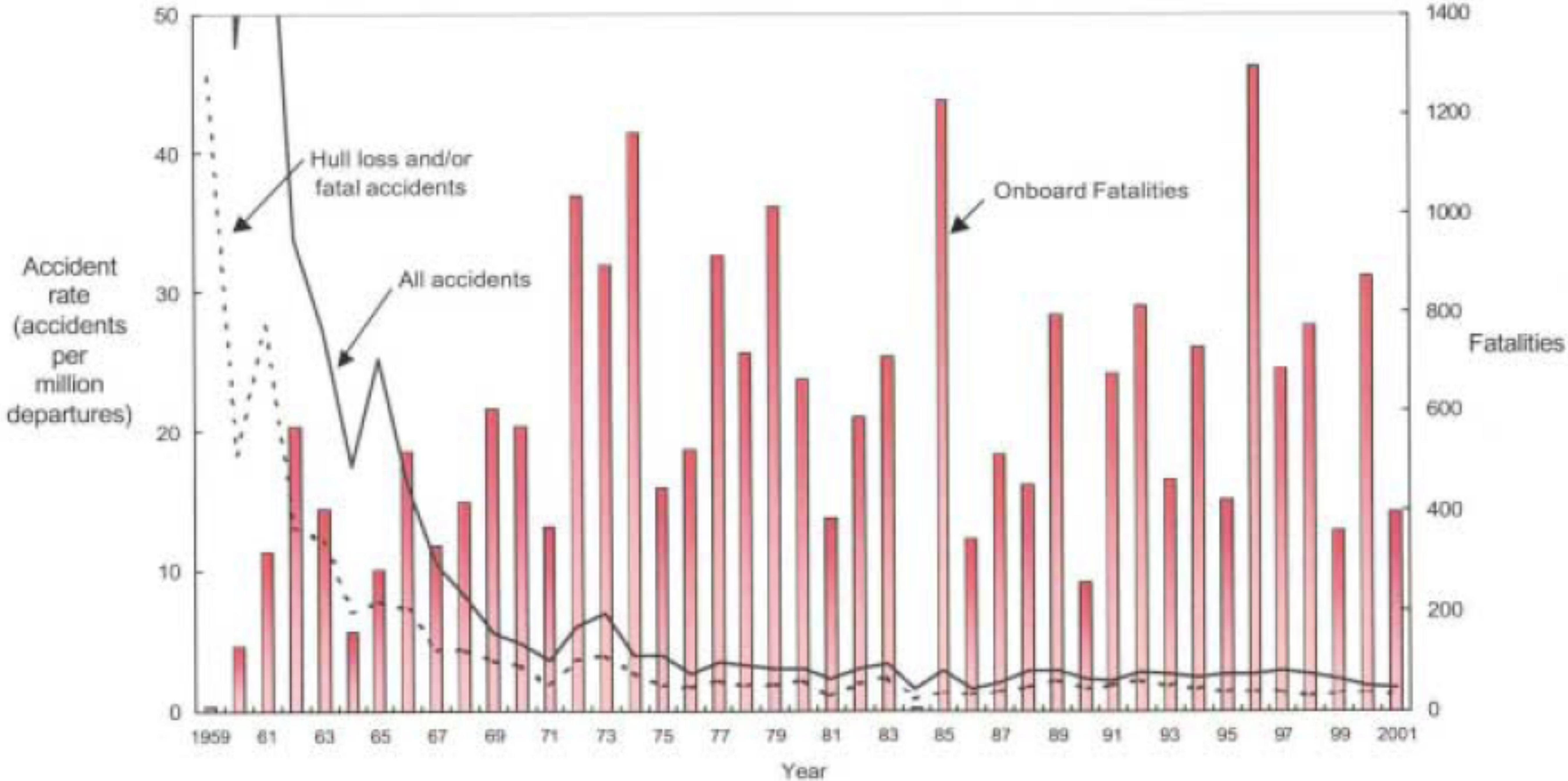
[1959-2001] 1,307 commercial jet aircraft losses



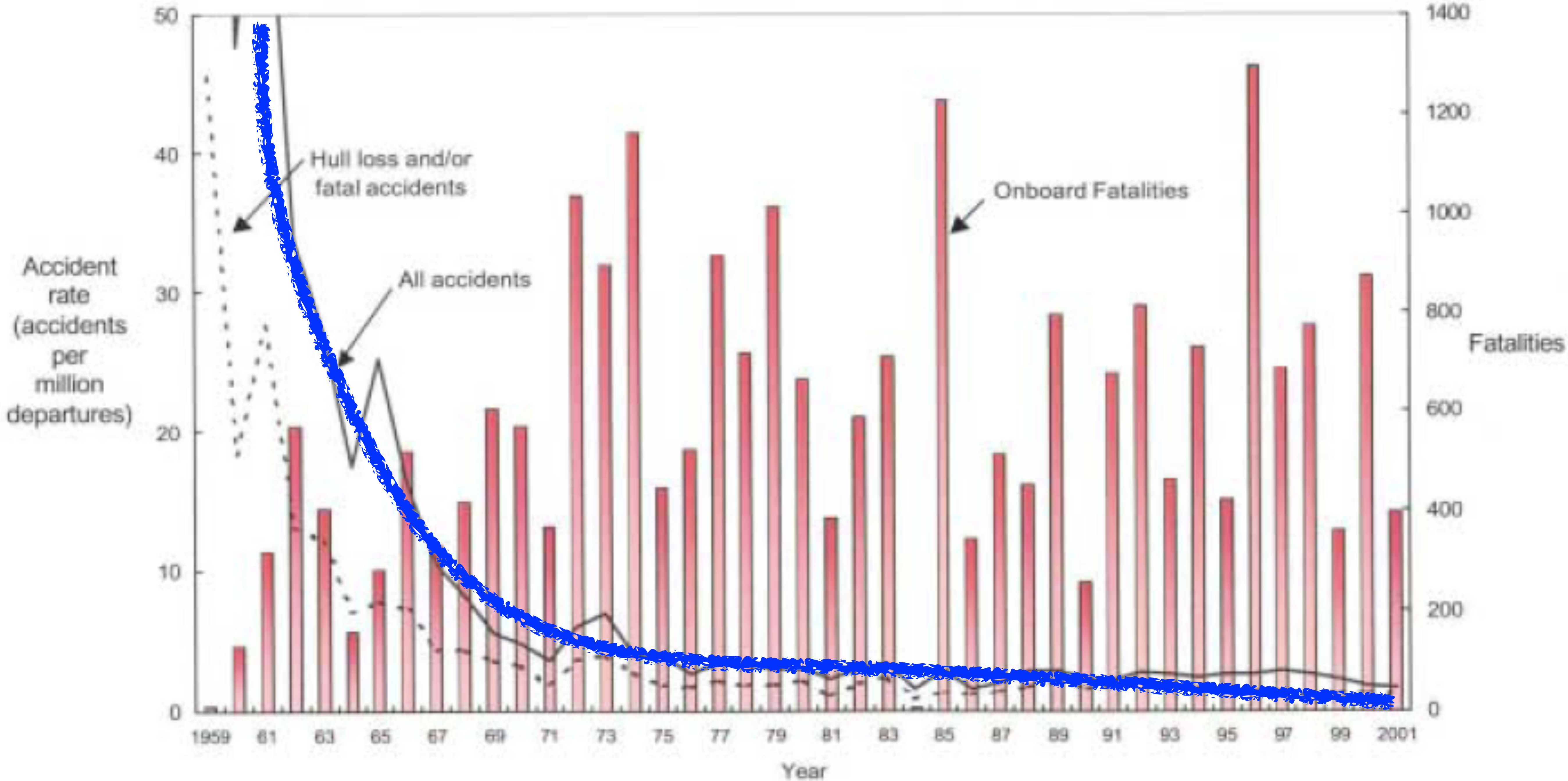
Today:

1 accident per 1,000,000 departures

Accident rates and fatalities/year

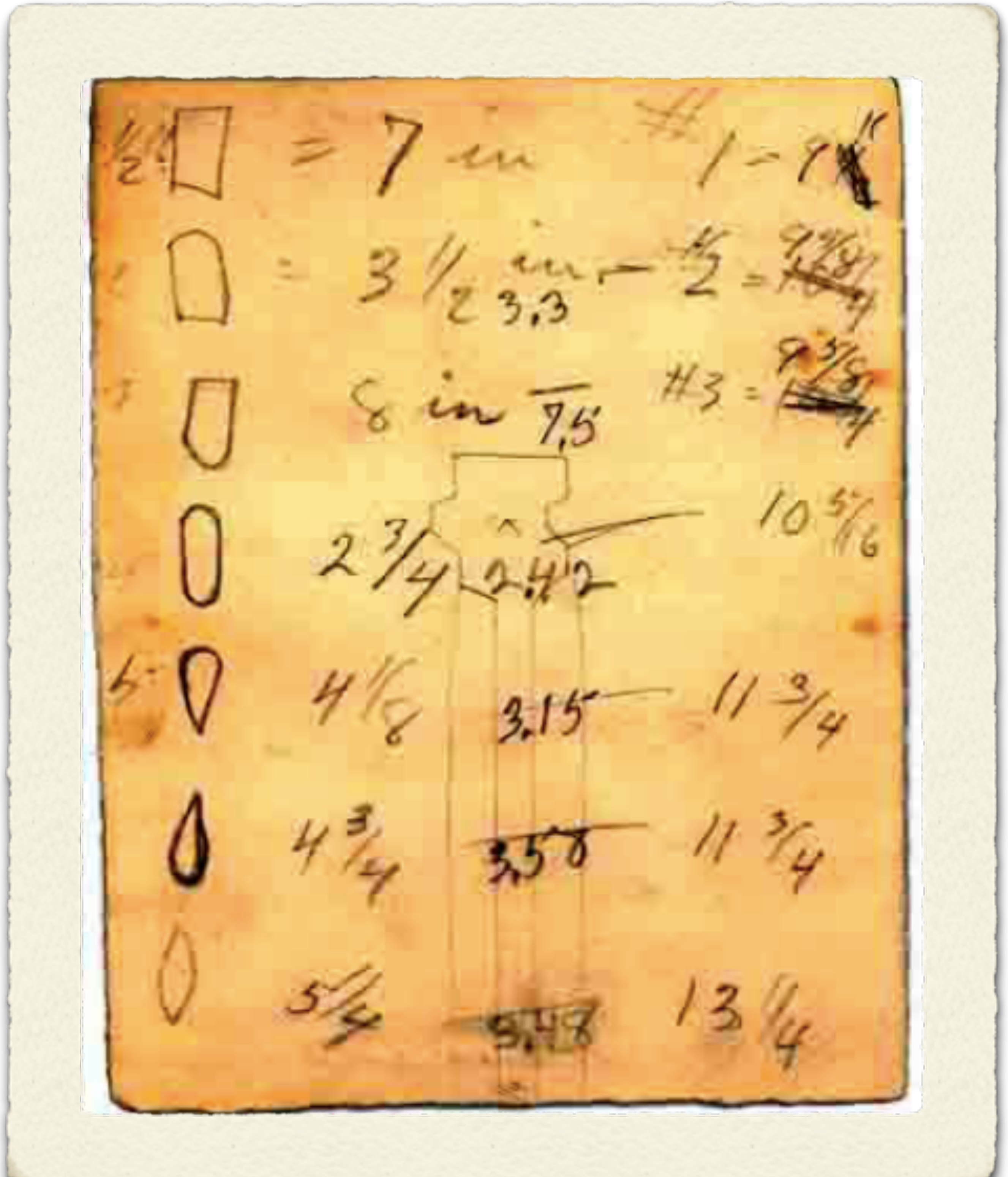


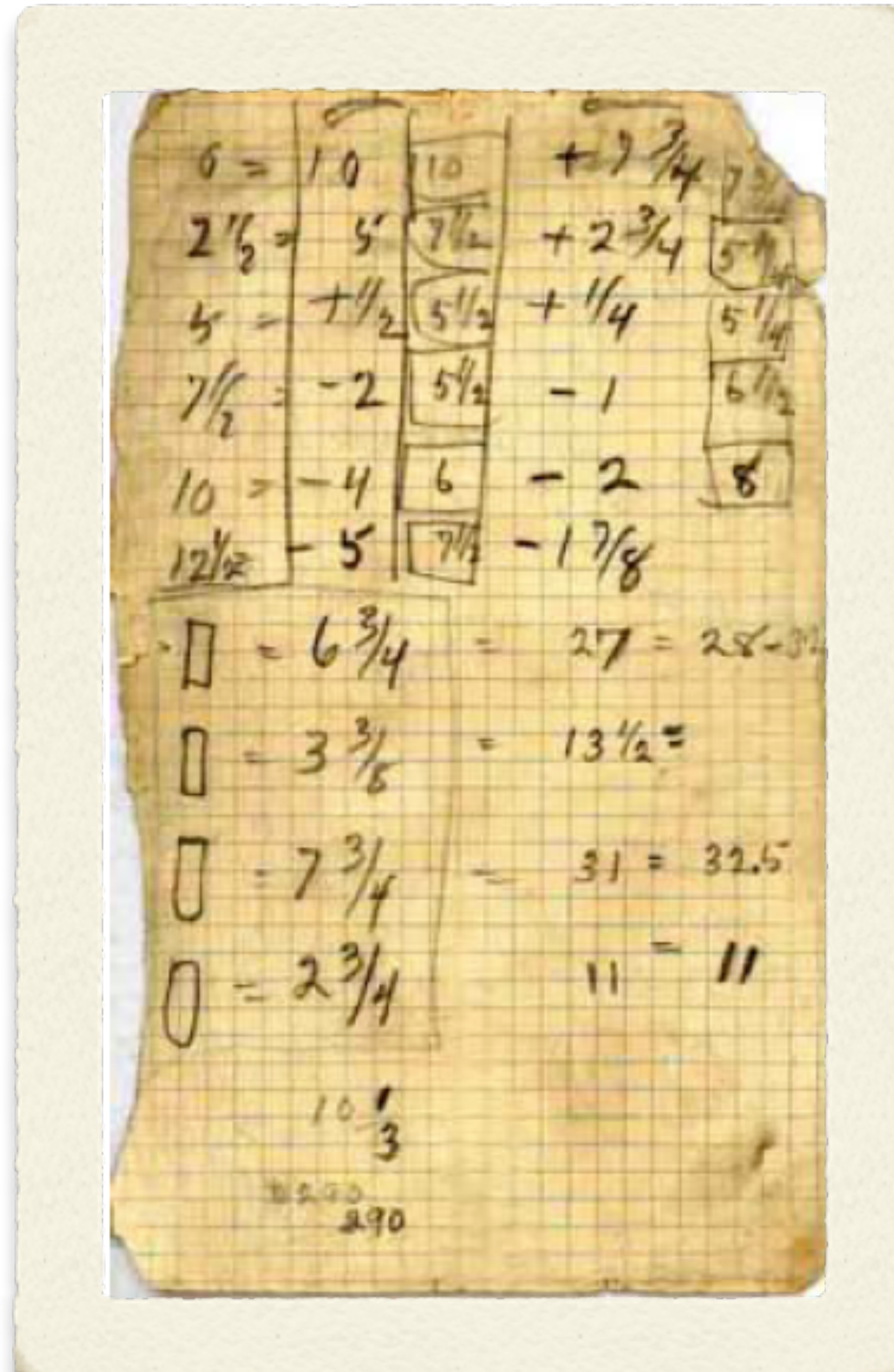
Accident rates and fatalities/year



Source: Flight Safety Foundation/Boeing Commercial Airplane Group

Learning from intuition & theory



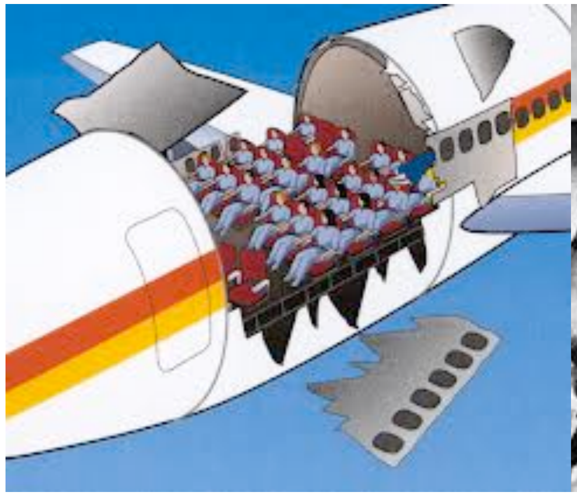


Franklin Institute Science Museum. Wilbur Wright's handwriting teach?...

Learning from experience

Increased practical understanding of mechanics — in particular fracture and fatigue

Bird strikes



Aloha airlines accident - fatigue cracks at corners

Novel convertible aircraft

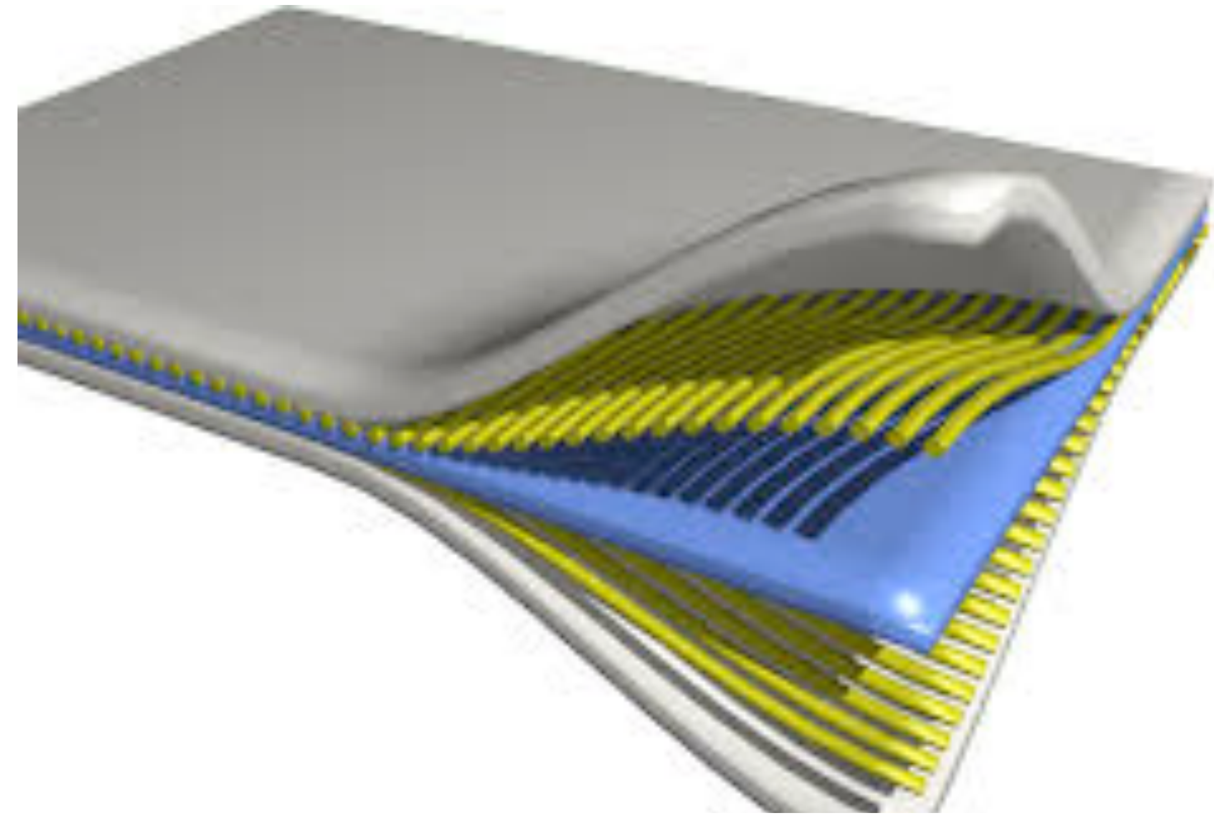
Learning from experi**ments**

World's largest wind tunnel (2014)

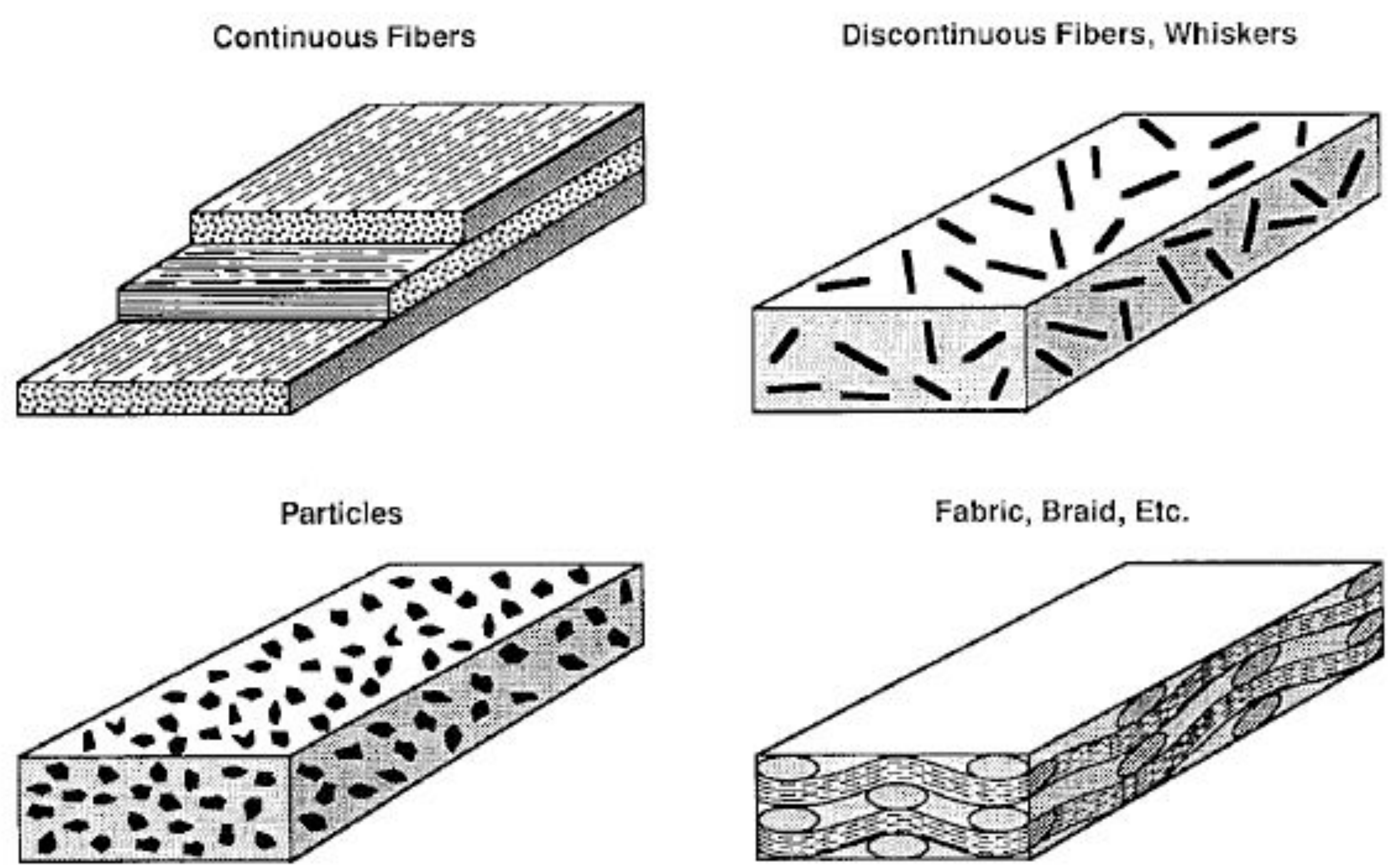
Replica of the 1901 Wright Wind Tunnel (constructed with assistance from Orville Wright)

New materials for more payload

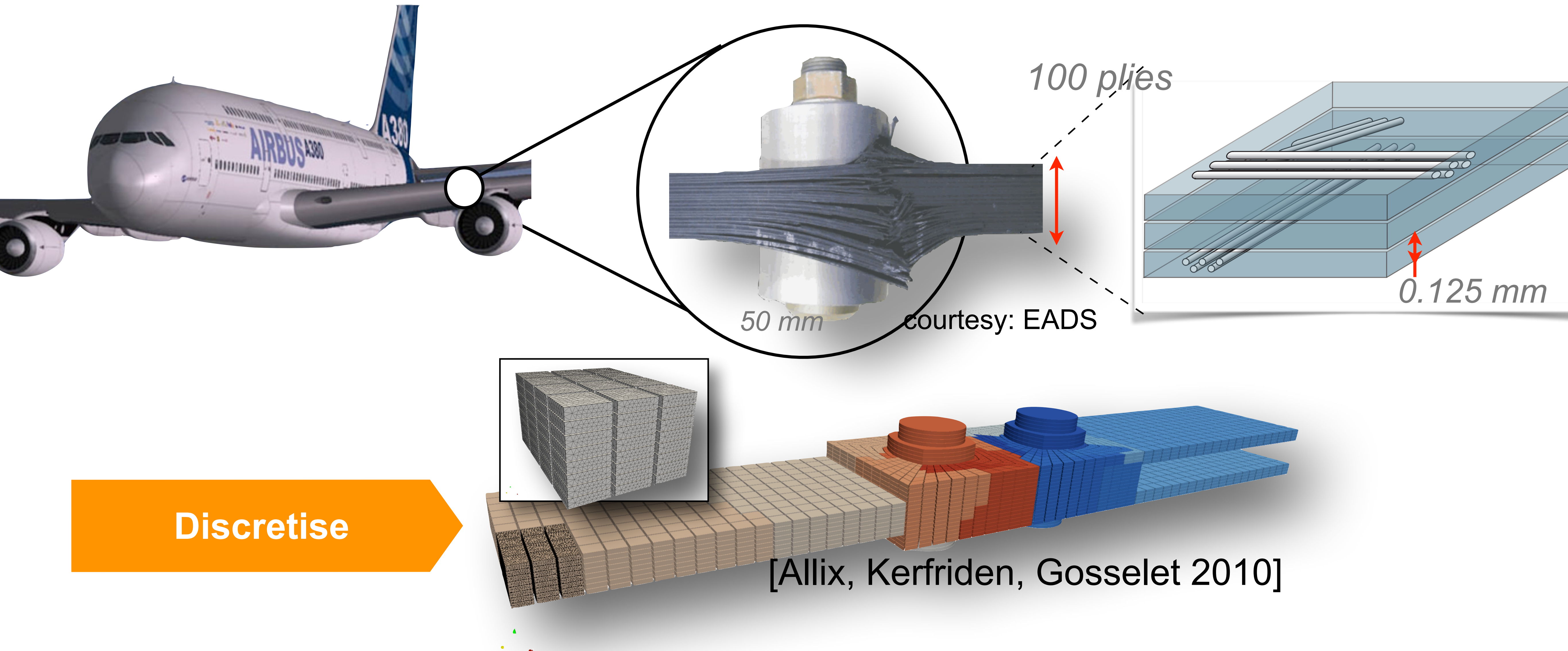
Introduction of composite materials have reduced the weight of structures by 20%



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

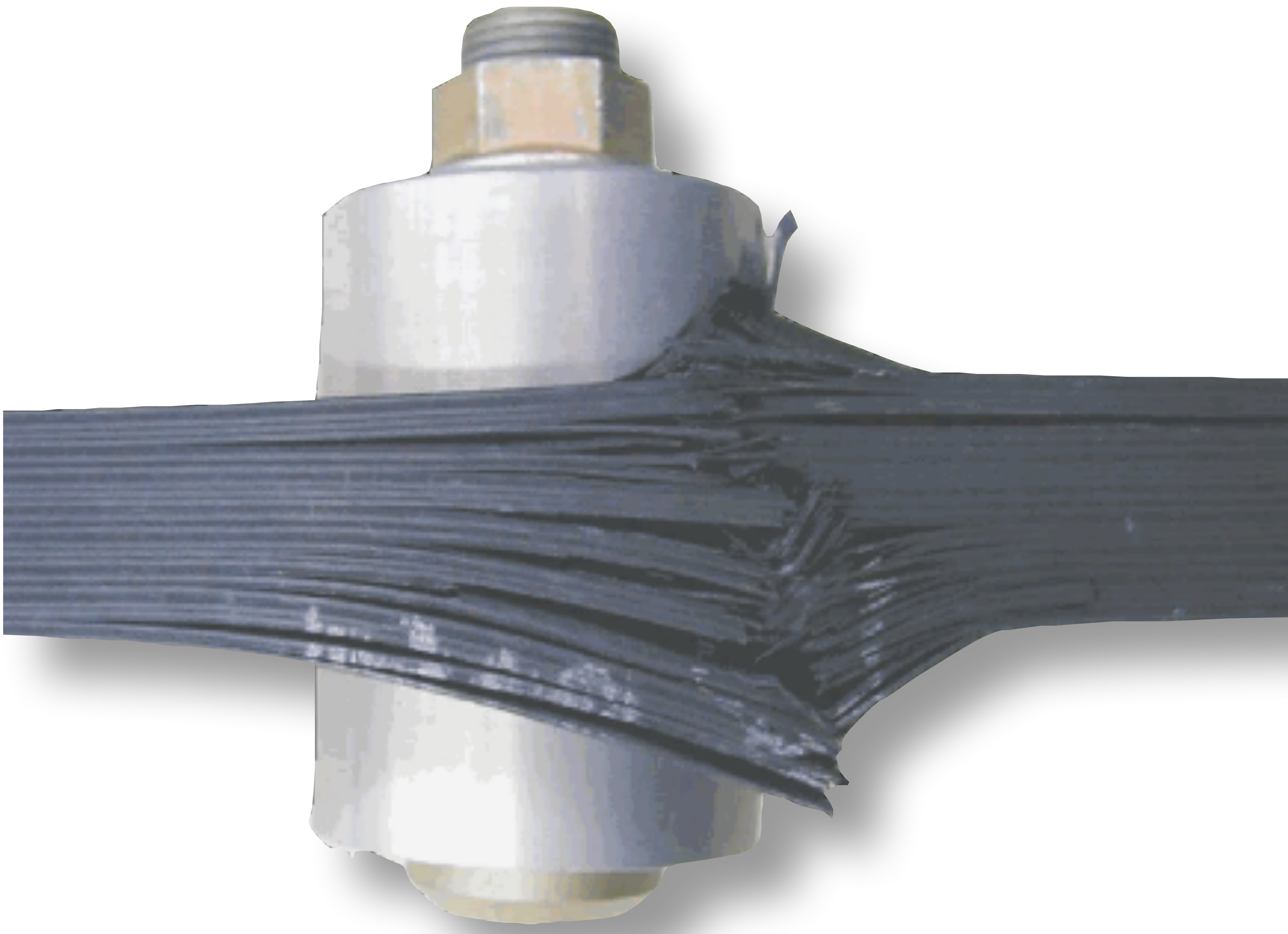


New kinds of experiments for new kinds of models

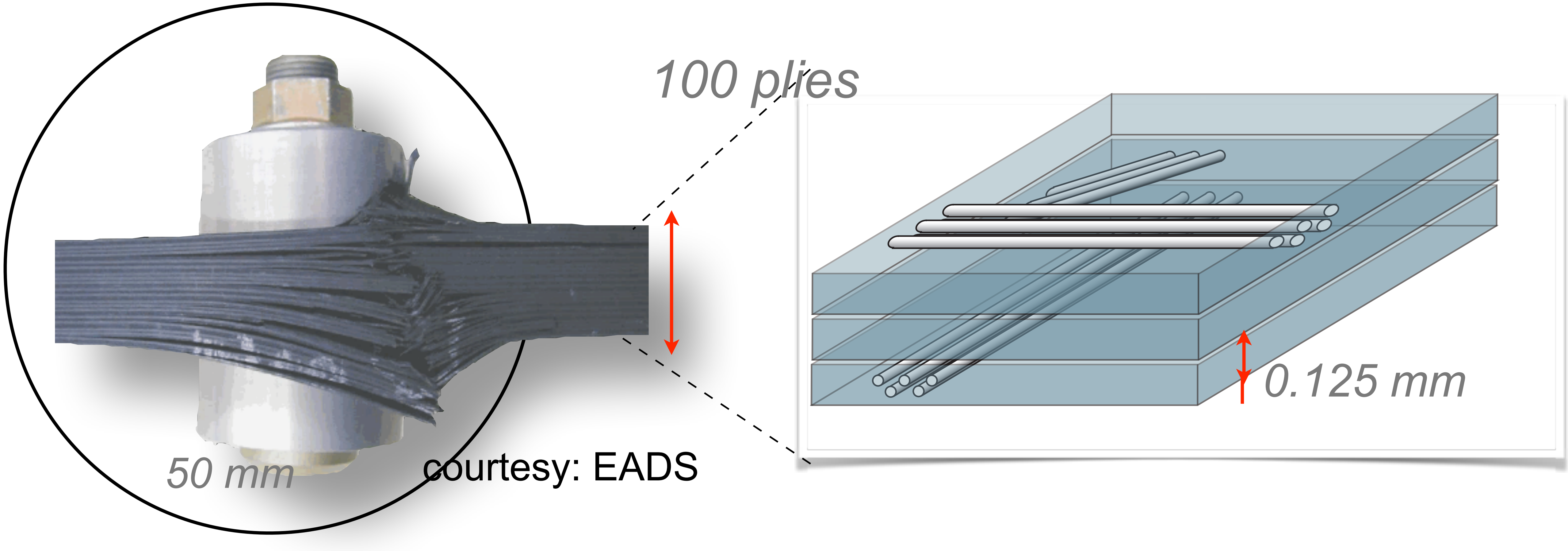


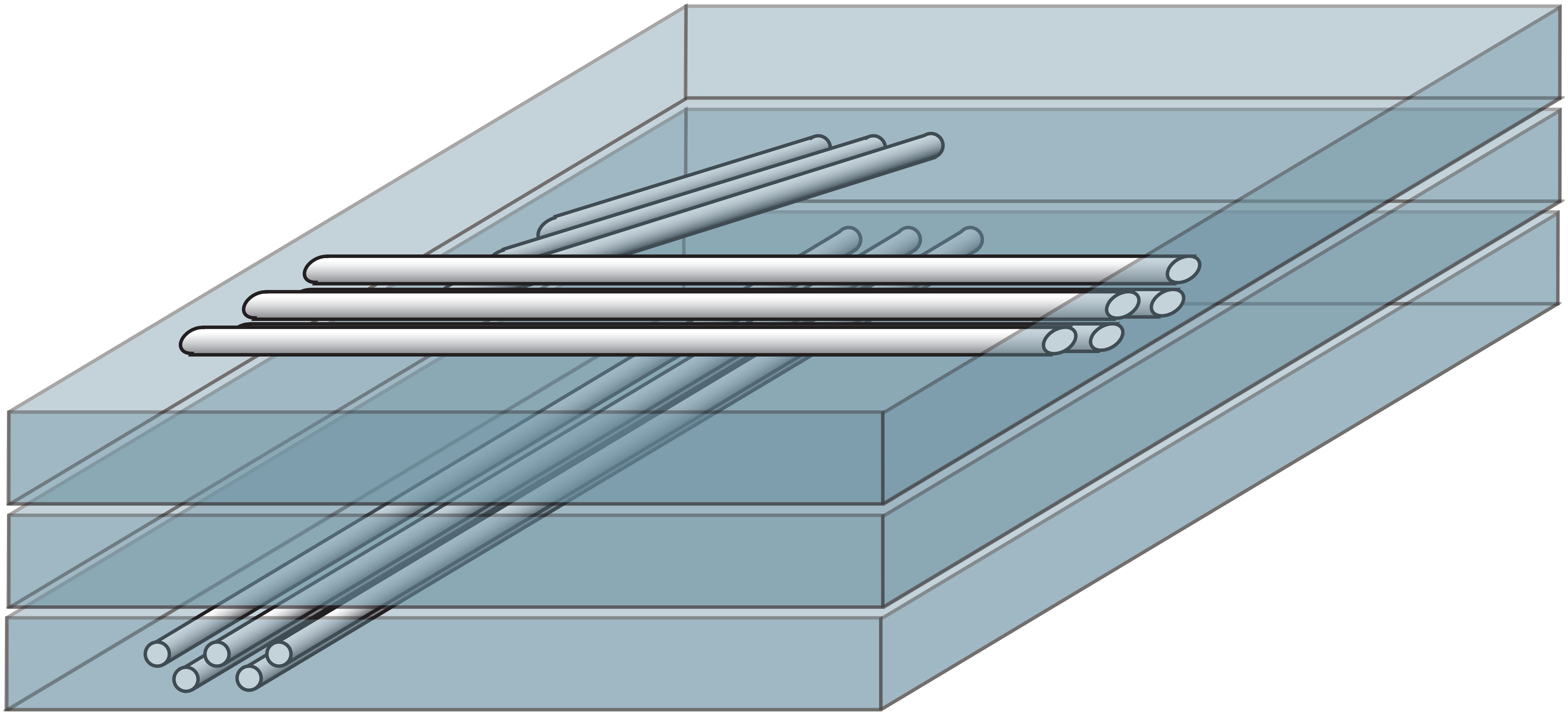
Kerfriden, Allix, Gosselet, Bordas *et al*, 2009, 2010, 2011, 2012, 2013, 2014

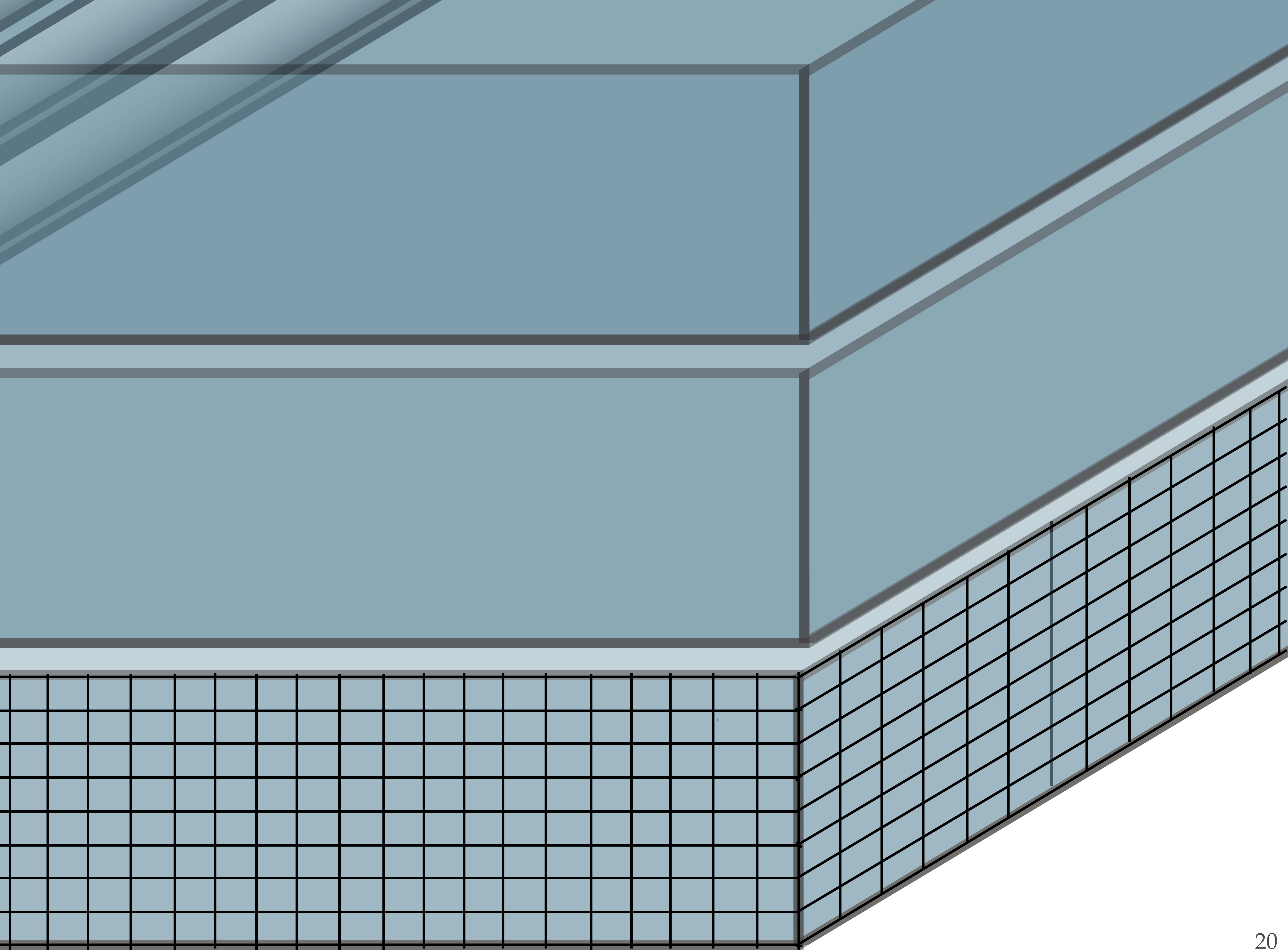
A bolted joint



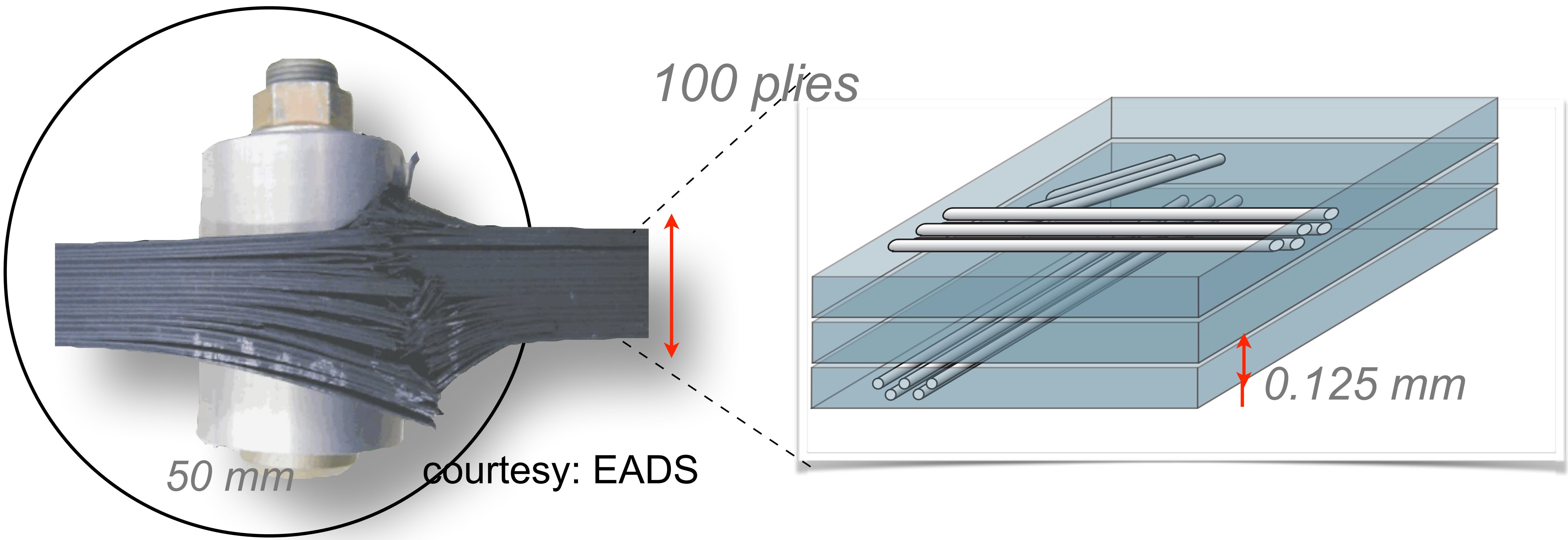
A bolted joint





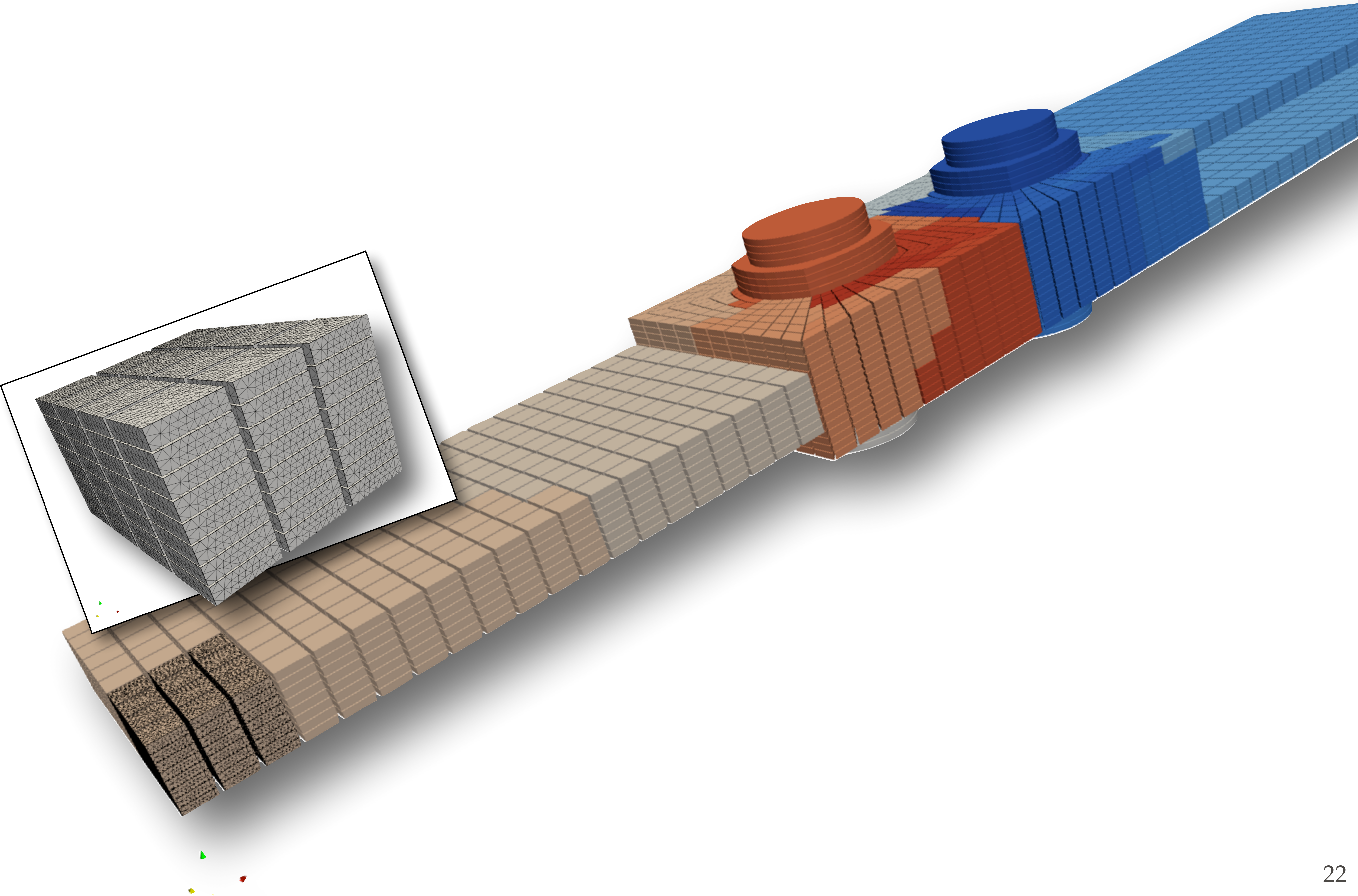


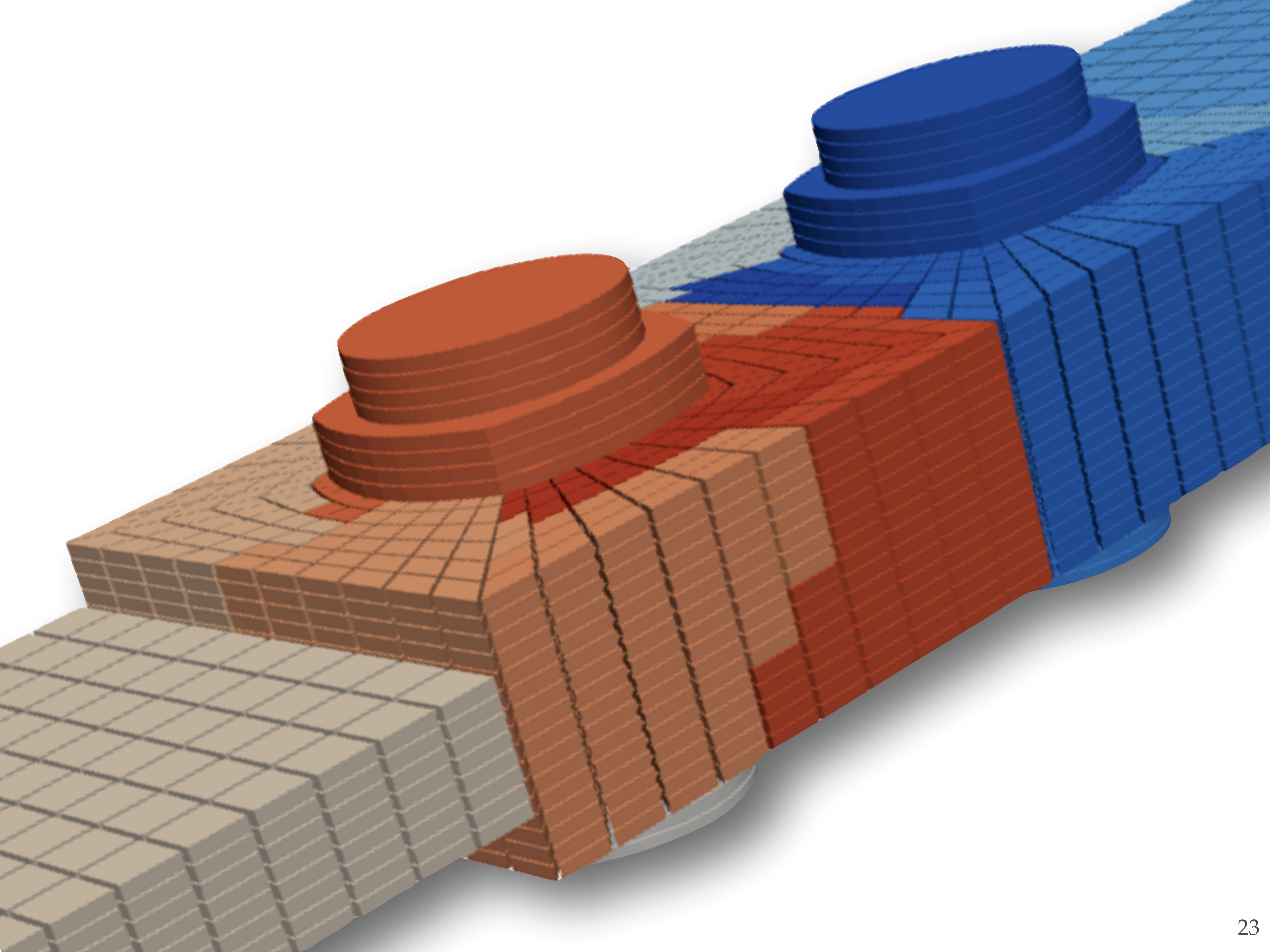
A bolted joint

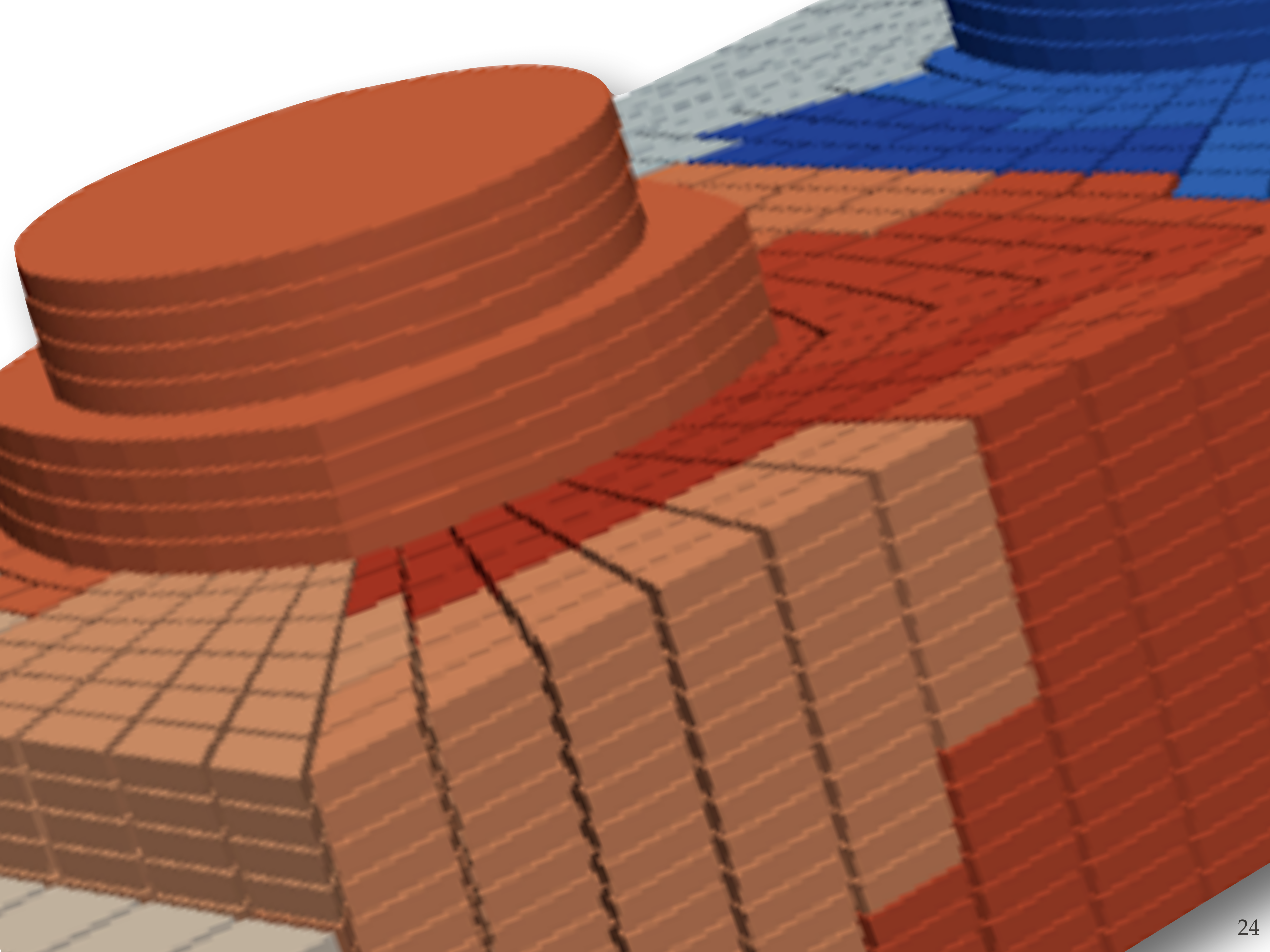


- 5 elements through the thickness of a ply => 0.025mm/element
- 50mm bolted joint area => 2,000 elements
- 50mm x 50mm x 100 plies => 2,000 x 2,000 x (100 x 5)

  => **2 billion elements**



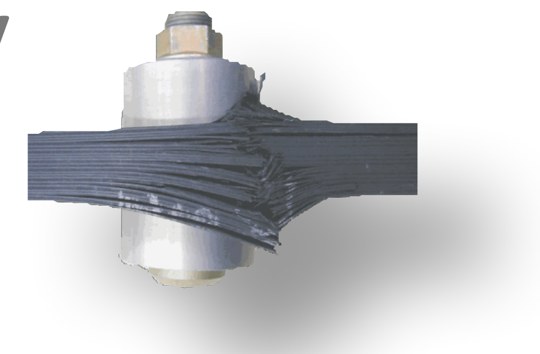




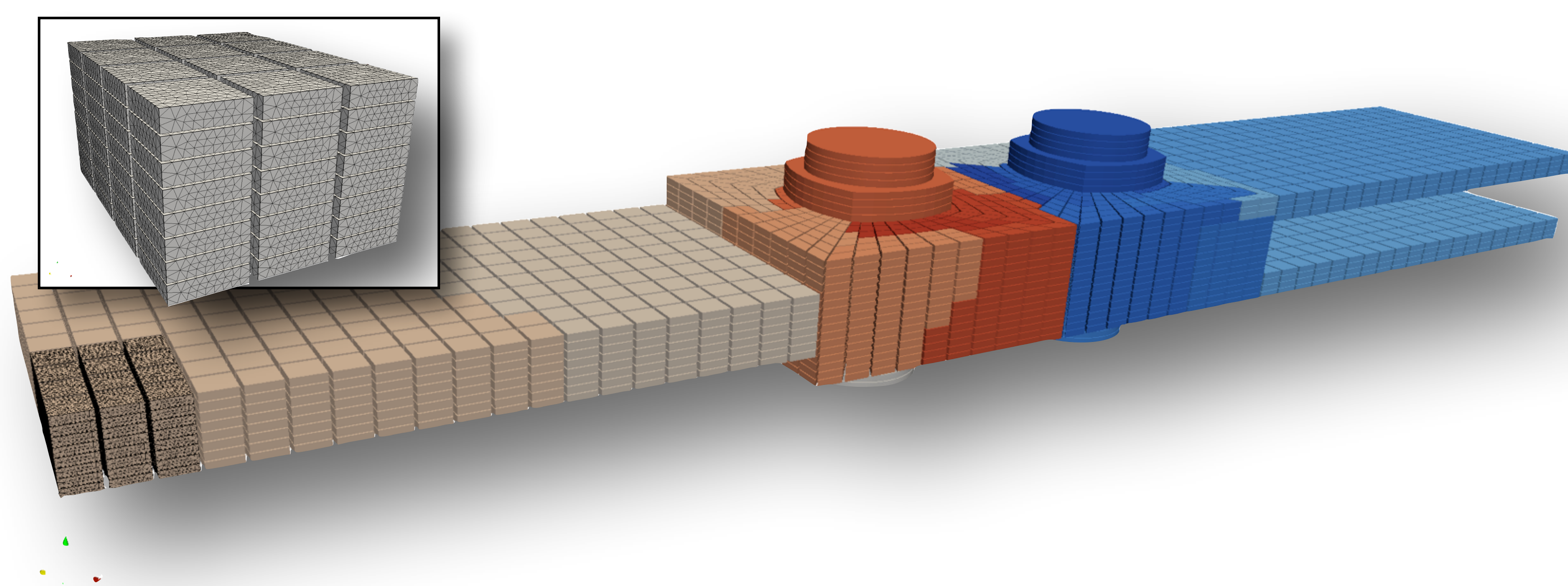
A380 giant

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

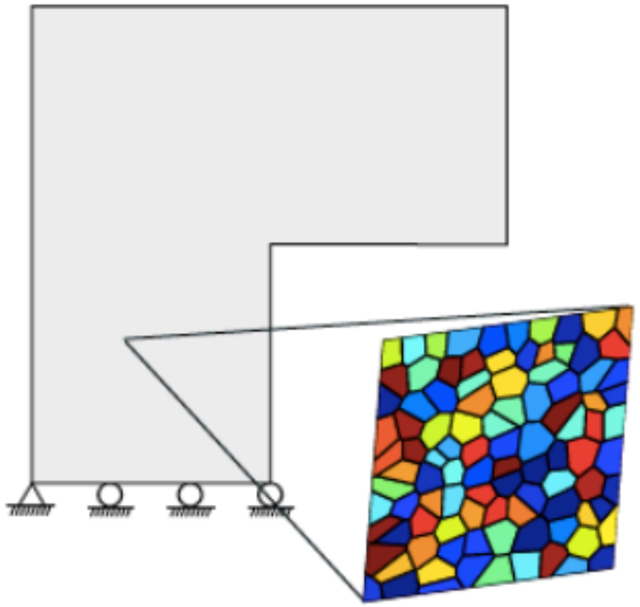
- Reduce the problem size
- Preserve essential features

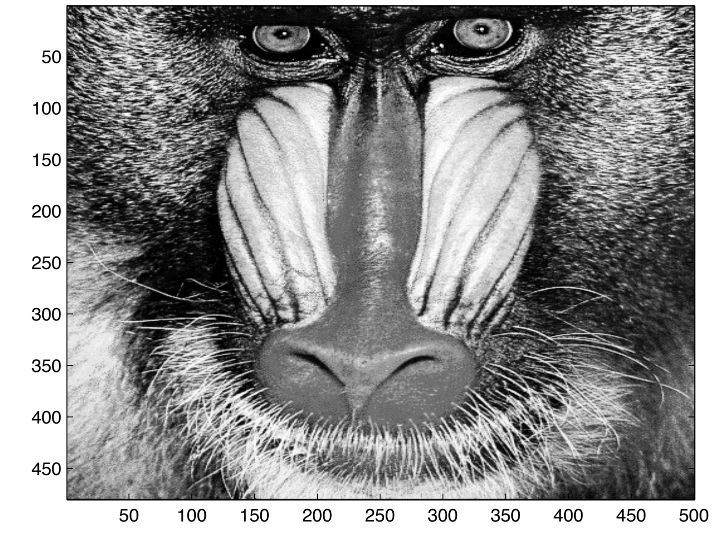
Reduce computational expense

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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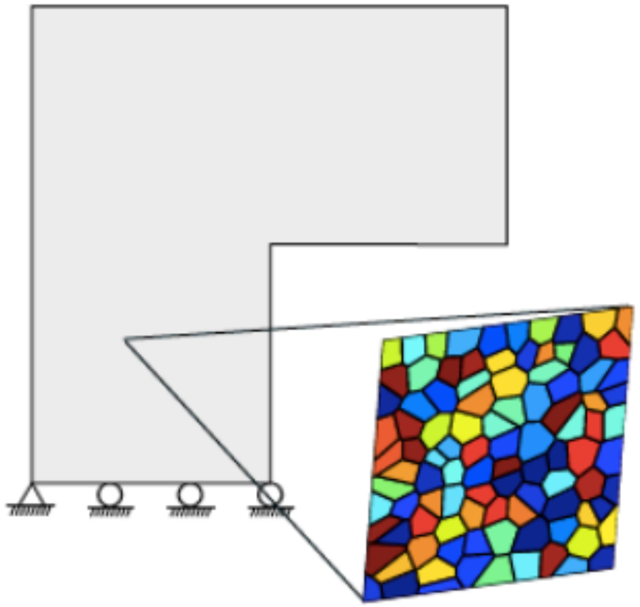
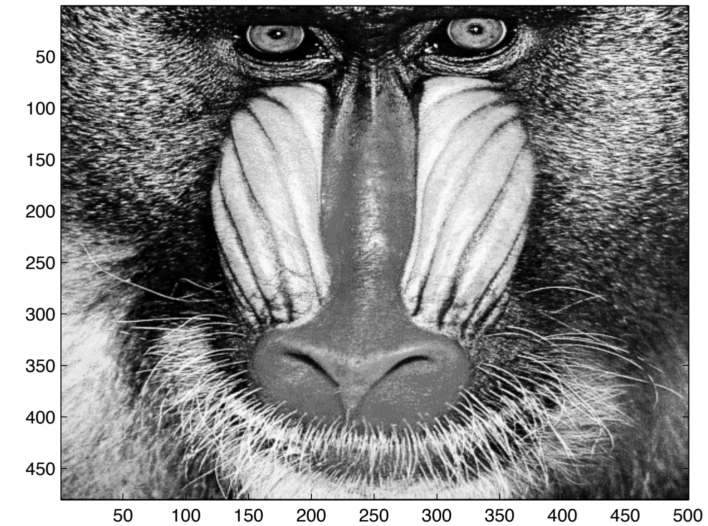
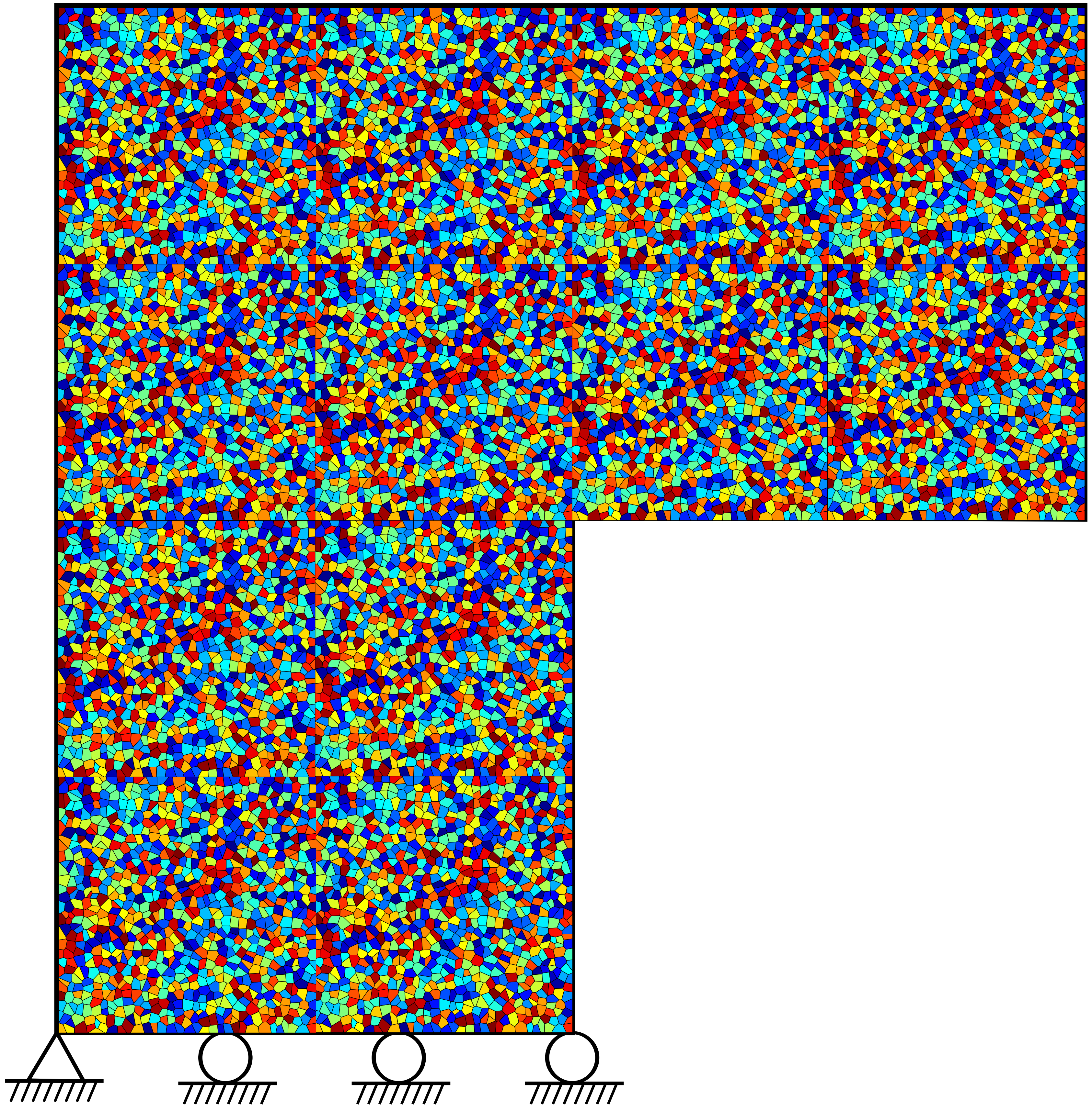


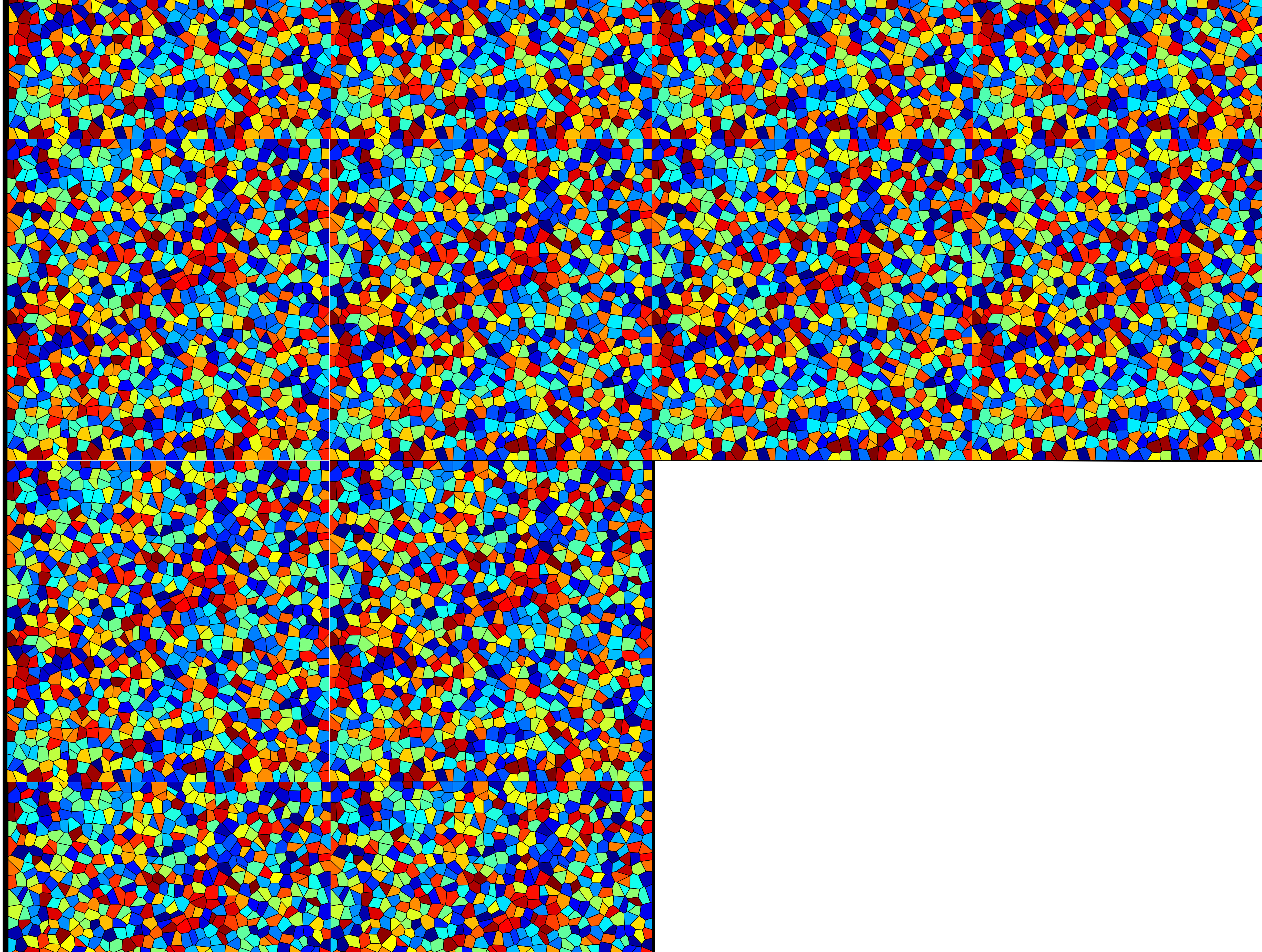


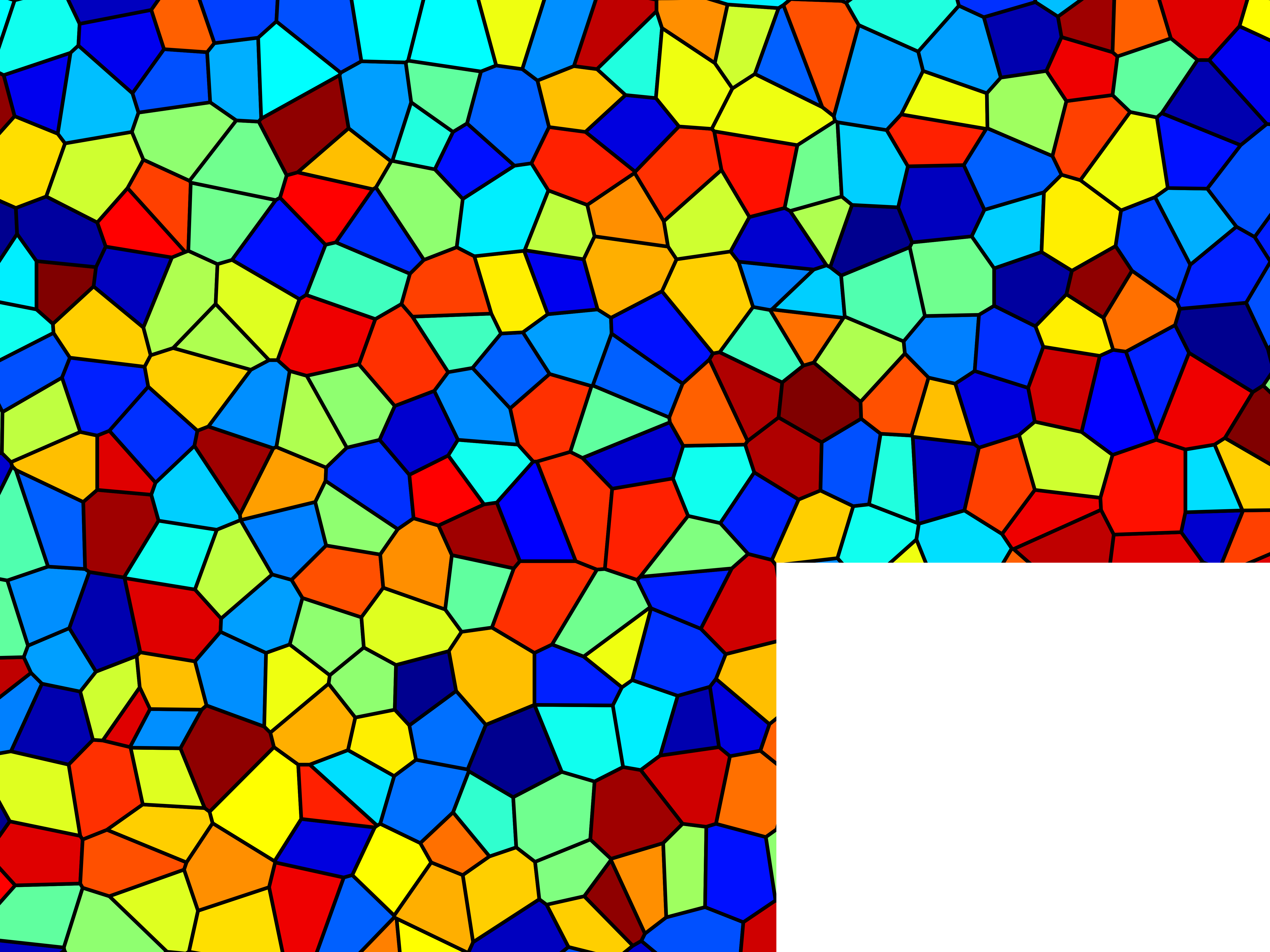
Physics-based model reduction methods

multi-scale methods

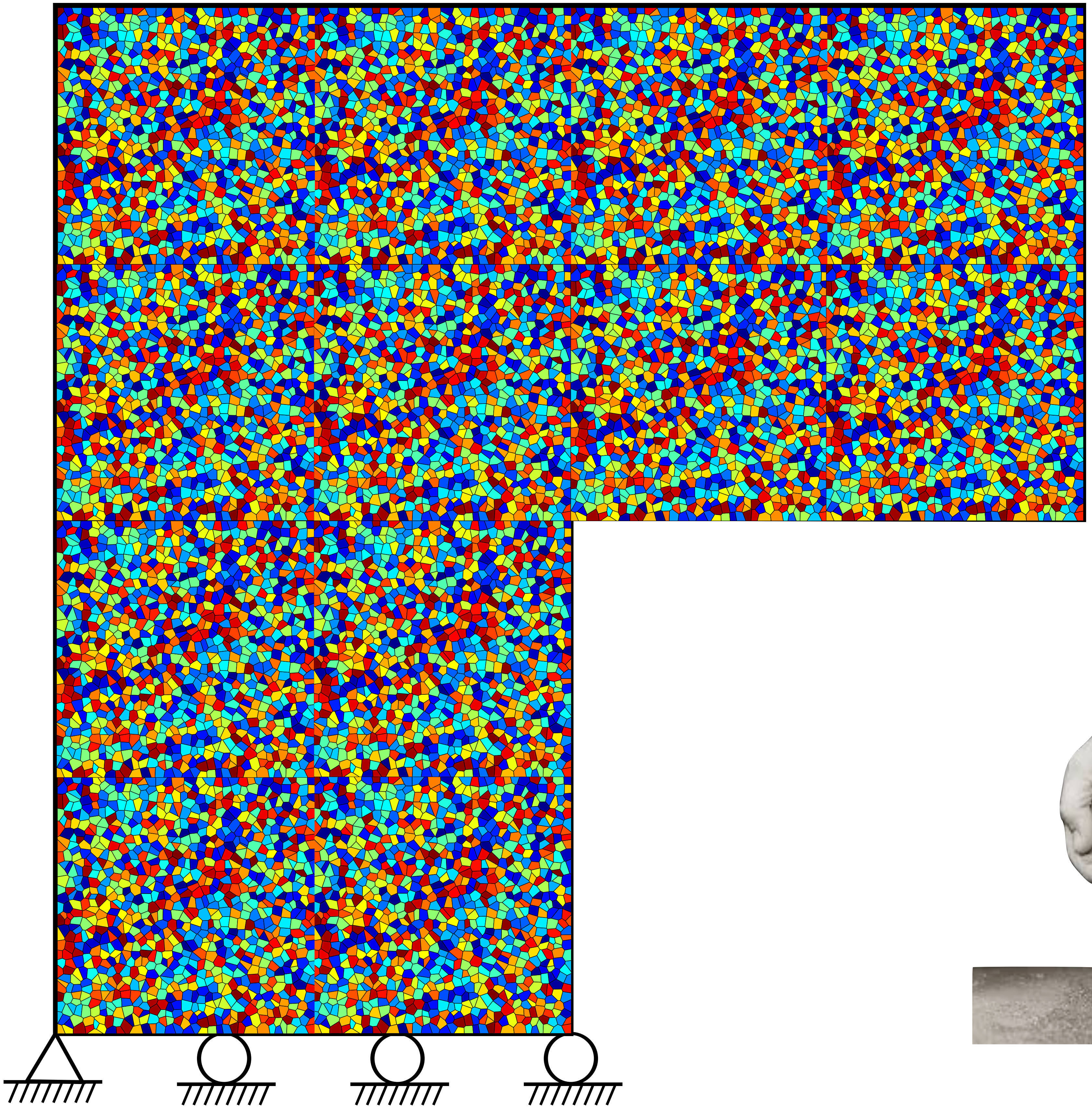
Full-scale





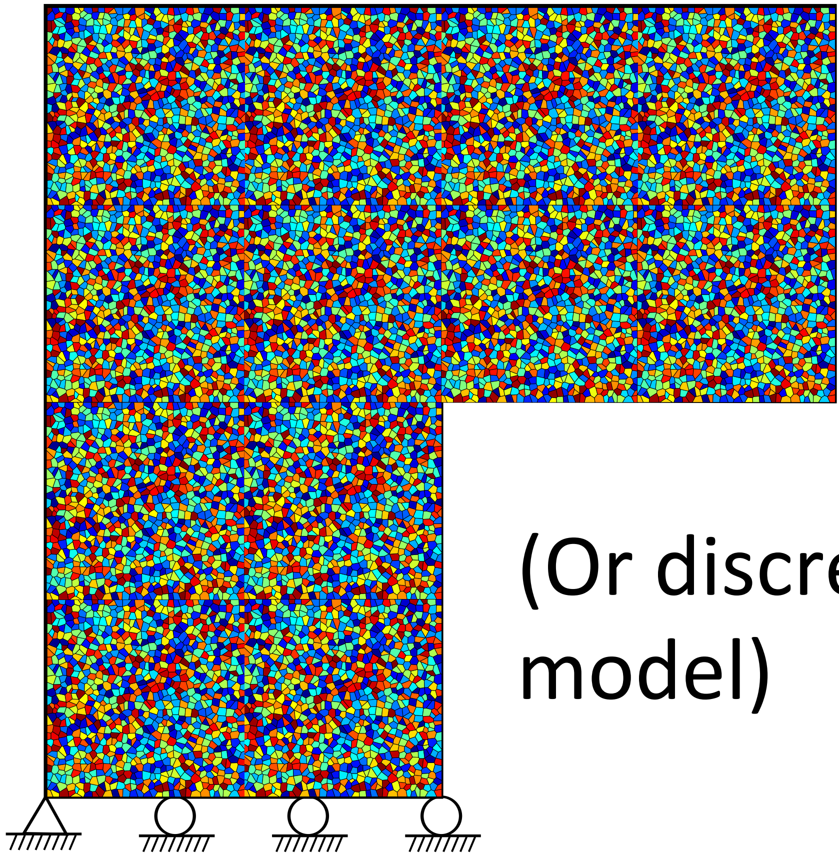


Full-scale



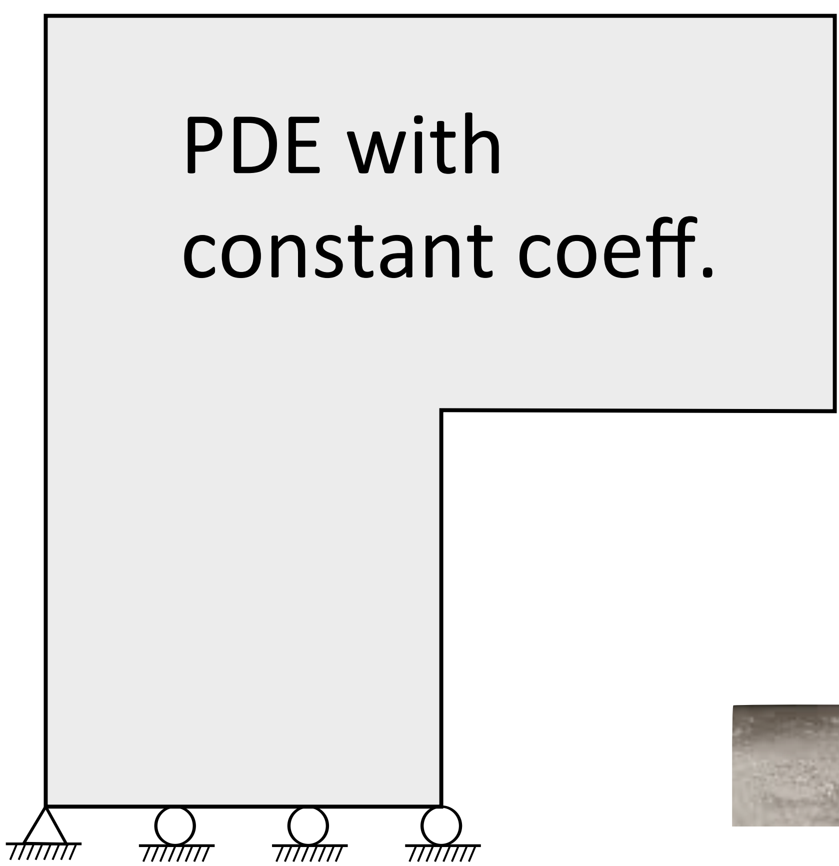
Multi-scale methods

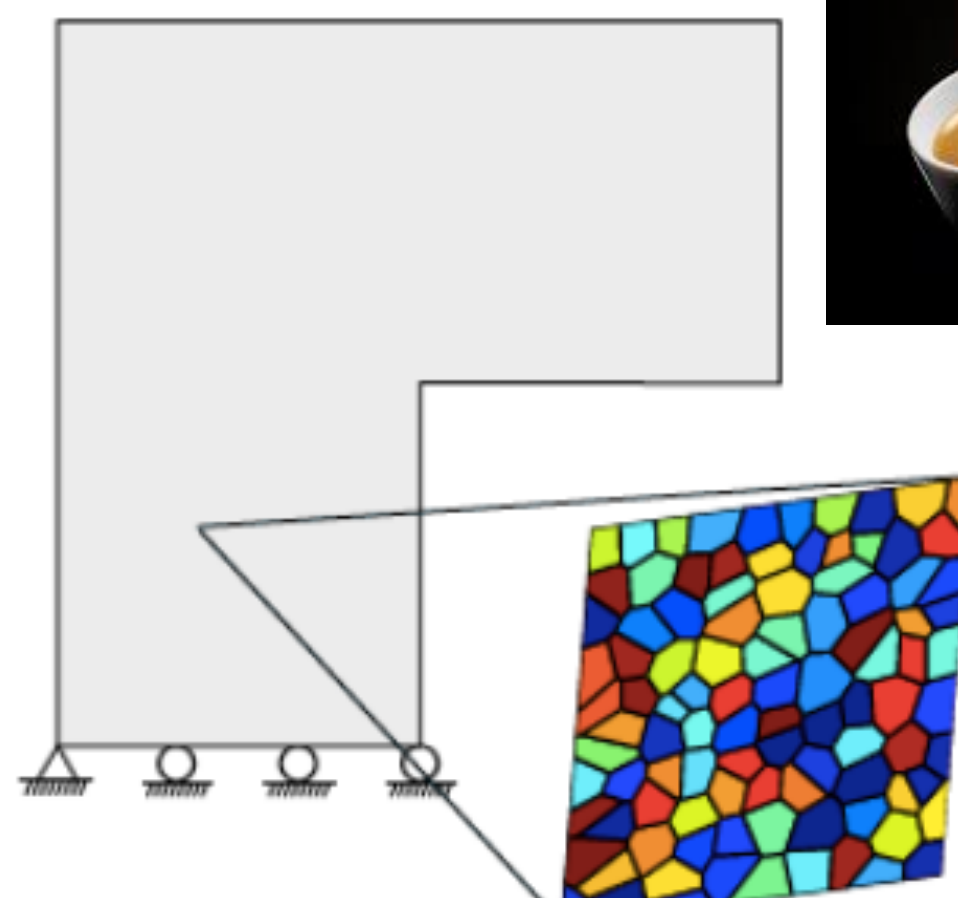
Replace the heterogeneous fine-scale model by an equivalent smoother model at the scale where the predictions are required



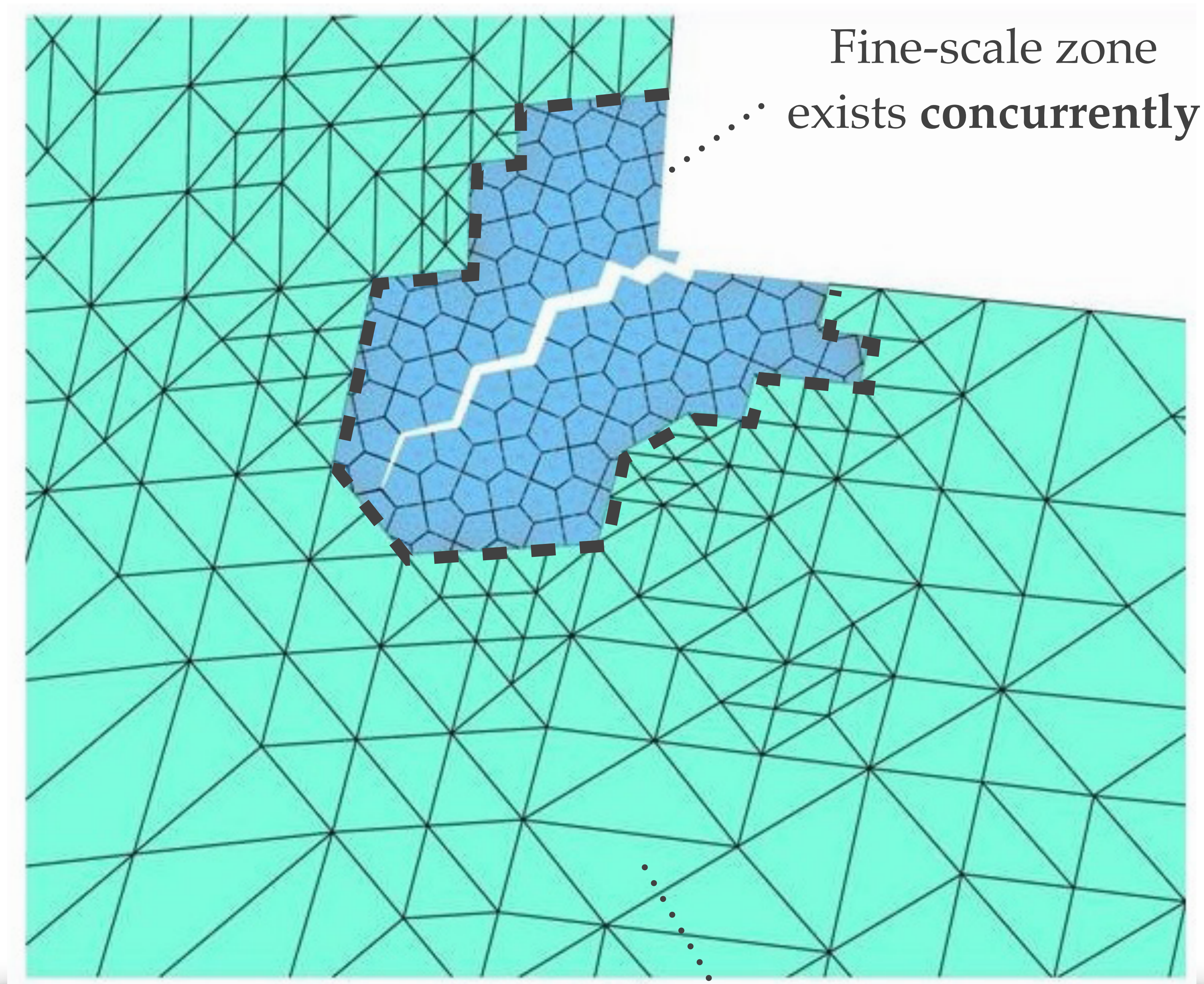
(Or discrete model)

↓ Homogenisation





Concurrent methods

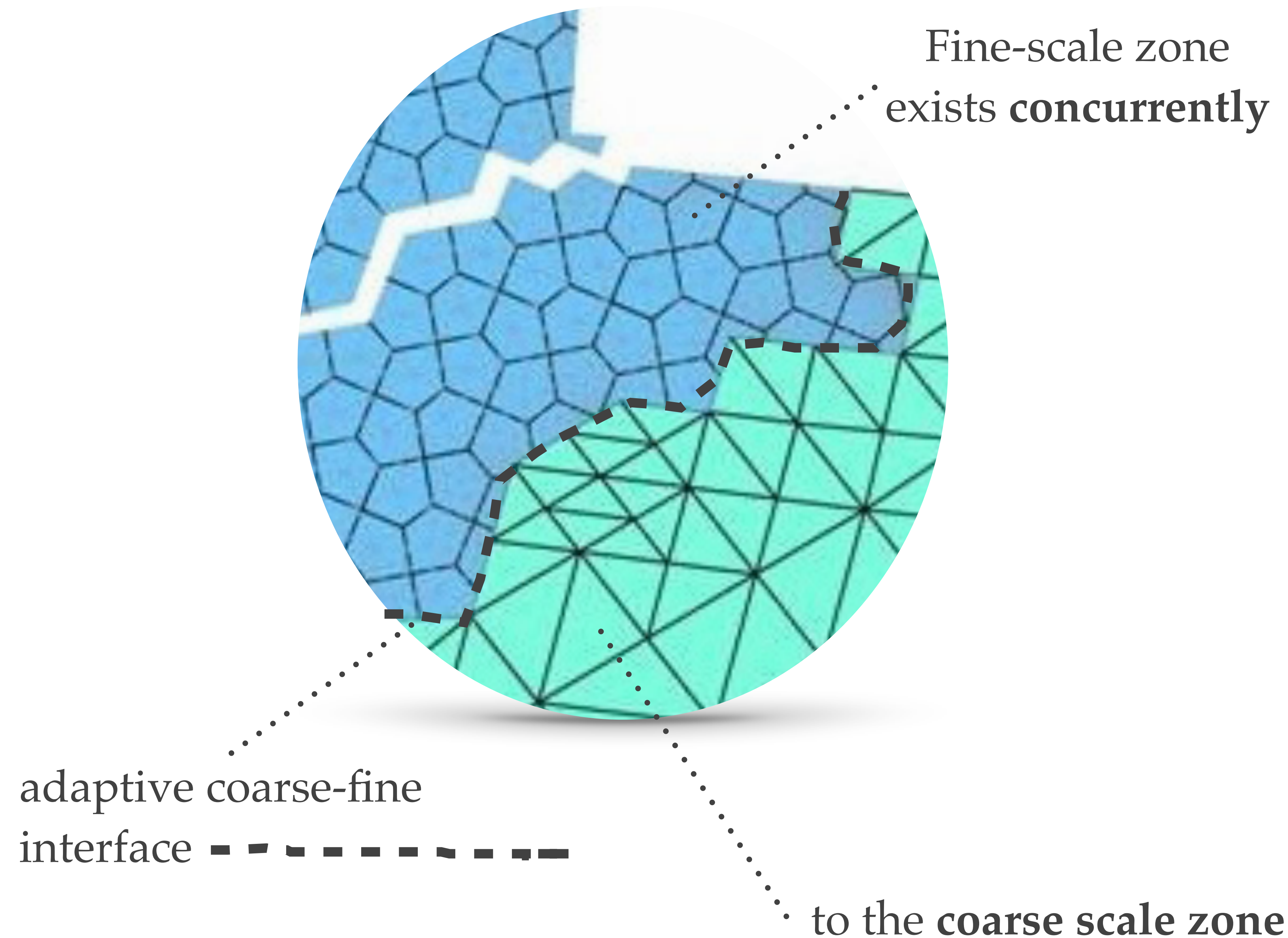


Fine-scale zone
exists **concurrently**

to the **coarse scale zone**

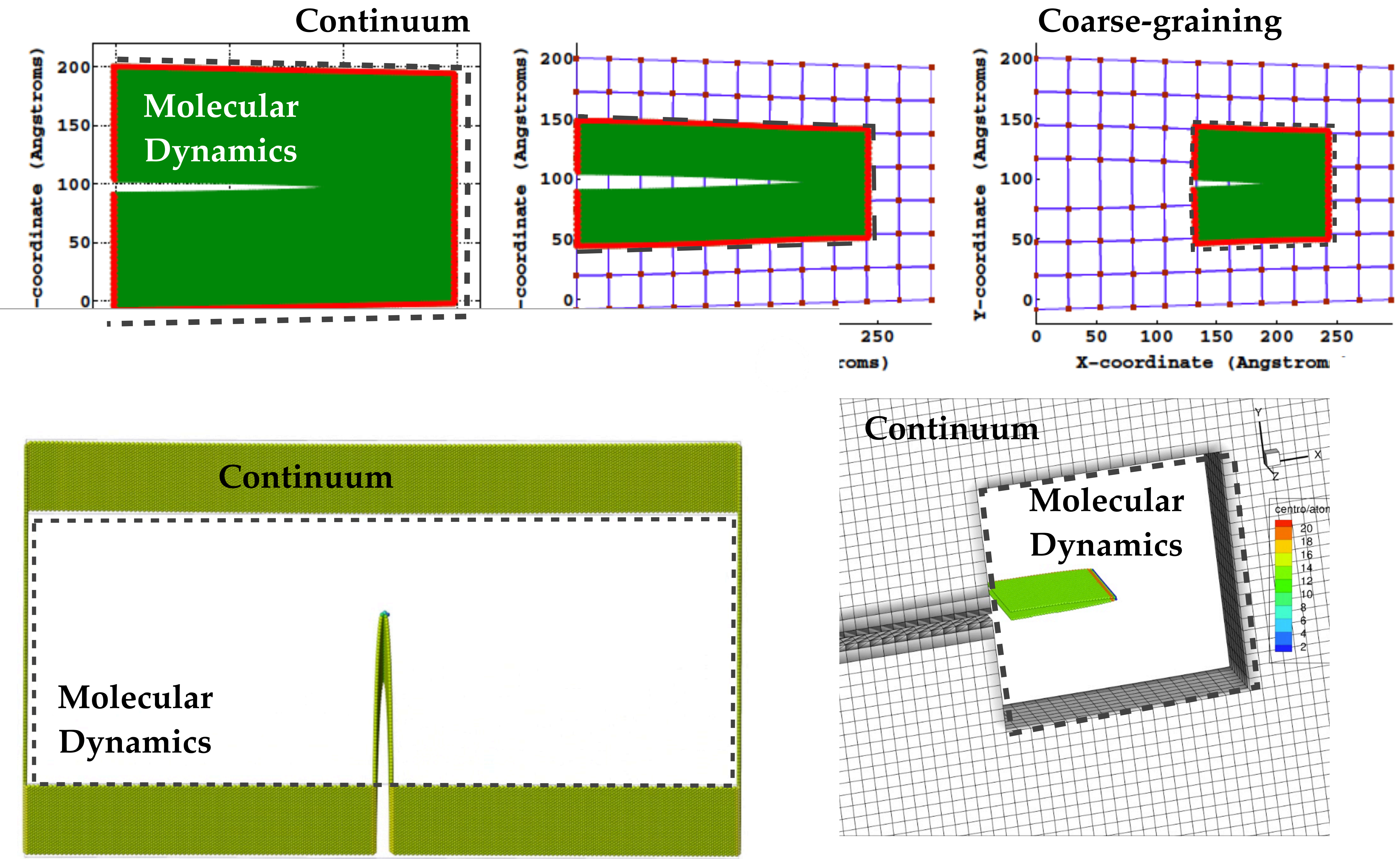
Akbari, Kerfriden, Bordas, 2014

Concurrent methods



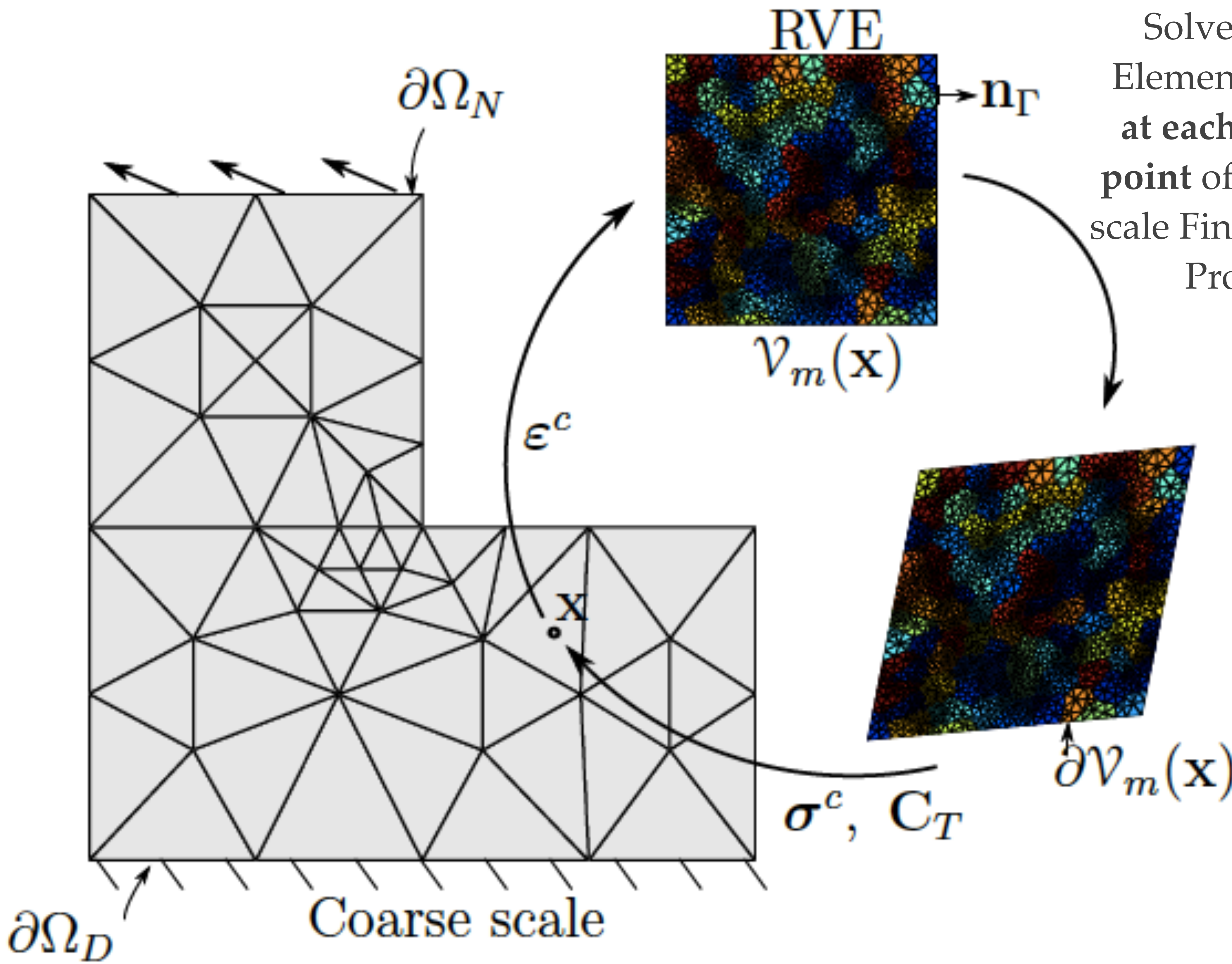
Akbari, Kerfriden, Bordas, 2014

Concurrent methods



Talebi, Ramaia, Rabczuk, Bordas, Kerfriden, 2014

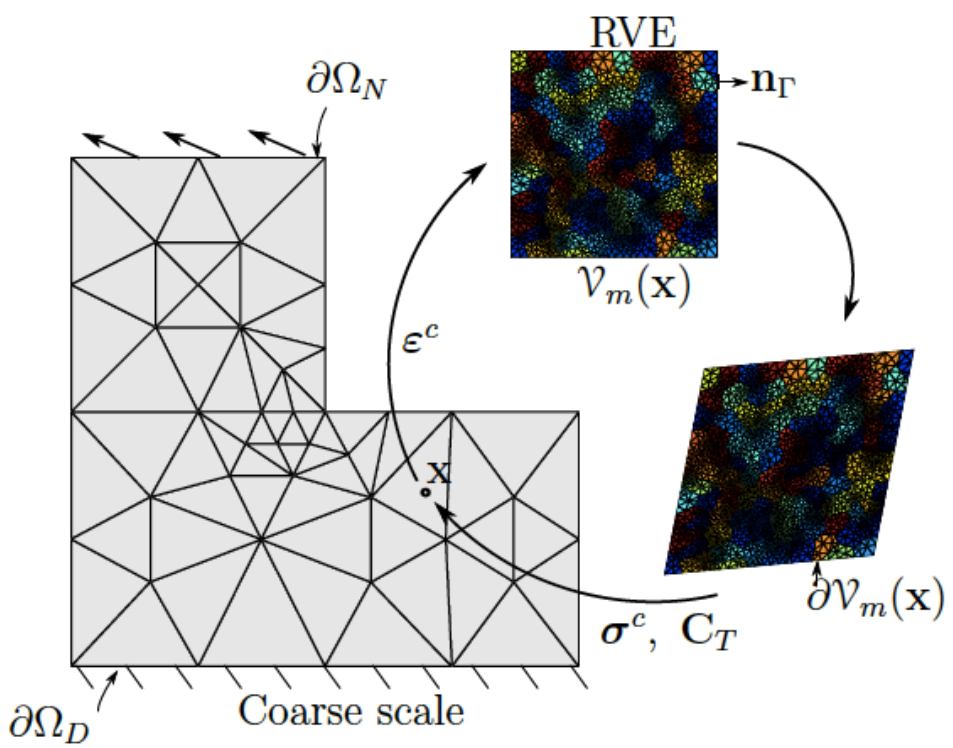
Hierarchical methods FE^2



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

Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2



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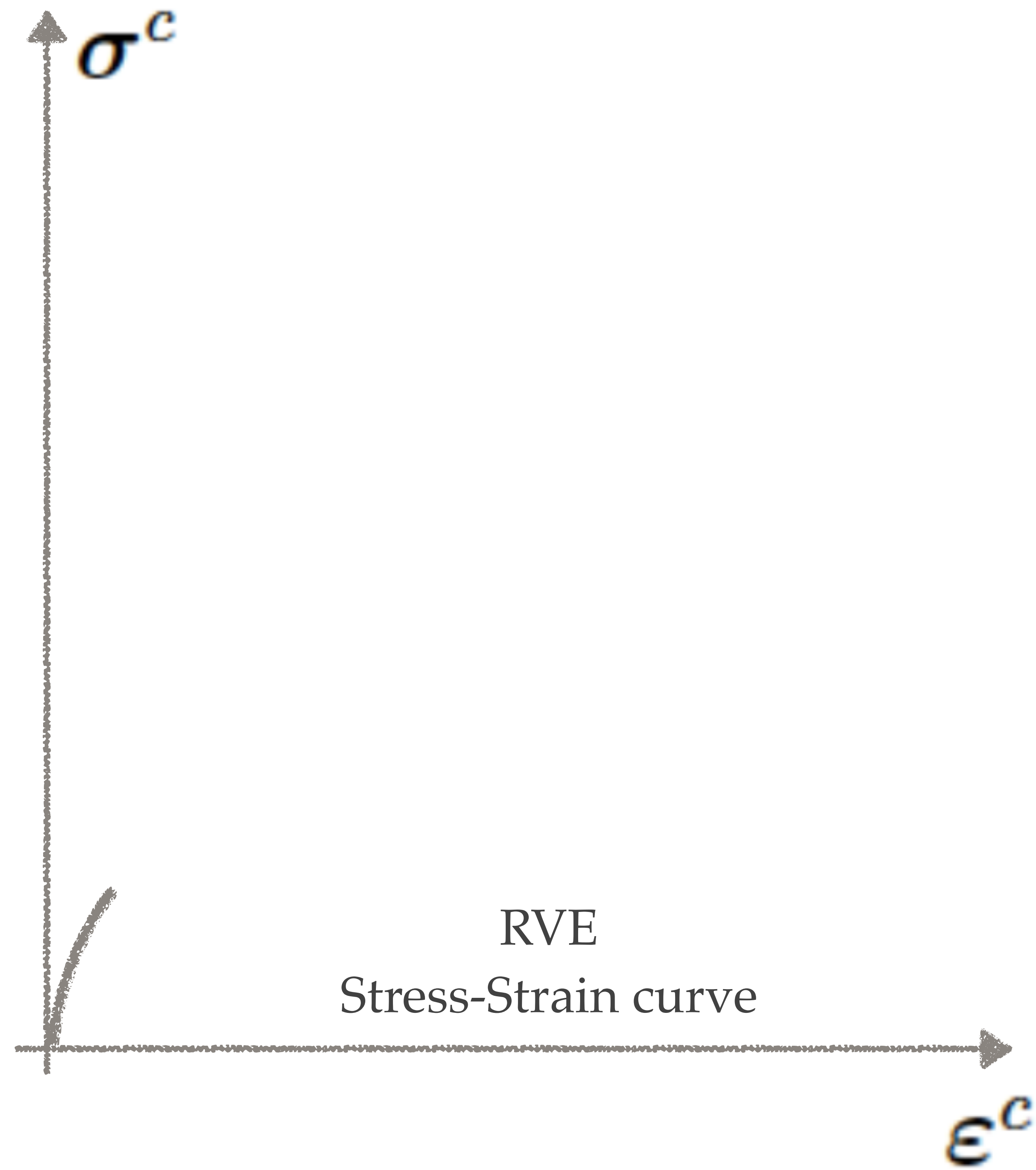
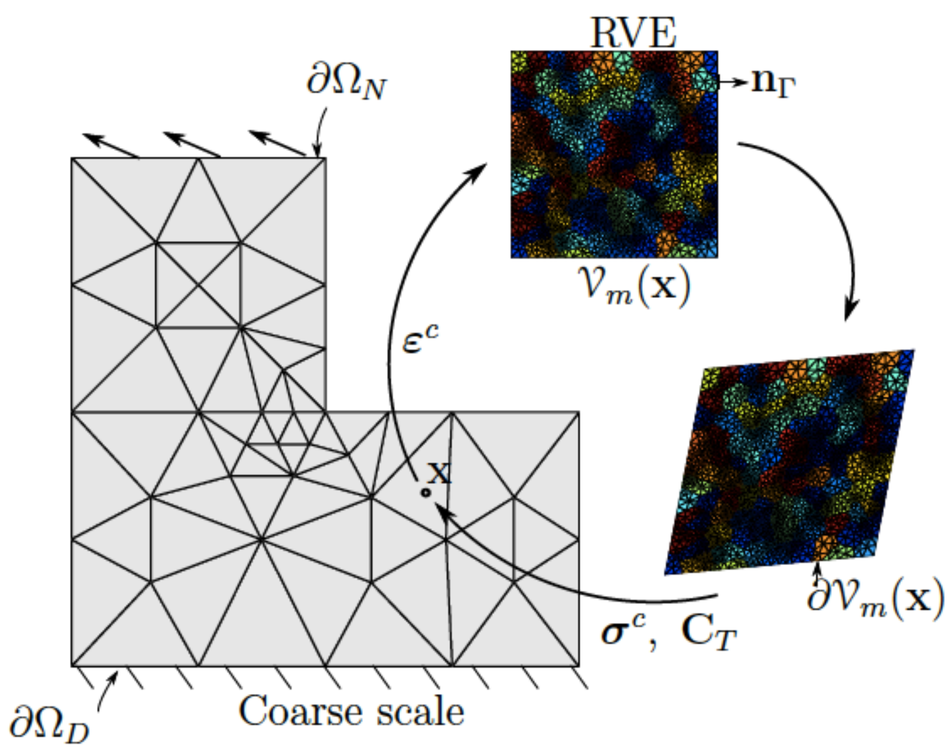
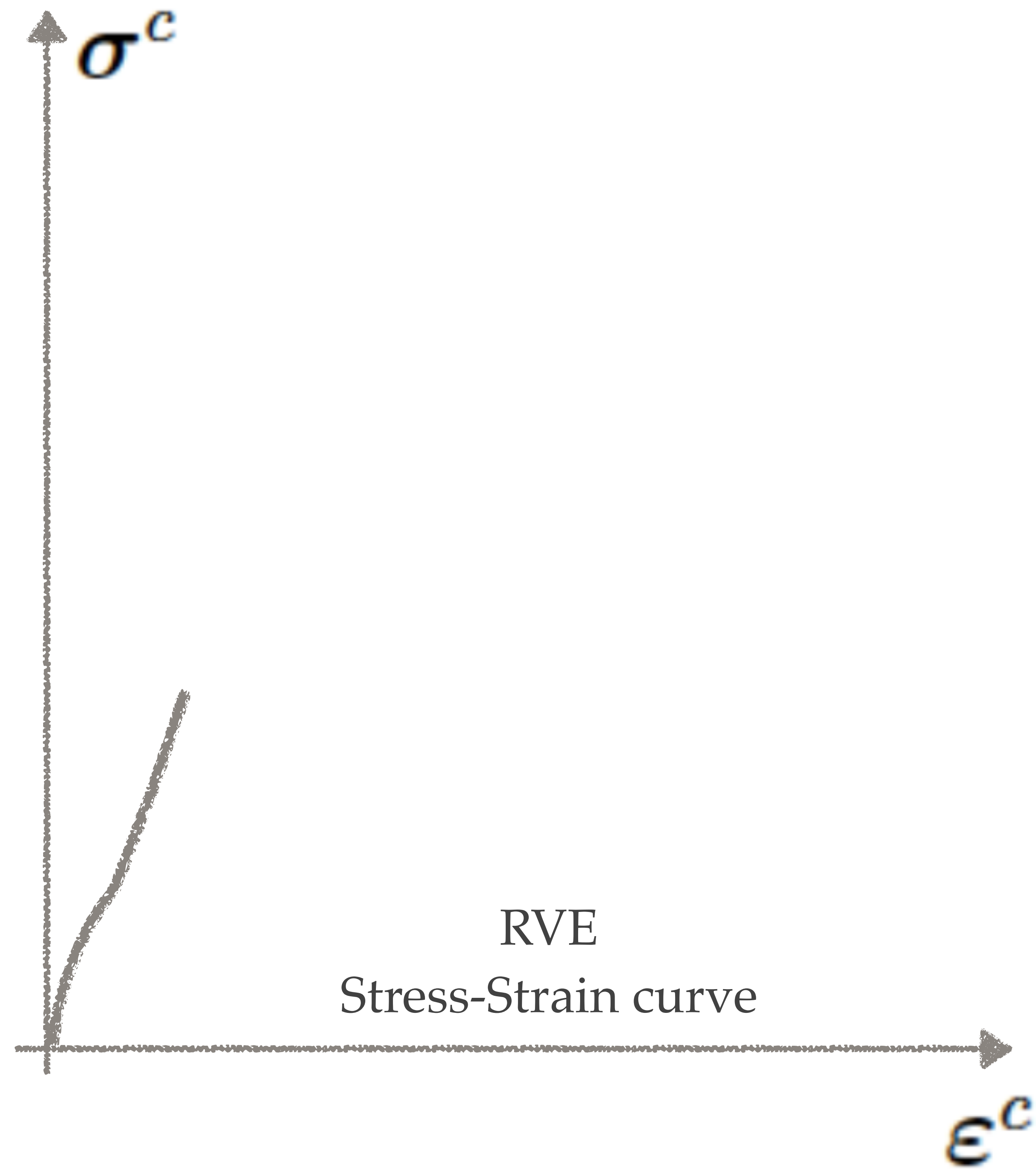


Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2





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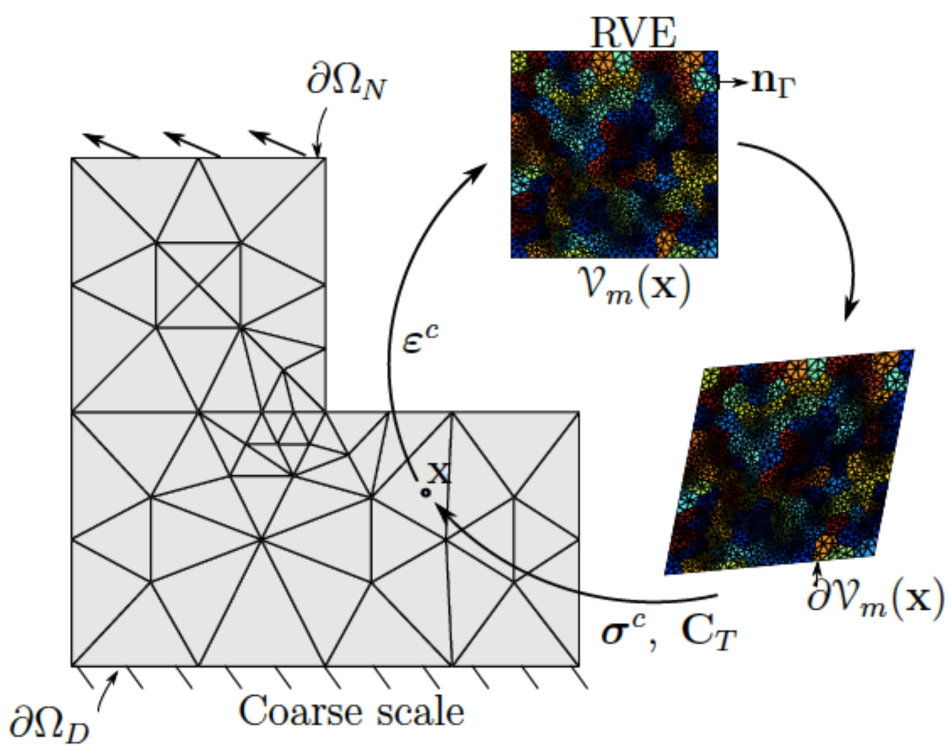
Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2



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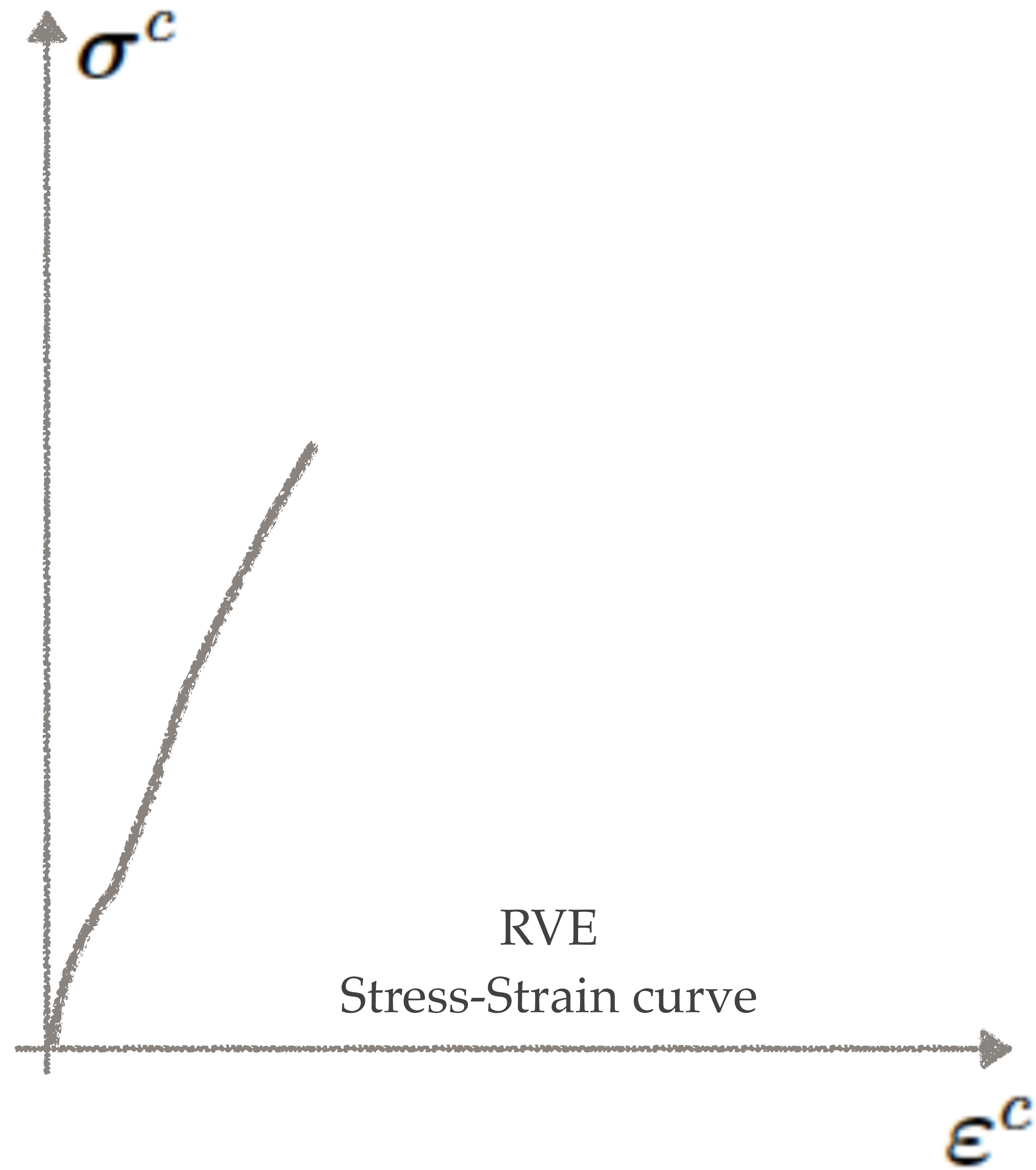
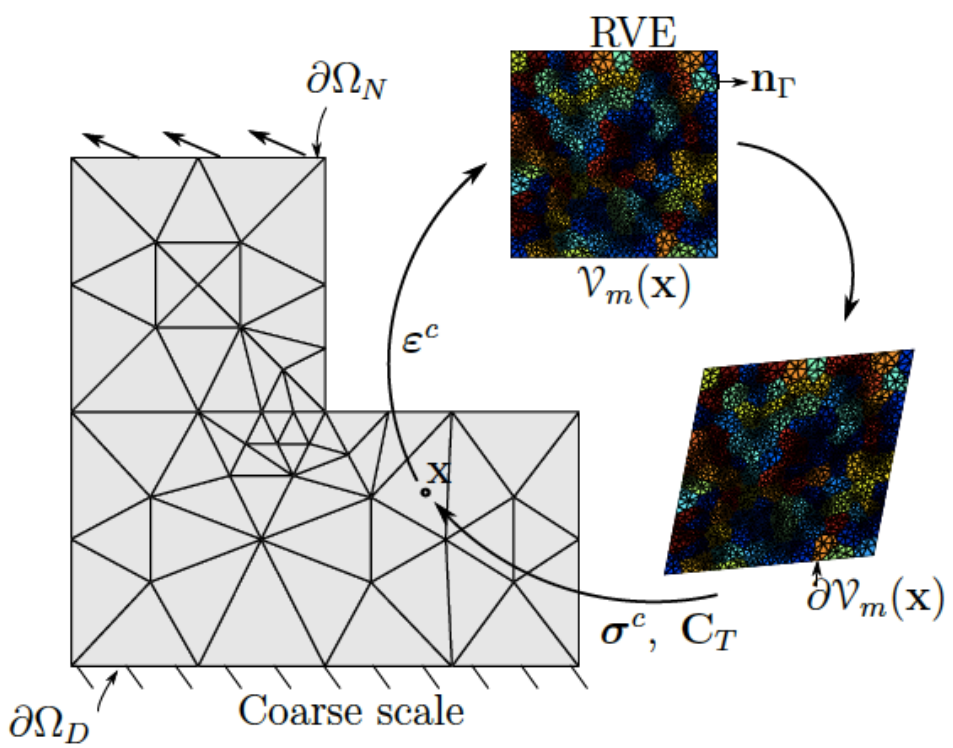
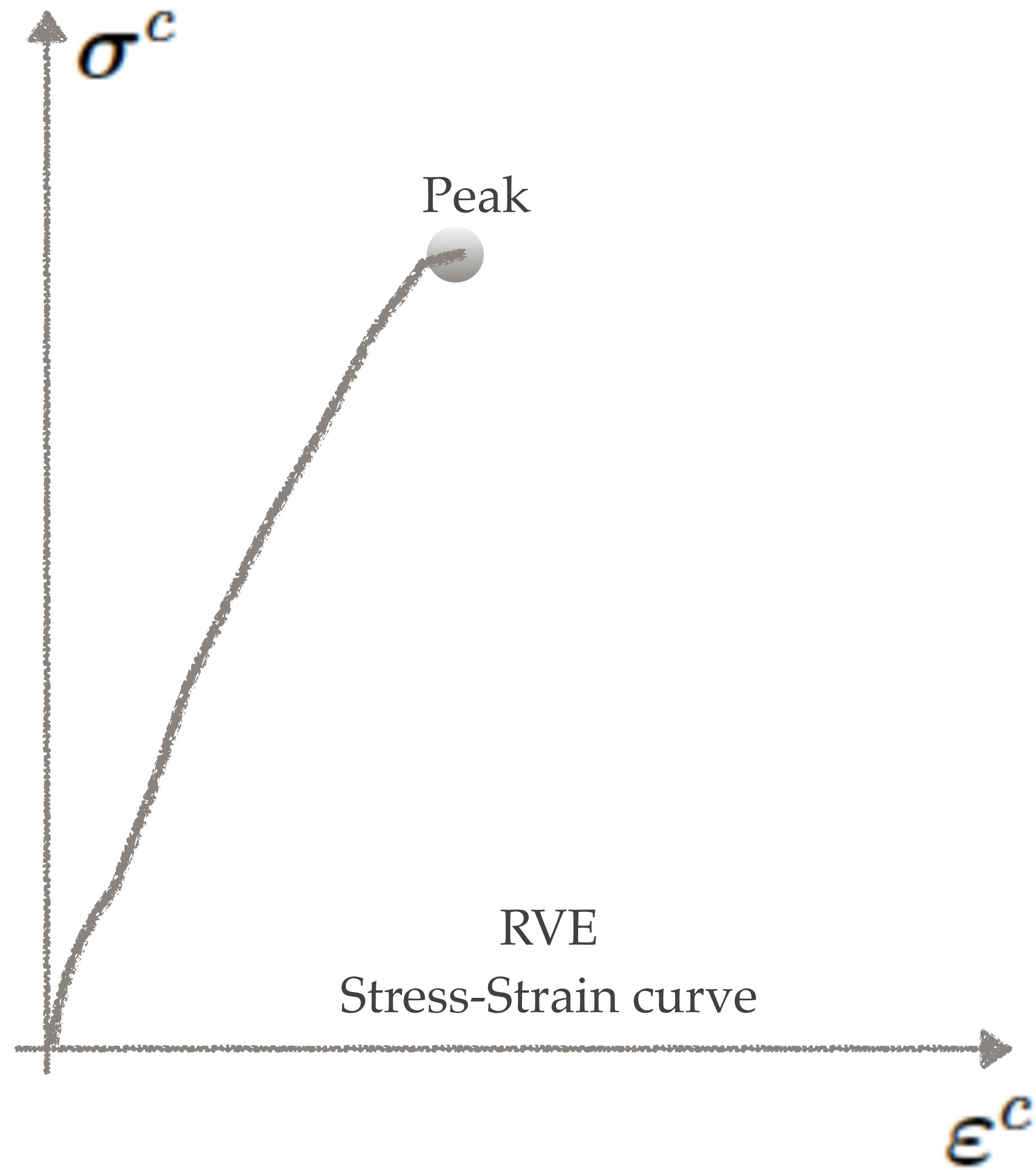


Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

Hierarchical methods FE^2

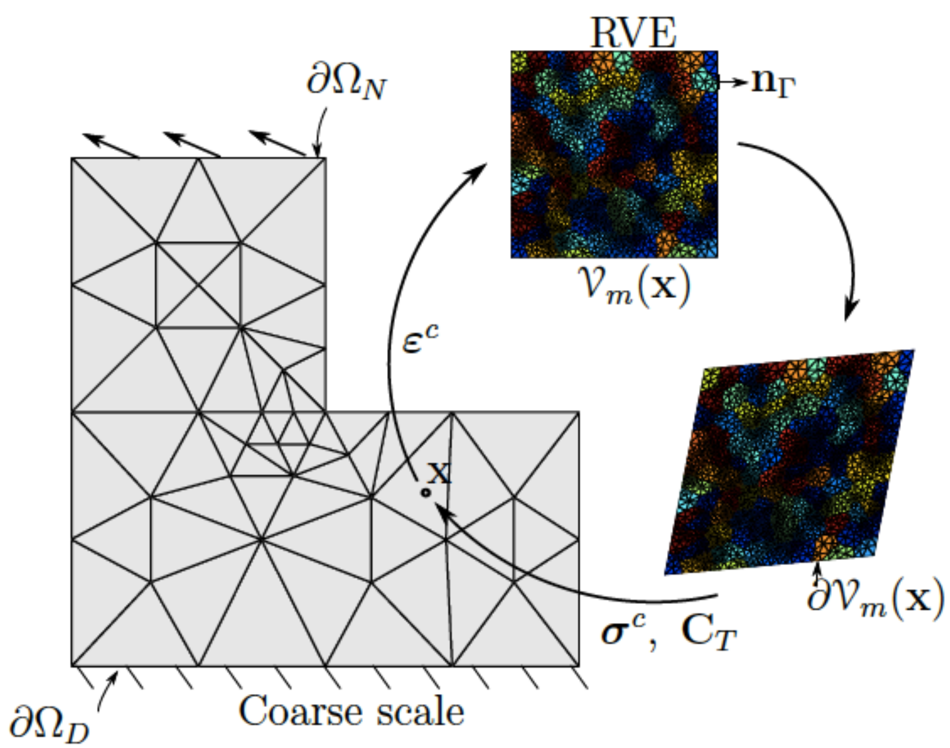


Peak

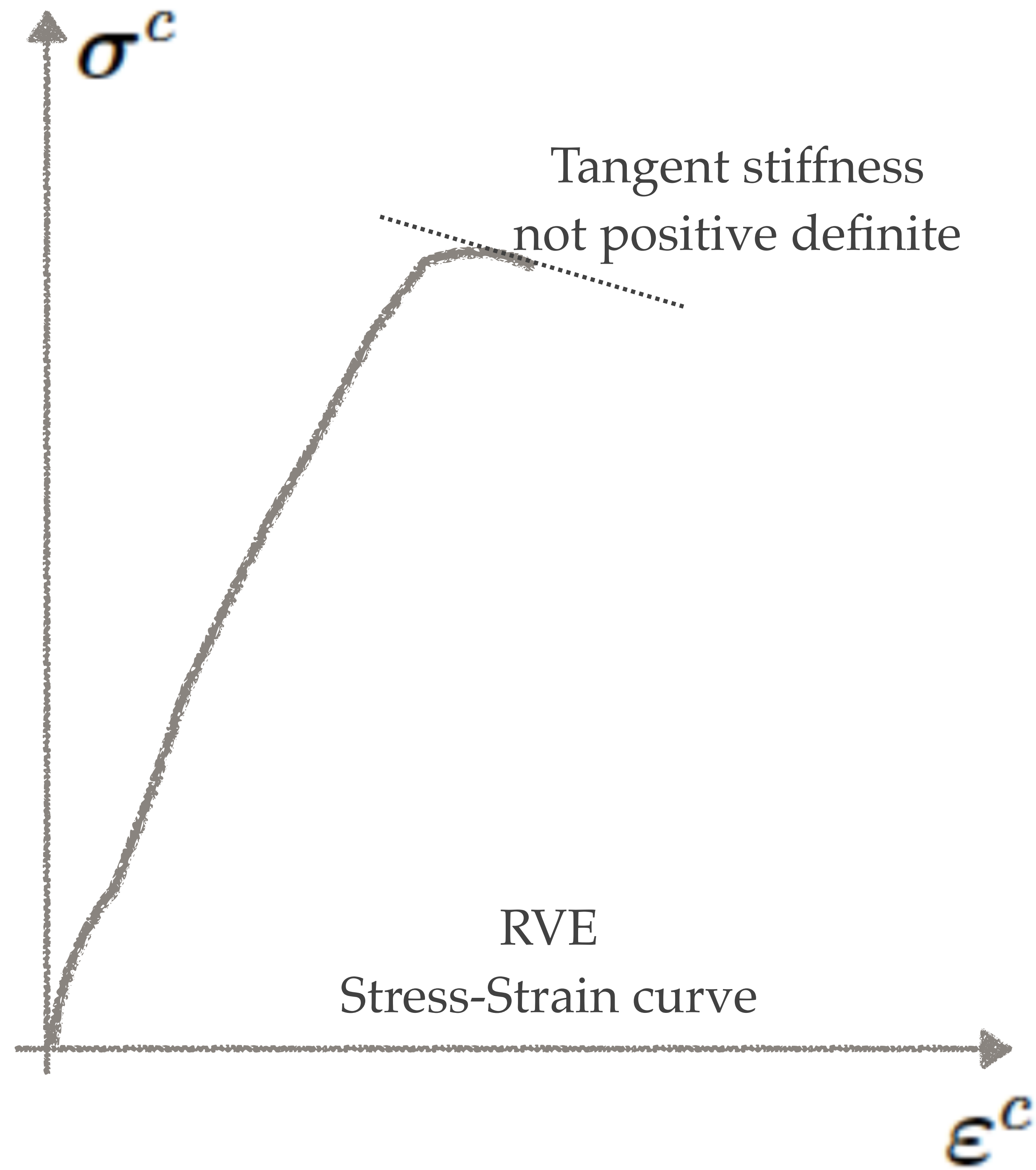


Feyel, Chaboche, 2000 - Akbari, Kerfriden, Bordas, 2014

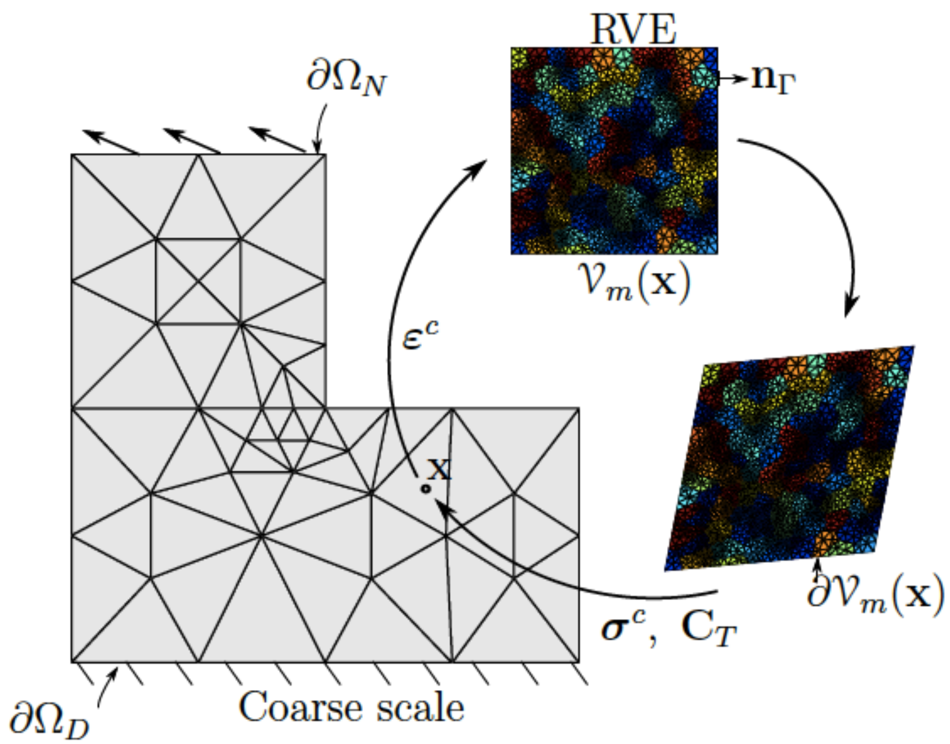
Hierarchical methods FE^2

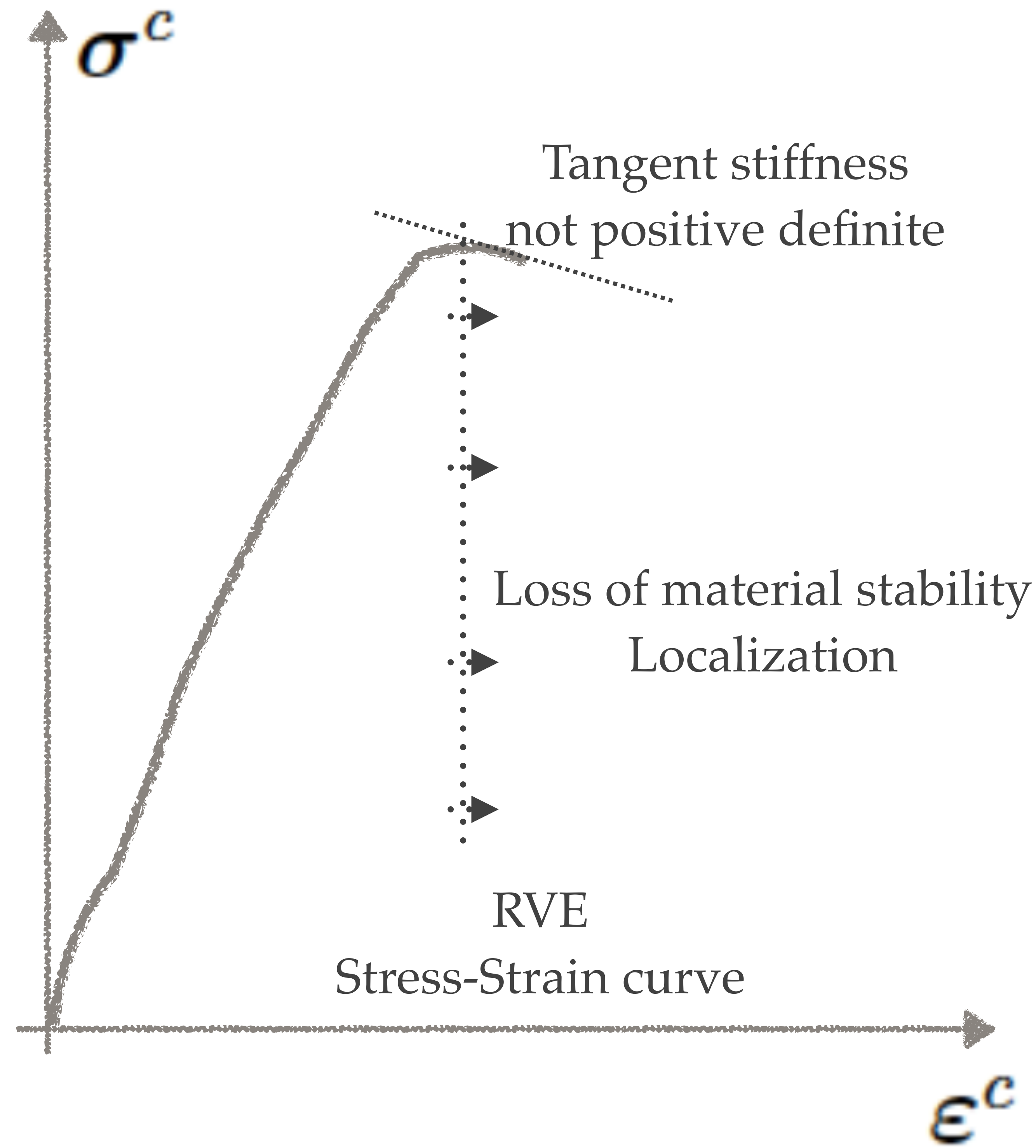


Unloading



Hierarchical methods FE^2



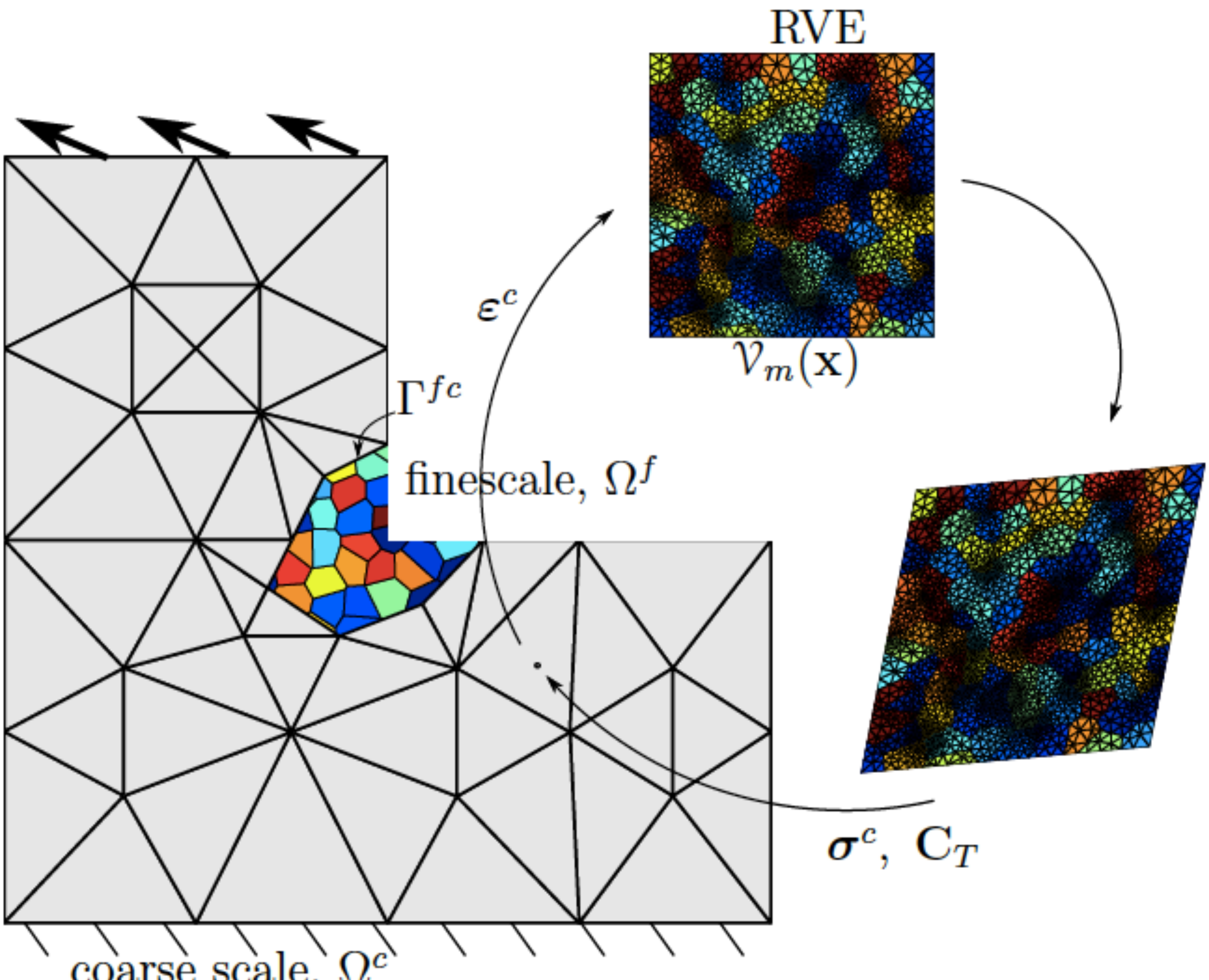


Unloading

RVE does not exist

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

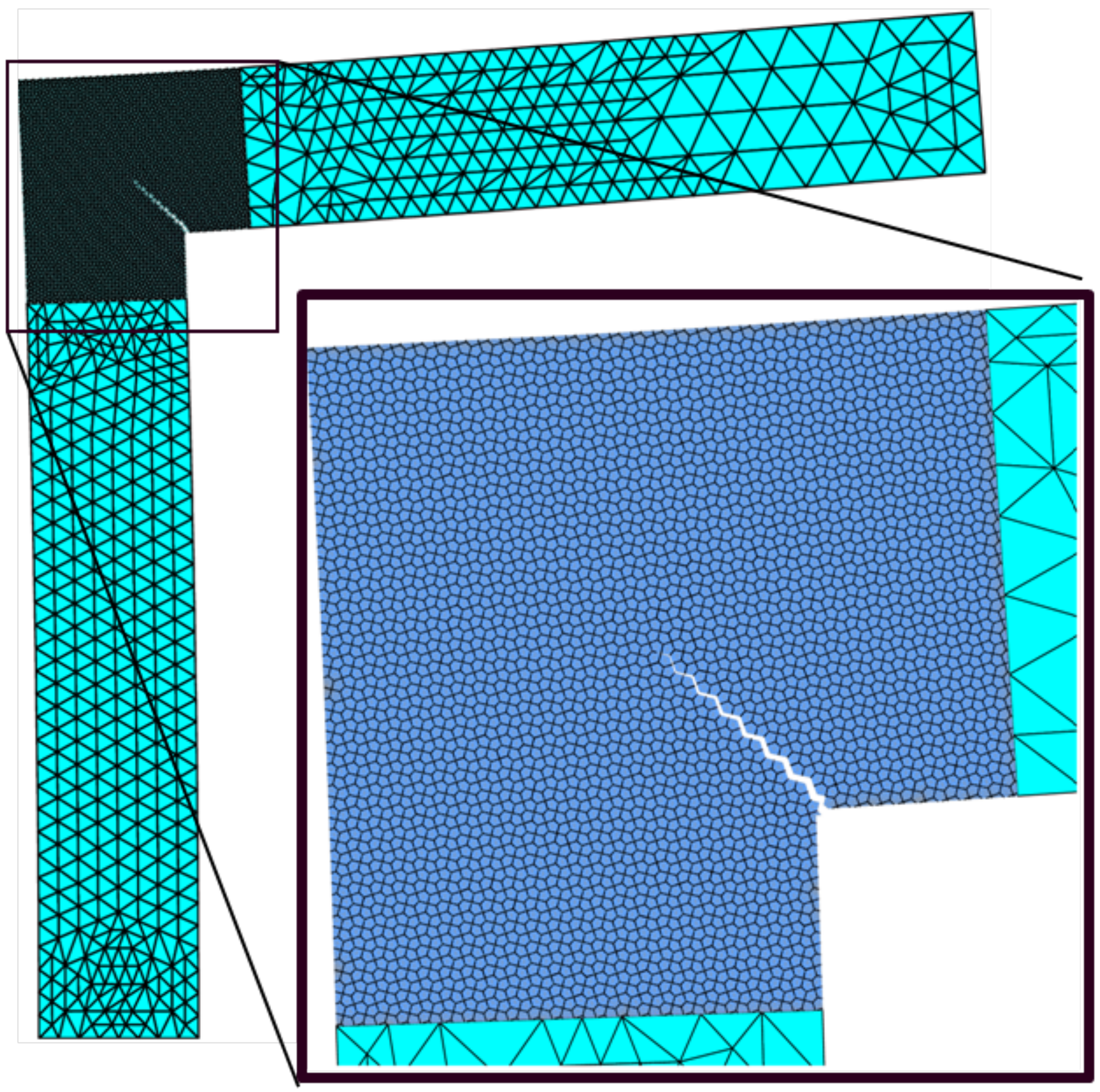
Hybrid methods



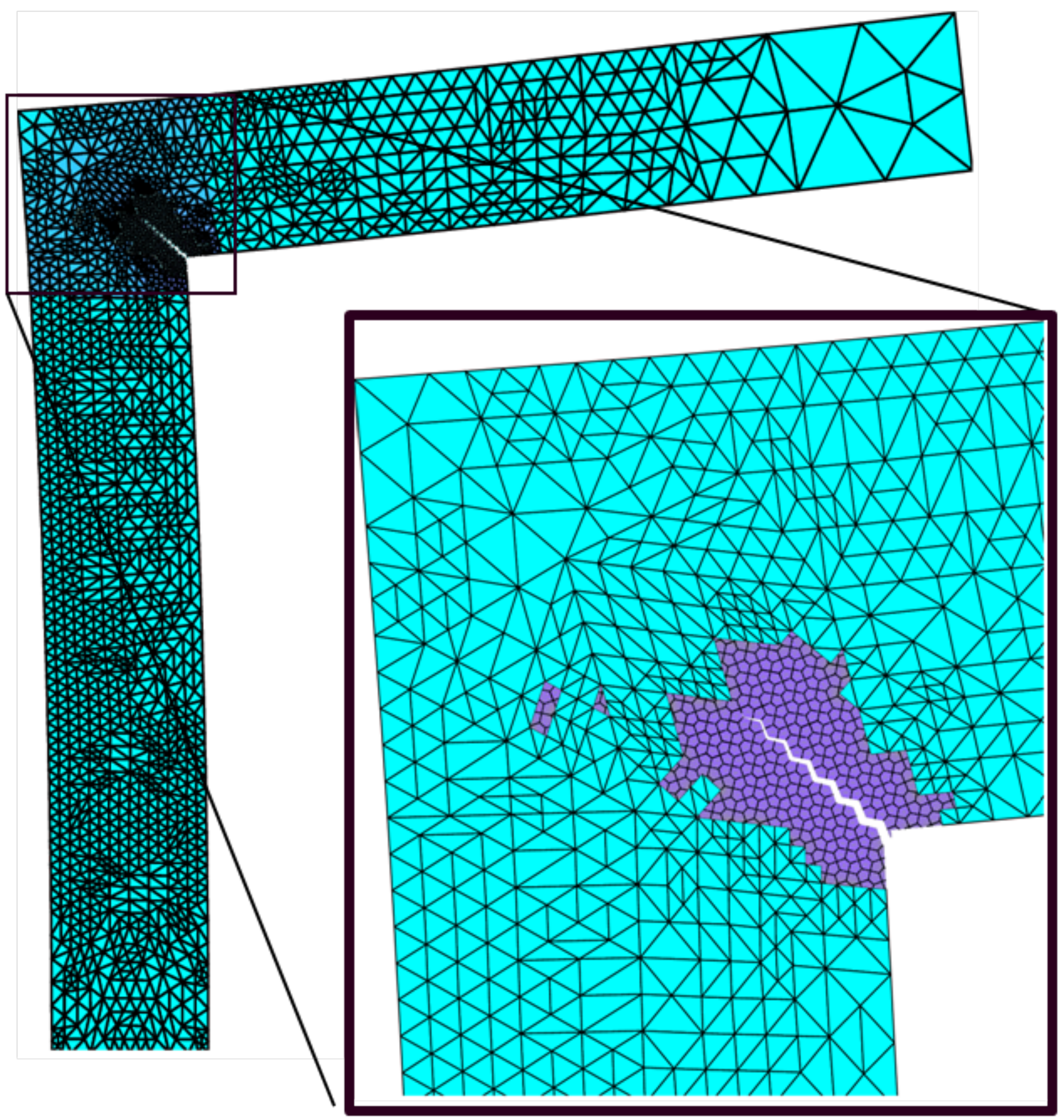
Akbari, Kerfriden, Bordas, 2014

Example

Direct Numerical Solution

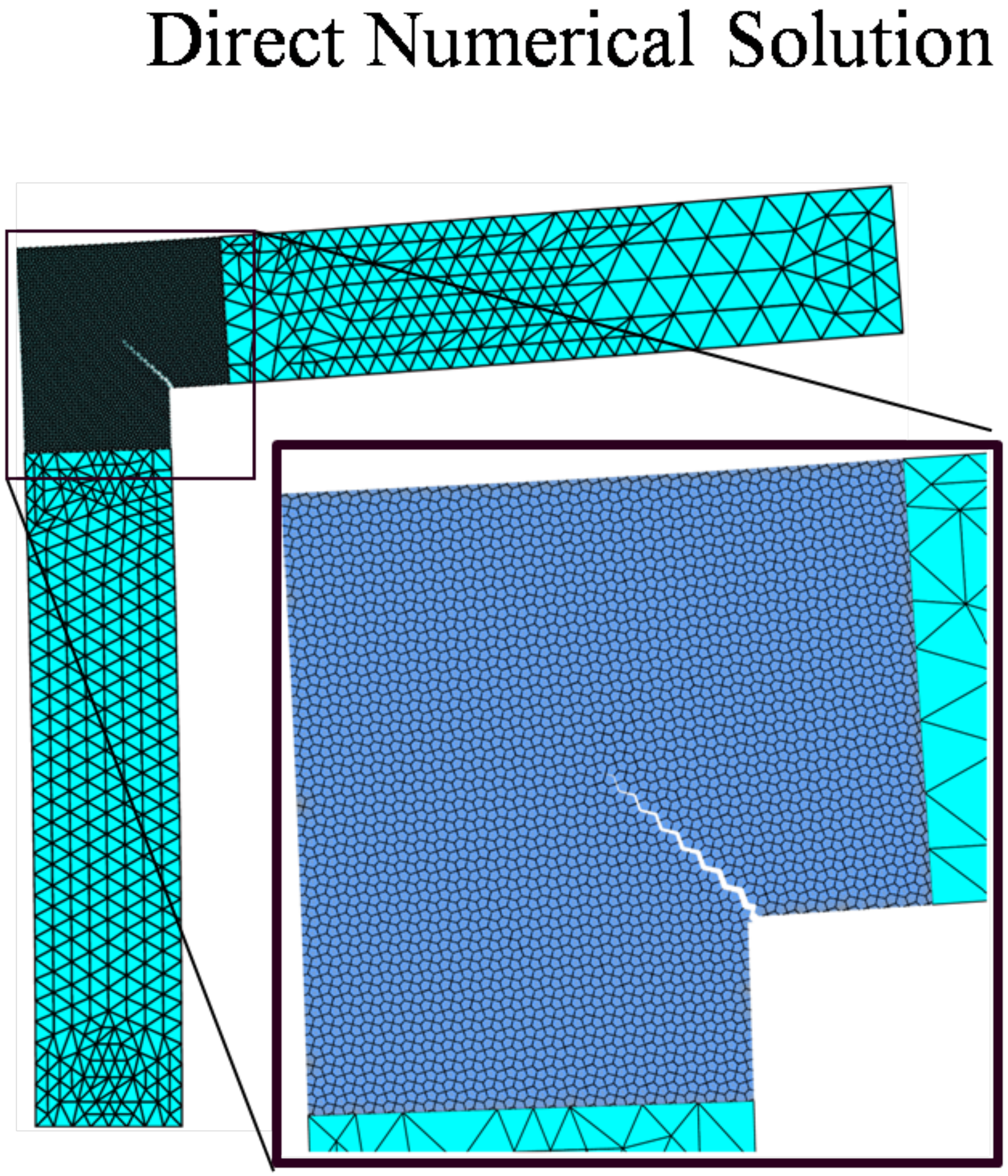


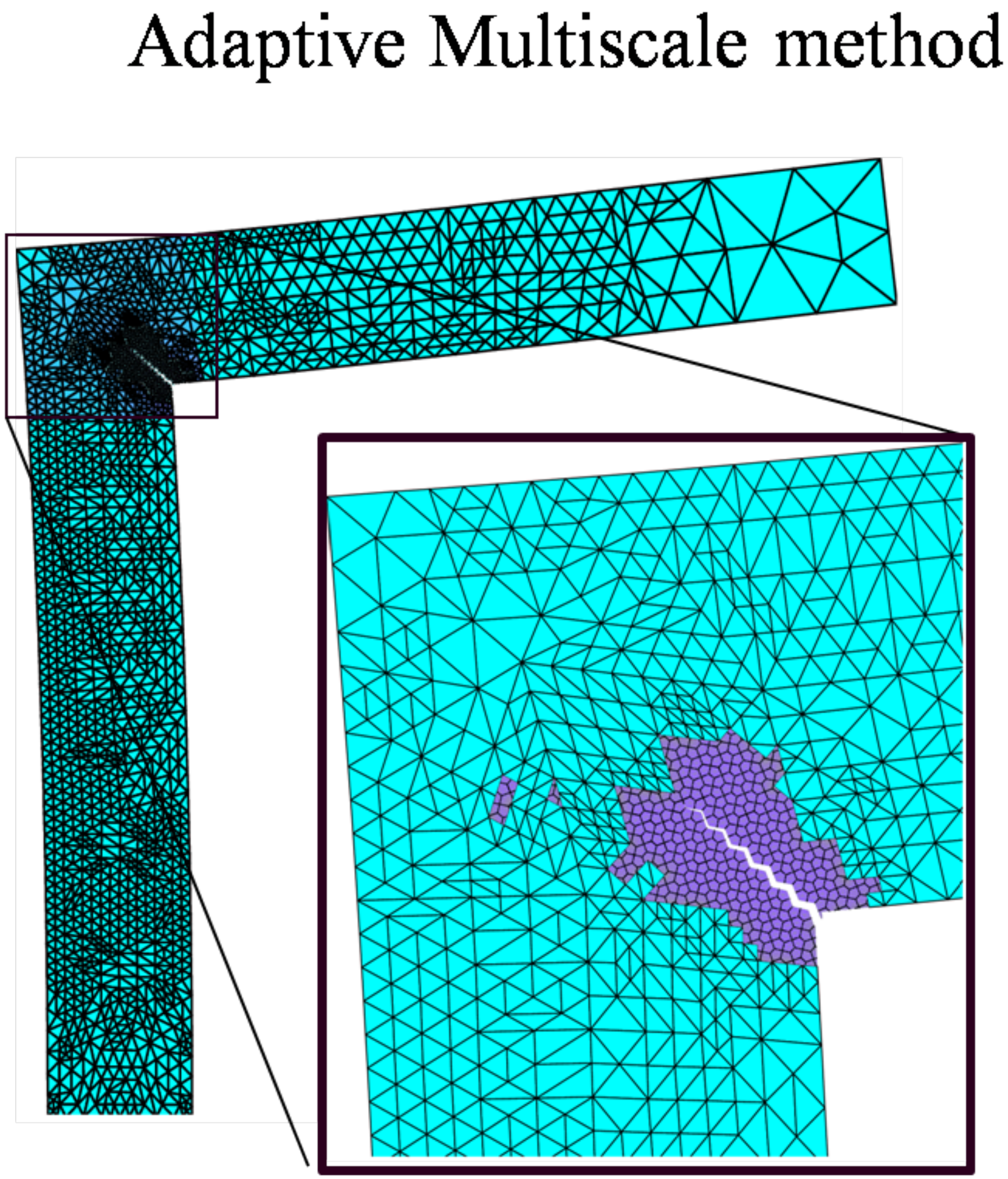
Adaptive Multiscale method



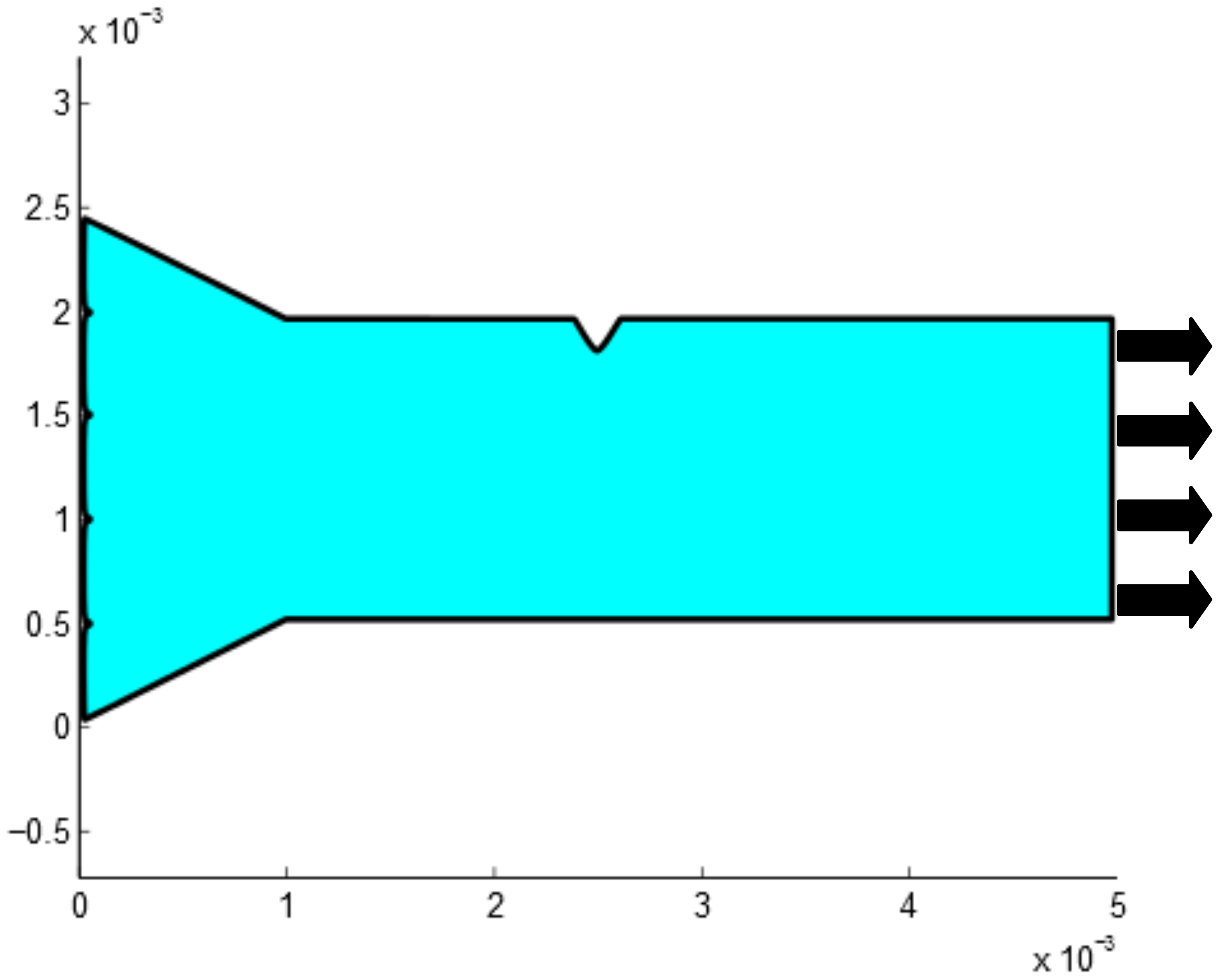
Example

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





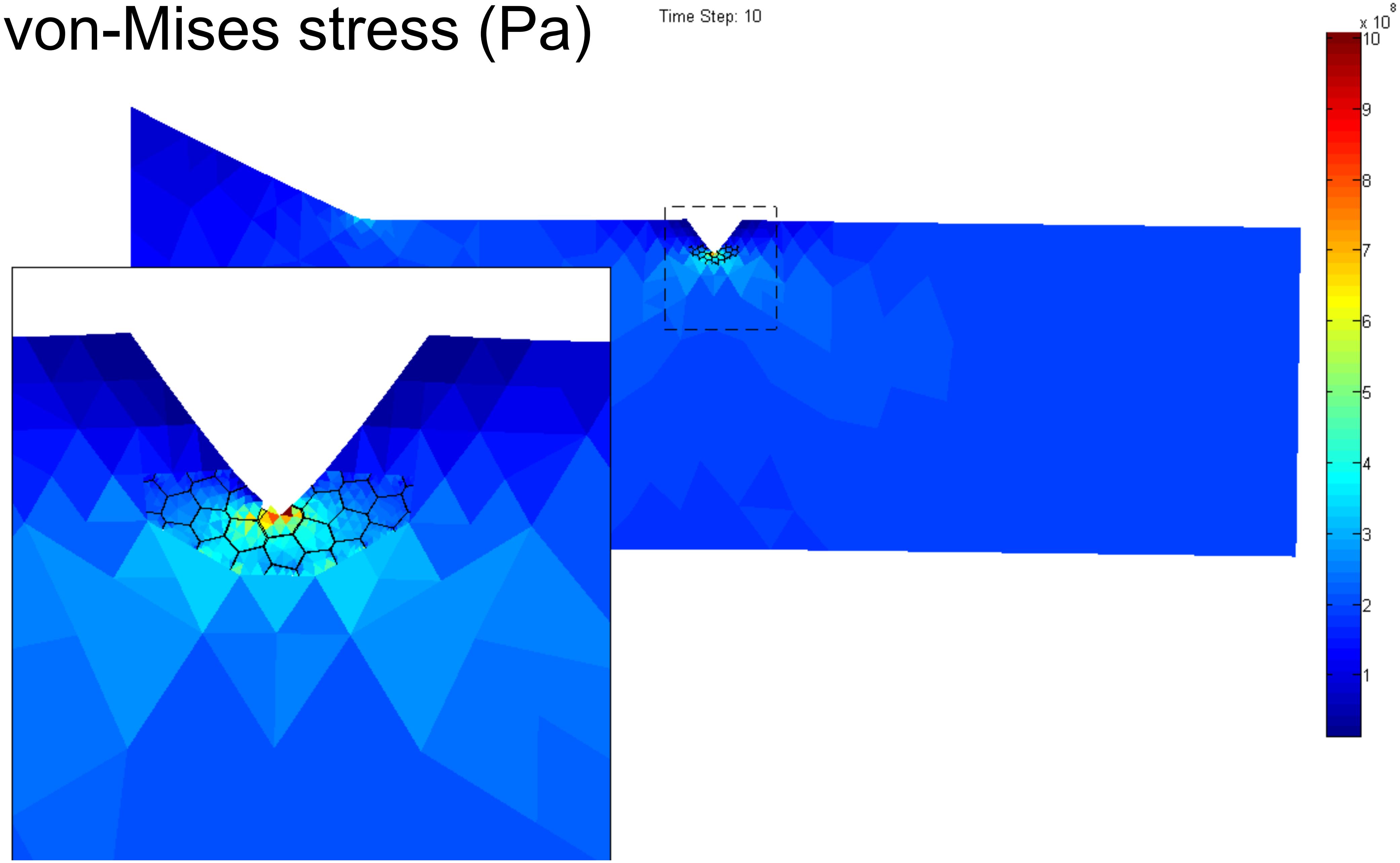
Results: uni-axial tension



❖ Sizes are in mm

Results: uni-axial tension

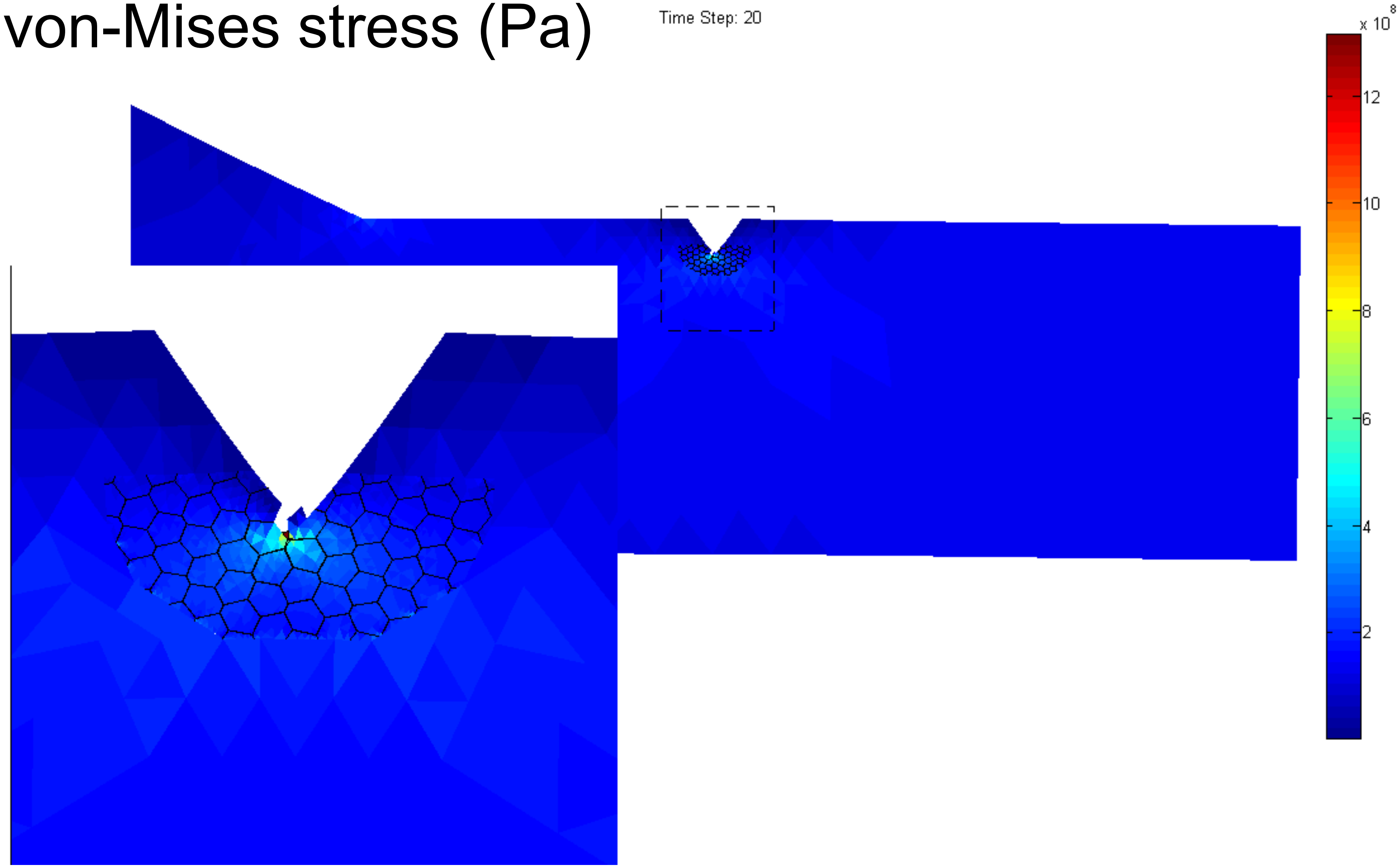
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

Results: uni-axial tension

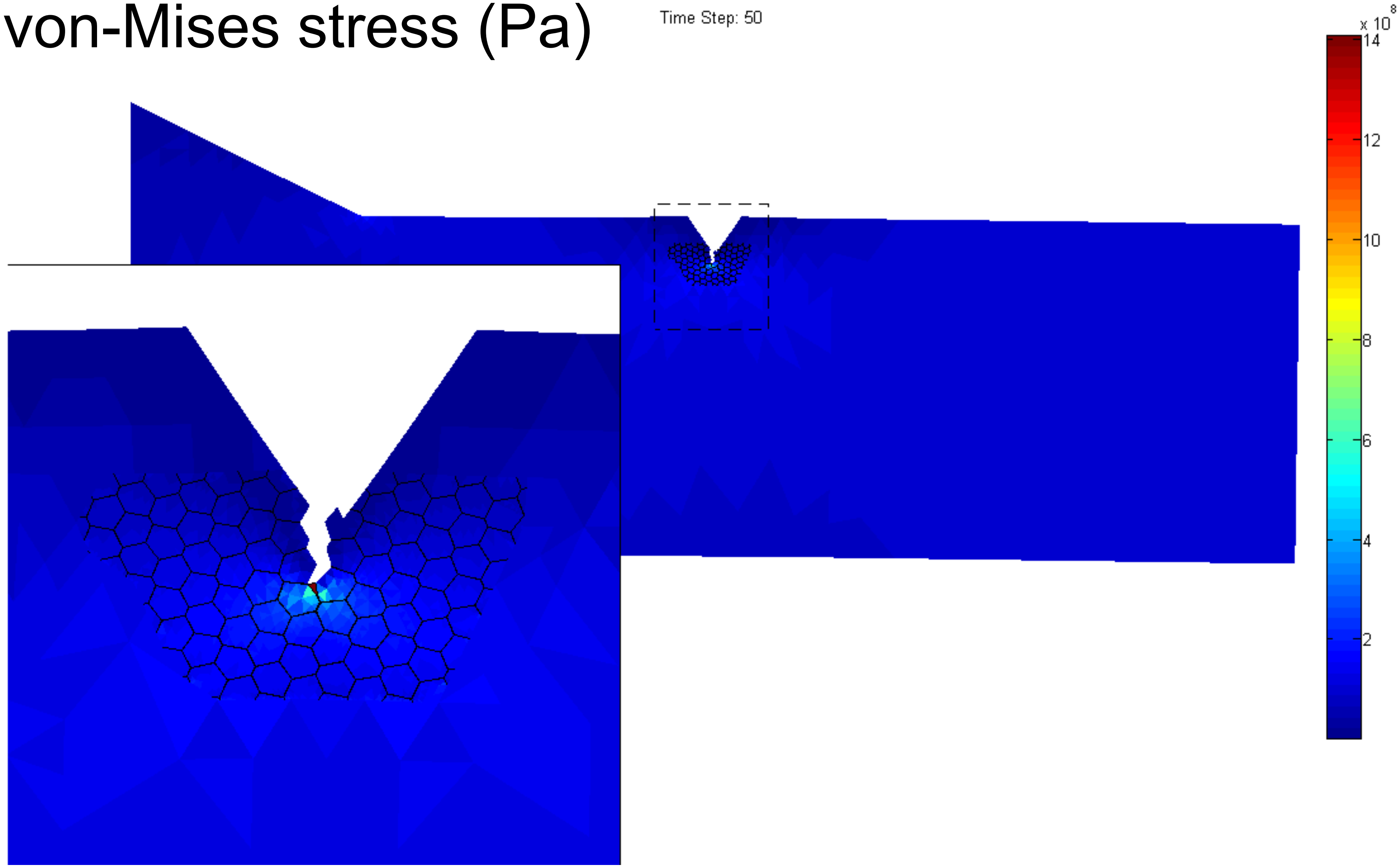
von-Mises stress (Pa)



❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)



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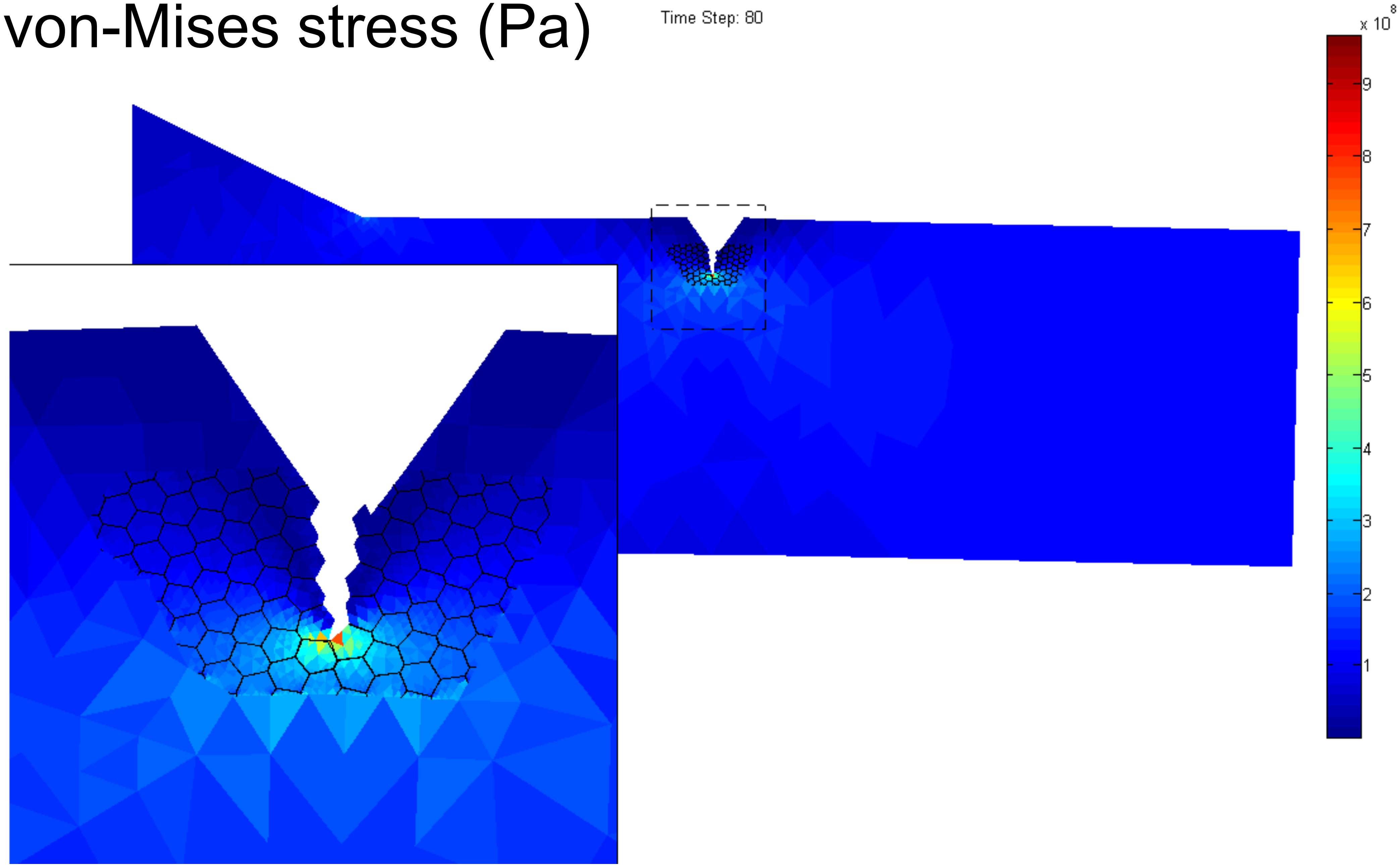

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Results: uni-axial tension

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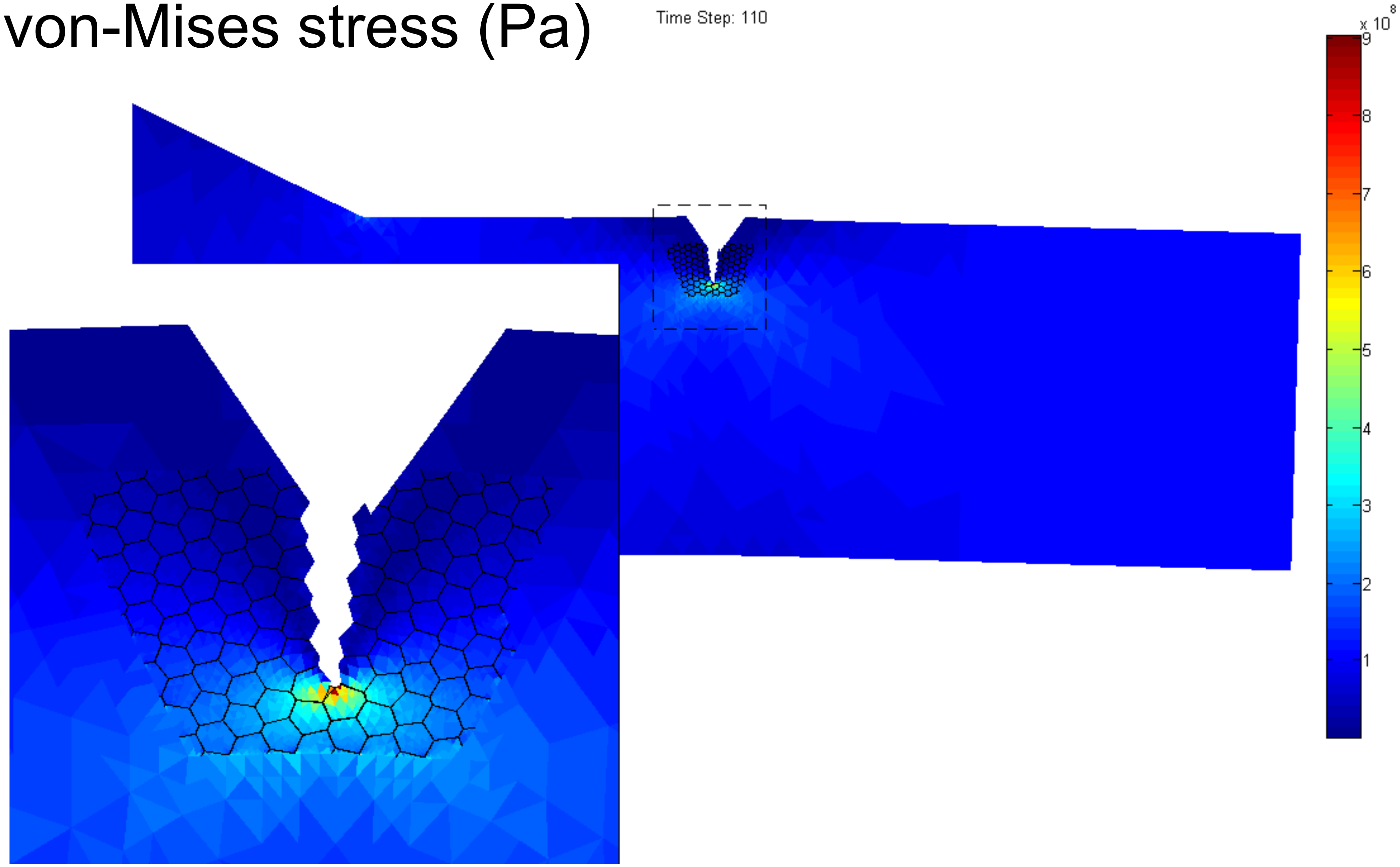
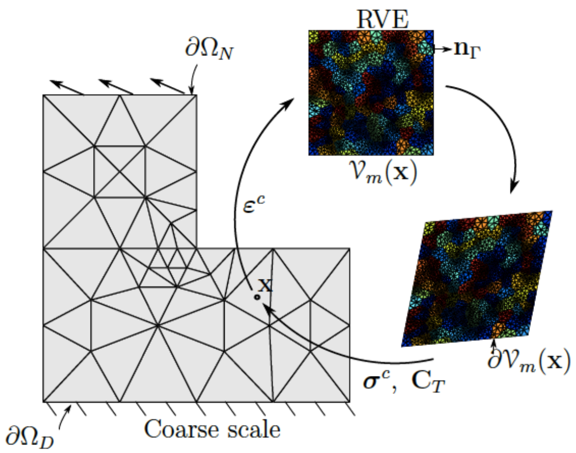
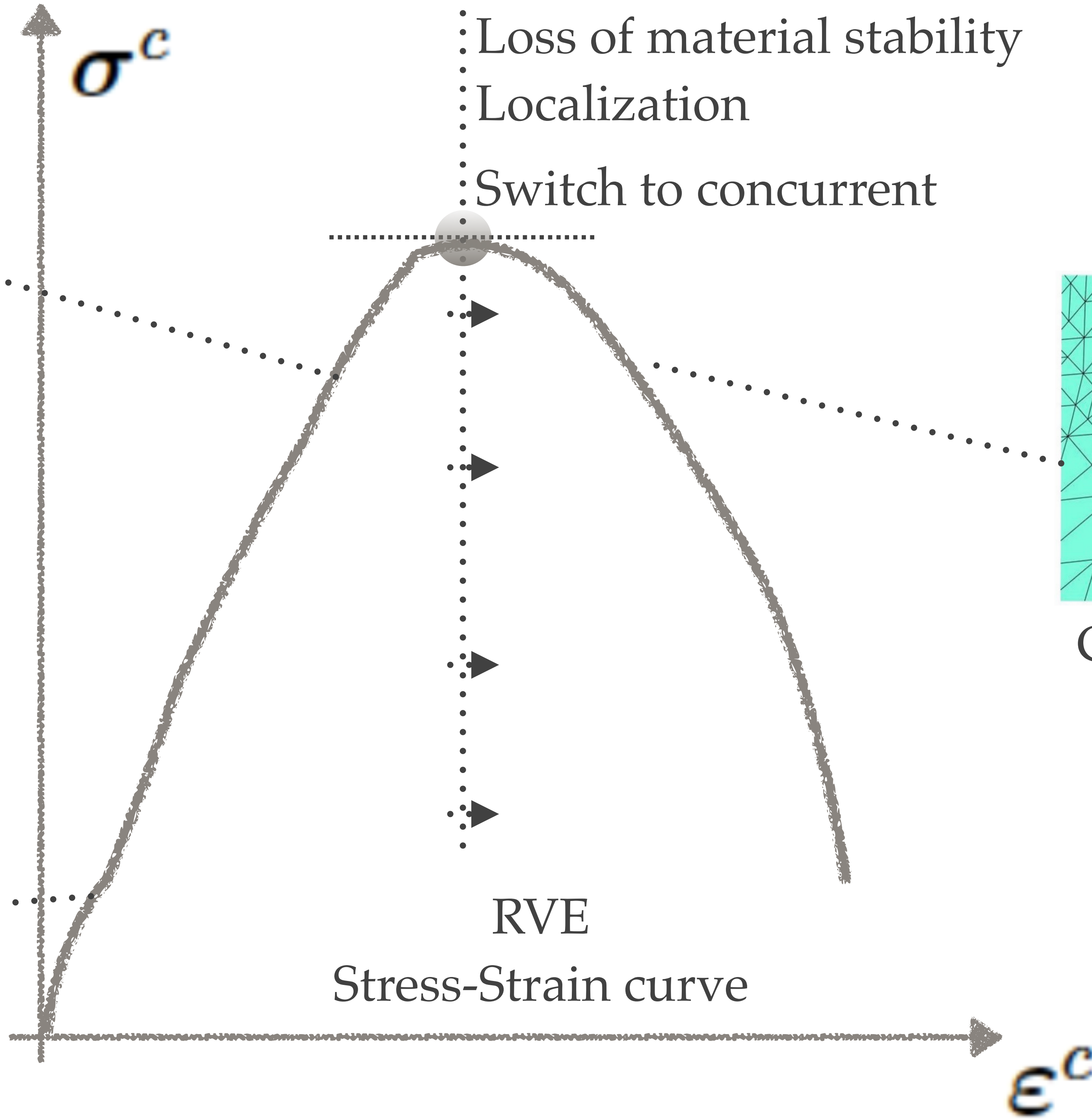


❖ 100X (magnification of displacement)

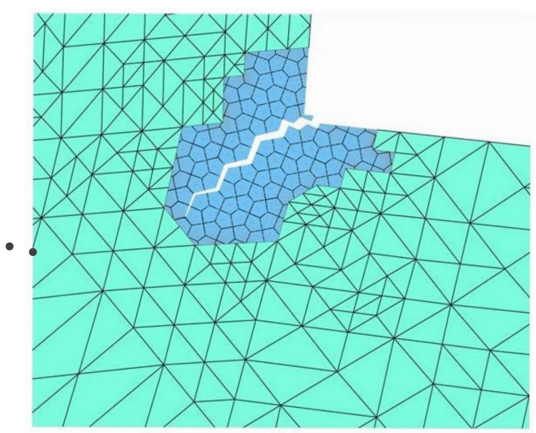
Adaptive multi-scale



Semi-concurrent
FE^2



Analytical
homogenisation



Concurrent

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

Open problem

- material parameter identification at small scales

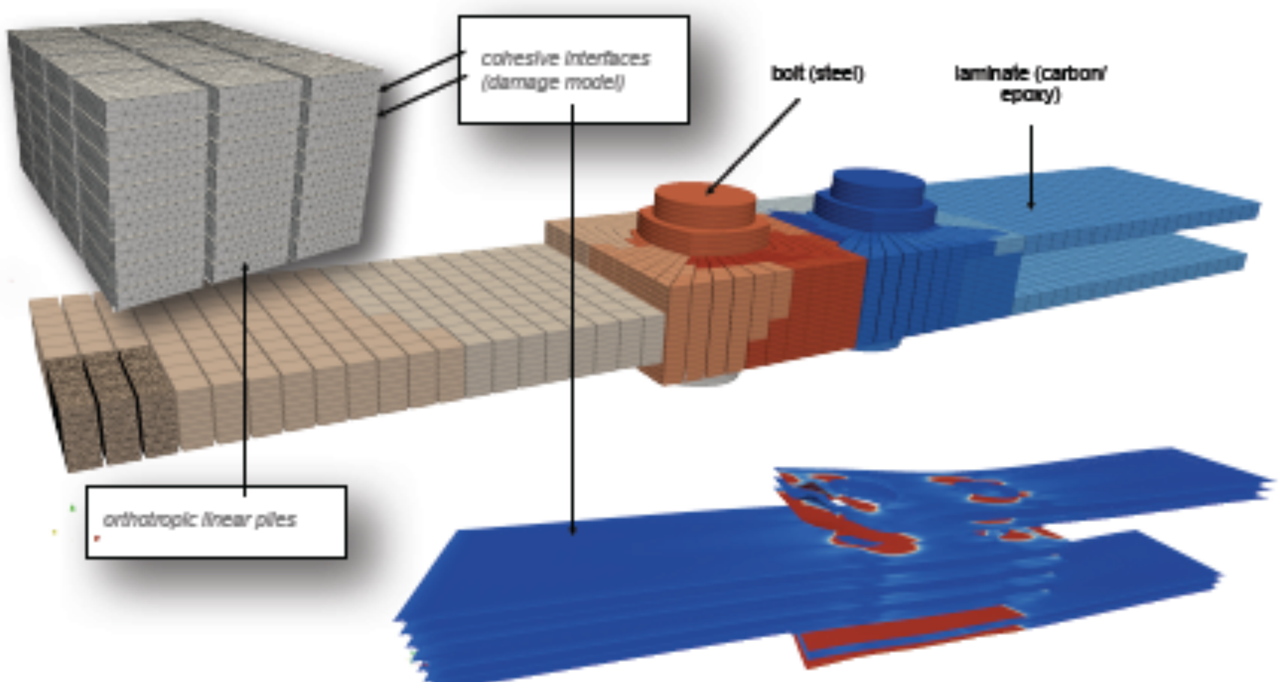
Possible approach

- small-scale experiments - costly

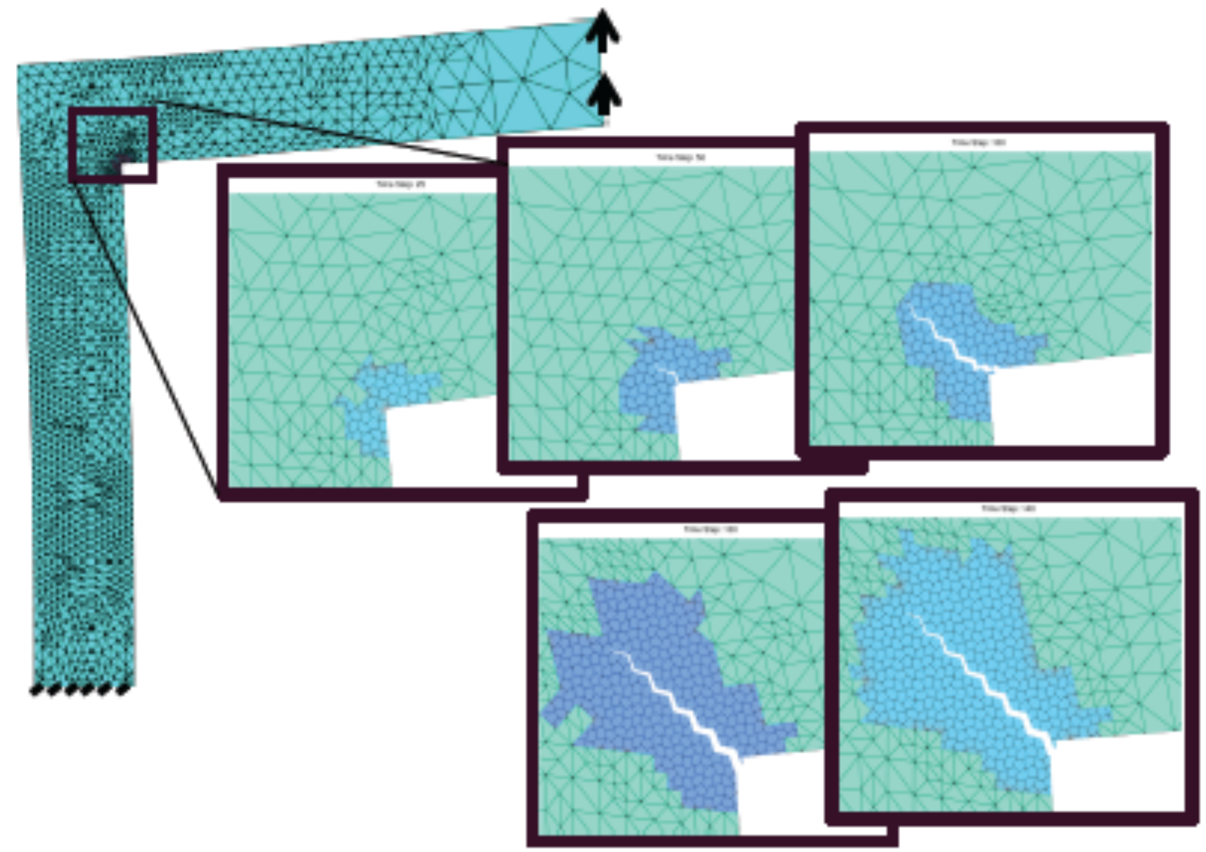
Model reduction - physics-based (1)

- Multilevel methods to reduce CPU time by orders of magnitude and devise robust, efficient code/model coupling

  - HPC Adaptive multiscale models/solvers with controlled accuracy



[Kerfriden et al., 2010]



[Akbari et al., 2013]

Open problem: adaptive error controlled algorithms for model and discretization error. Use the right model at the right place/time.

Challenge

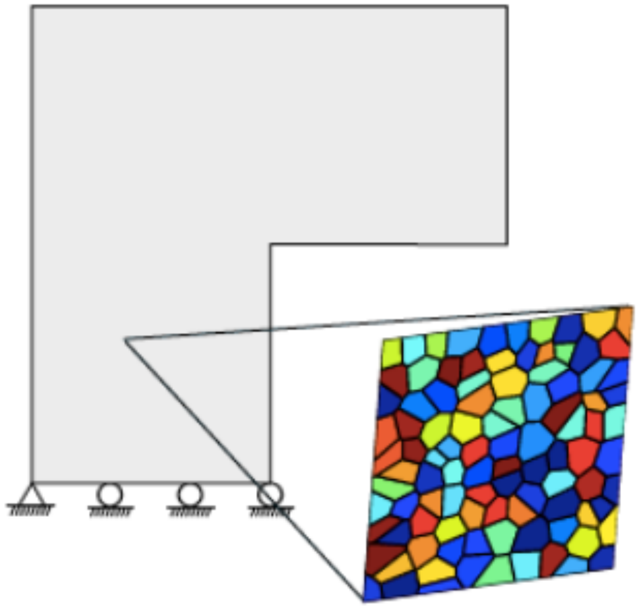
- Reduce the problem size
- Preserve essential features

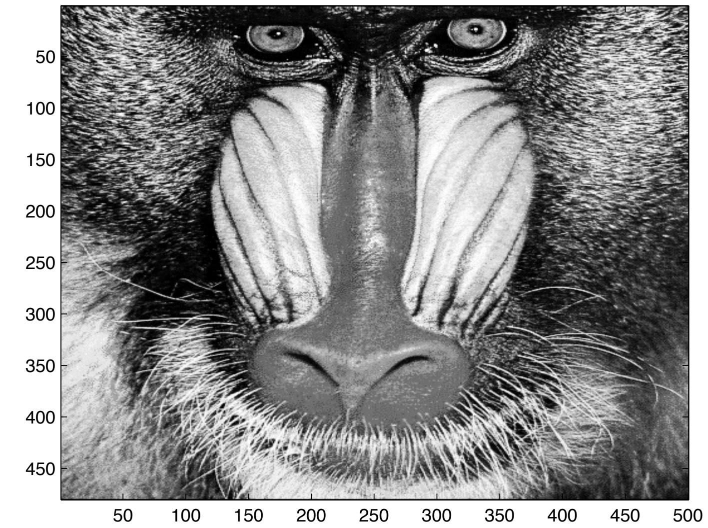
Reduce computational expense

Control the error

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

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





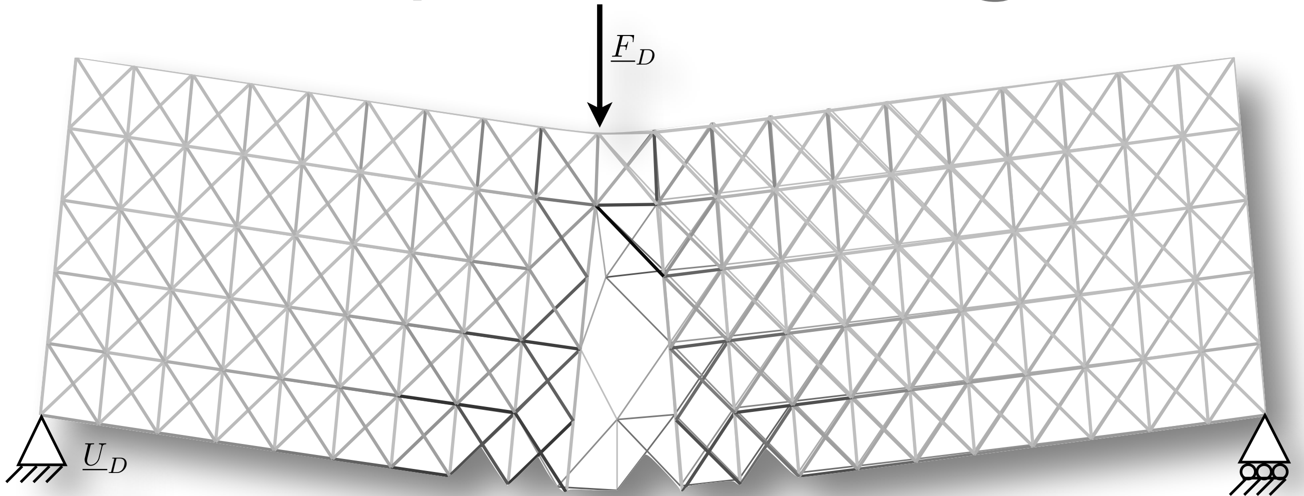
Algebraic model reduction methods

Use precomputed solutions to accelerate online simulations

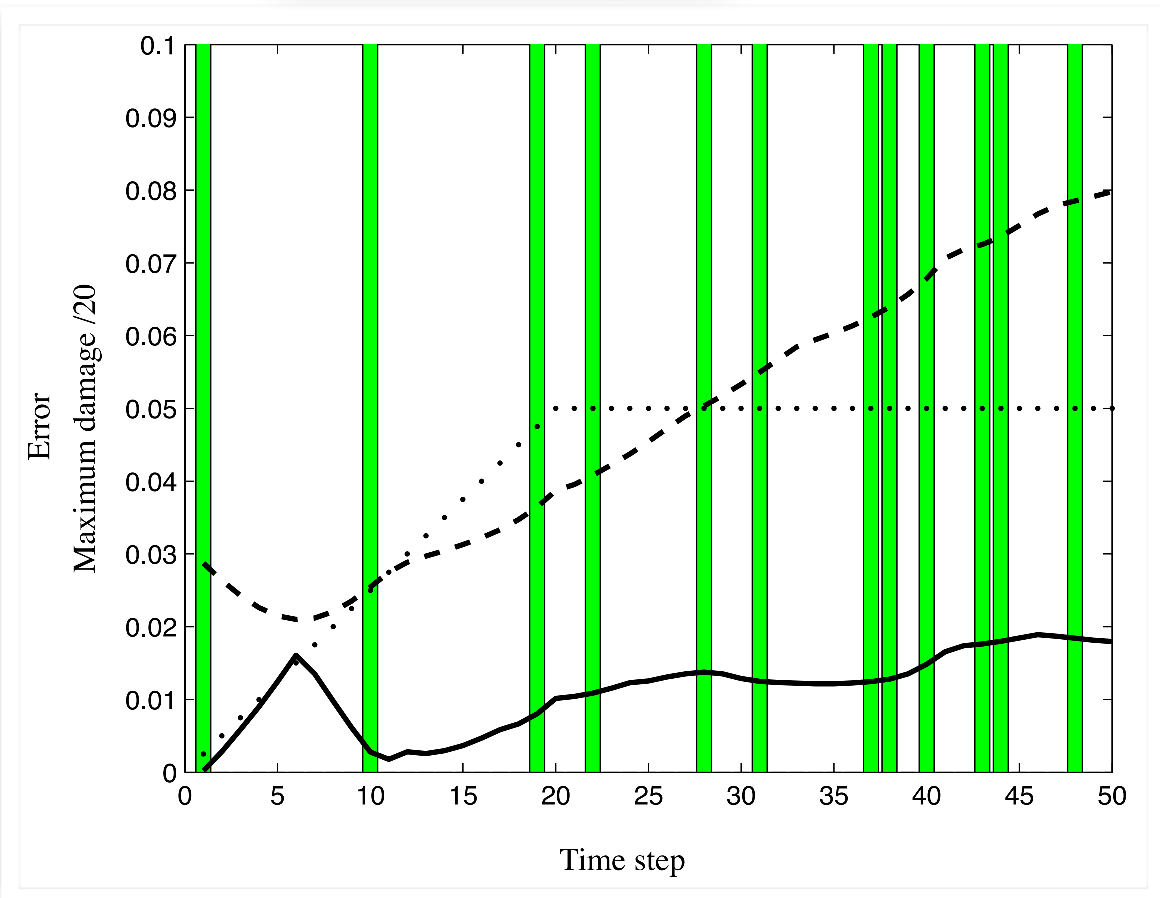
Example - parametric problems

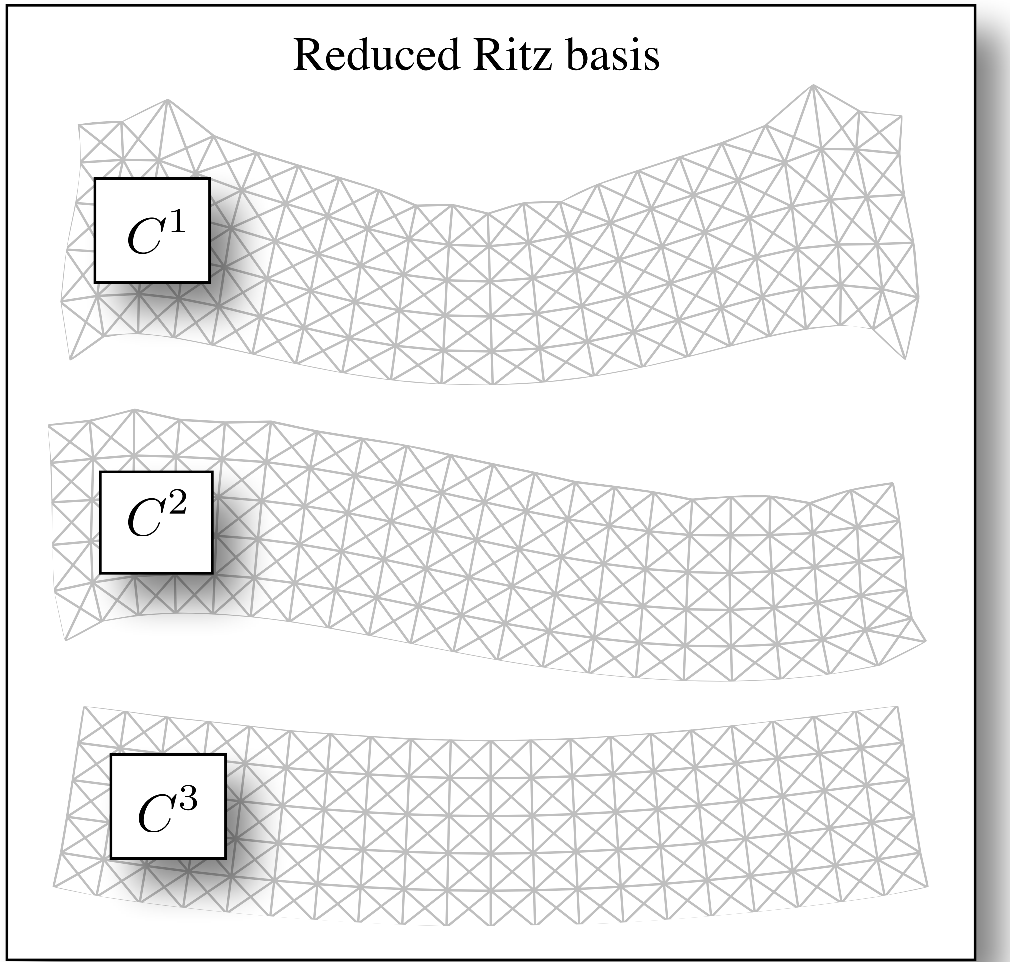
Method of separated representation

Proper orthogonal decomposition (POD)



This solution is not in the snapshot !





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.

Illustration of the method of separated representation

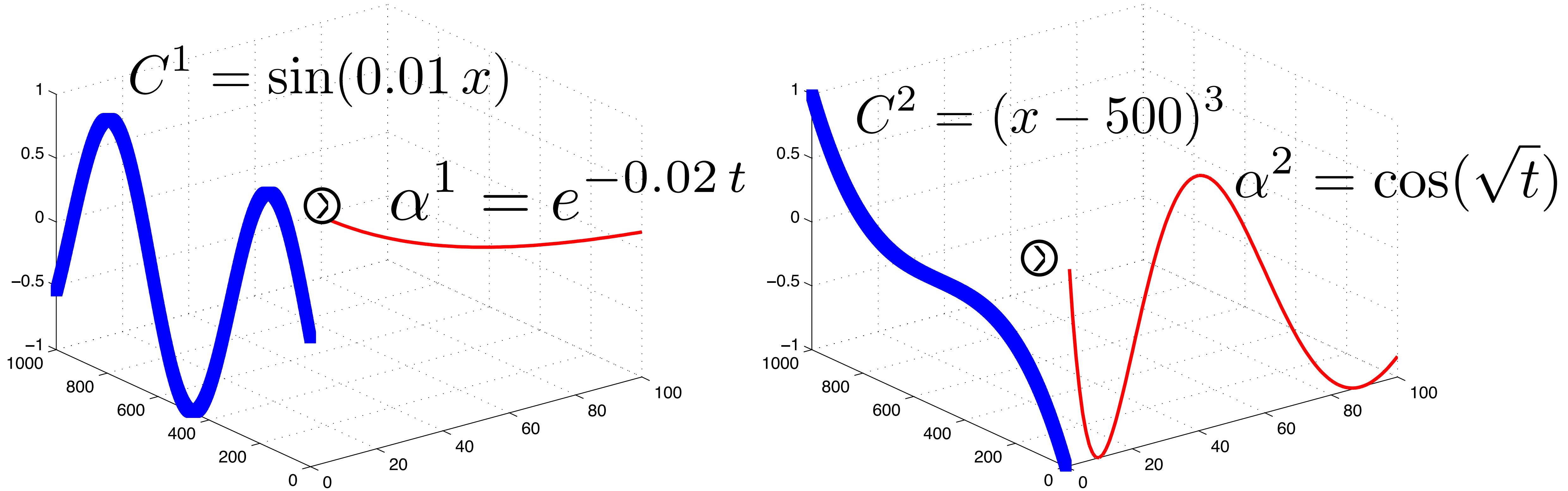


Illustration of the method of separated representation

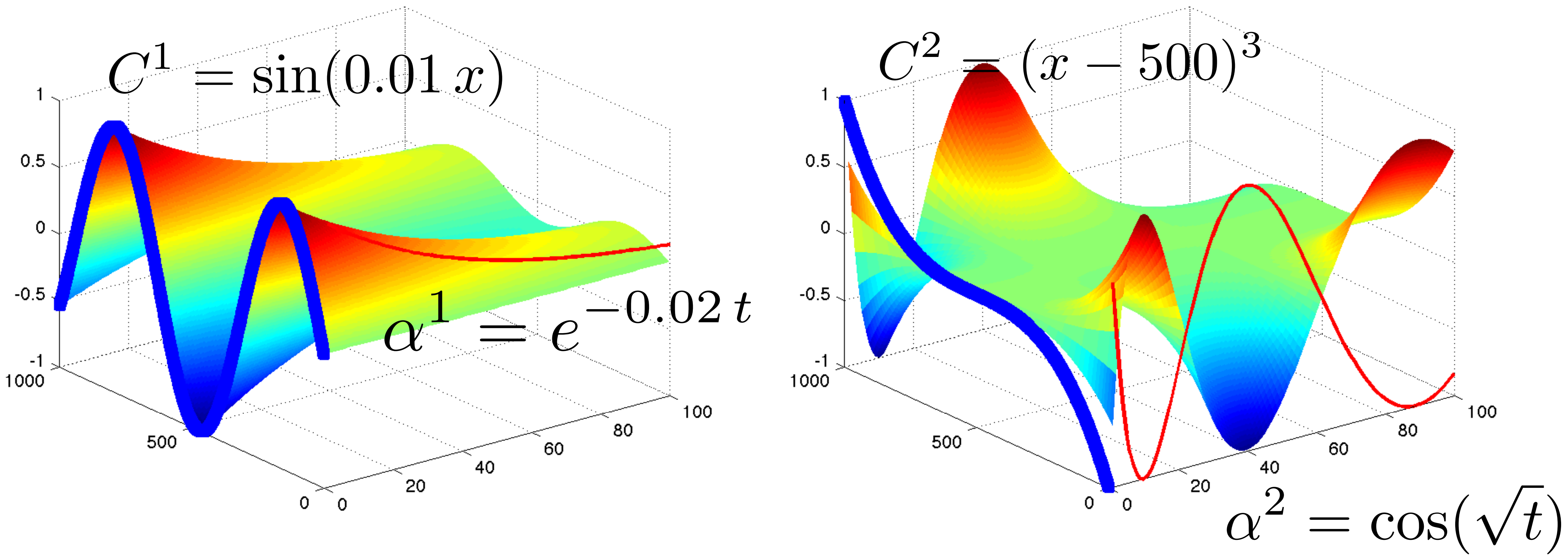
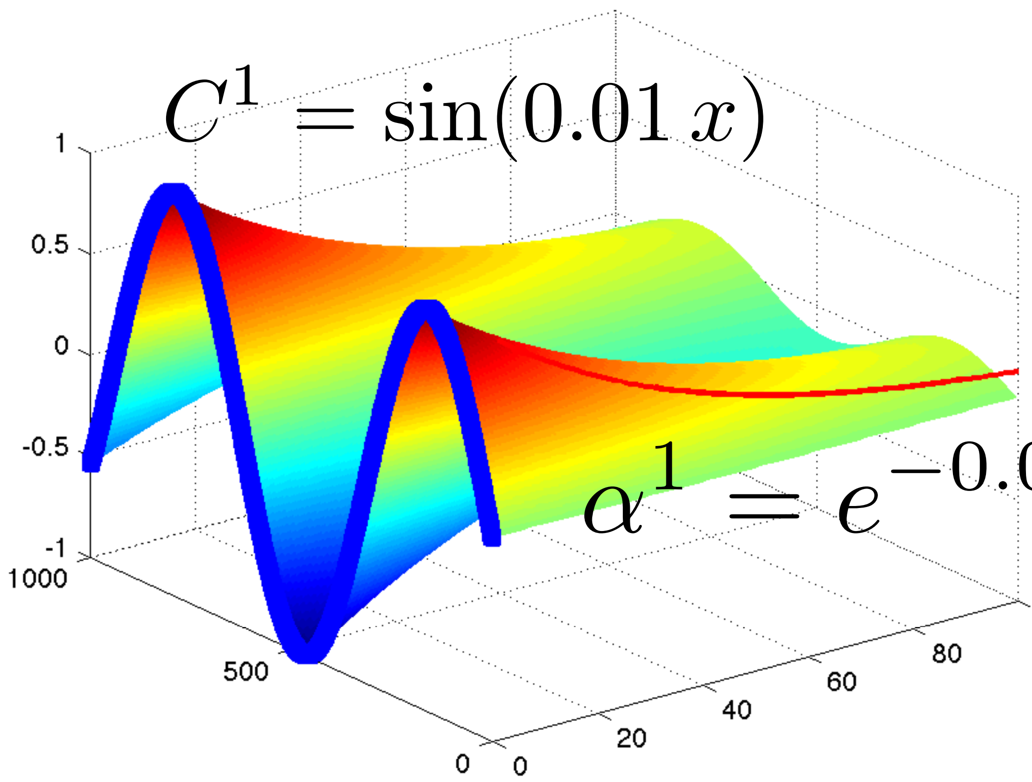


Illustration of the method of separated representation

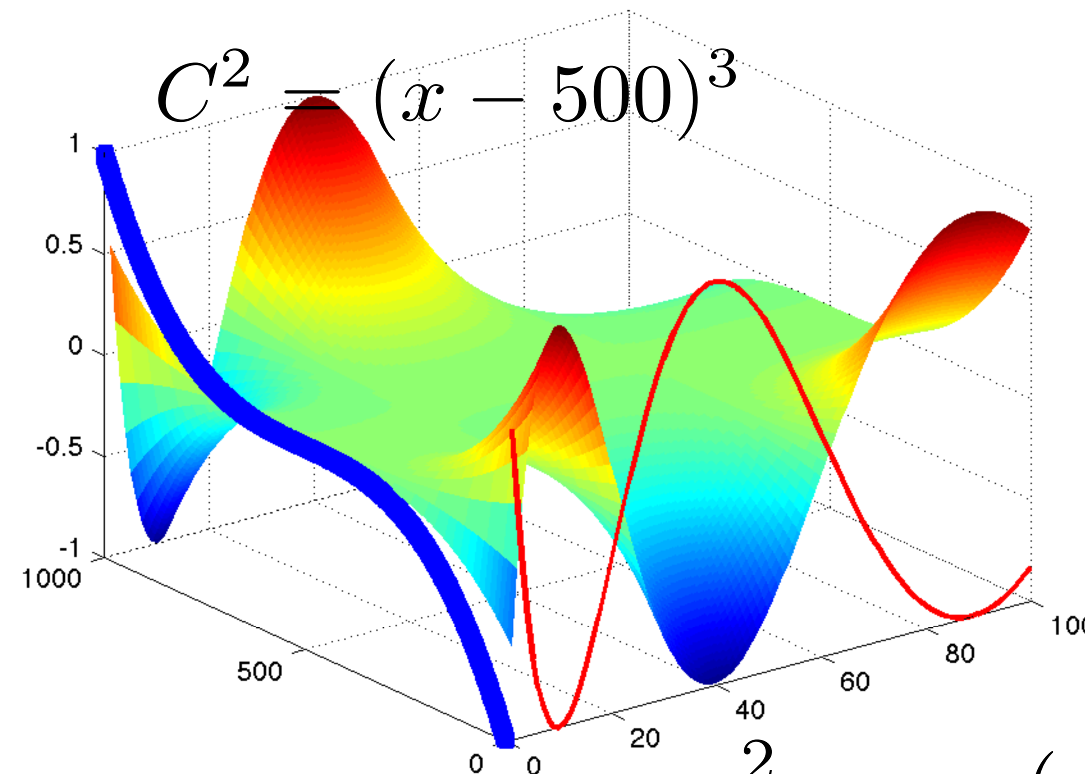
$$C^1 = \sin(0.01\,x)$$

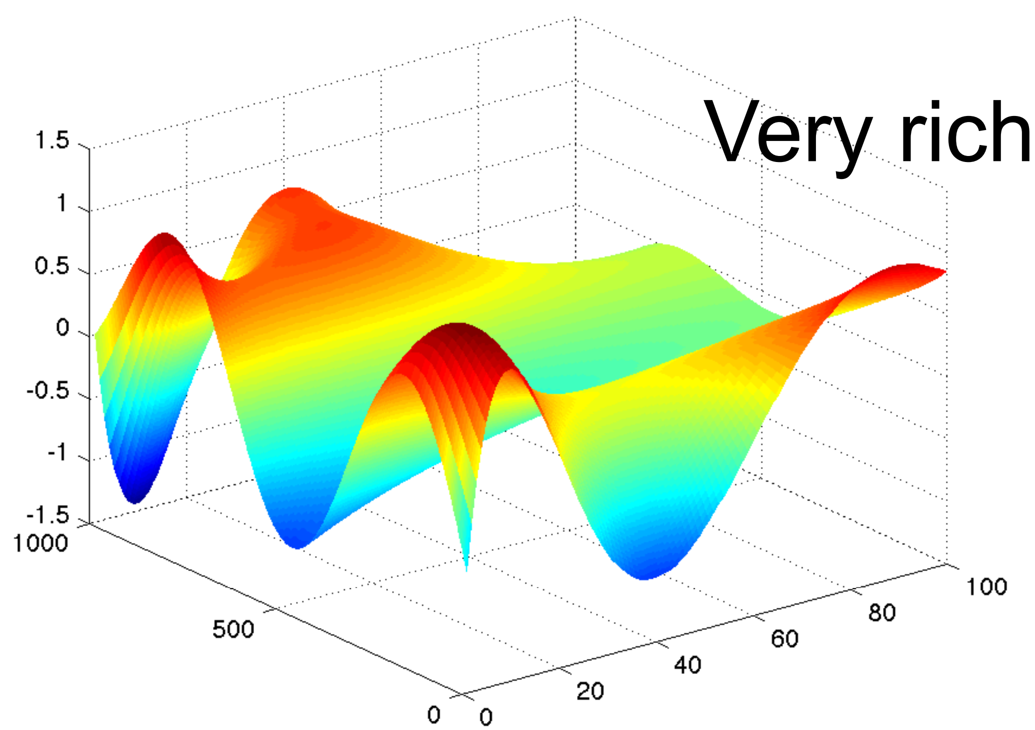
$$\alpha^1 = e^{-0.02\,t}$$



$$C^2 = (x-500)^3$$

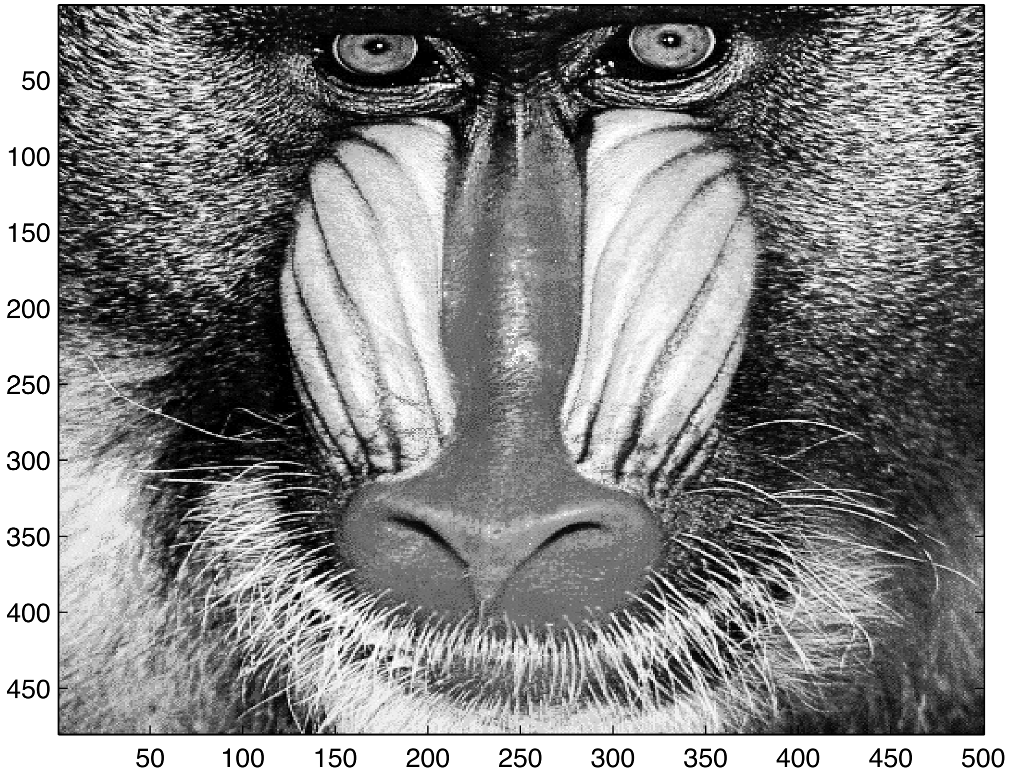
$$\alpha^2 = \cos(\sqrt{t})$$

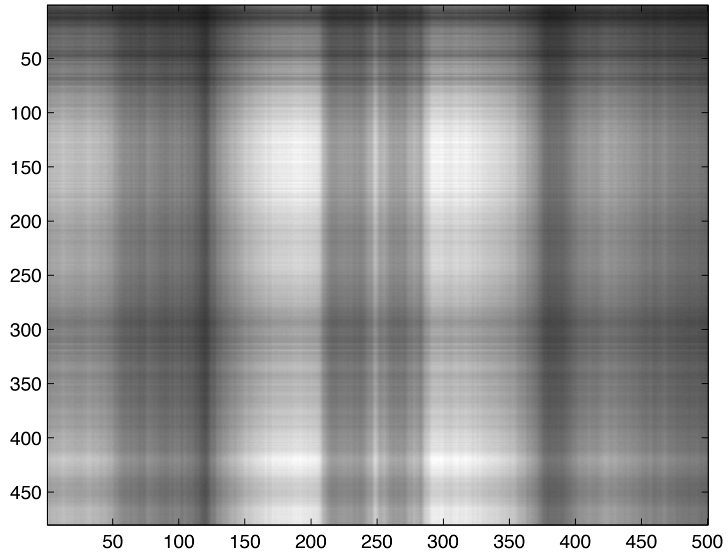




Very rich approximation!

Data compression: get the nose with the POD!





$n_c = 1$

$$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} \underline{C}_x^i(x_i)\, \underline{C}_y^i(y_i)$$

$$(C_x^i, C_y^i)_{i \in [\![1, n_c]\!]} = \operatorname{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$$

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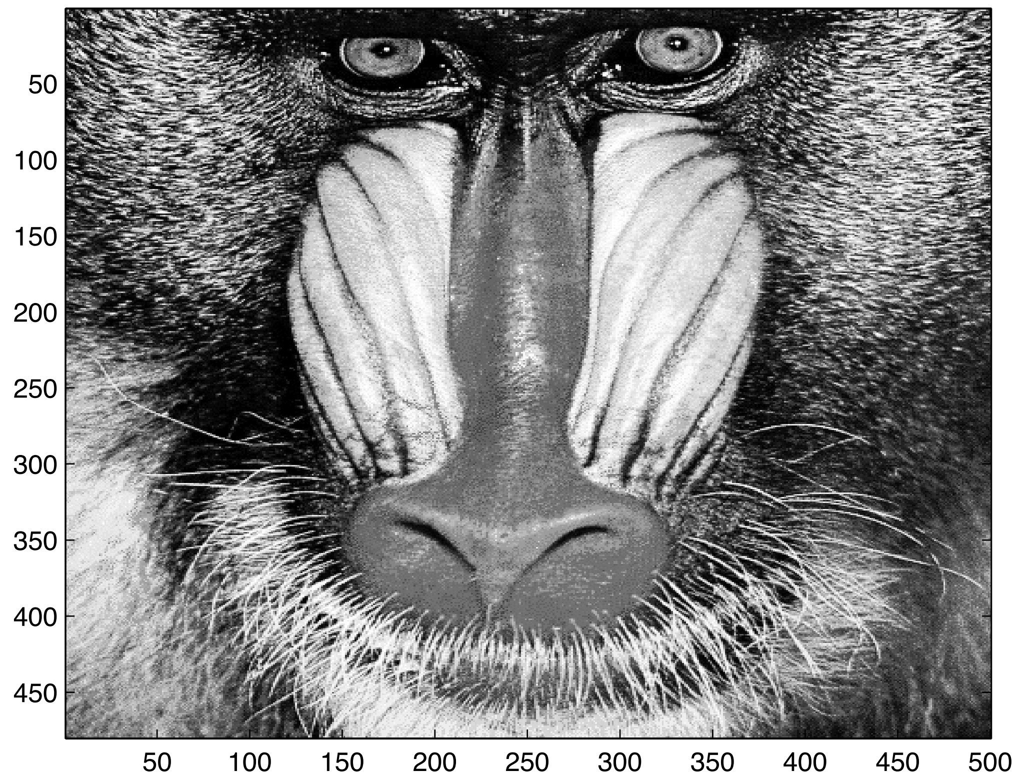
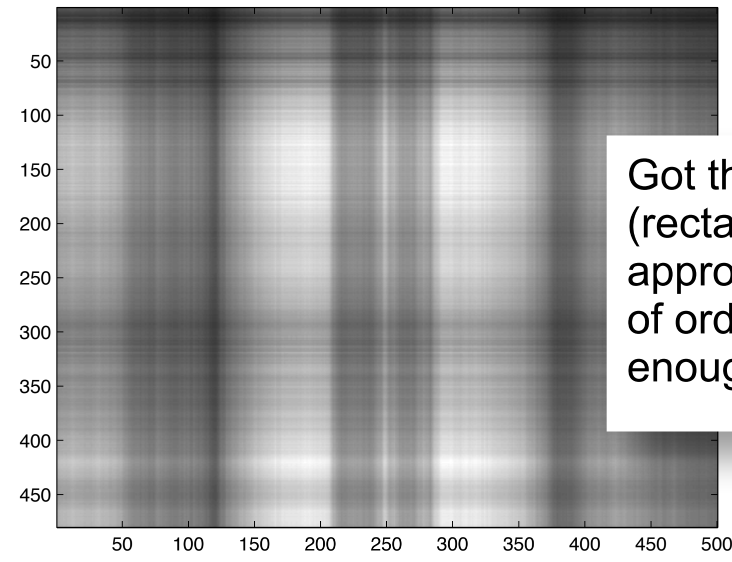
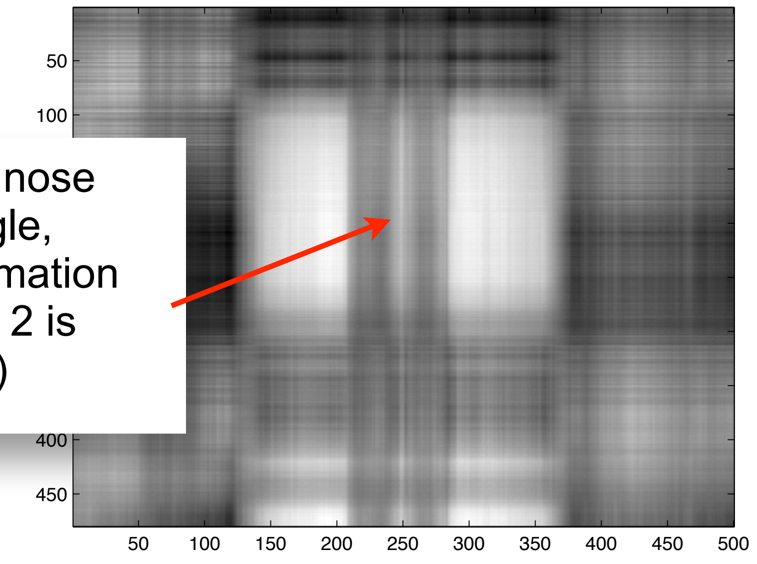
Data compression: get the nose with the POD!





$n_c = 1$



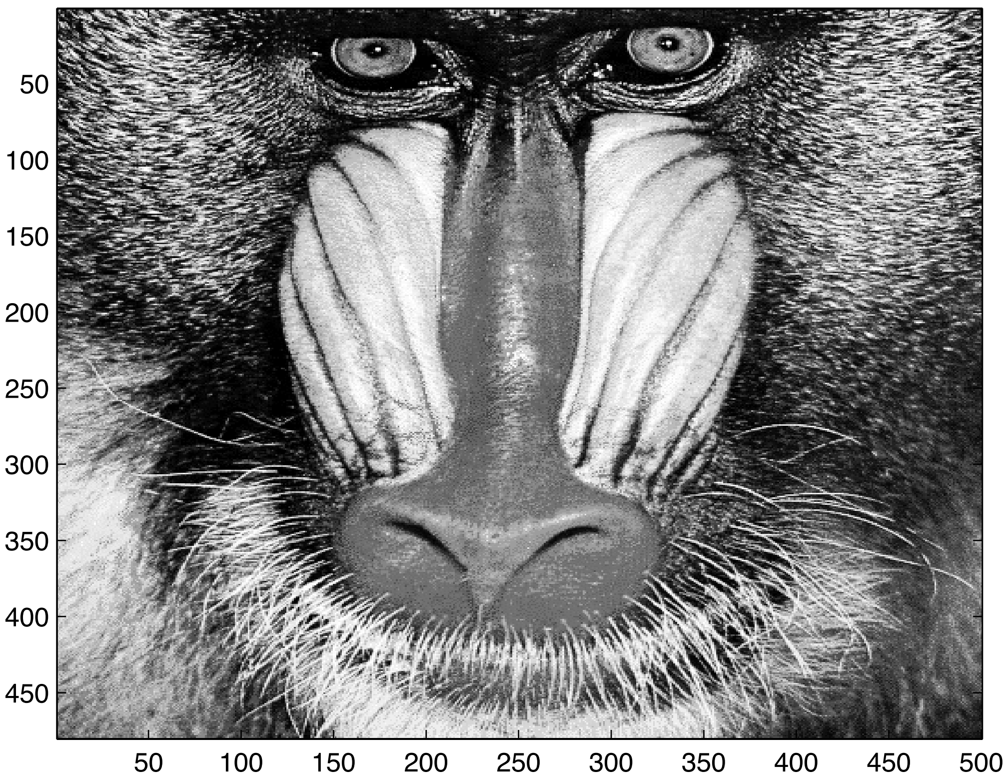
$n_c = 2$

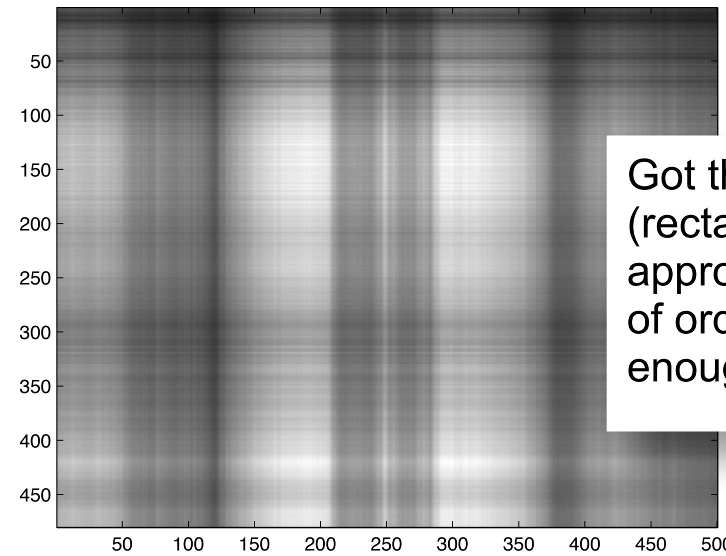
Got the nose (rectangle, approximation of order 2 is enough)

$$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} \underline{C}_x^i(x_i)\, \underline{C}_y^i(y_i)$$

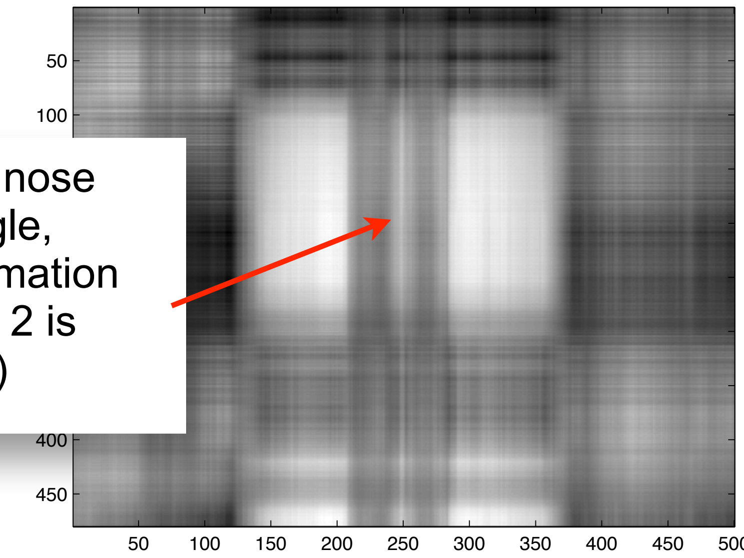
$$(C_x^i, C_y^i)_{i \in [\![1, n_c]\!]} = \operatorname{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$$

Data compression: get the nose with the POD!



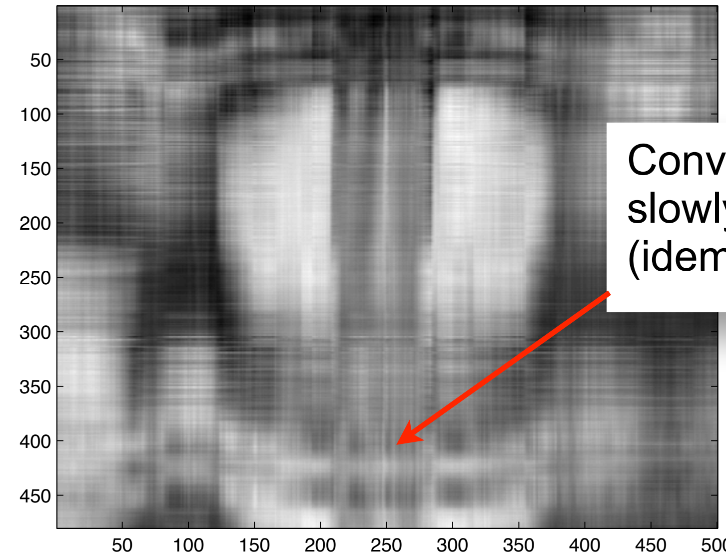


$n_c = 1$

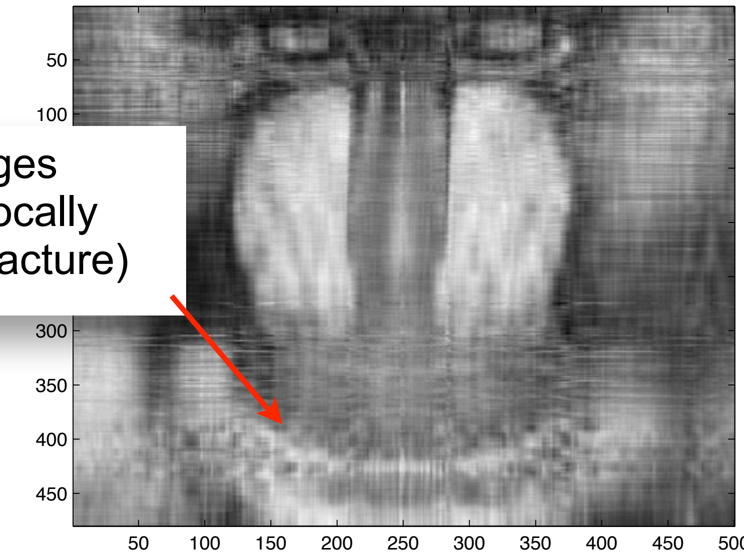


$n_c = 2$

Got the nose (rectangle, approximation of order 2 is enough)

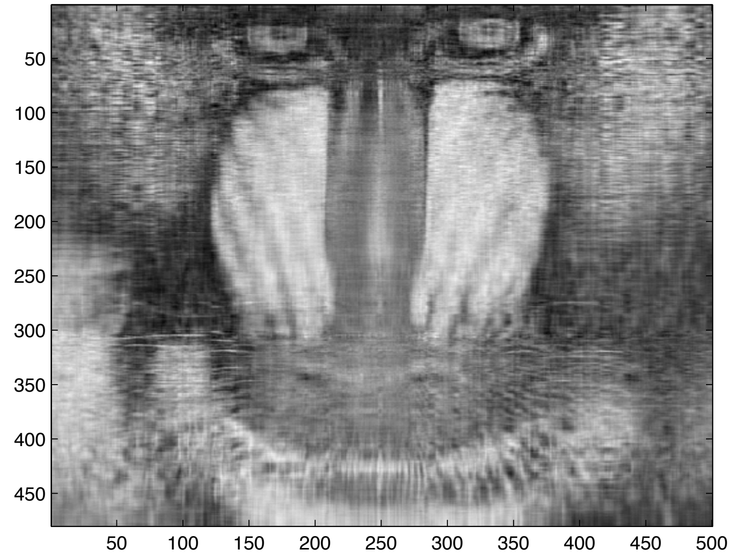


$n_c = 5$



$n_c = 10$

Converges slowly locally (idem fracture)

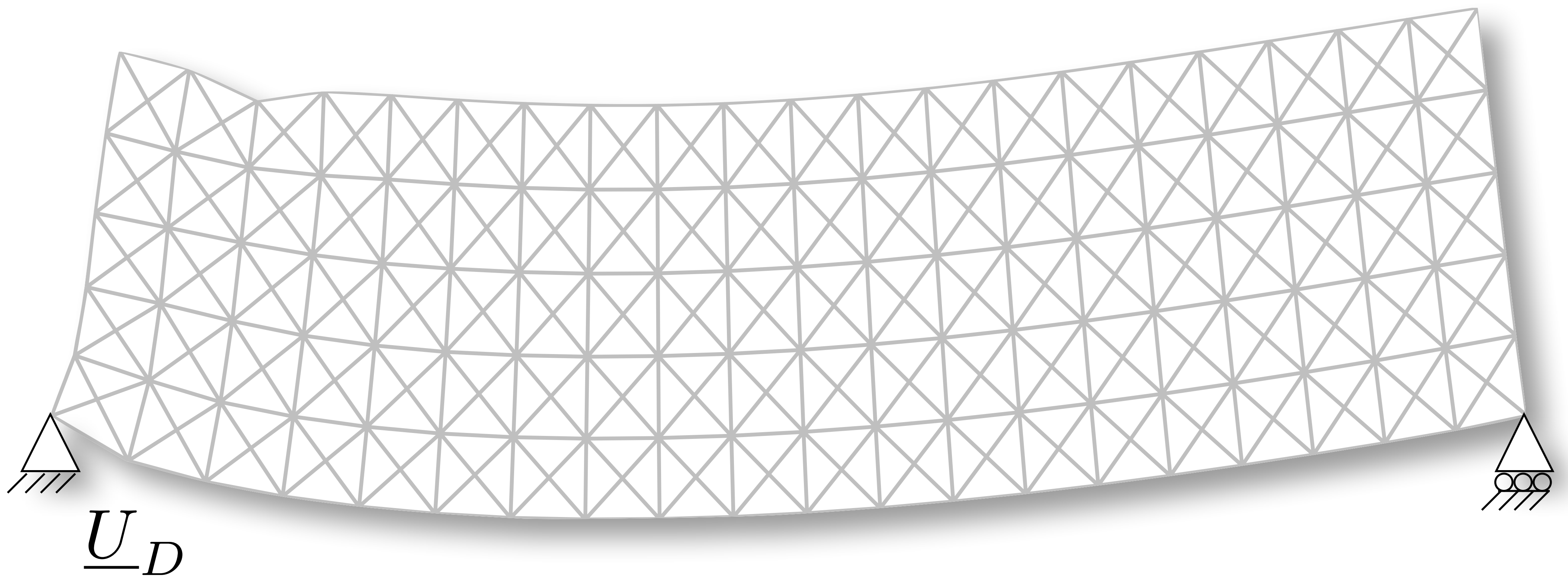


$n_c = 20$

$$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} \underline{C_x^i}(x_i)\, \underline{C_y^i}(y_i)$$

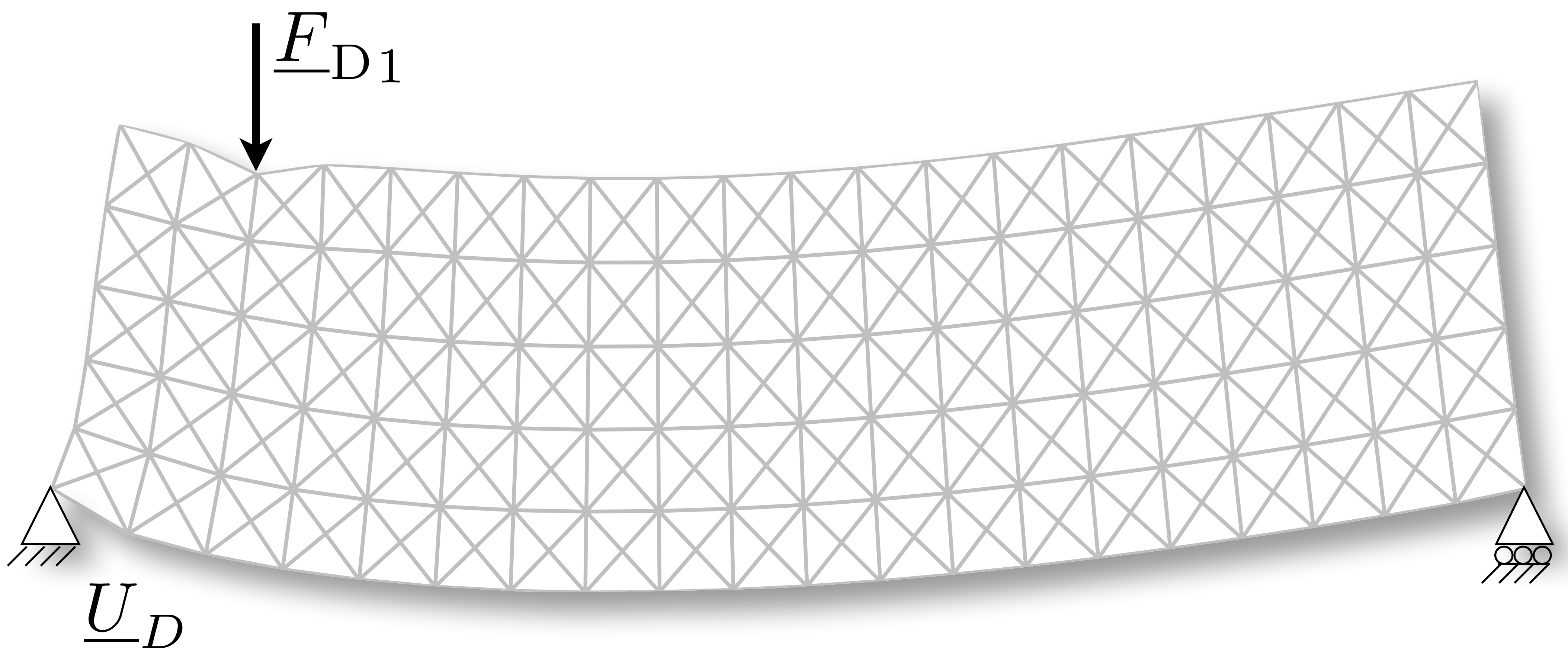
$$(C_x^i, C_y^i)_{i \in [\![1, n_c]\!]} = \operatorname{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$$

Lattice beam problem



Aim: accelerate the simulation using pre-computations

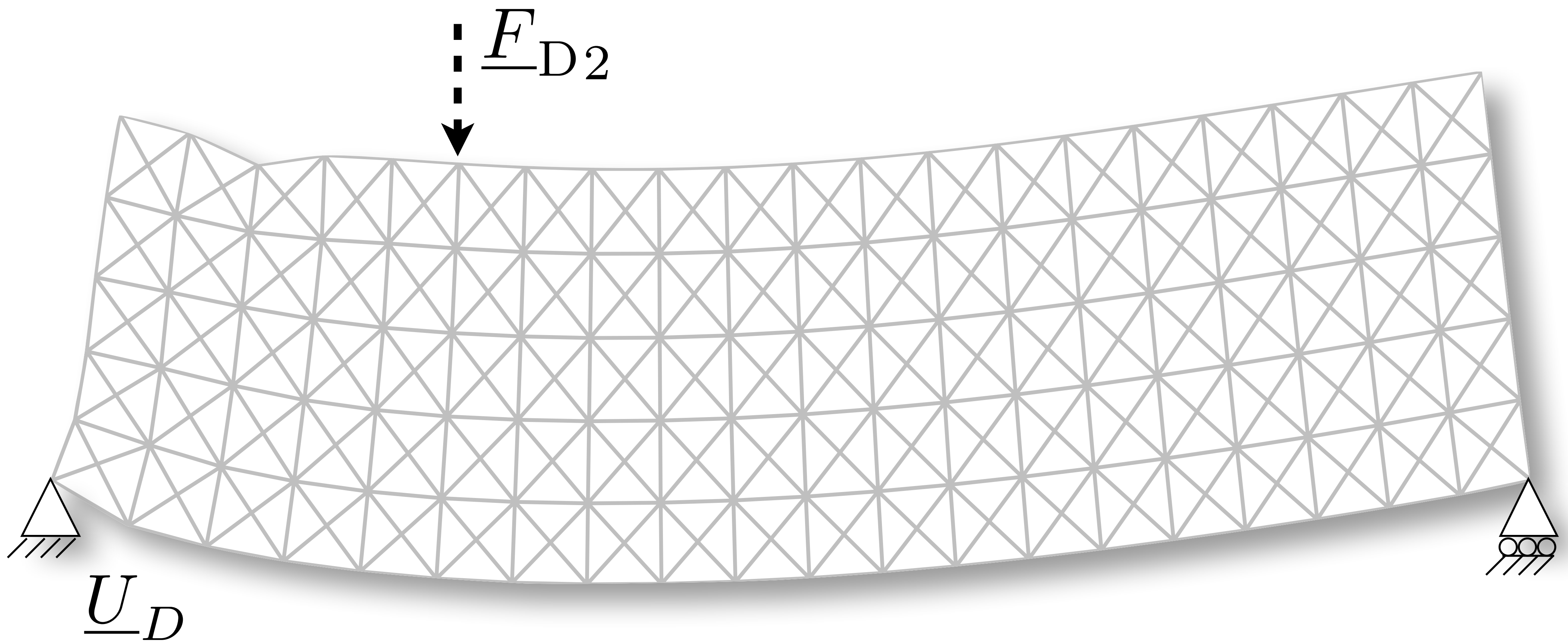
Lattice beam problem



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

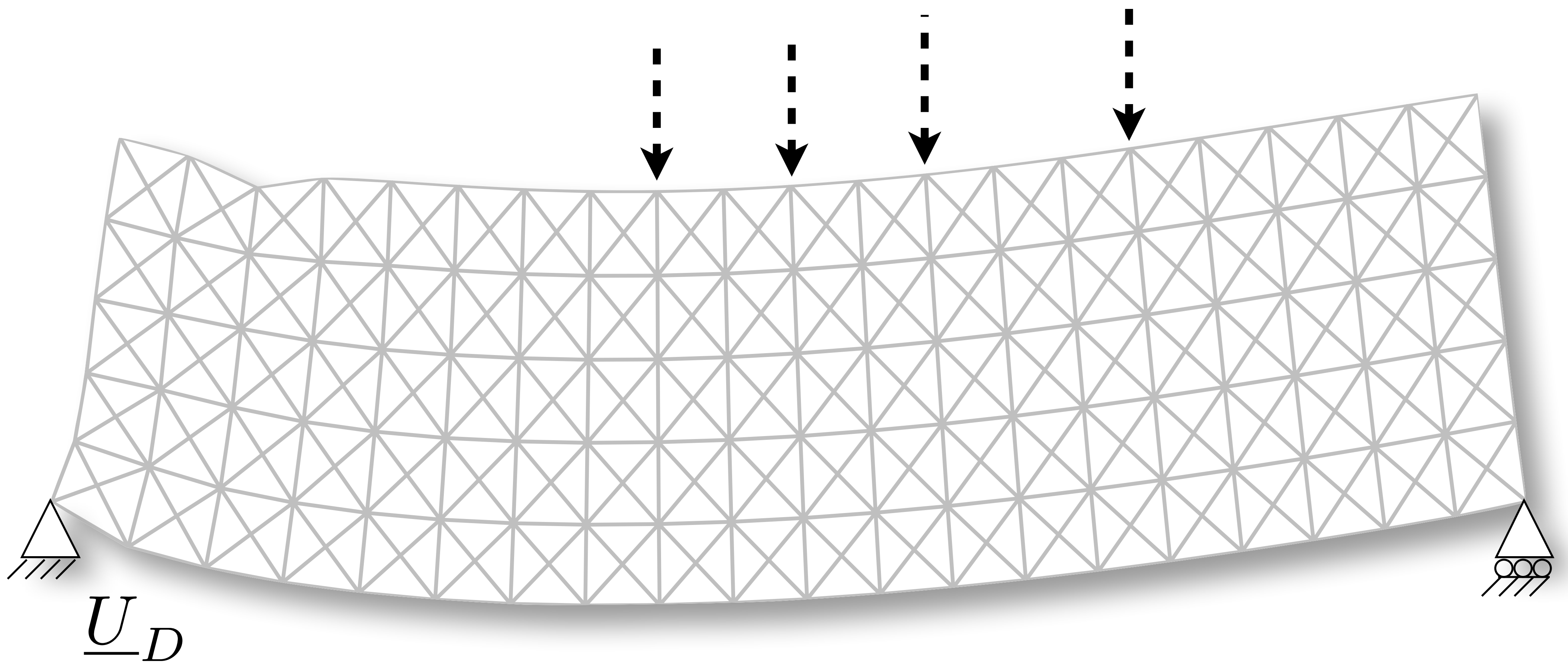
Compute solutions for several loading conditions

Lattice beam problem



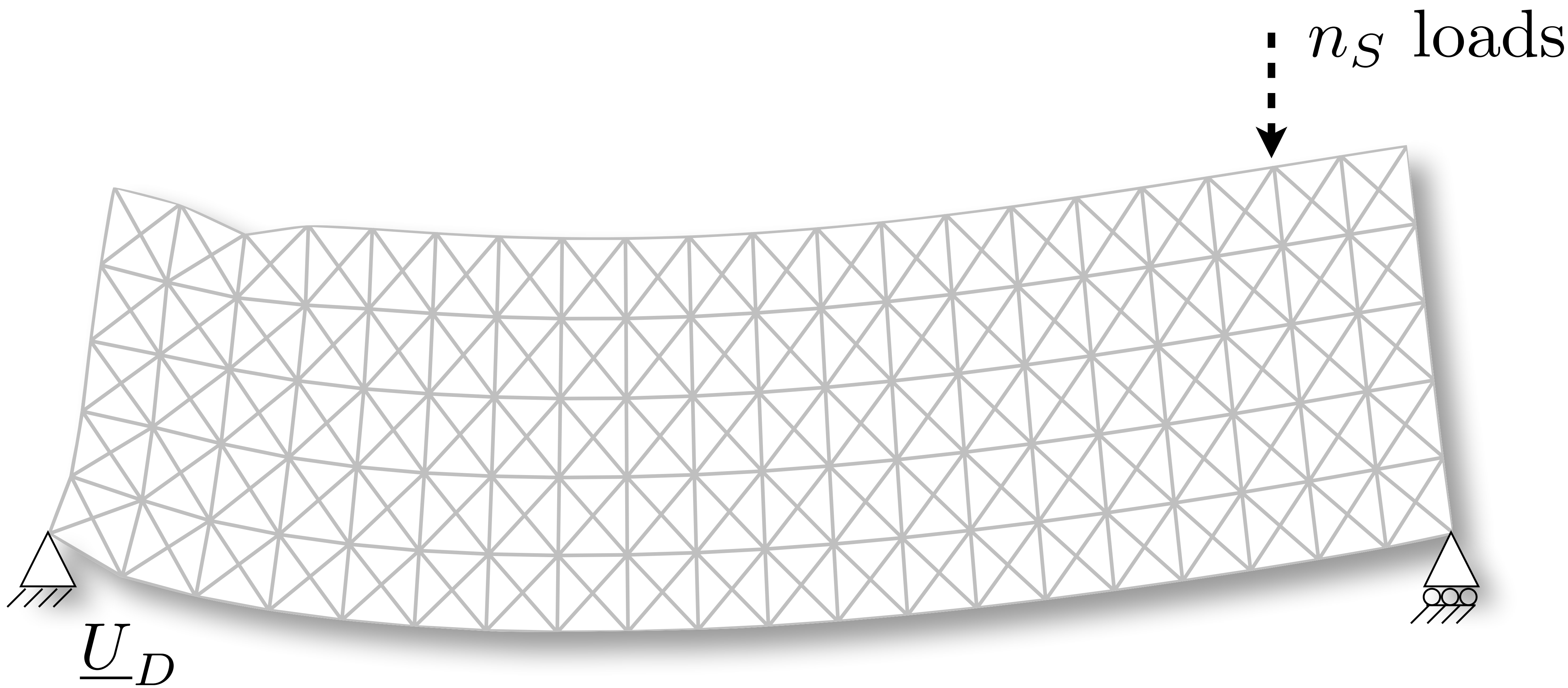
$$\underline{\underline{\mathbf{S}}} = \left(\; \underline{\mathbf{S}}^1 \quad \underline{\mathbf{S}}^2 \right.$$

Lattice beam problem



$$\underline{\underline{\mathbf{S}}} = \Big(\; \underline{\mathbf{S}}^1 \quad \underline{\mathbf{S}}^2 \quad \dots$$

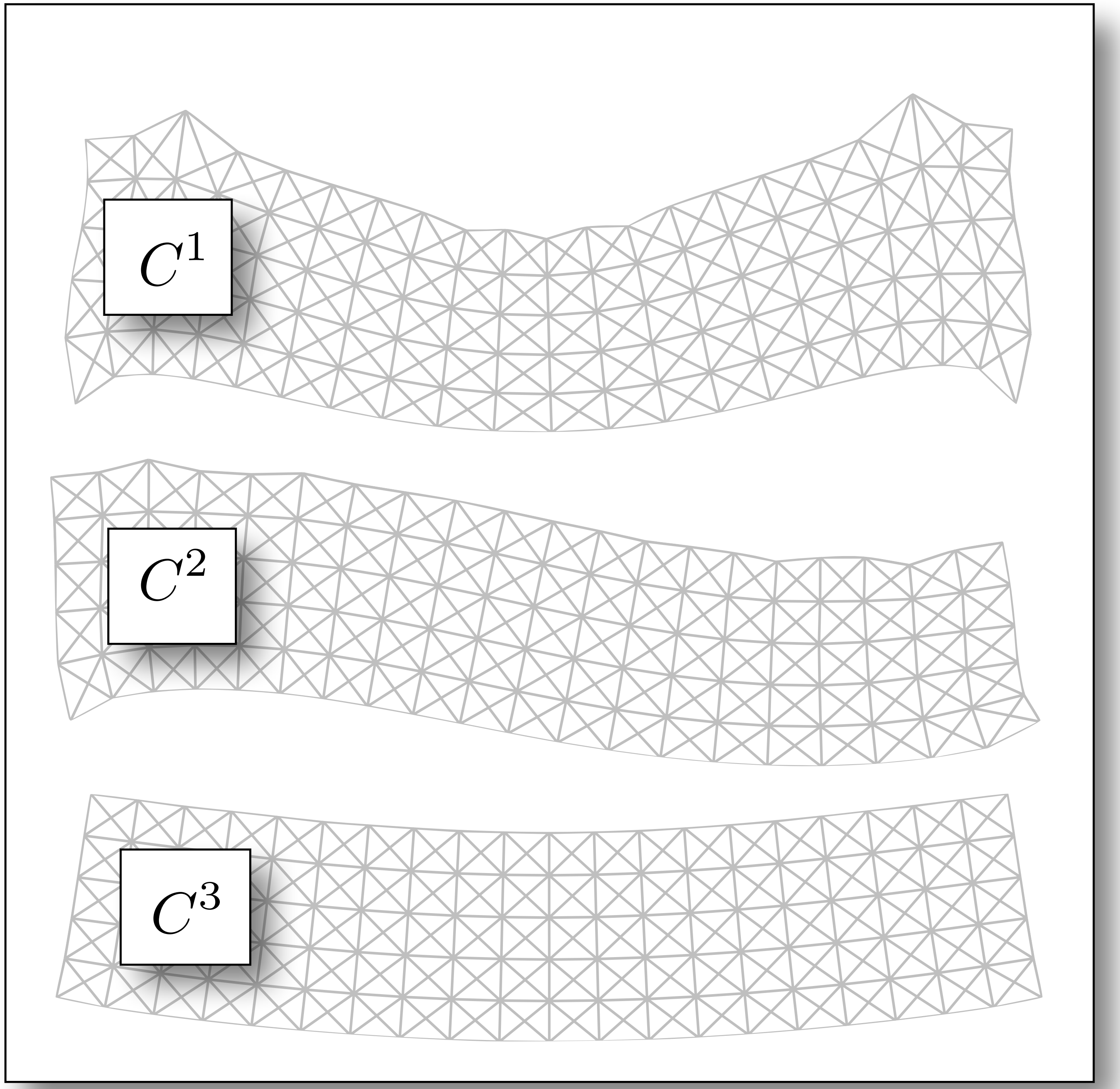
Lattice beam problem



$$\underline{\underline{\mathbf{S}}} = \begin{pmatrix} \underline{\mathbf{S}}^1 & \underline{\mathbf{S}}^2 & \dots & \underline{\mathbf{S}}^{n_S} \end{pmatrix}$$

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

Reduced basis



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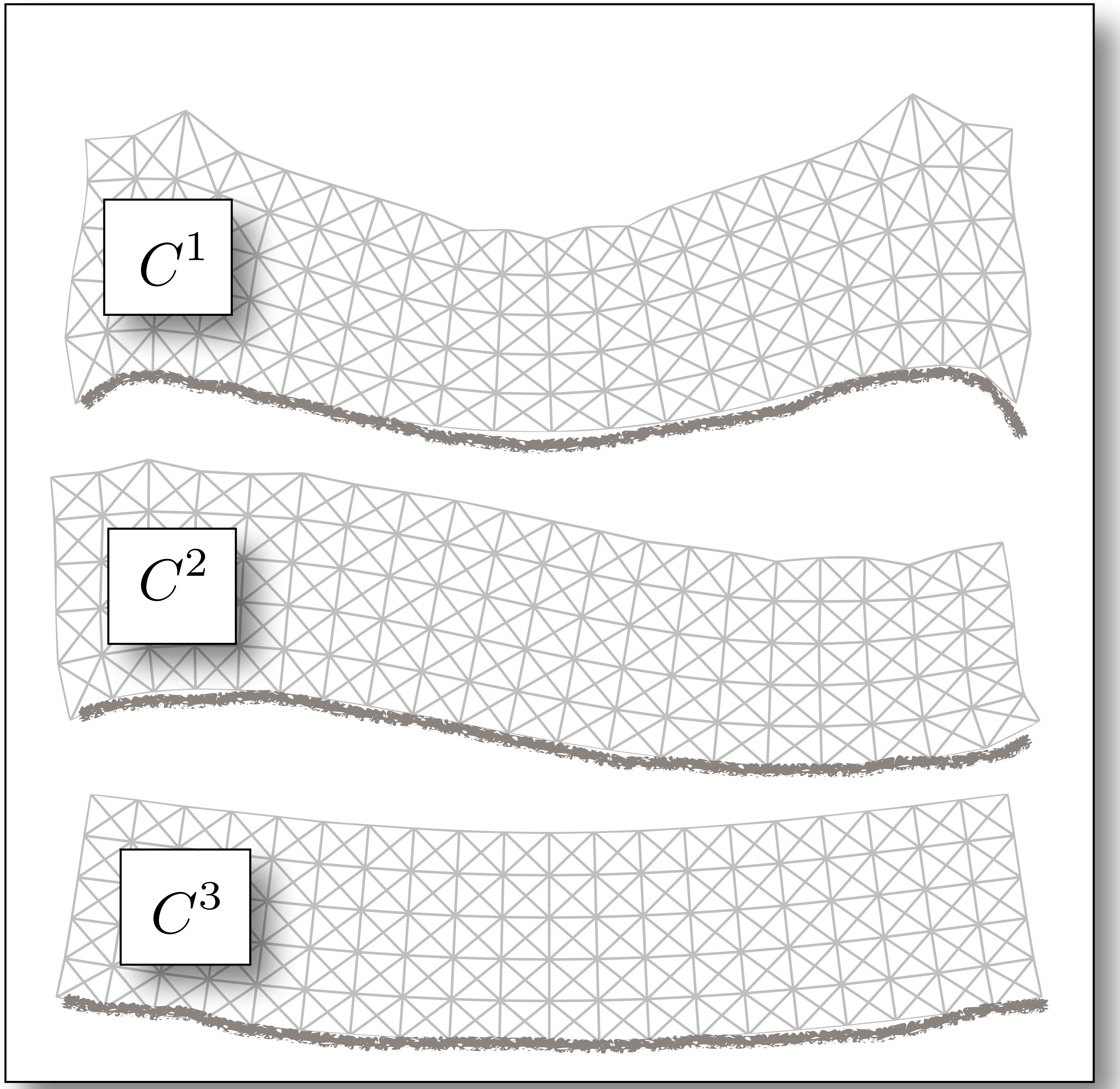
Reduced basis



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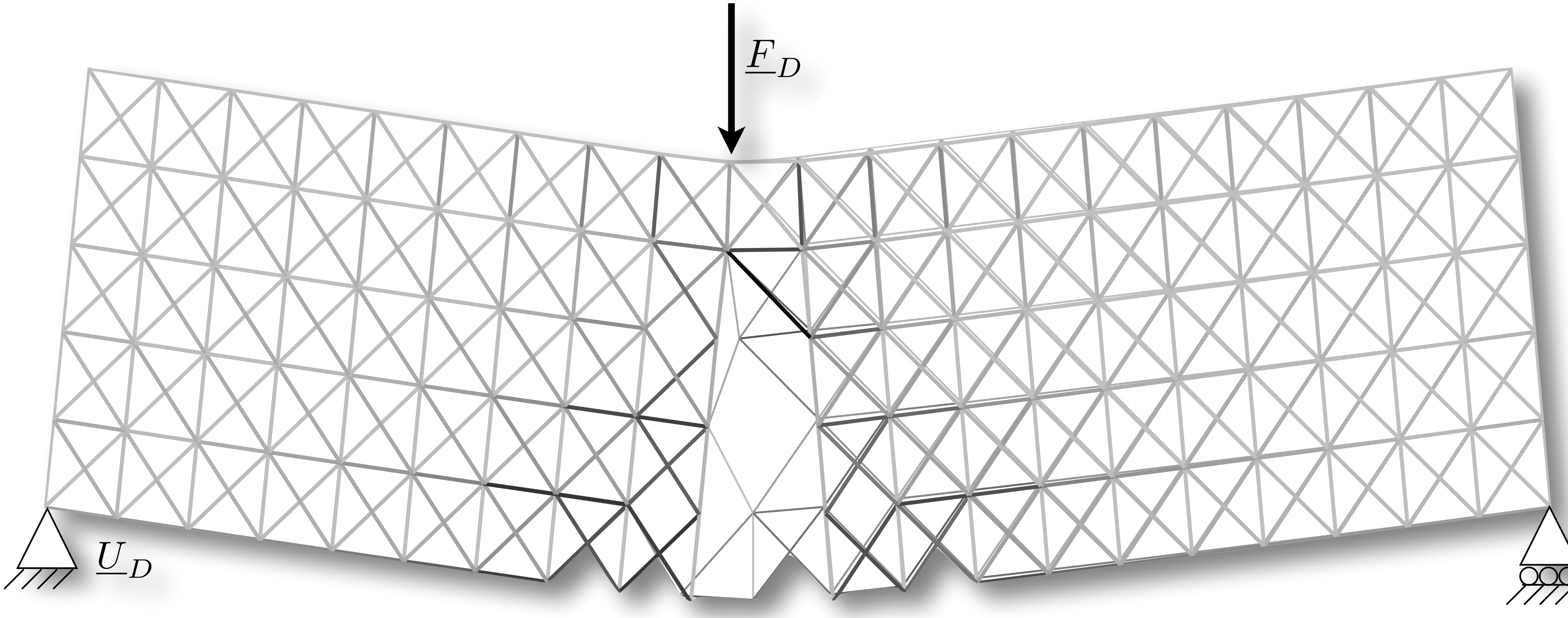
Beyond the elastic limit



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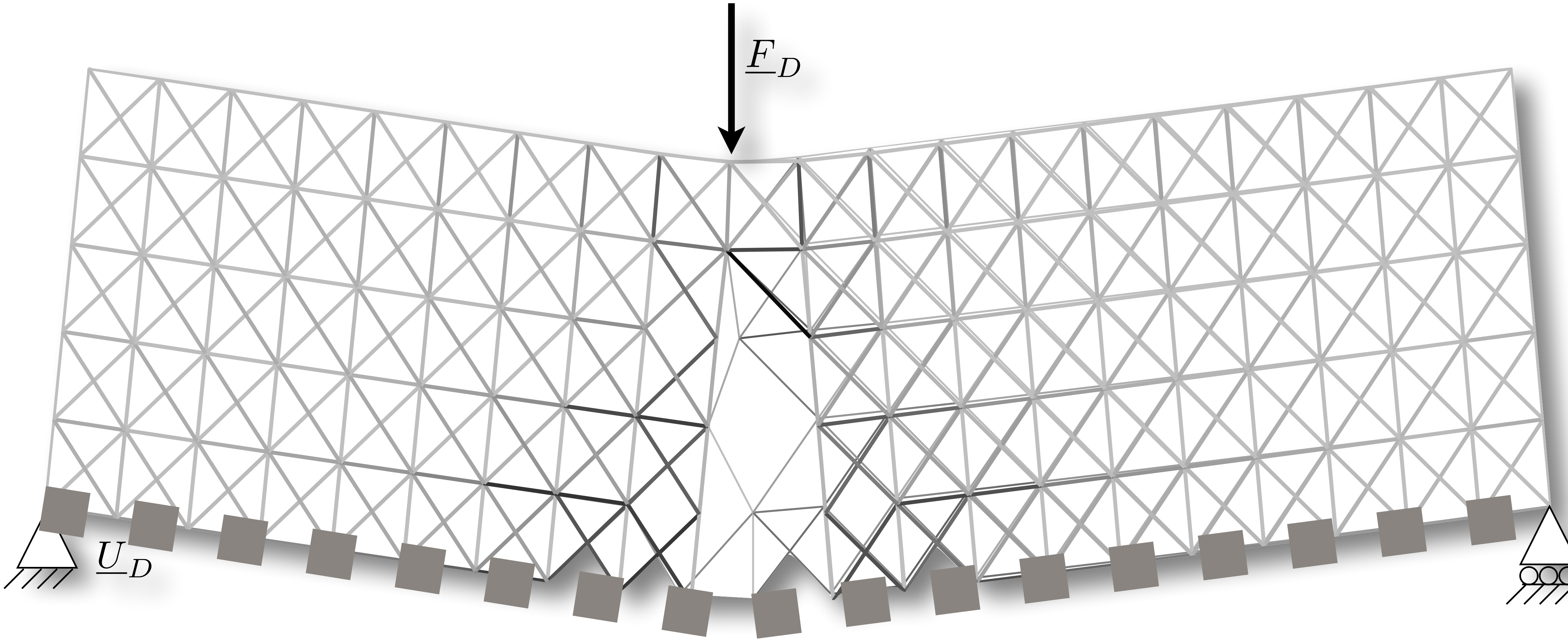
Beyond the elastic limit



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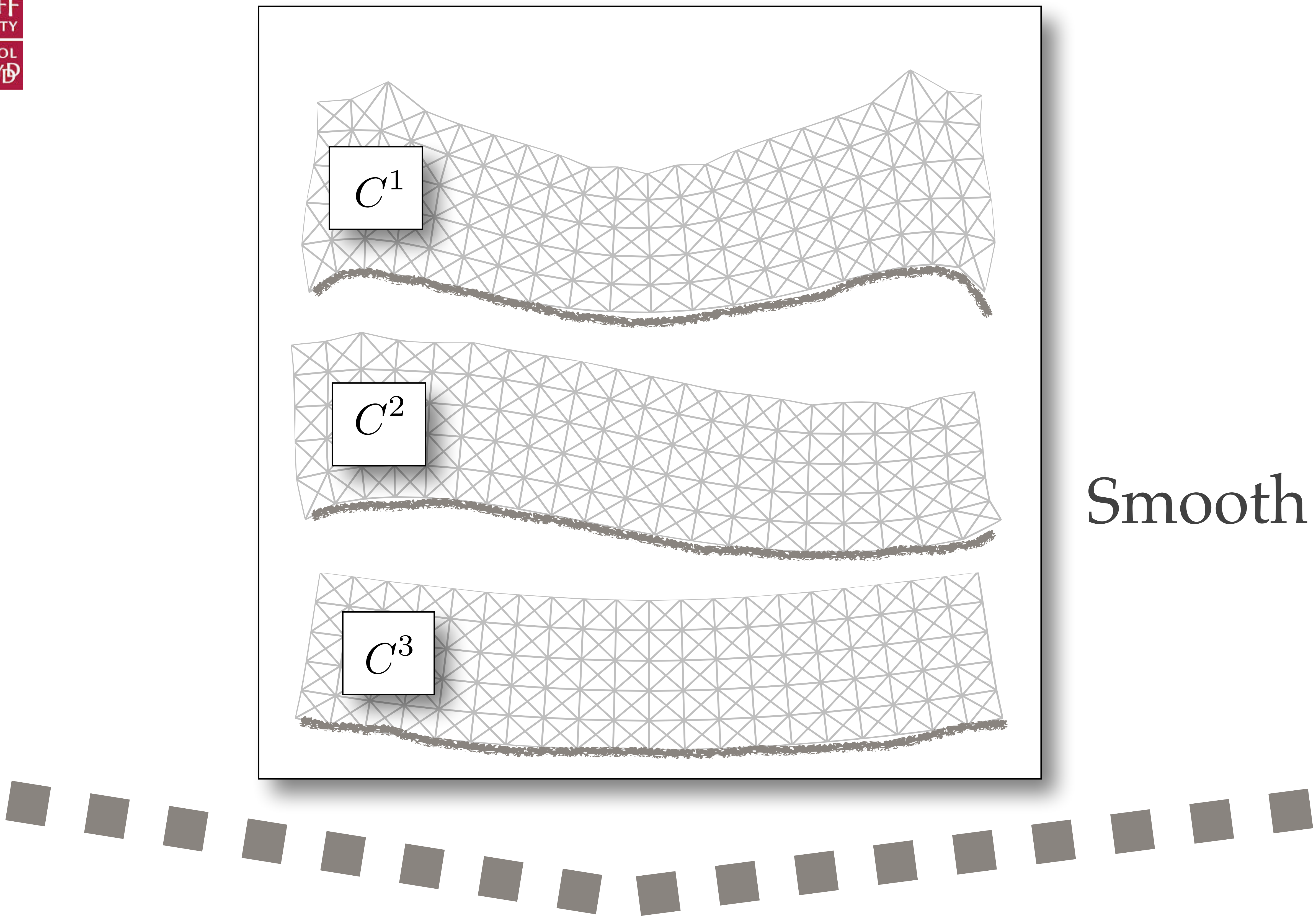
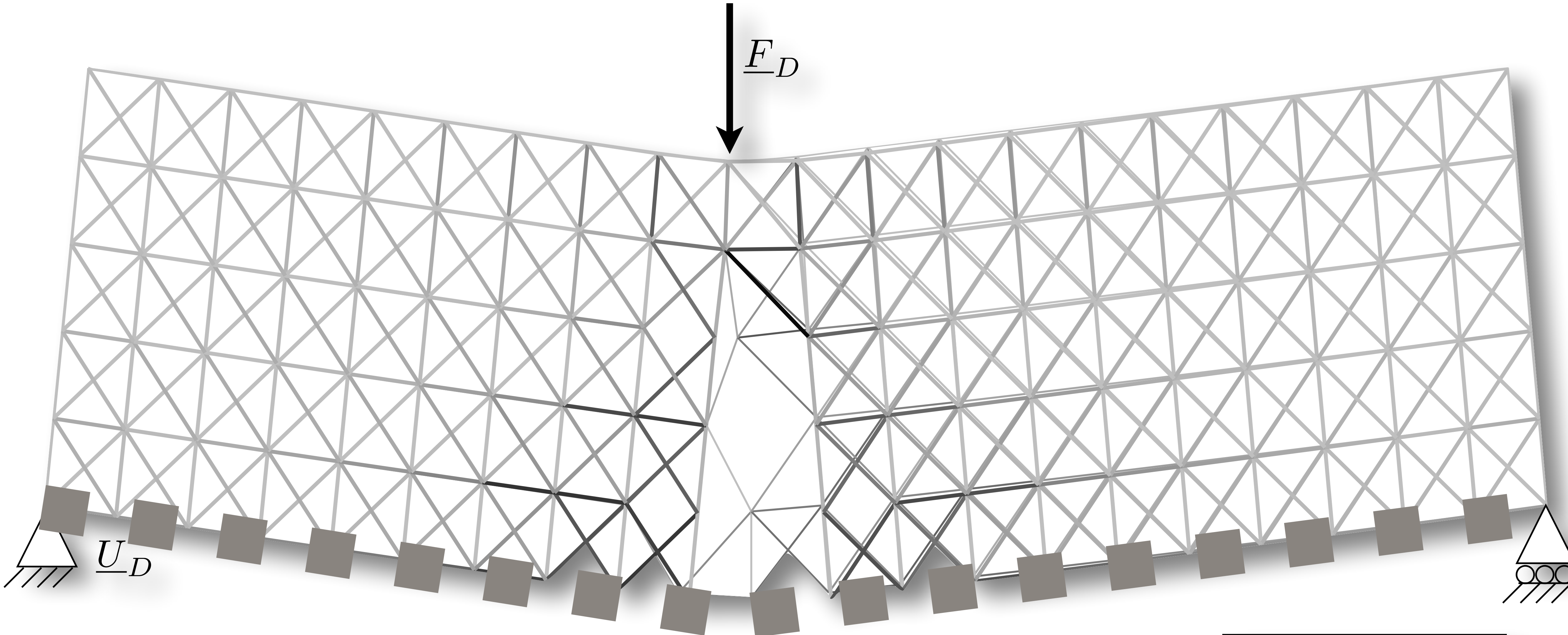
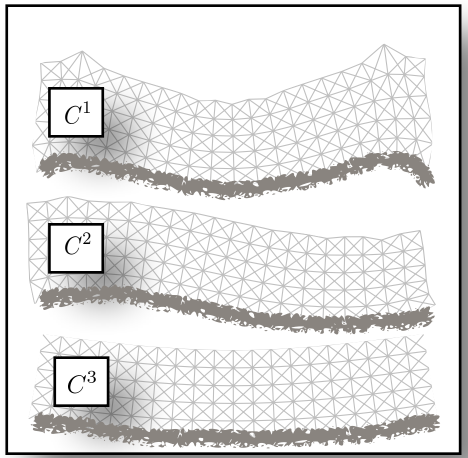


Smooth

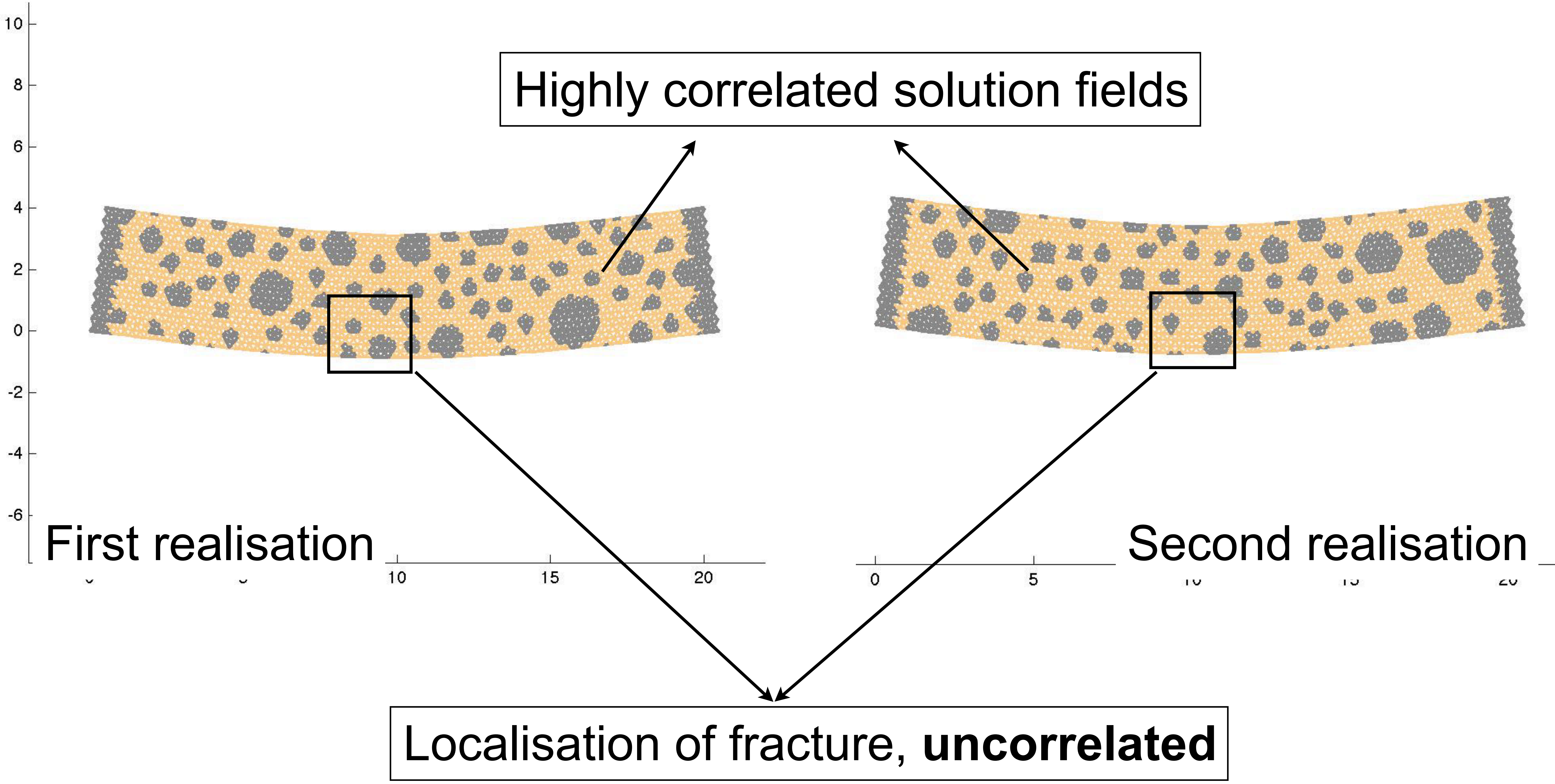
Kink



This solution is not in the snapshot !



Parametric / stochastic multiscale fracture mechanics



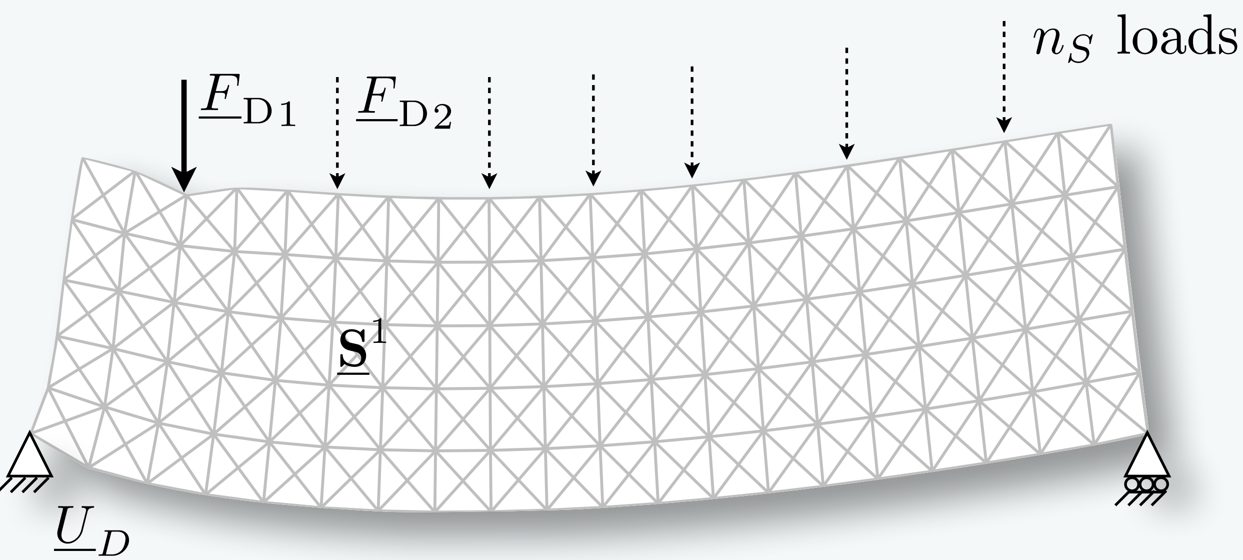
- Search for the solution in space / time / parameter in a product space:

$$\underline{\bar{\mathbf{U}}} : \quad \mathcal{U}_{\text{sep}} = \mathbb{R}^n \times \mathcal{T} \times \mathcal{P} \to \mathbb{R}^n$$
$$\underline{\bar{\mathbf{U}}}(t,\mu) = \sum_{i=1}^{n_C} \underline{\mathbf{C}}_i \, \beta_i(t) \gamma_i(\mu) \,,$$

$$\underline{\mathbf{C}}^i \in \mathbb{R}^n$$
$$\beta^i : \mathcal{T} \to \mathbb{R}, \quad \forall i \in [\![1, n_C]\!] \,,$$
$$\gamma^i : \mathcal{P} \to \mathbb{R}, \quad \forall i \in [\![1, n_C]\!] \,,$$

- Optimality of an expansion of order n_c with respect to a particular metric defined on $\mathcal{U}_{\text{sep}}$
  - ➡ different metrics lead to different methods, which have their pro/cons
  - ➡ Choice strongly dependent on the context
  - Data compression: **POD** (Proper Orthogonal Decomposition) is a classical choice in dimension 2
  - Data compression in many dimensions: **multilinear POD**
  - Solver in many dimensions without *a priori* knowledge of the solution: **PGD**
  - Model order reduction: **Snapshot POD, Snapshot PGD**
  - Initialiser, preconditioners: **low-order POD**, **low-order PGD**, **Snapshot POD**

a posteriori model order reduction. **Idea**: search for the **solution as a linear**



(1) Solve FINE for n_S parameters (EXPENSIVE!)

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

(2) Singular value decomposition

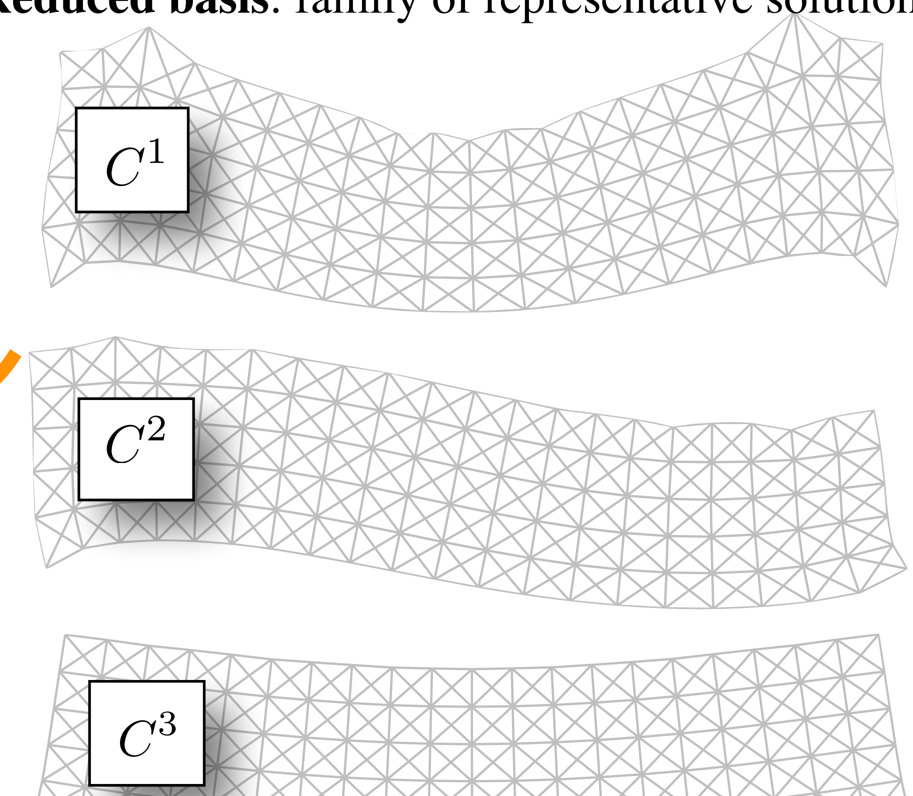
$$\underline{\underline{\mathbf{S}}} = \underline{\underline{\mathbf{U}}}\,\underline{\underline{\mathbf{\Sigma}}}\,\underline{\underline{\mathbf{V}}}^T = \sum_{k=1}^{n_S} \Sigma^k\, \underline{\mathbf{U}}^k\, \underline{\mathbf{V}}^{k\,T}$$

n_S solutions, sorted by relevance

where $(\Sigma^k)_{k\in[\![1\ n_S]\!]}$ in decreasing order

(3) Truncation

Reduced basis: family of representative solutions



$$\underline{\underline{\mathbf{C}}} = \left(\underline{\mathbf{U}}^1 \quad \underline{\mathbf{U}}^2 \quad \dots \quad \underline{\mathbf{U}}^{n_C} \right)$$

Initial set of equations

$$\underline{\mathbf{F}}_{\mathrm{Int}}(\underline{\mathbf{U}}) + \underline{\mathbf{F}}_{\mathrm{Ext}} = 0$$

(4) Galerkin orthogonality

$$\underline{\underline{\mathbf{C}}}^T\, \underline{\mathbf{F}}_{\mathbf{int}}\left(\underline{\underline{\mathbf{C}}}\,\underline{\alpha}\right) + \underline{\underline{\mathbf{C}}}^T\, \underline{\mathbf{F}}_{\mathbf{ext}} = 0$$

Approximation of the solution in a space of small dimension (n_c)

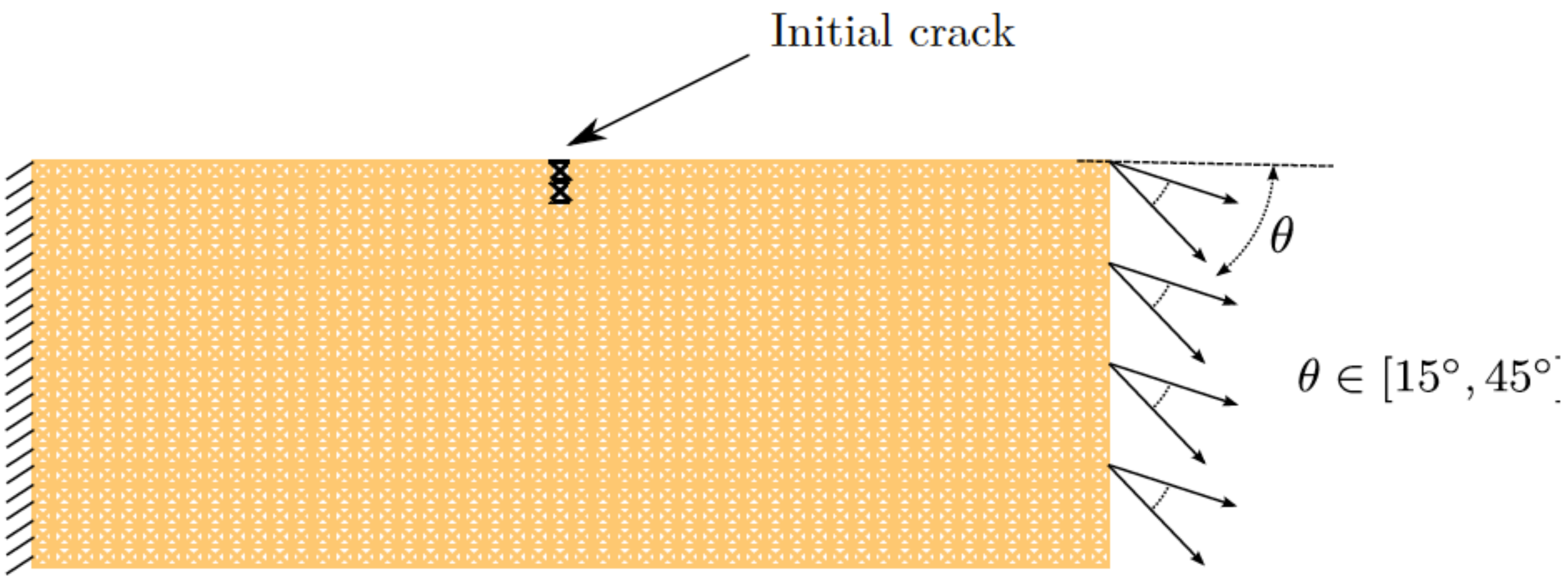
Family of representative solutions

$$\underline{\mathbf{U}} = \underline{\underline{\mathbf{C}}}\,\underline{\alpha}$$

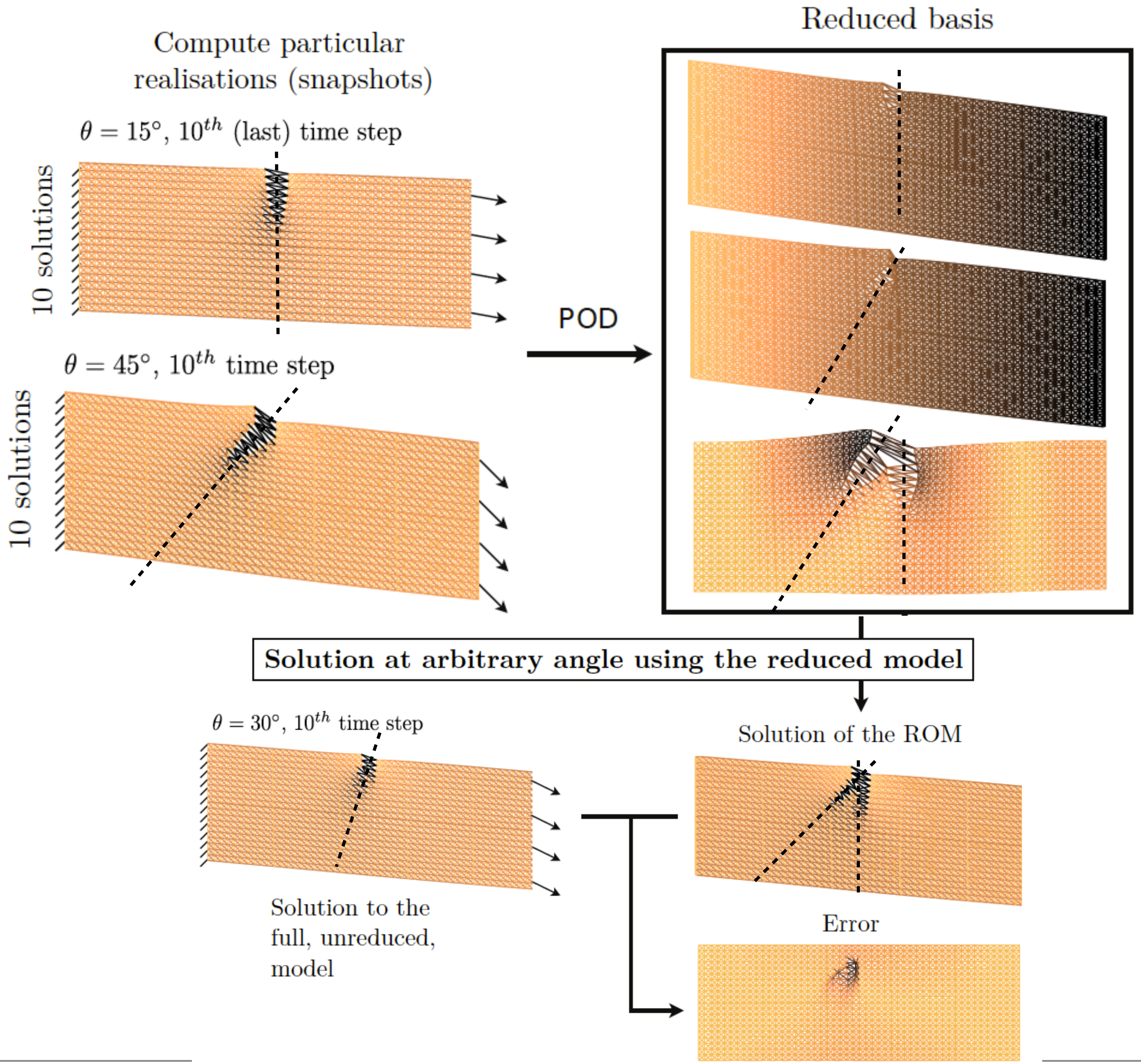
Solution

Coefficients

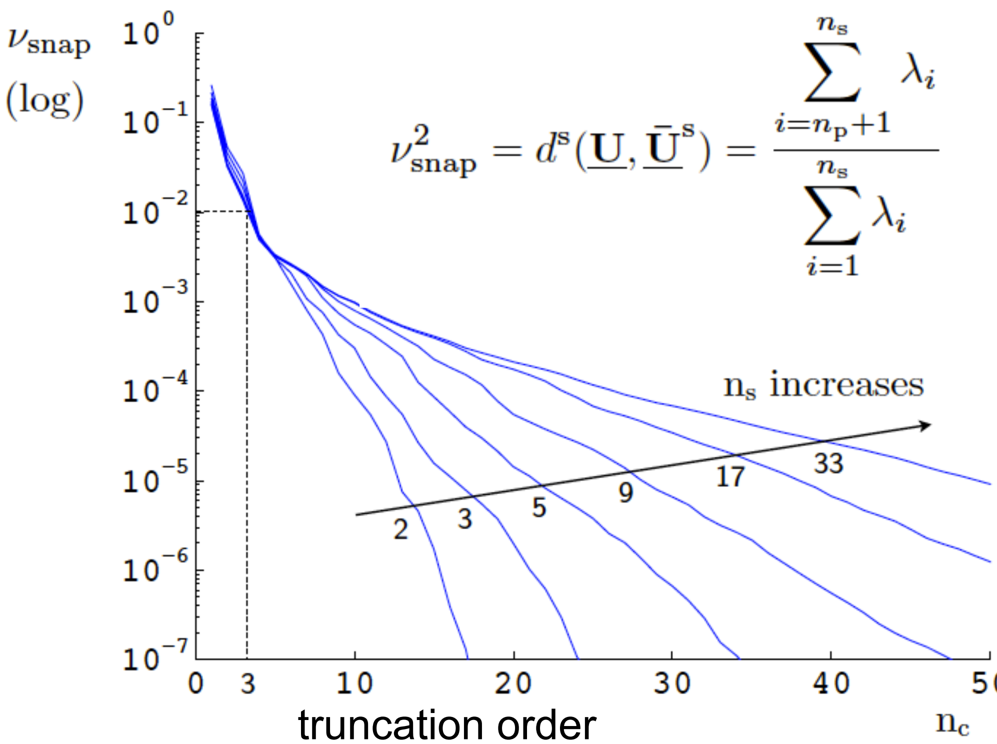
Application to a parametric fracture problem



Application to a parametric fracture problem

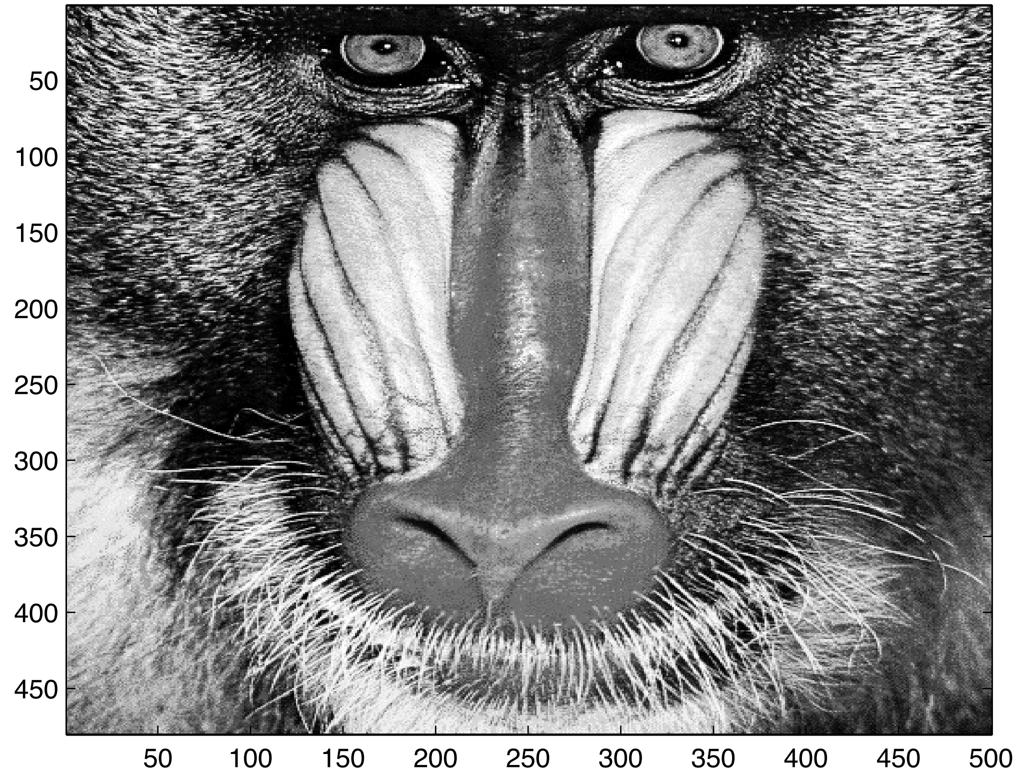


- The POD solution is not able to reproduce the solution in the cracked area
- Due to lack of correlation introduced by crack growth
- Leads to a local projection error



ν_{snap} (log)
$\nu^2_{\text{snap}} = d^{\text{s}}(\underline{\mathbf{U}}, \underline{\bar{\mathbf{U}}}^{\text{s}}) = \frac{\sum_{i=n_{\text{p}}+1}^{n_{\text{s}}} \lambda_i}{\sum_{i=1}^{n_{\text{s}}} \lambda_i}$
n_s increases
2
3
5
9
17
33
truncation order
n_c

Return of the monkey



- What can we do to address this lack of separation of scales/ reducibility?

Model reduction in mechanics (non exhaustive)

- Model order reduction in a domain decomposition context
  - Craig-Bampton [Craig and Bampton ’68, Rixen et al. ’04]
  - LaTIn method / PGD [Ladevèze et al. ’03, Ladevèze et al. ’10]
  - Partitioned Component Mode Synthesis [Park and Park ’04, Markovic and Ibrahimbegovic ’09]
  - Partitioned POD [Kerfriden et al. ’11]
- Model order reduction of substructures not requiring a fine analysis *a priori*
  - Modal truncation [Barbone et al. ’03, Rickelt and Reese ’04]
  - POD [Rickelt and Reese ’06]
- Patches
  - Finite element enrichment of PGD models by VMM [Ammar et al. ’11]
  - XFEM discontinuities in soft tissues [Niroomandi et al. ’11]
- Model order reduction for heterogeneous/nonlinear materials fracture
  - *A priori* Hyperreduction for plasticity [Ryckelynck et al. ’08] and damage [Kerfriden et al. ’10]
  - Adaptive POD and morphing in the XFEM context [Galland et al. ’09]
  - Reduced model multiscale method [Yvonnet et al. ’07]
  - LaTIn method [Ladevèze et al. ’03]

How we got to this point...

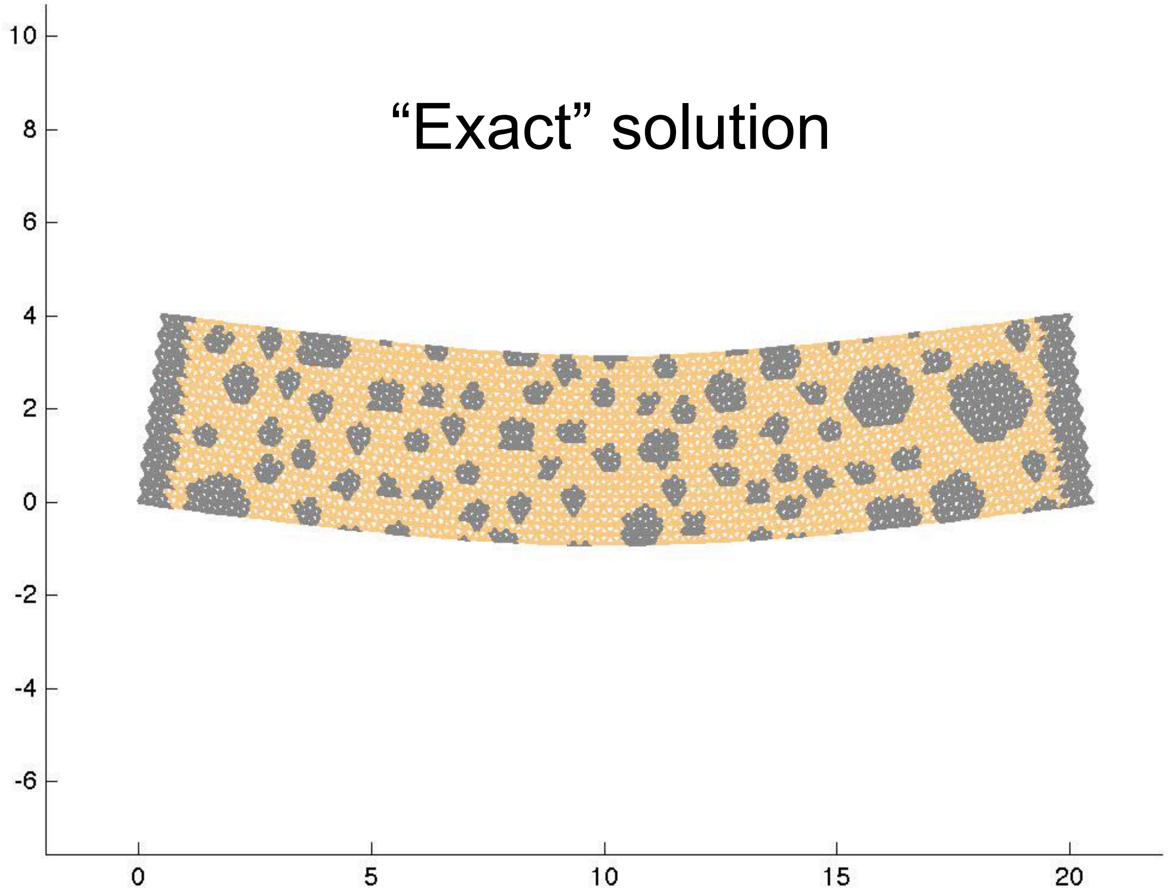
P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems. *Computer Methods in Applied Mechanics and Engineering*, 200(5-8):850–866, 2011.

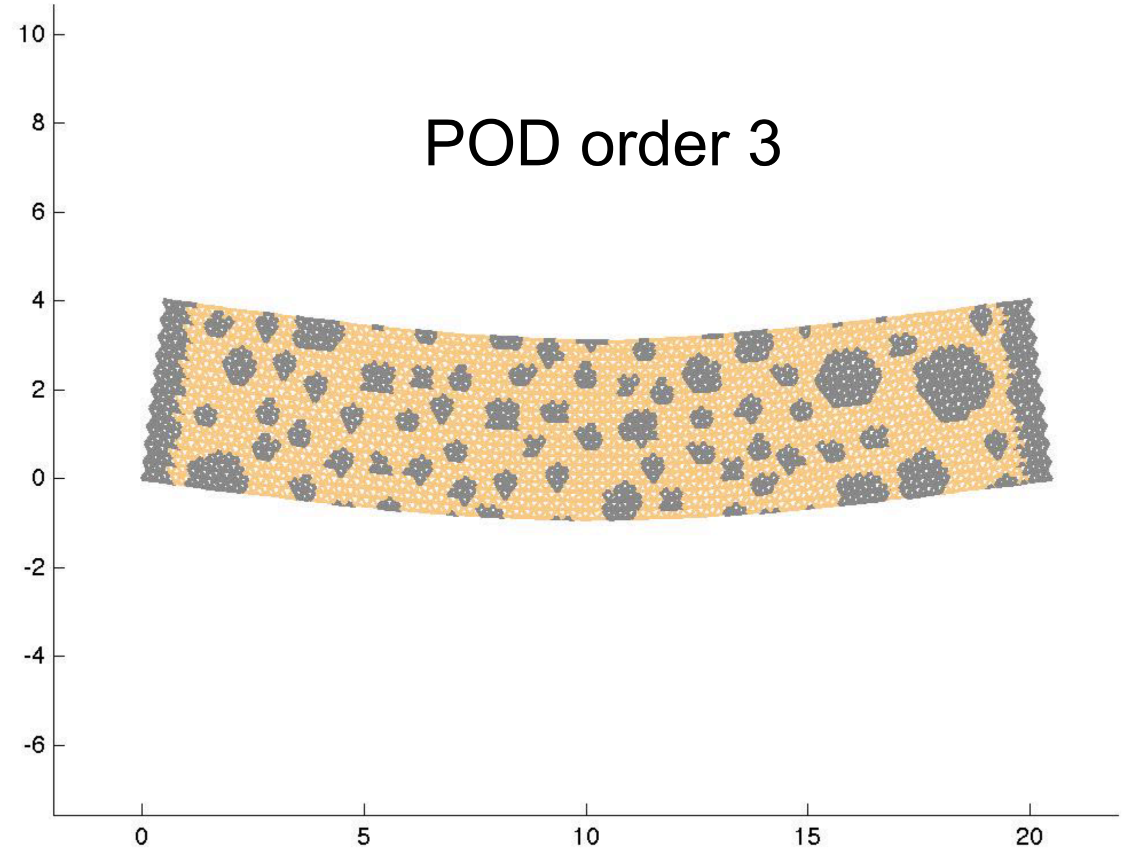
P. Kerfriden, J.C. Passieux, and S. Bordas. Local/global model order reduction strategy for the simulation of quasi-brittle fracture. *International Journal for Numerical Methods in Engineering*, 89(2):154–179, 2011.

P. Kerfriden, K.M. Schmidt, T. Rabczuk, and Bordas S.P.A. Statistical extraction of process zones and representative subspaces in fracture of random composites. *Accepted for publication in International Journal for Multiscale Computational Engineering, arXiv:1203.2487v2*, 2012.

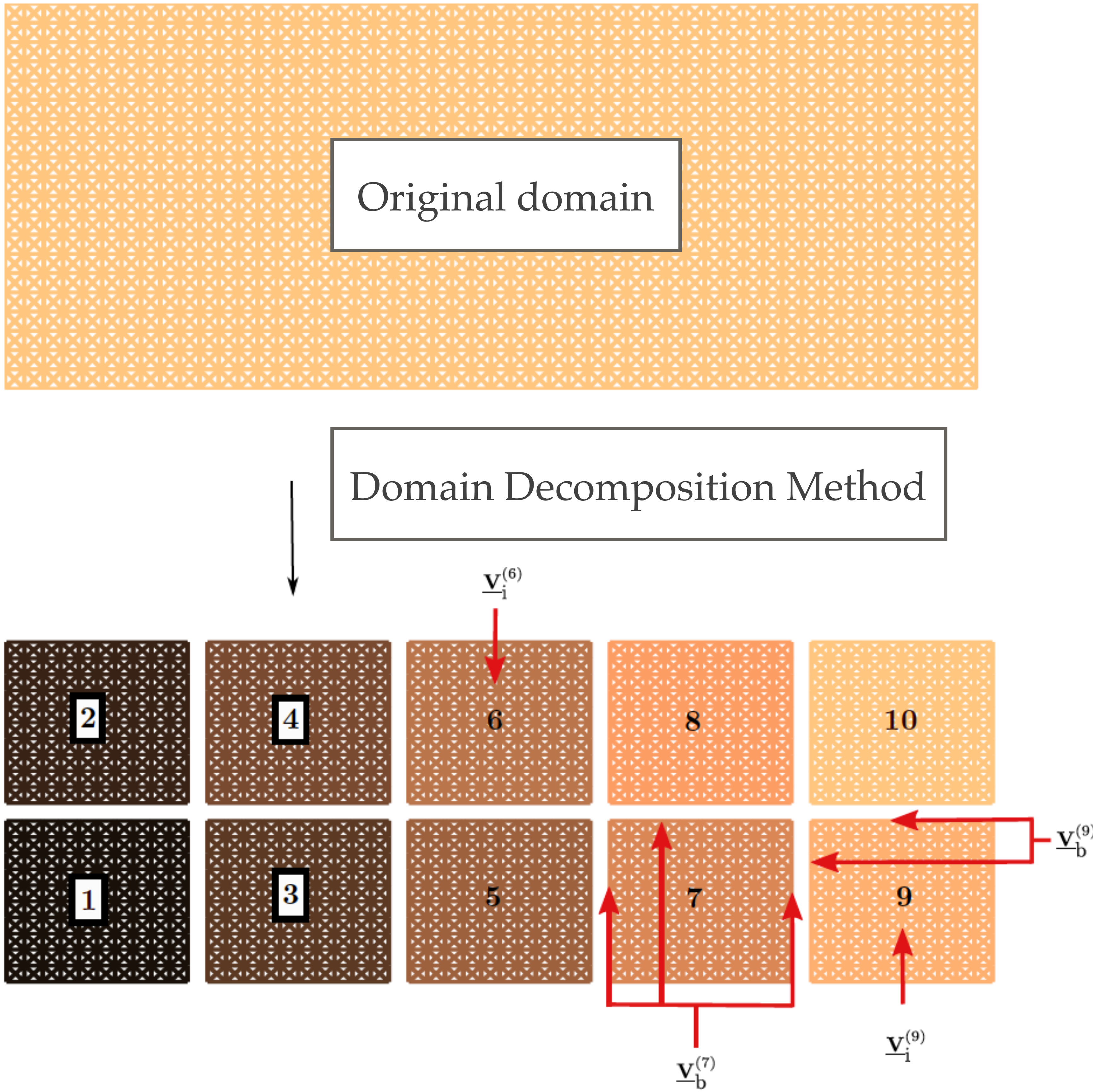
Data compression: fracture

Snapshot POD (snapshot space is spanned by the ensemble of solutions at all time steps)





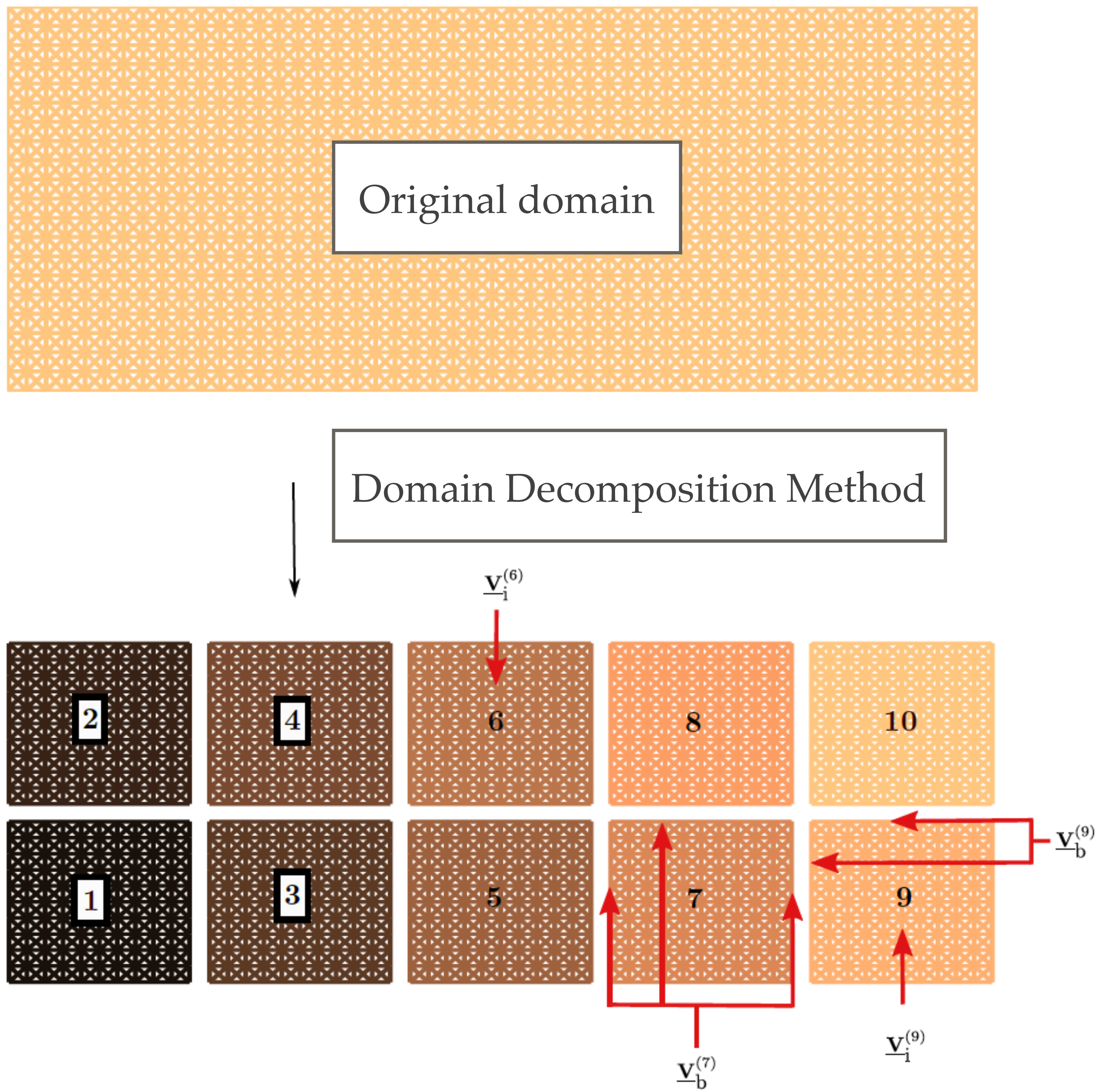
Partitioned POD/DDM

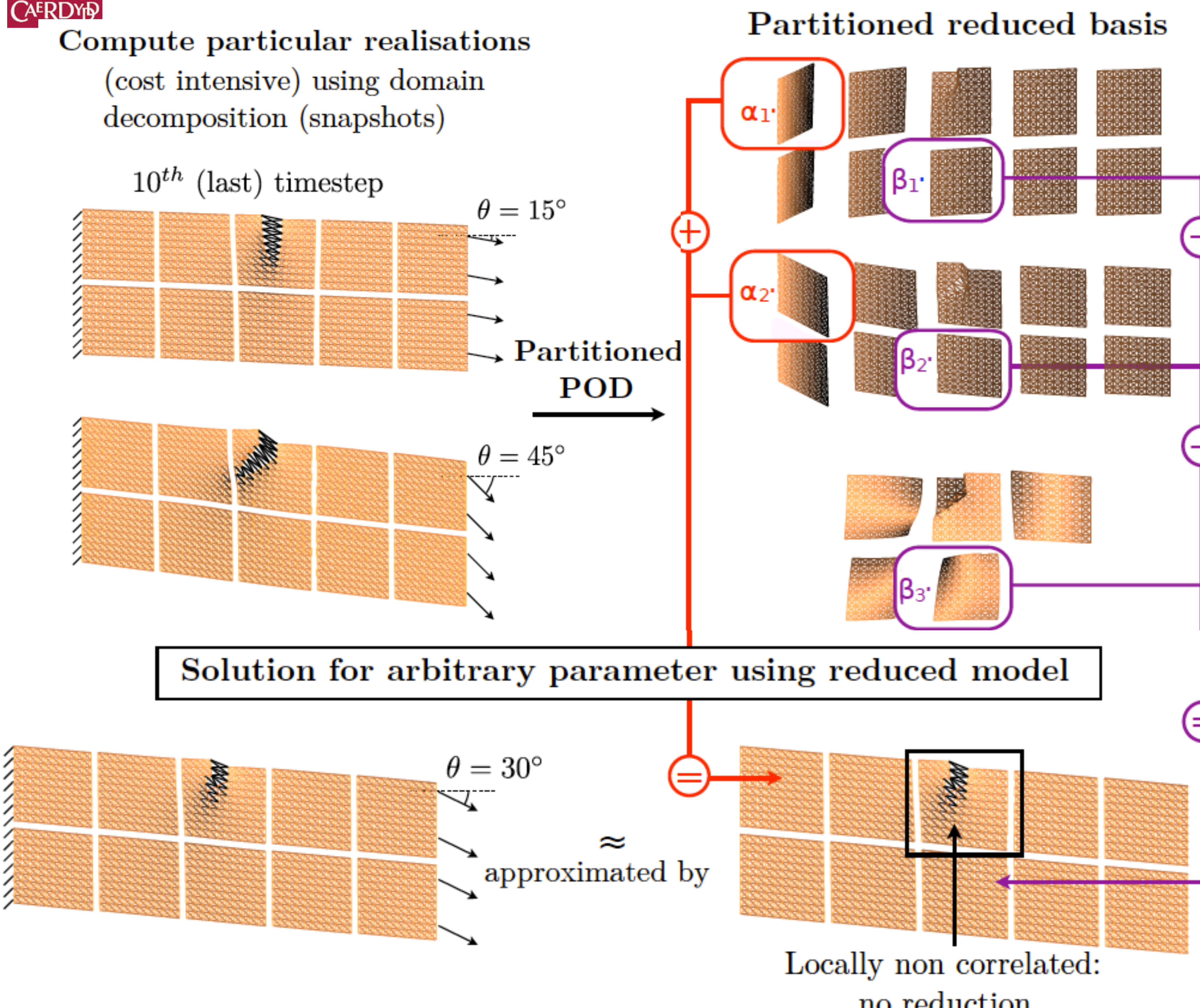


Partitioned POD/DDM

Domain Decomposition Method

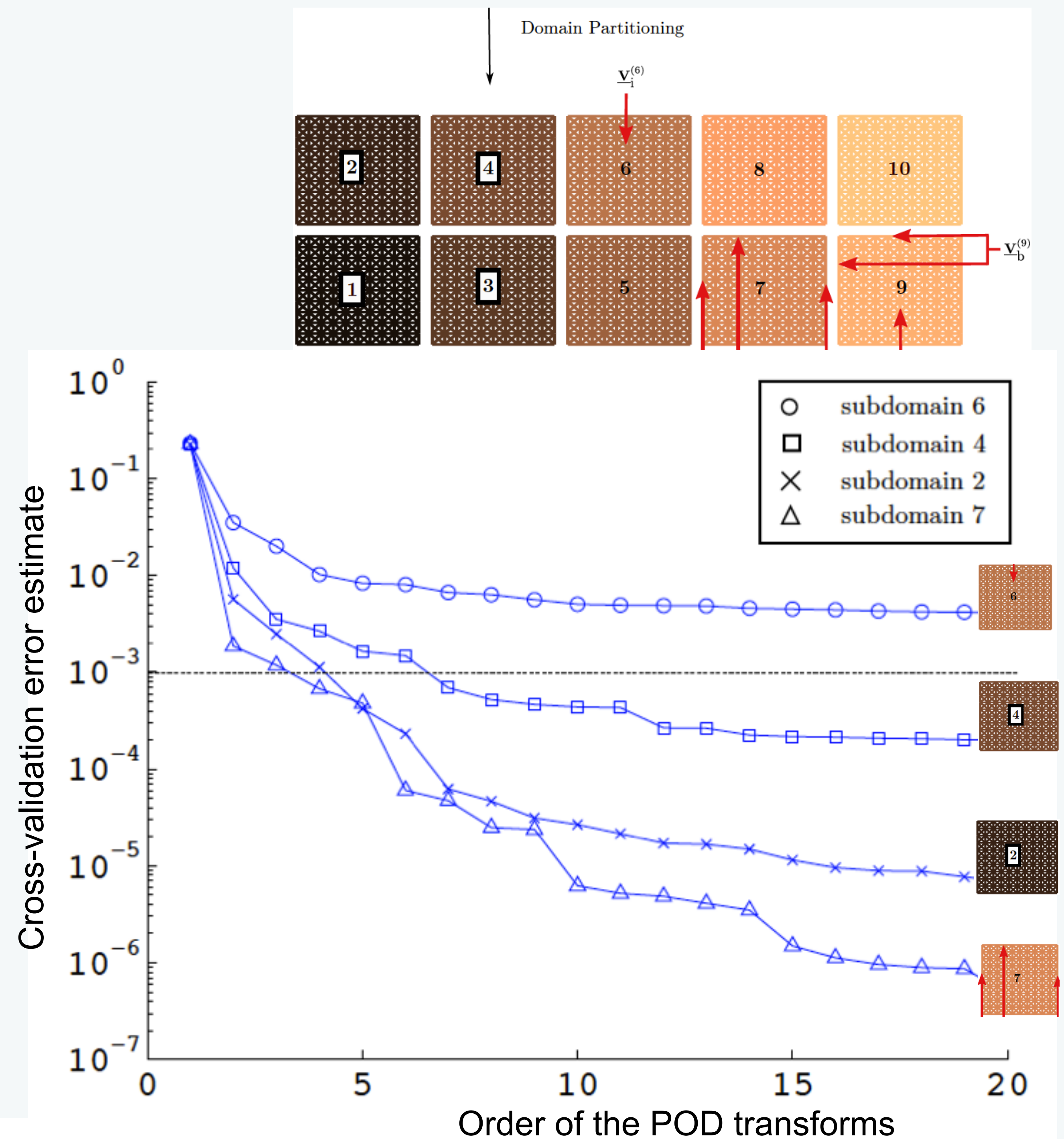
Partitioned POD/DDM





- 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

Choice of the reduced subdomains: local error estimation by



$$\left(\tilde{\nu}^{(e)}_{\mathrm{snap}}\right)^2 = \frac{\displaystyle\sum_{\mu\in\mathcal{P}^s}\sum_{t_n\in\mathcal{T}^h}\left\|\underline{\mathbf{U}}_{\mathrm{i}}(t_n,\mu) - \sum_{j=1}^{n_c^{(e)}}\left(\tilde{\underline{\mathbf{C}}}_{\mathrm{i},j}^{(e),(\mu)\,T}\,\underline{\mathbf{U}}_{\mathrm{i}}(t_n,\mu)\right)\tilde{\underline{\mathbf{C}}}_{\mathrm{i},j}^{(e),(\mu)}\right\|_2^2}{\displaystyle\sum_{t_n\in\mathcal{T}^h}\sum_{\mu\in\mathcal{P}^s}\|\underline{\mathbf{U}}_{\mathrm{i}}(t_n,\mu)\|_2^2}$$

- Reduced subspaces are independent and we assume a snapshot is *a priori* available
  - (1) Dimension of the local space for each subdomain?
  - (2) Is a given subdomain is reducible?
- (1) and (2) will be treated by cross-validation (e.g. W. J. Krzanowski. Cross-validation in principal component analysis. Biometrics, 43(3):575-584, 1987.)
  - **Training set**: snapshot
  - **Validation set**: set of additional finescale solutions
  - Independent training/validation avoids overfitting
  - Cross validation **emulates independence**. Error calculated using the local reduced basis obtained by a snapshot POD transform of all the available snapshot solutions except the one corresponding to the value of the summation variable.
- **NOTE:** If the snapshot is not assumed *a priori* then
  - Assess whether the snapshot contains sufficient information, and generate additional, suitable, data if required
  - Most analysis (mostly by statisticians) assume the snapshot is known *a priori*. Recent review: Hervé Abdi and Lynne J. Williams. Principal component analysis. Wiley Interdisciplinary Reviews: Computational Statistics, 2(4):433{459, 2010.

System approximation

$$\underline{\underline{\mathbf{C}}}^T \underline{\mathbf{F}}_{\text{int}}\left(\underline{\underline{\mathbf{C}}}\,\underline{\alpha}\right) + \underline{\underline{\mathbf{C}}}^T \underline{\mathbf{F}}_{\text{ext}} = 0$$

EXPENSIVE! REQUIRES INTEGRATION OVER THE WHOLE DOMAIN

- Governing equations

- Linearisation (or higher order Taylor) of the non-linear terms in the set of equations
  - Reduced linear operators computed “offline” once and for all
  - Reused “online” in the Newton solver
  - Usability of such techniques is “local” along the trajectory of the reduced state variables

- $$\underline{\mathbf{F}}_{\text{int}}\left(\underline{\underline{\mathbf{C}}}\,\underline{\boldsymbol{\alpha}}(t_n,\mu)\right) = \sum_{i=1}^{n_{\text{d}}} \underline{\mathbf{D}}_i\, \beta_i(t_n,\mu) = \underline{\underline{\mathbf{D}}}\,\underline{\boldsymbol{\beta}}(t_n,\mu) \qquad \underline{\boldsymbol{\beta}}(t_n,\mu) = \underset{\underline{\boldsymbol{\beta}}^\star}{\operatorname{argmin}} \left\| \underline{\underline{\mathbf{D}}}\,\underline{\boldsymbol{\beta}}^\star(t_n,\mu) - \underline{\mathbf{F}}_{\text{int}}\left(\underline{\underline{\mathbf{C}}}\,\underline{\boldsymbol{\alpha}}(t_n,\mu)\right) \right\|_{\underline{\underline{\mathbf{P}}}}$$

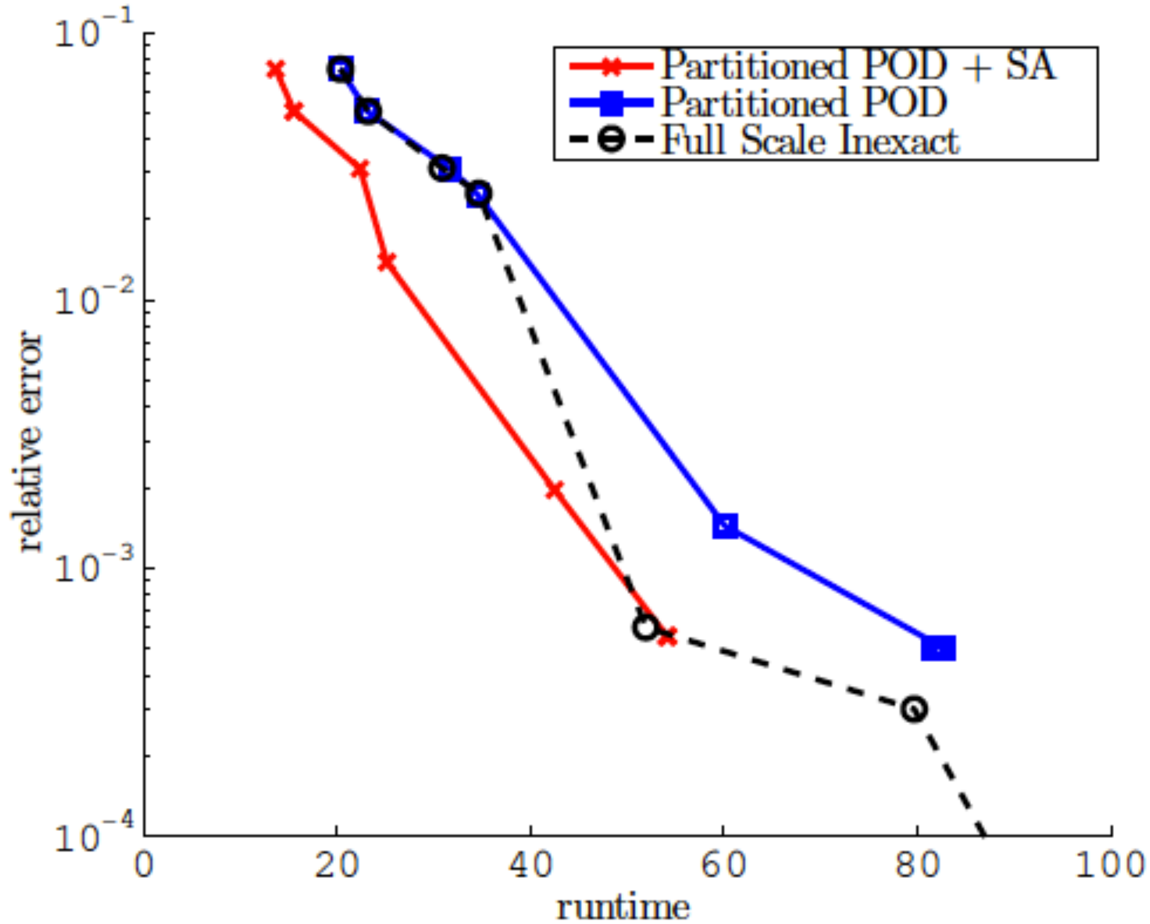
$$\underline{\underline{\mathbf{D}}}\left(\underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{P}}}\,\underline{\underline{\mathbf{D}}}\right)^{-1} \underline{\underline{\mathbf{D}}}^T \underline{\underline{\mathbf{P}}}\,\underline{\mathbf{F}}_{\text{int}}\left(\underline{\underline{\mathbf{C}}}\,\underline{\alpha}\right) + \underline{\mathbf{F}}_{\text{ext}} = \underline{\mathbf{R}}(\underline{\alpha})$$

  - “Collocation” methods look for a solution which is optimal with respect to a few equations of the system (least squares or Galerkin frameworks can be used).

Performance: load angle 40 | 27 - 121 nodes

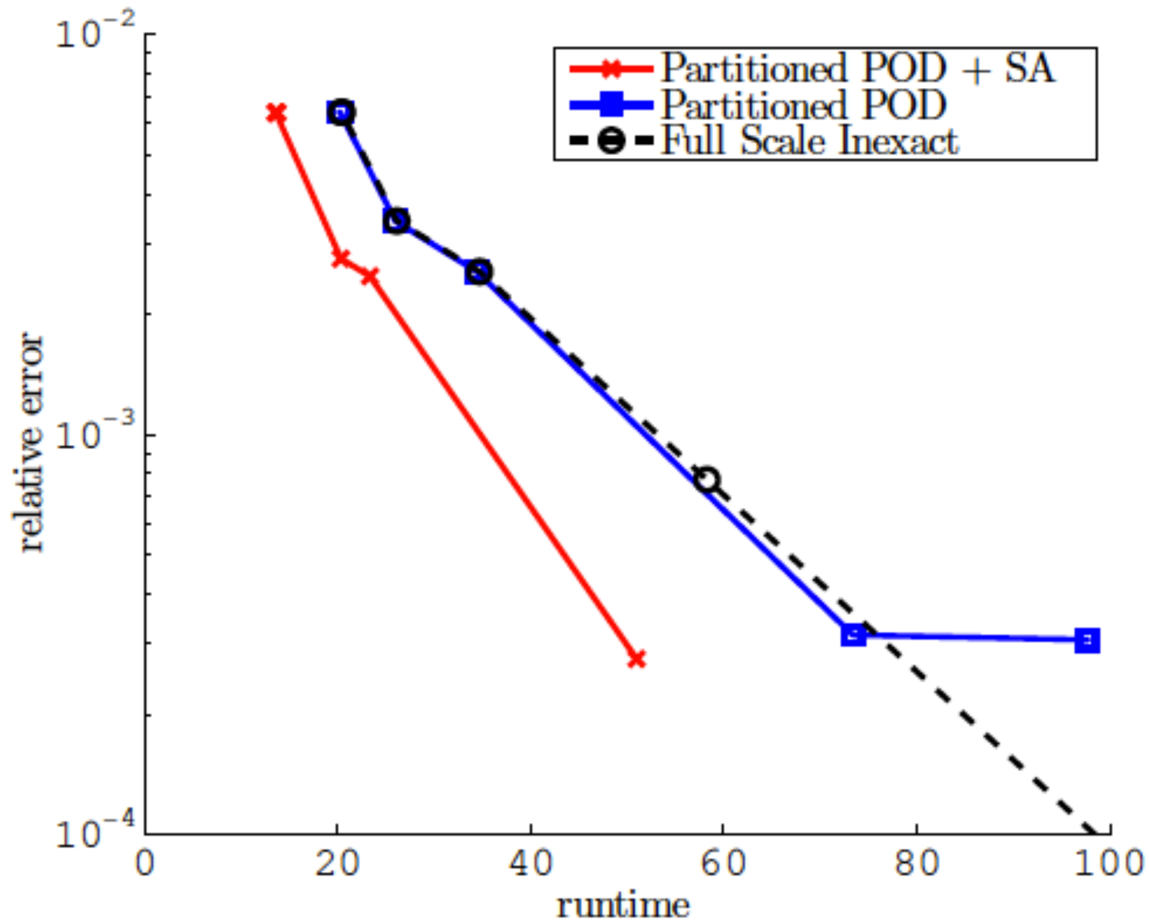
$$\nu^{\mathrm{app},(\mu)}\left(\underline{\mathbf{U}}^{\mathrm{app}}\right)^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\mathrm{app}}(t_n,\mu) - \underline{\mathbf{U}}^{\mathrm{ex}}(t_n,\mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\mathrm{ex}}(t_n,\mu)\|_2^2}$$

40^o



(a) Relative error for the different models using 121 nodes per subdomain

27^o



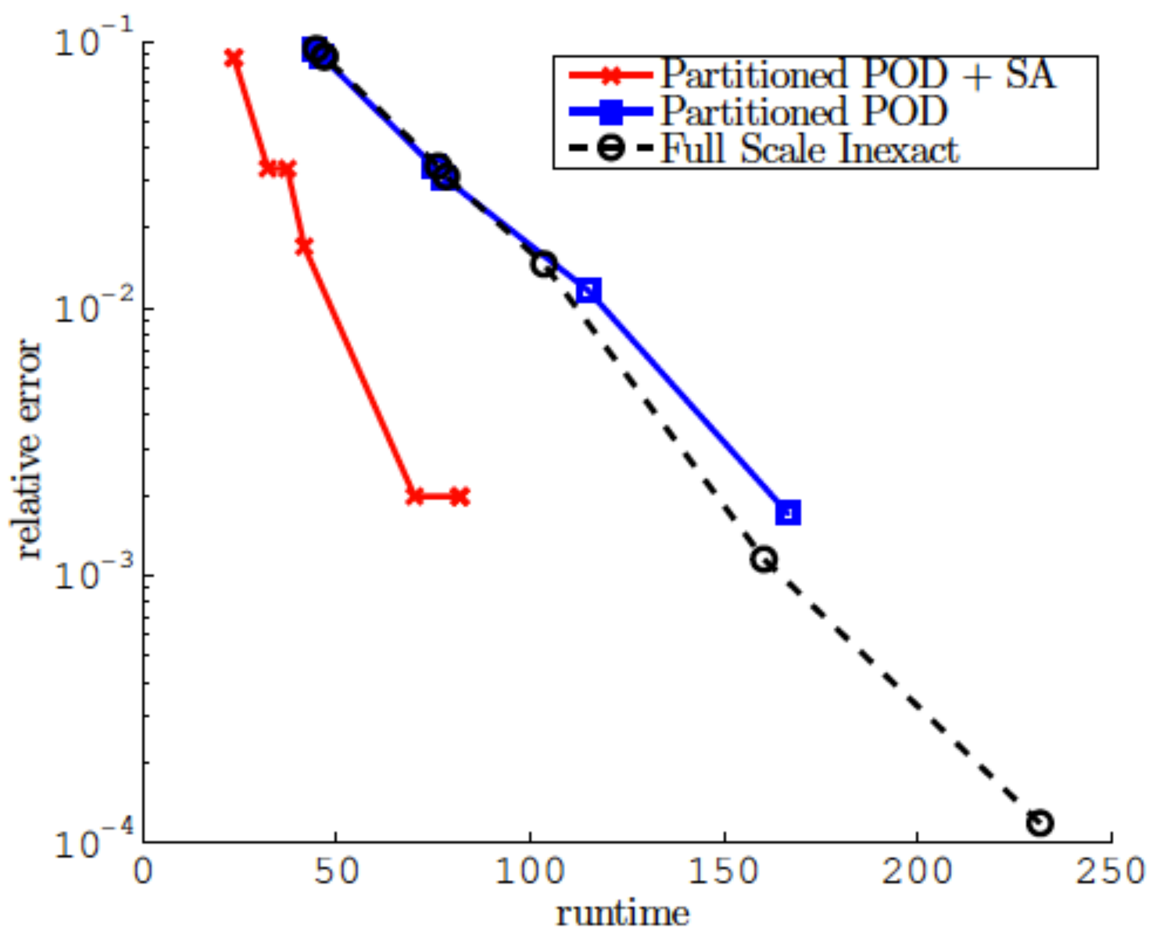
(a) Relative error for the different models using 121 no per subdomain

Performance: load angle 40 | 27 - 256 nodes

- Relative error

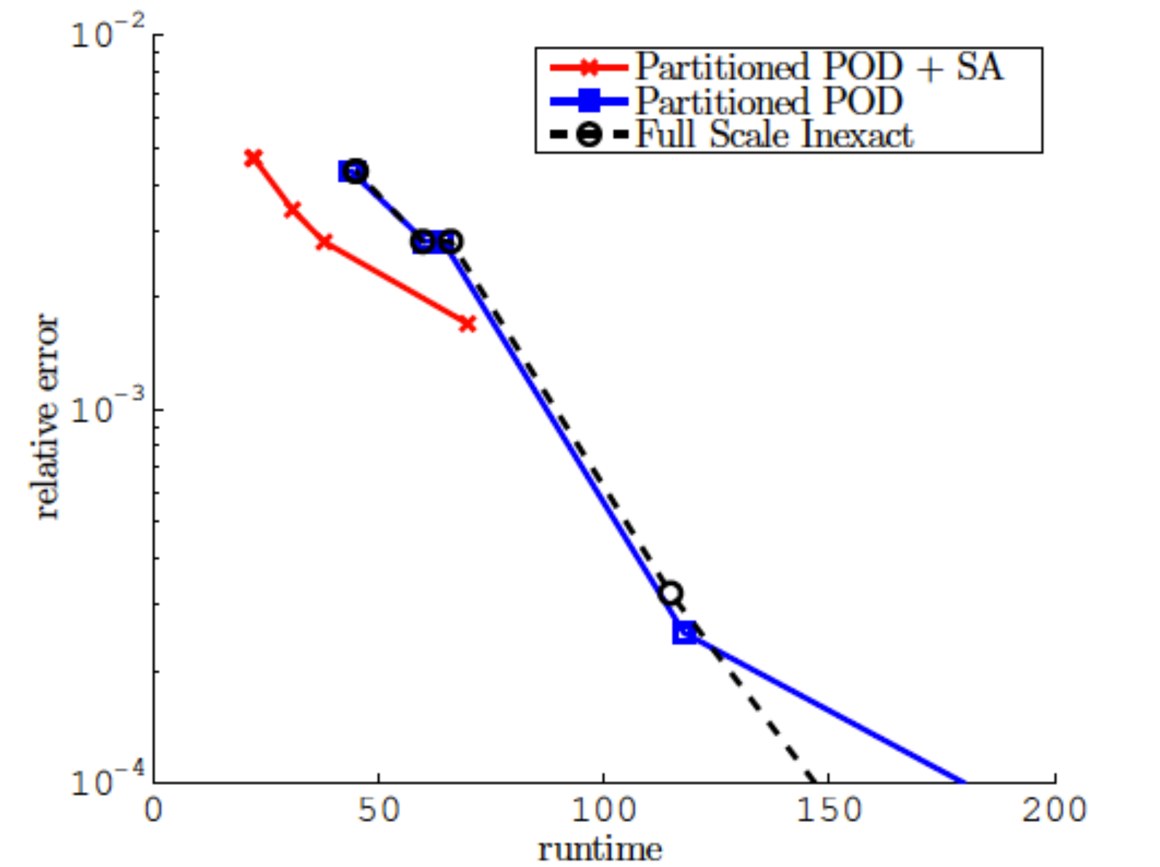
$$\nu^{\text{app},(\mu)}\left(\underline{\mathbf{U}}^{\text{app}}\right)^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{app}}(t_n,\mu) - \underline{\mathbf{U}}^{\text{ex}}(t_n,\mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{ex}}(t_n,\mu)\|_2^2}$$

40^o



(b) Relative error for the different models using 256 nodes per subdomain

27^o

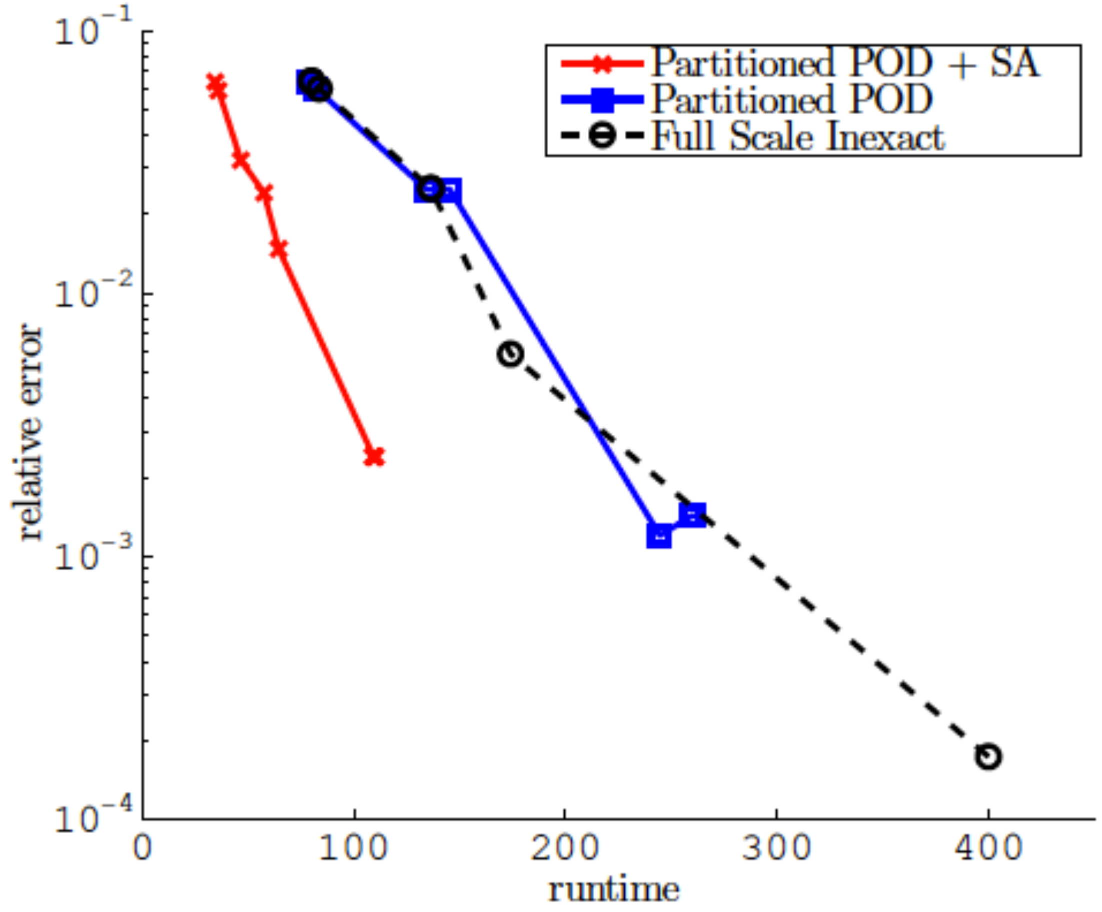


(b) Relative error for the different models using 256 nodes per subdomain

Performance: load angle 40 | 27 - 441 nodes

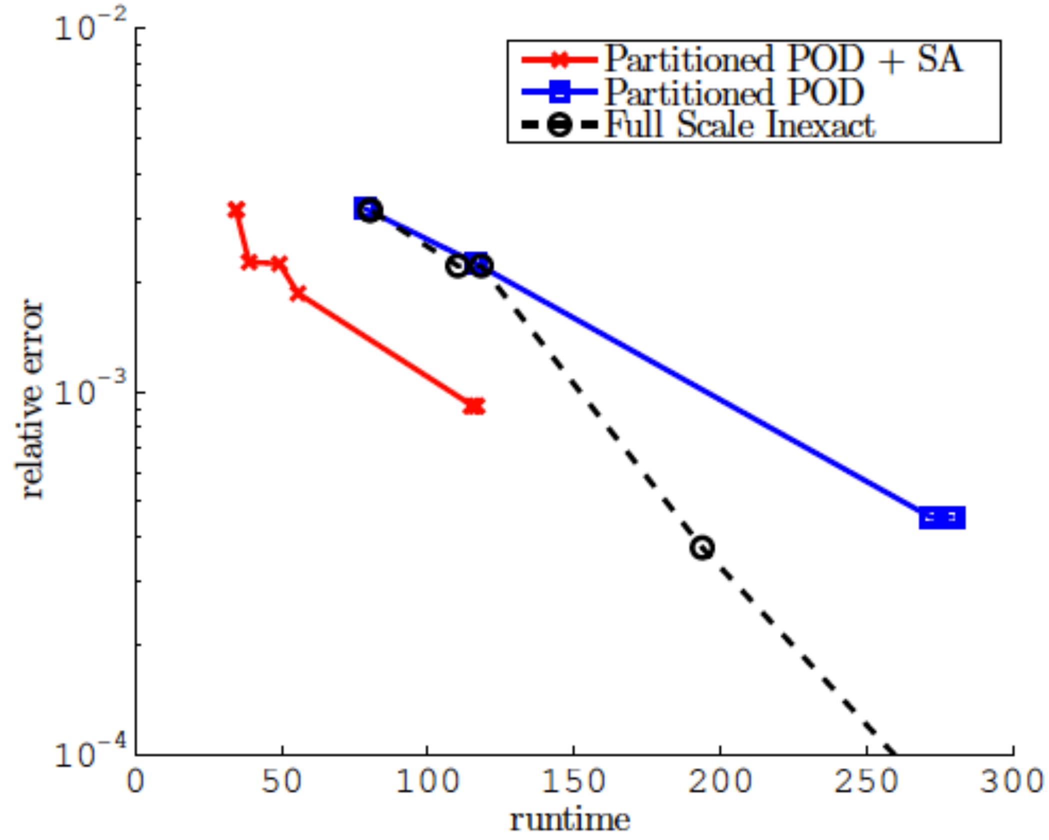
$$\nu^{\mathrm{app},(\mu)}\left(\underline{\mathbf{U}}^{\mathrm{app}}\right)^2 = \frac{\sum\limits_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\mathrm{app}}(t_n,\mu) - \underline{\mathbf{U}}^{\mathrm{ex}}(t_n,\mu)\|_2^2}{\sum\limits_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\mathrm{ex}}(t_n,\mu)\|_2^2}$$

40^o



(c) Relative error for the different models using 441 nodes per subdomain

27^o



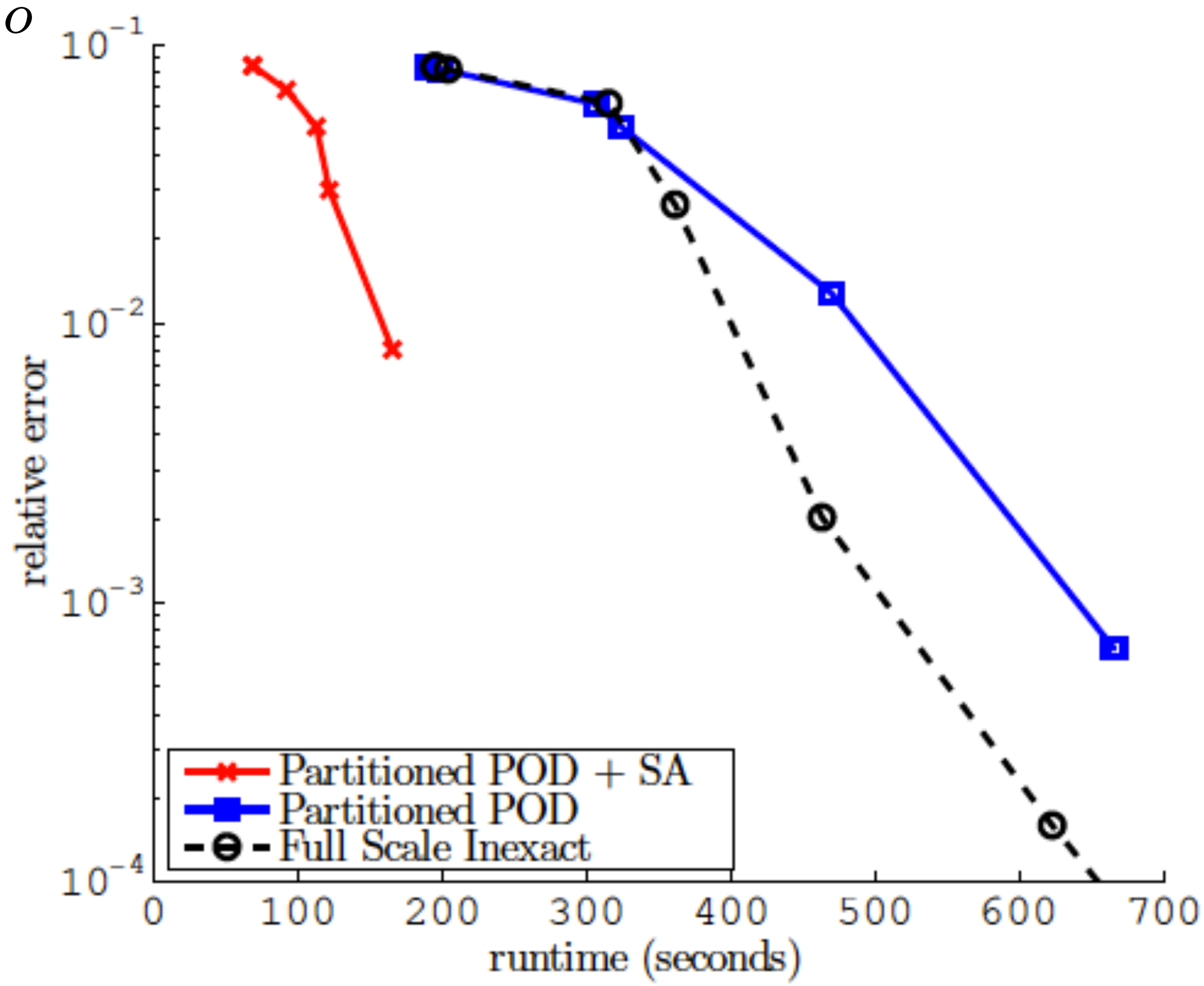
(c) Relative error for the different models using 441 nodes per subdomain

Performance: load angle 40 | 27 - 961 nodes

- Relative error

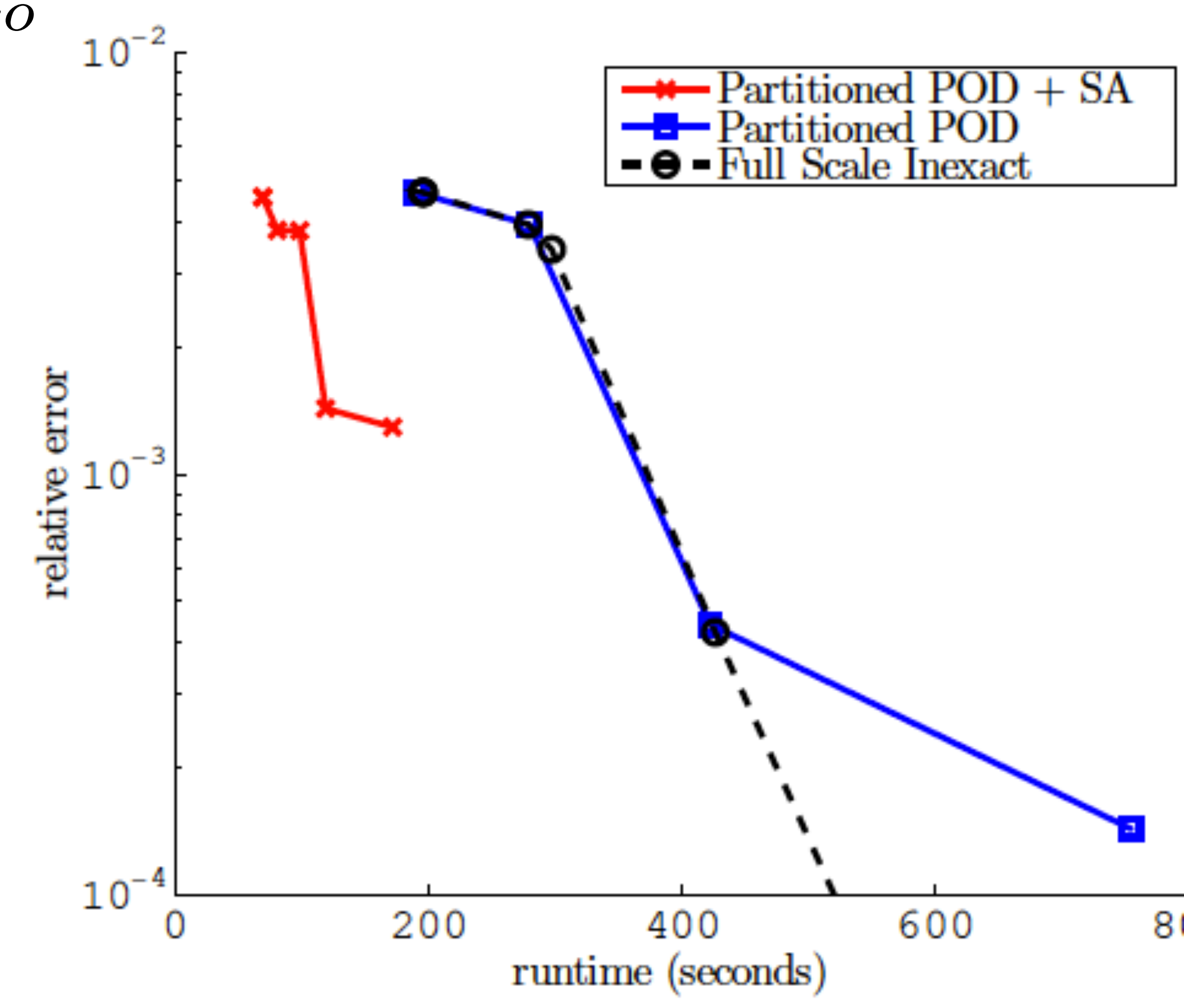
$$\nu^{\text{app},(\mu)}\left(\underline{\mathbf{U}}^{\text{app}}\right)^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{app}}(t_n,\mu) - \underline{\mathbf{U}}^{\text{ex}}(t_n,\mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{ex}}(t_n,\mu)\|_2^2}$$

40^o



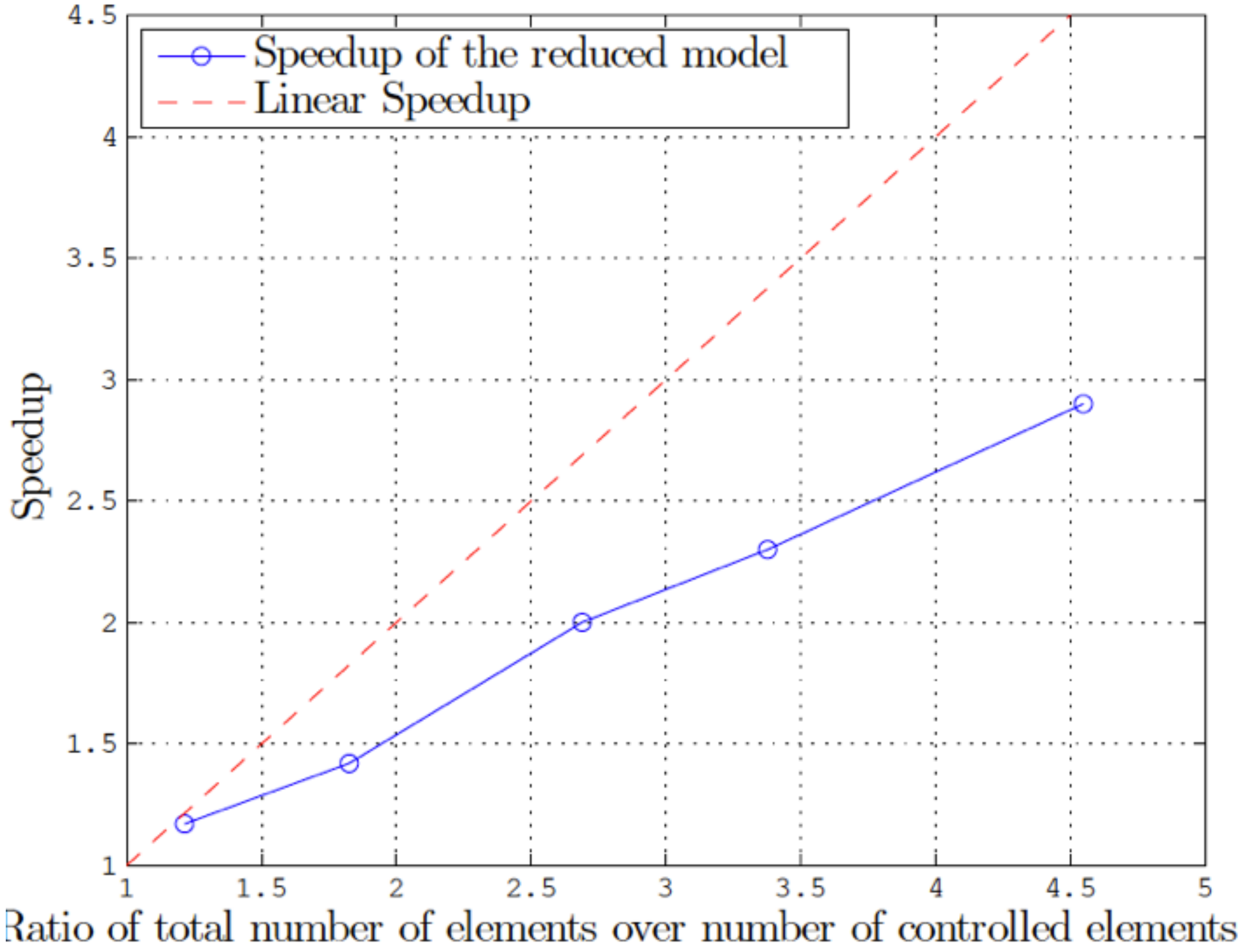
(d) Relative error for the different models using 961 nodes per subdomain

27^o



(d) Relative error for the different models using 961 per subdomain

Role of system approximation



Conclusions and perspectives

- Domain coupling using the primal Schur-complement domain decomposition method.
- Local subproblems have been reduced by projection in low-dimensional subspaces obtained by the snapshot POD.
- This approach permits to flexibly reduce the computational cost associated with highly nonlinear problems. In particular:
    - the **local reduced spaces are generated independently**, and have independent dimensions, which allows us to focus the numerical effort where it is most needed.
    - subdomains that are close to highly damaged zones need a richer model to account for the effect of topological changes. The local **POD transforms automatically generate local reduced spaces of larger dimension in these zones**.
    - the domain decomposition framework enables us to **switch from reduced local solvers to full local solvers** in a transparent manner. This is particularly useful for the subdomains that contain process zones, as a solution obtained by projection would be more expensive than a direct solution for a desirable accuracy.
    - the transition between ``offline'' and ``online'' computations becomes flexible. The **reduced models can be used in the zones where the local reduced spaces converge quickly** when enriching the snapshot space, while still computing snapshots and refining the reduced models via a direct local solver in the remaining subdomains.

Perspectives (1/2)

- Further work related to domain decomposition
  - **load balancing** mismatch would occur when using such a strategy in parallel. CPUs which support domains that are not reduced, or domains for which the corresponding subproblems need to be projected in a space of relatively high dimension, would require to perform more operations. <u>The domain partitioning itself should be performed jointly with the model reduction in order to distribute the load evenly</u>.
  - **the interface problem itself was not reduced** here, to guarantee the interface kinematic compatibility.
    - Suboptimal reduced order model. Would generate expensive communications in parallel
    - A reduction of the interface problem using the POD can be done but is neither elegant nor easy
    - Dual Schur-complement domain decomposition method would allow the kinematic approximation of the subproblems to include the interface. However, this would only deflect the difficulty to the necessary reduction of the interface Lagrange multiplier space. This issue is our current direction of research.

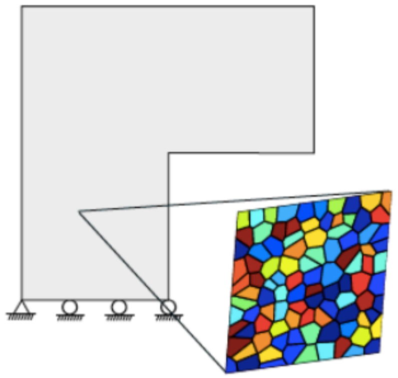
Perspectives (2)

- A Quarteroni, G Rozza, and A Manzoni. Certified reduced basis approximation for parametrized partial differential equations and applications. *Journal of Mathematics in Industry*, 1(3):1–44, 2011.

research area

  - We have used a cross validation technique. OK if sufficiently fine snapshot space.
  - We cannot find zones of “non-smoothness” in the parameter space automatically.
- We used global Euclidian norms to evaluate the error. Needs refinement to tackle goals and quantities of interest.

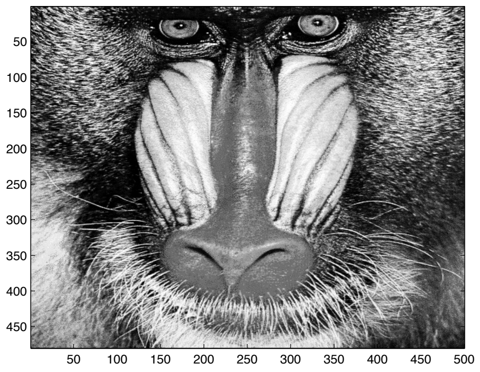
- Use model reduction to identify “fracture zones” / localisation bands, etc.



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

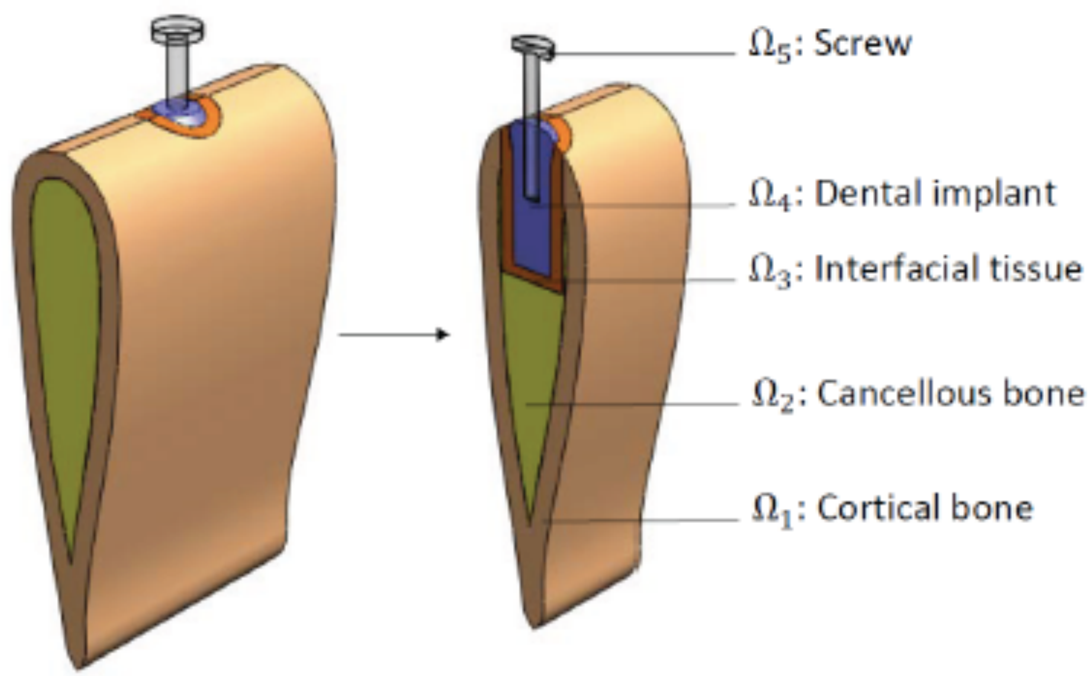
- how to define the reduced area?

- precomputation time (offline)

Model reduction - algebraic

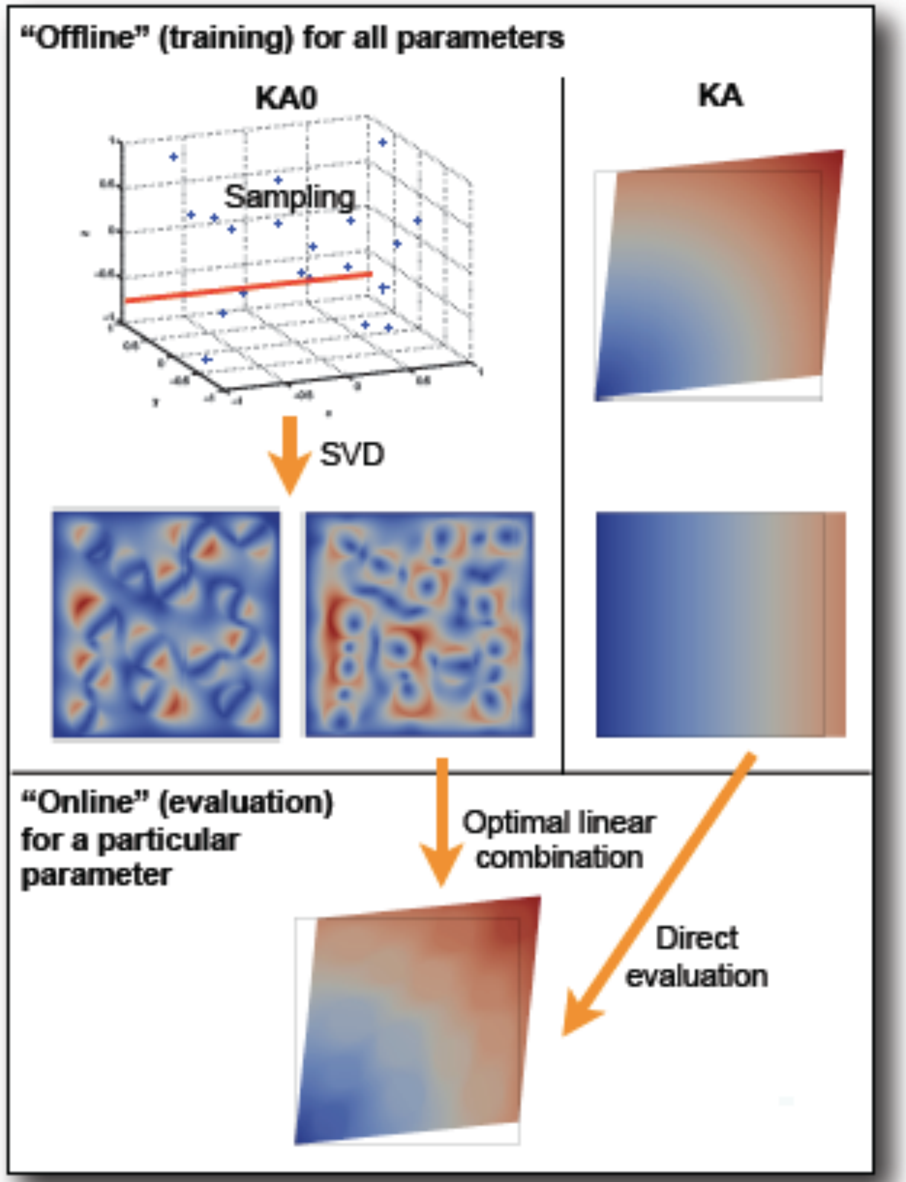
- Multilevel methods to reduce CPU time by orders of magnitude and devise robust, efficient code/model coupling

  - Virtual chart with controlled accuracy via ROM for multiscale modelling and real-time optimisation



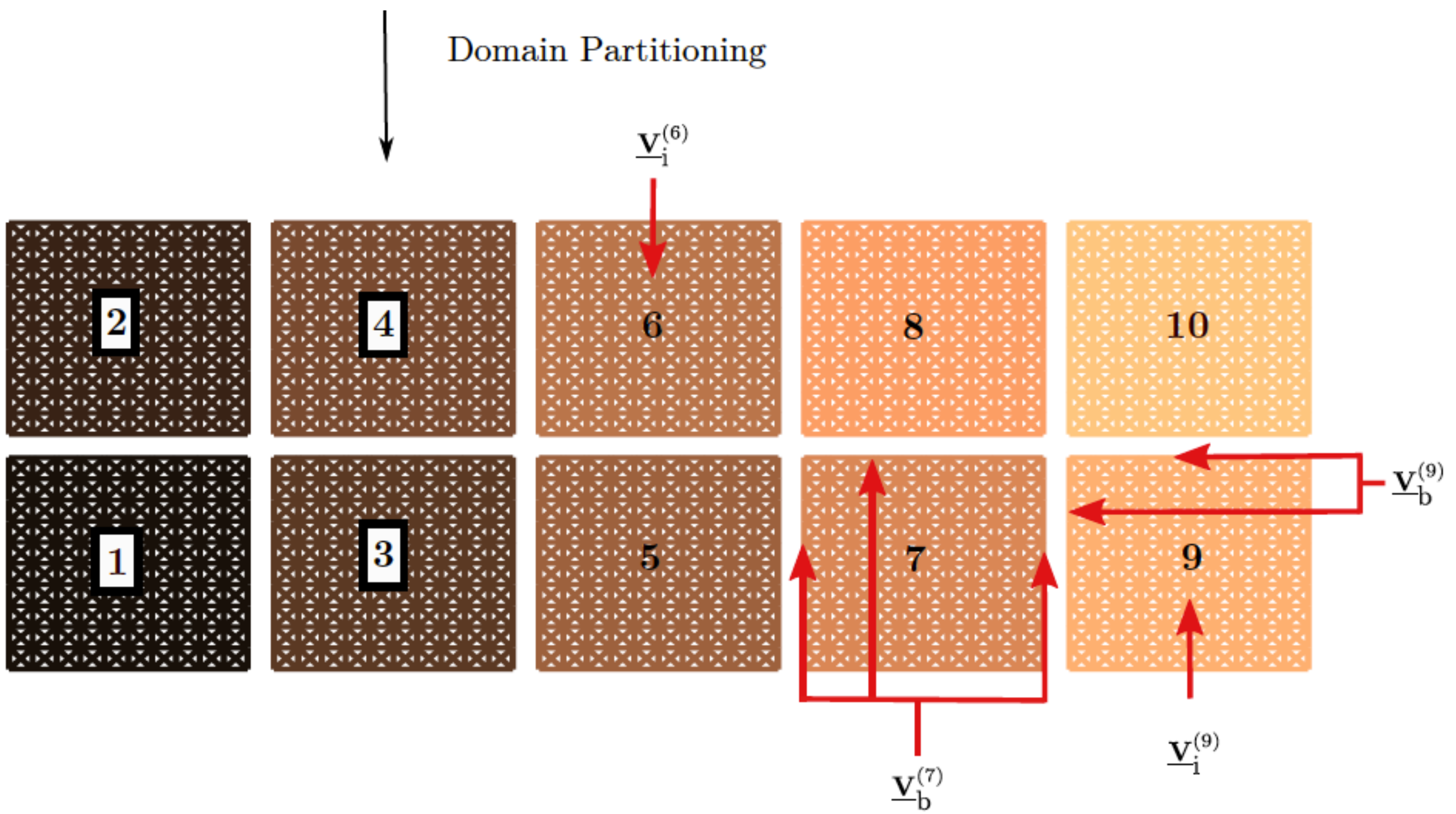
[Hoang et al., 2013]

"offline" / "online" strategy



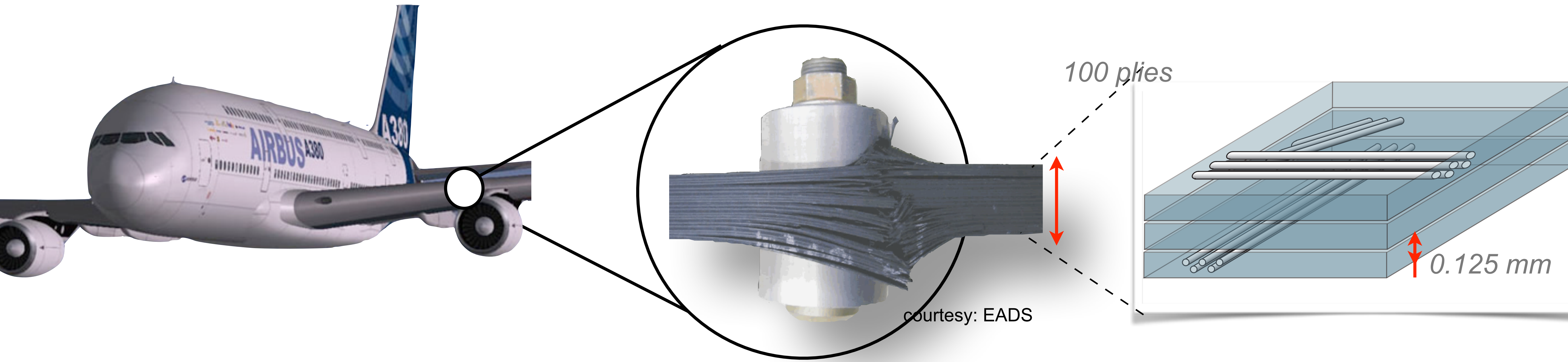
[Kerfriden et al., 2013]

Open problem: algebraic model reduction for non-linear problems with localisation - fracture, moving interfaces


Domain Partitioning
$\underline{\mathbf{v}}_{\mathrm{i}}^{(6)}$
2
4
6
8
10
1
3
5
7
9
$\underline{\mathbf{v}}_{\mathrm{b}}^{(9)}$
$\underline{\mathbf{v}}_{\mathrm{i}}^{(9)}$
$\underline{\mathbf{v}}_{\mathrm{b}}^{(7)}$

Future?

Material complexity

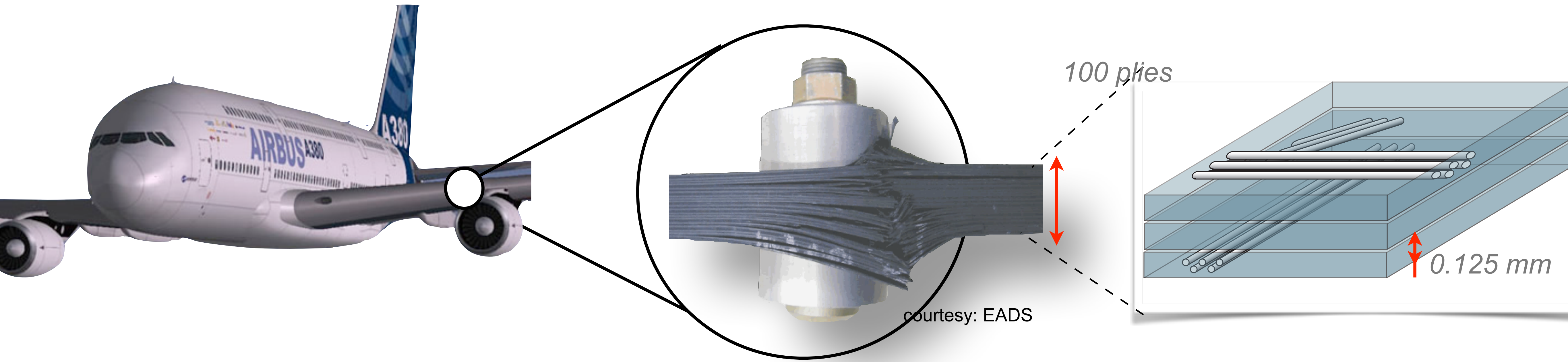


Heterogeneous & multi-functional materials

Can we optimise the material microstructure given macroscopic objective functions

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

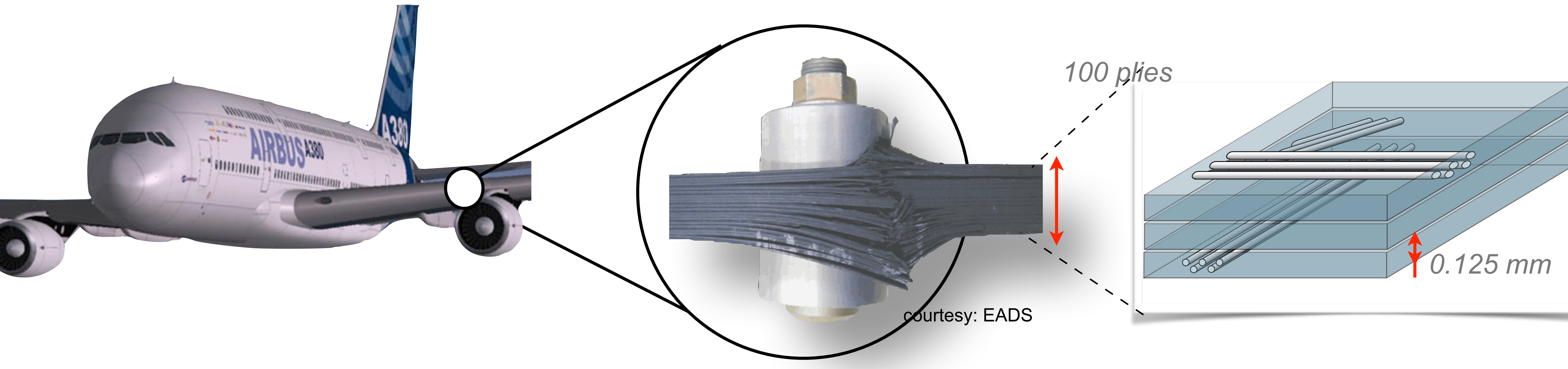
Material complexity



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, …)

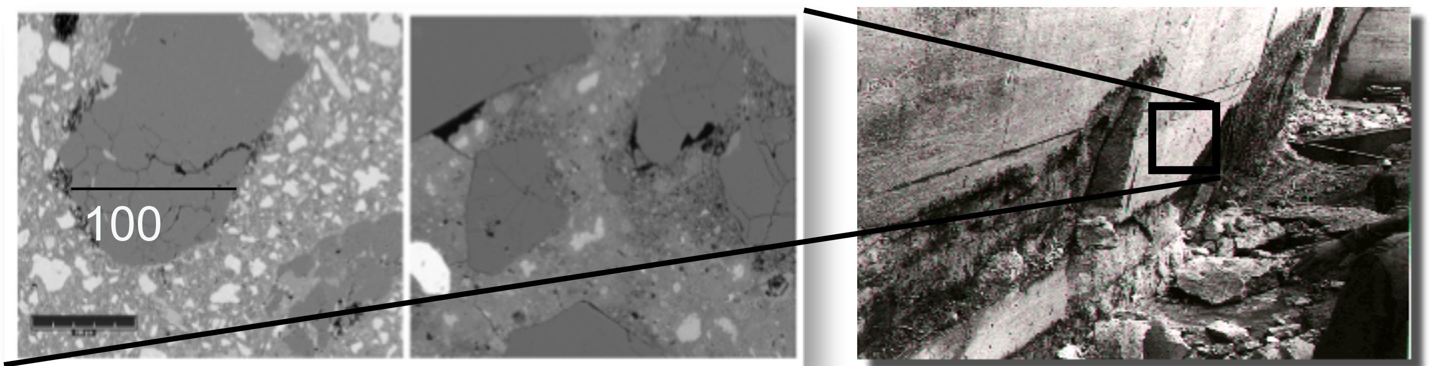
Digital twin concept

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

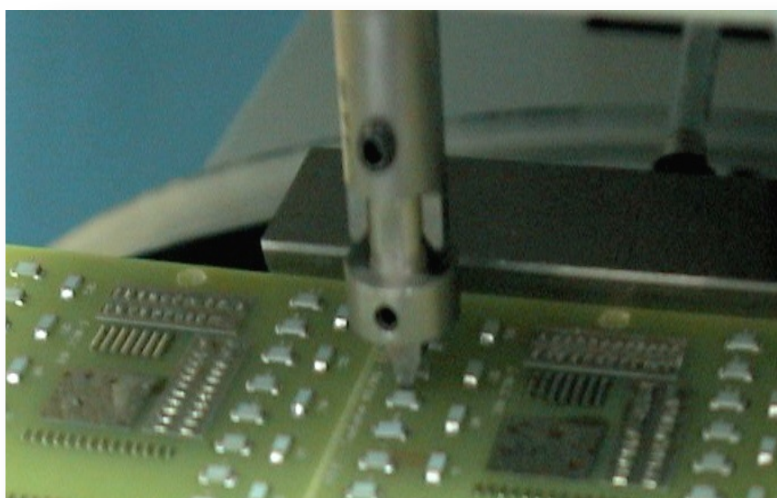
Requires real-time data assimilation, and model update…

Industrial and clinical applications

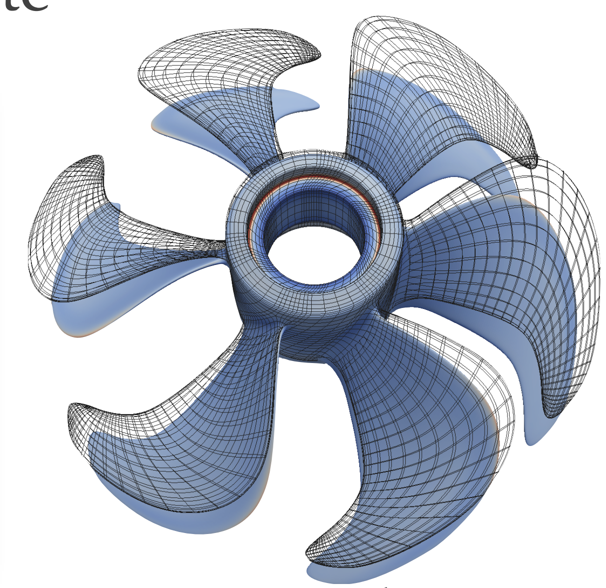
Industrial and clinical applications



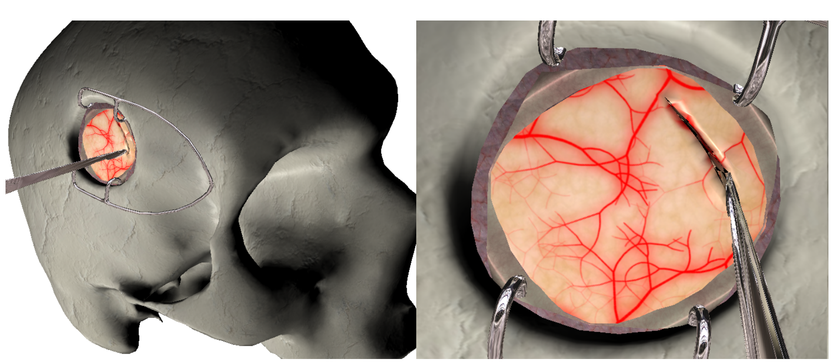
Alkali-silica reaction in concrete



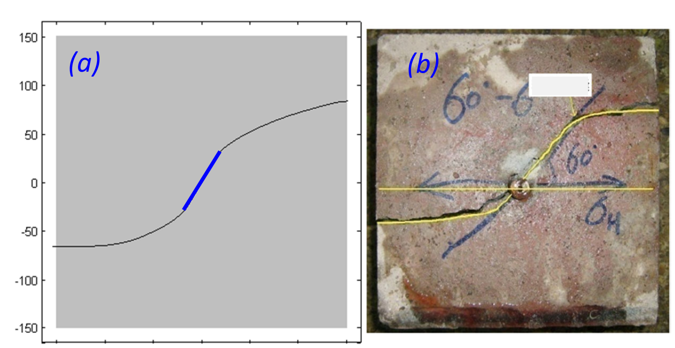
Solder joint durability
in the car industry



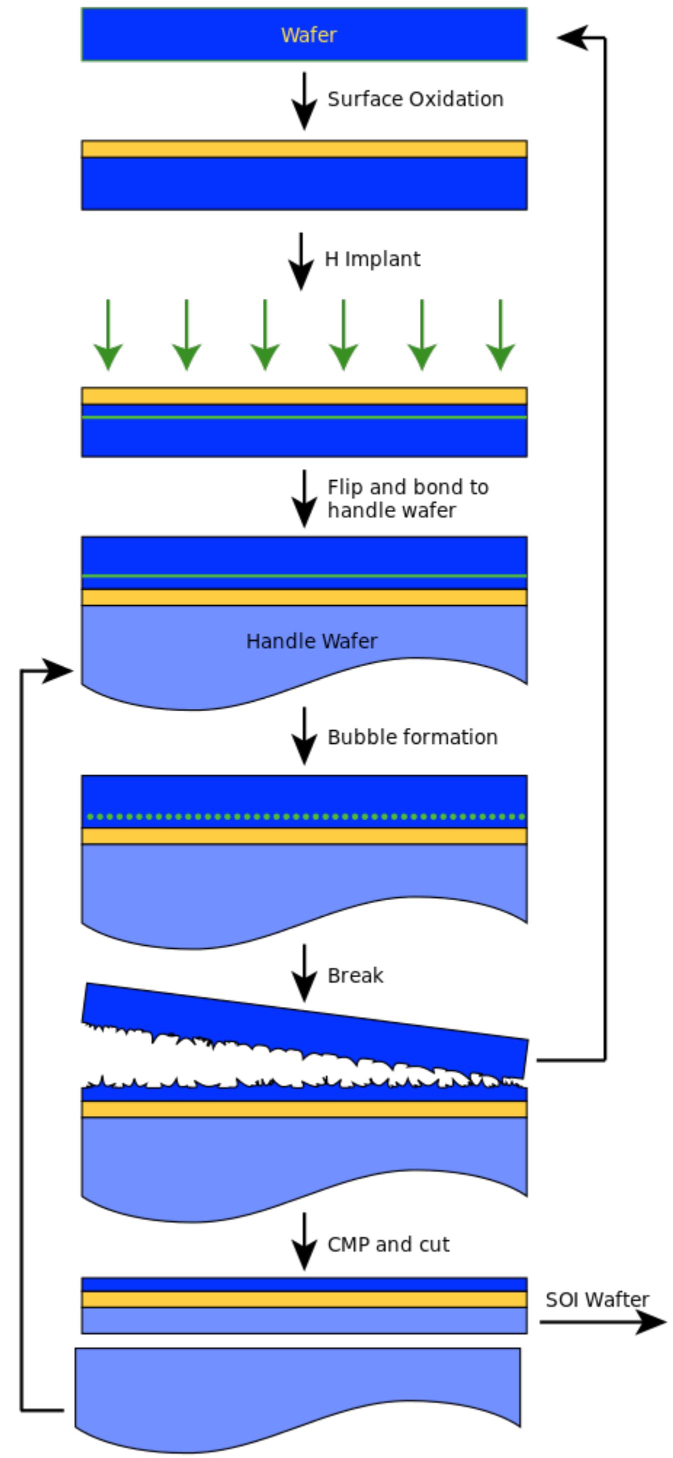
Turbine shape
optimisation



Surgical simulation



Hydraulic fracture



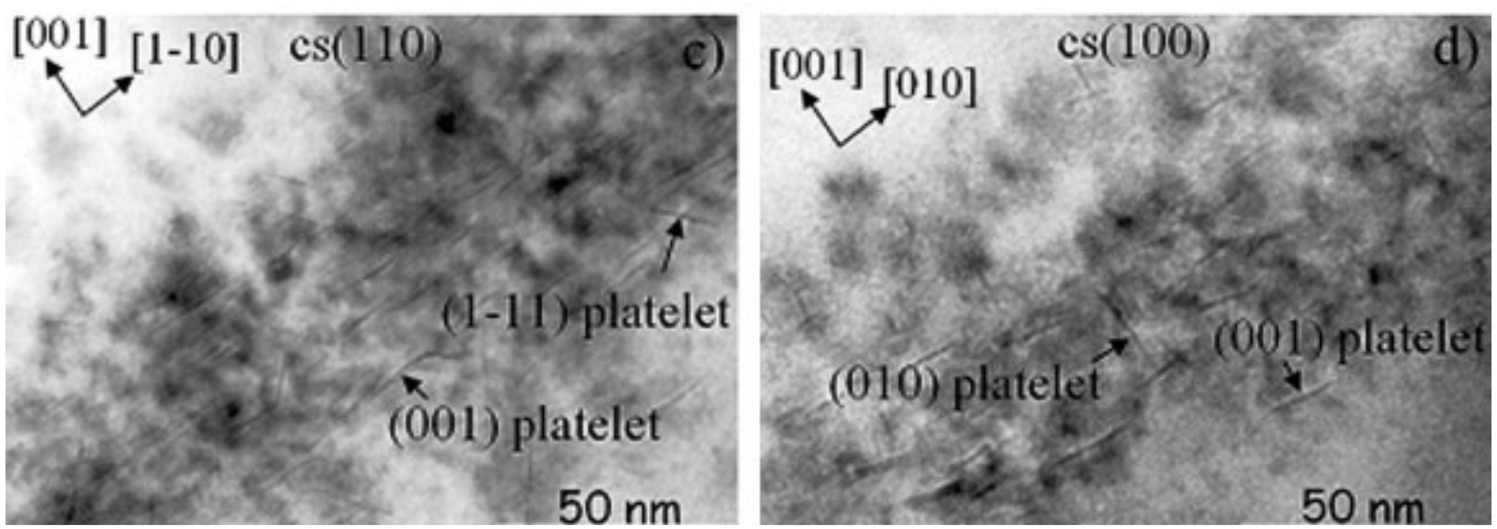
Silicon wafer
cutting

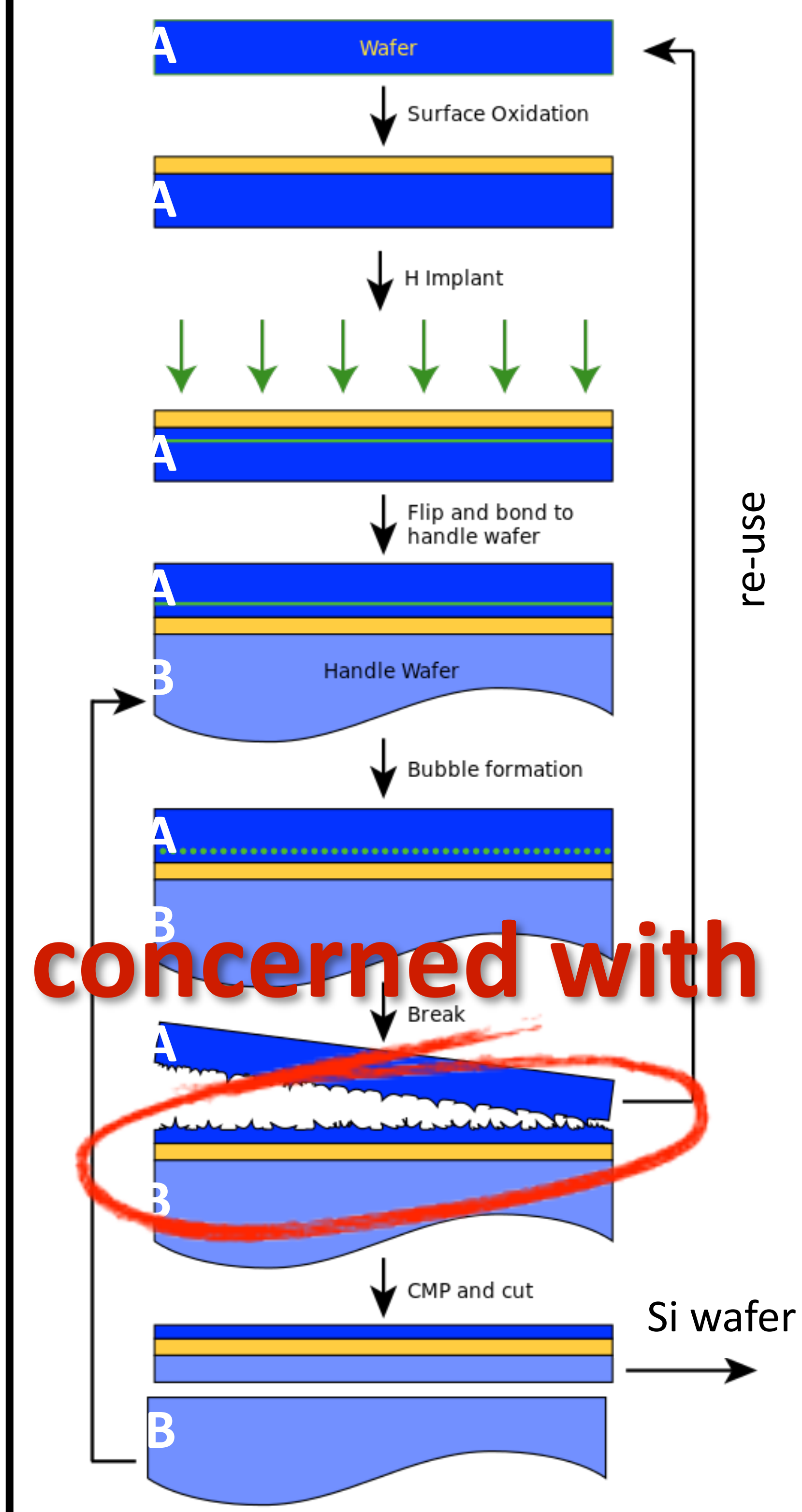
Numerical Modeling of SOI Wafer Splitting

Physical process

Manufacturing process: *SmartCut™*

- H^+ ionization of a thin surface of Si
- Bonding to a handle-wafer (stiffener)
- High temperature thermal annealing
- Nucleation and growth of cavities filled with H_2
- Pressure driven micro crack growth
- Coalescence and post-split fracture roughness





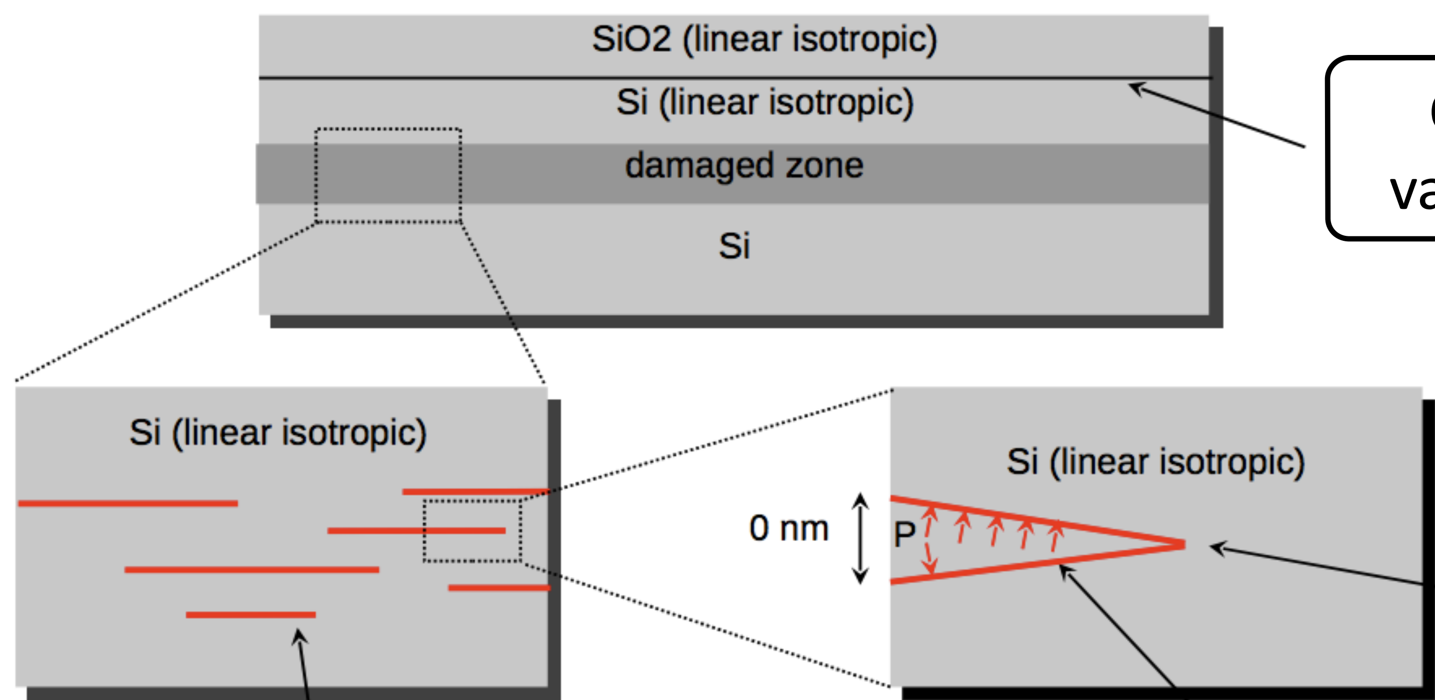
Model

Modeling cavities by zero thickness surfaces

- discontinuities in the displacement field

Linear elastic fracture mechanics (LEFM)

- infinite stress at crack tip, i.e. *singularity*

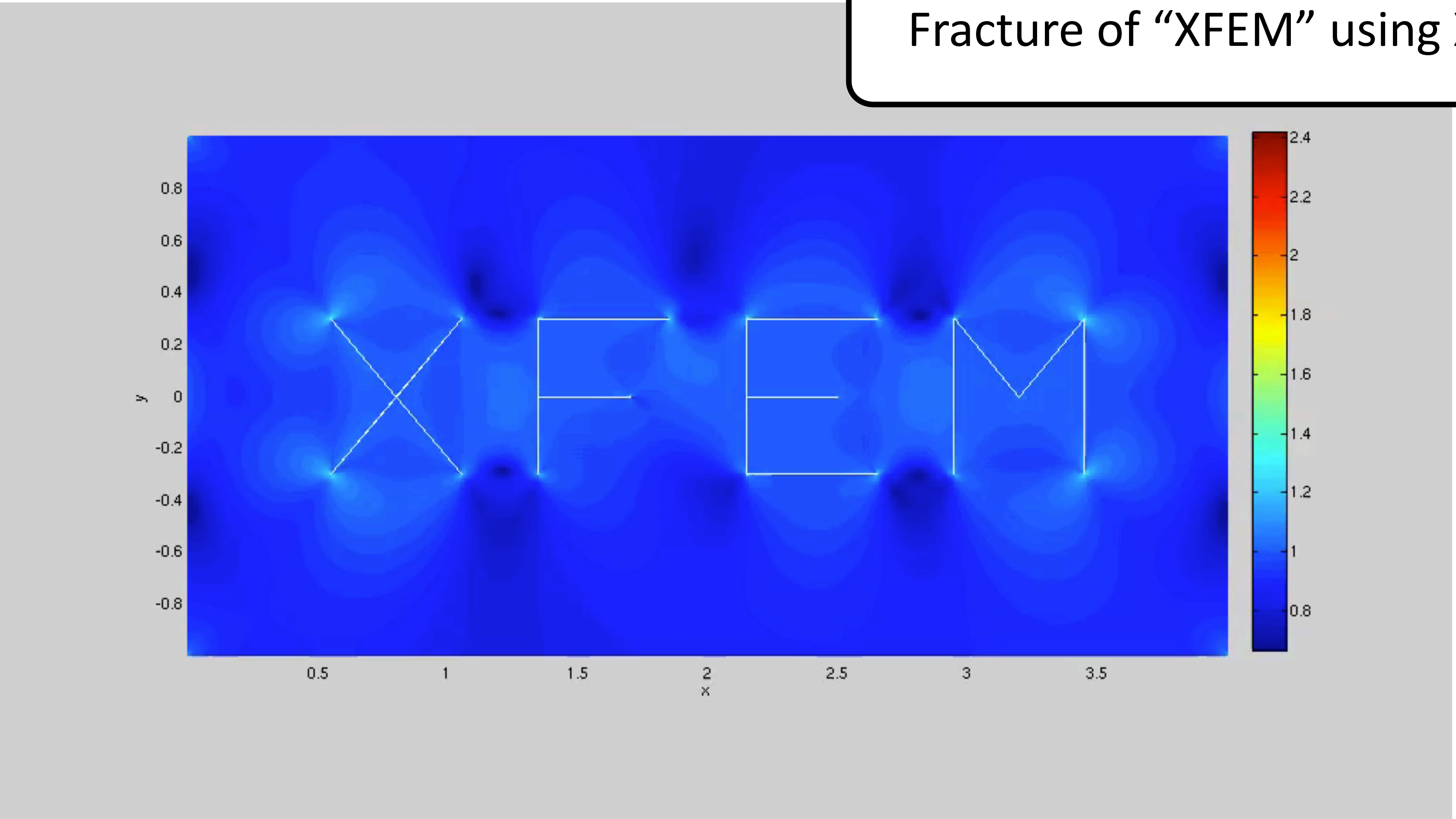


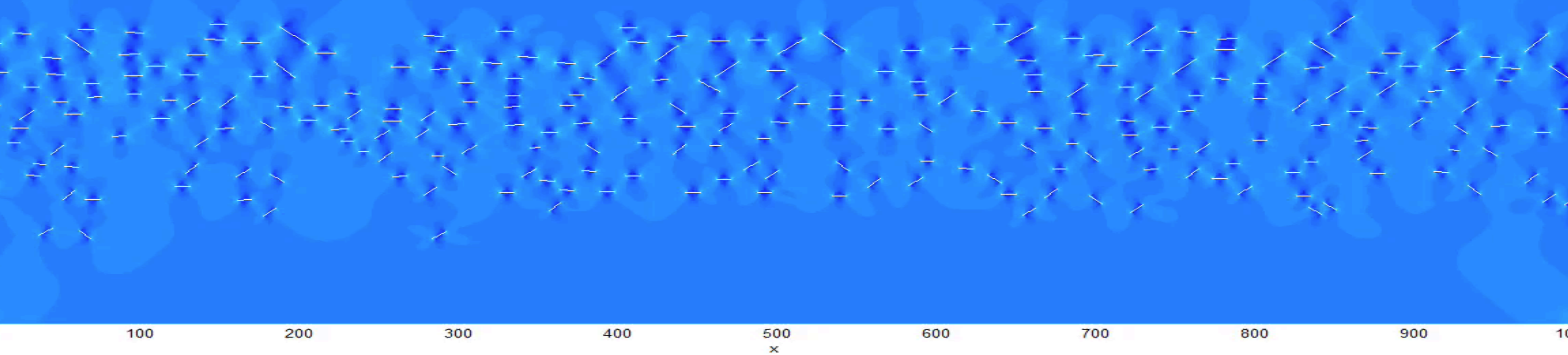
Discretization: XFEM

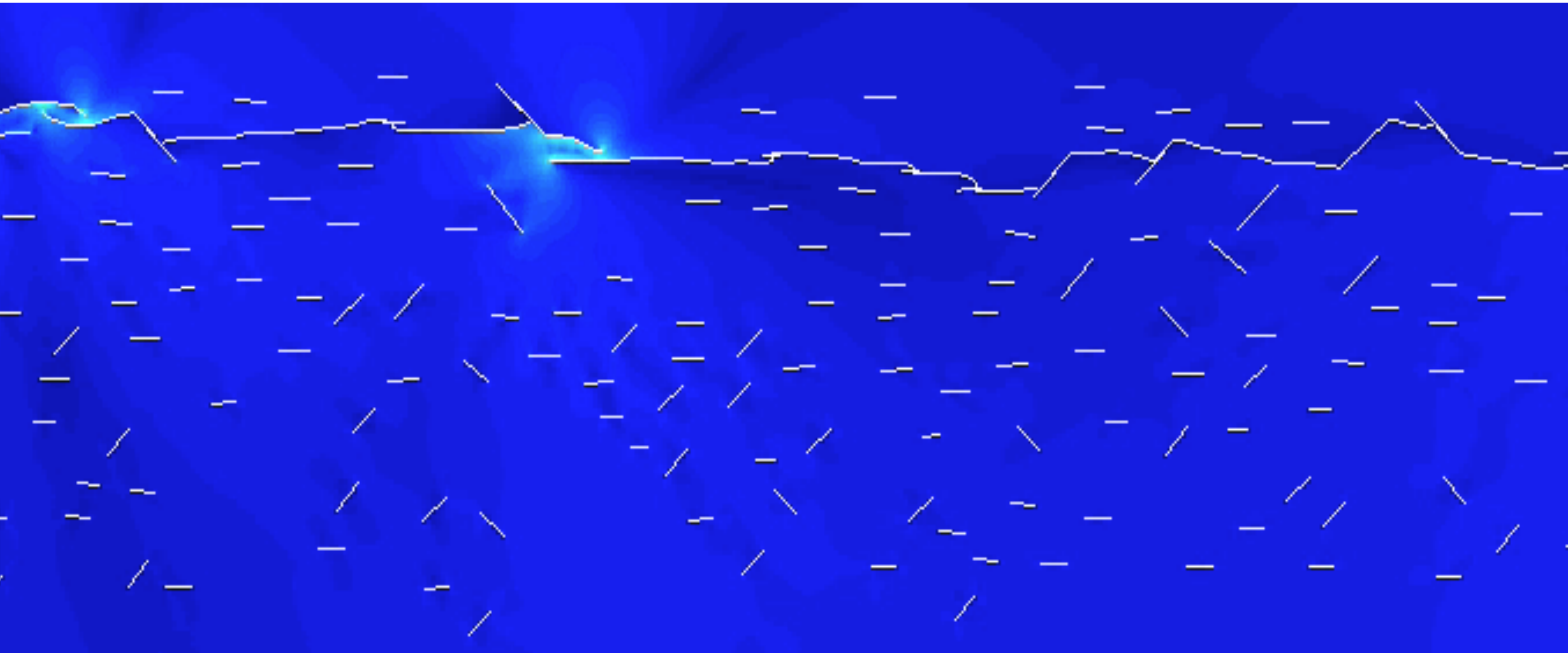
Extended Finite Element Method (XFEM)

- Introduced by Ted Belytschko (1999) for elastic problems

Fracture of "XFEM" using XFEM




100
200
300
400
500
600
700
800
900
x

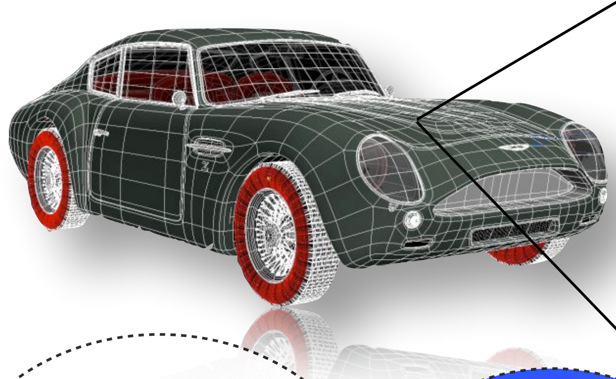


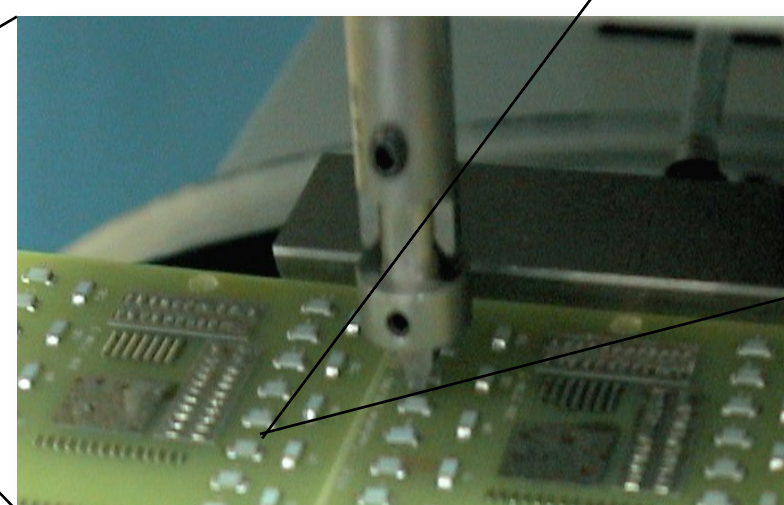
Solder joint durability - role of Pb

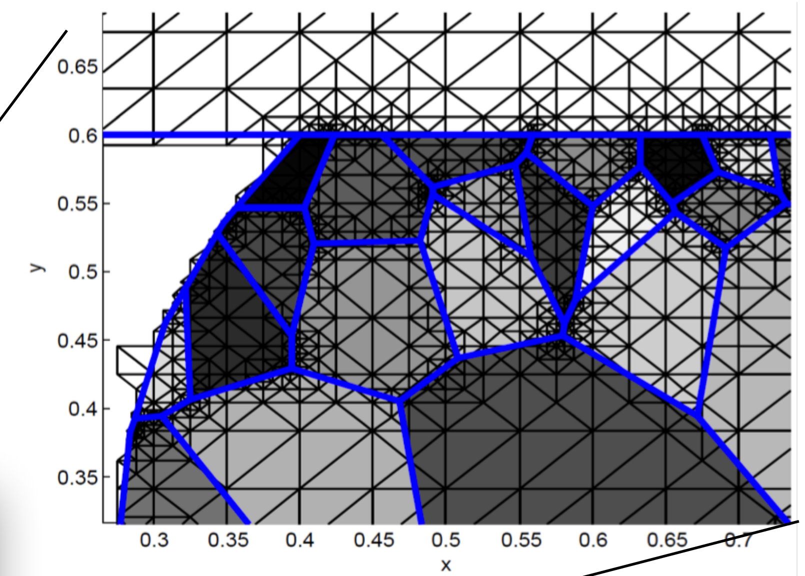
Challenges

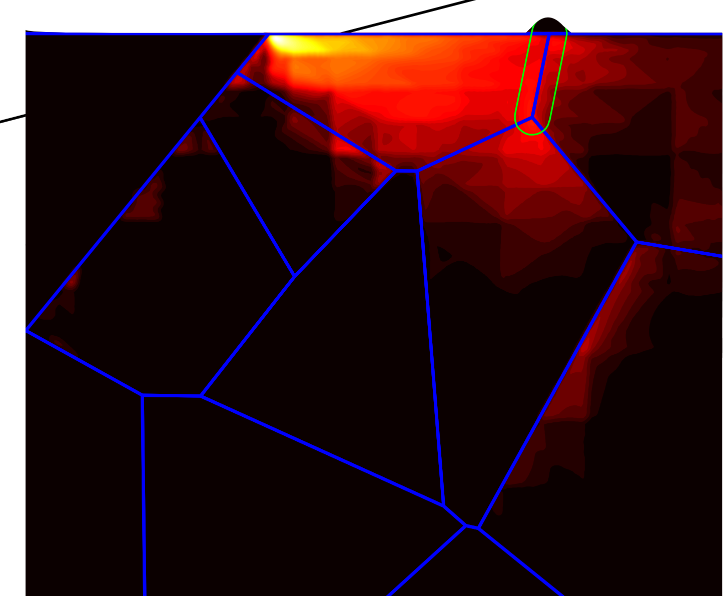
- microstructure/meshing - statistical variability
- robustness -> preconditioning
  - maintain accuracy

BOSCH









0.1mm

Advanced discretisation

Model reduction

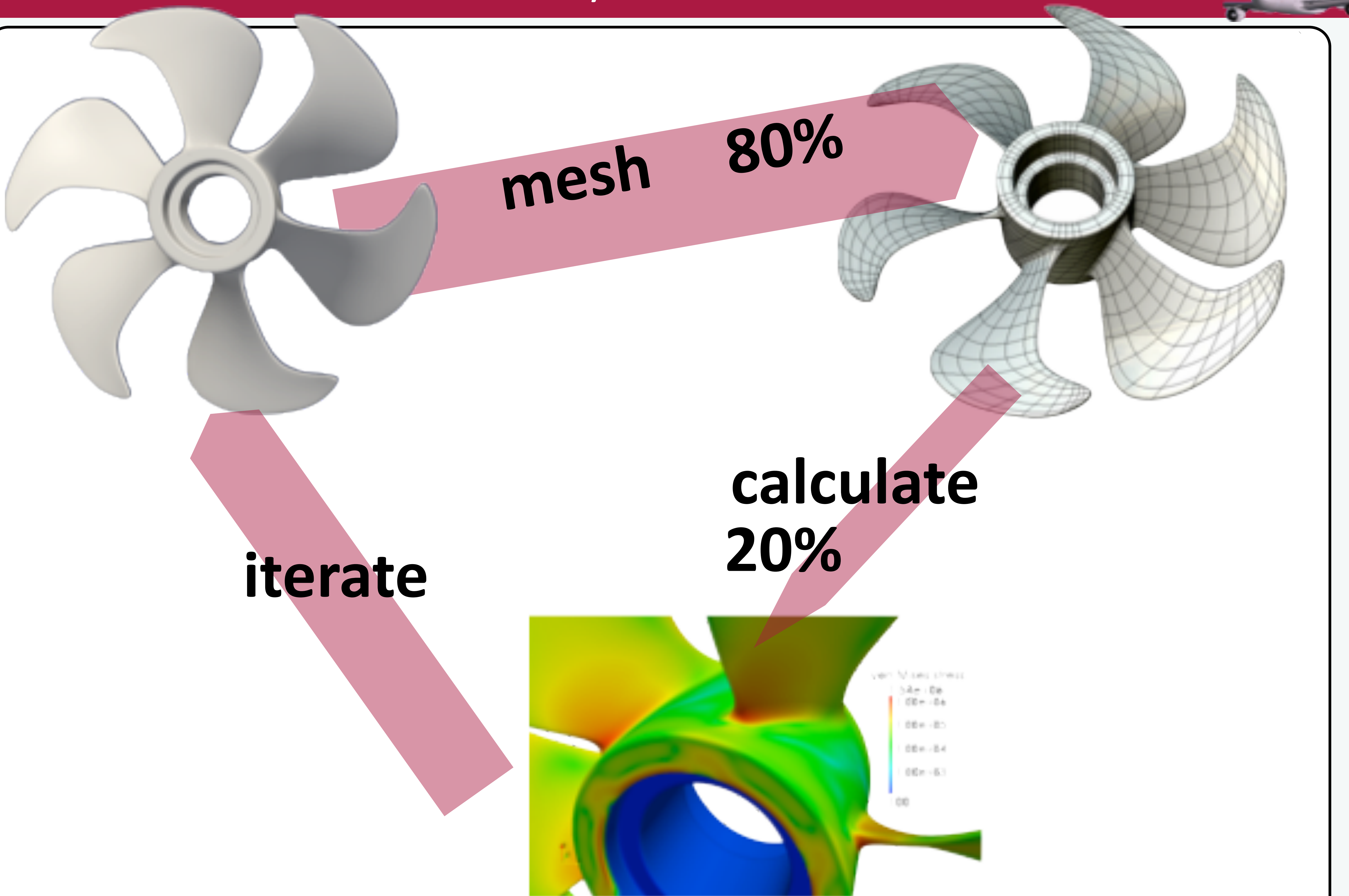
Computational time?

Conclusions : (1) microstructures play a determining role on thermo-mechanical fatigue life; (2) Pb increases the life span (of the solder)

thesis Menk

Industrial applications of isogeometric analysis (IGA)

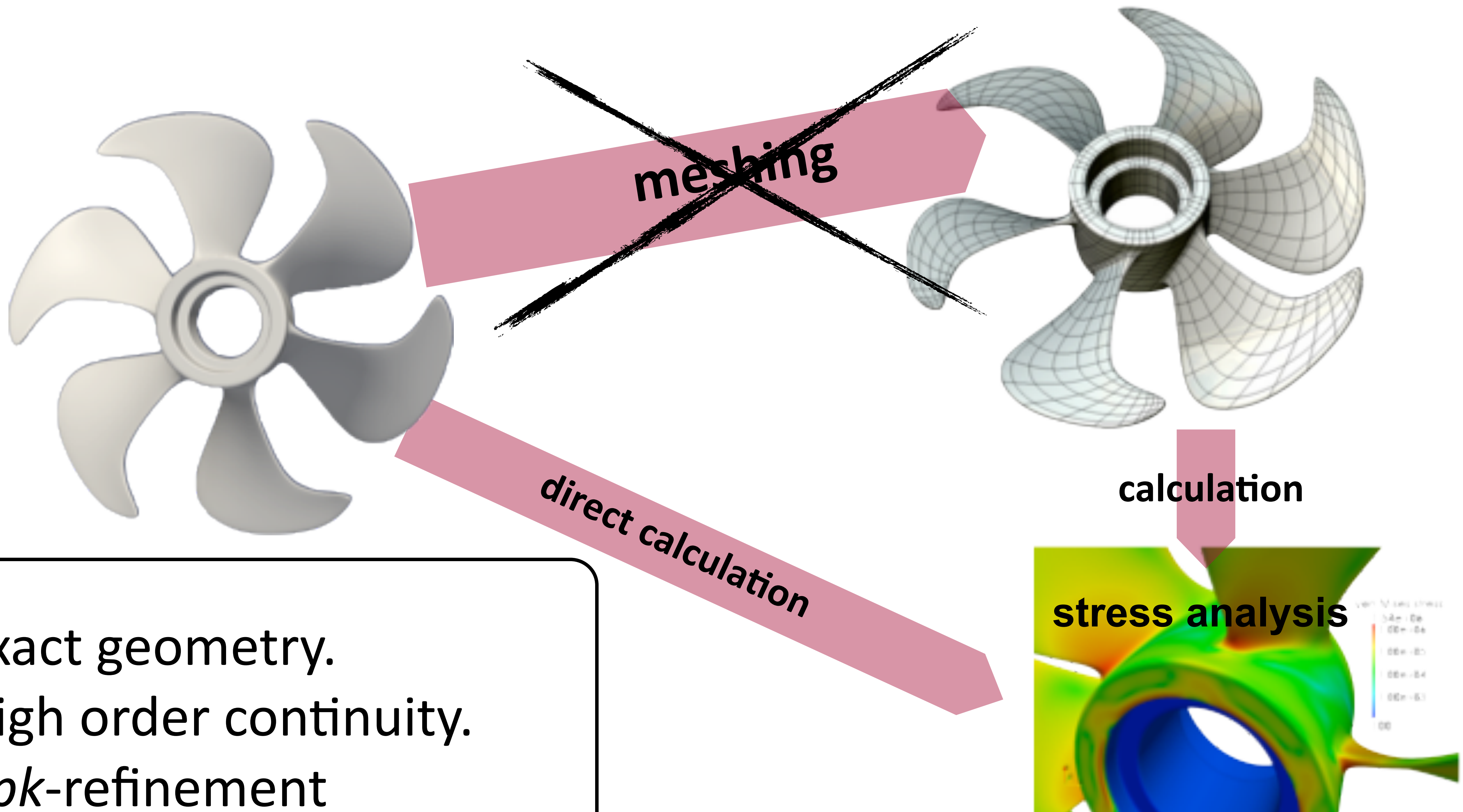
CAD to Analysis



vM stress distribution

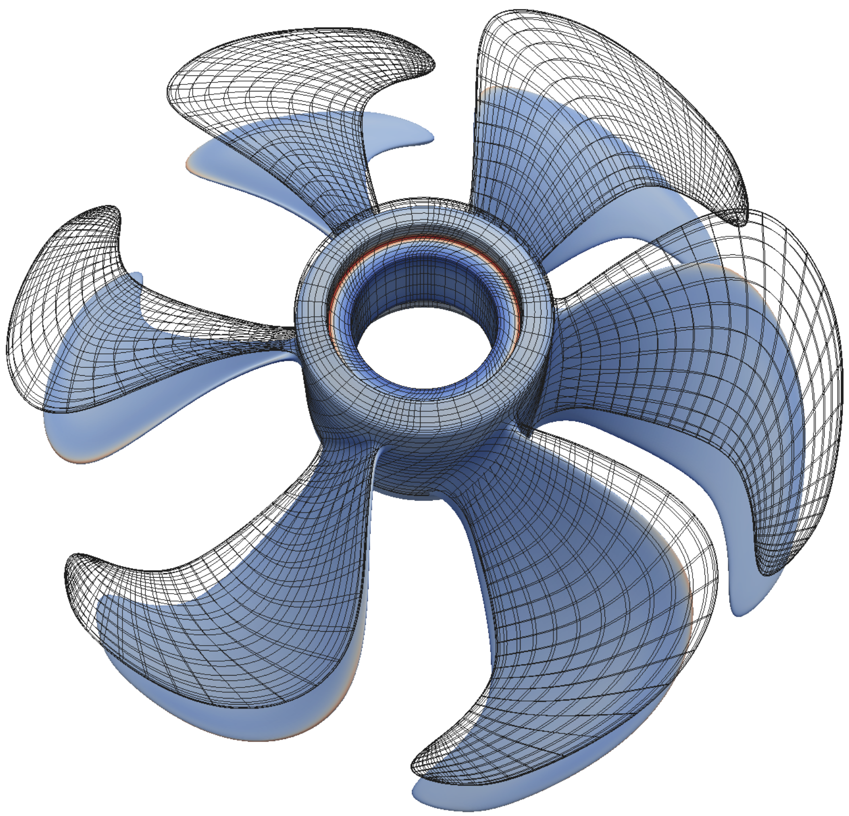
Isogeometric analysis (with BEM)

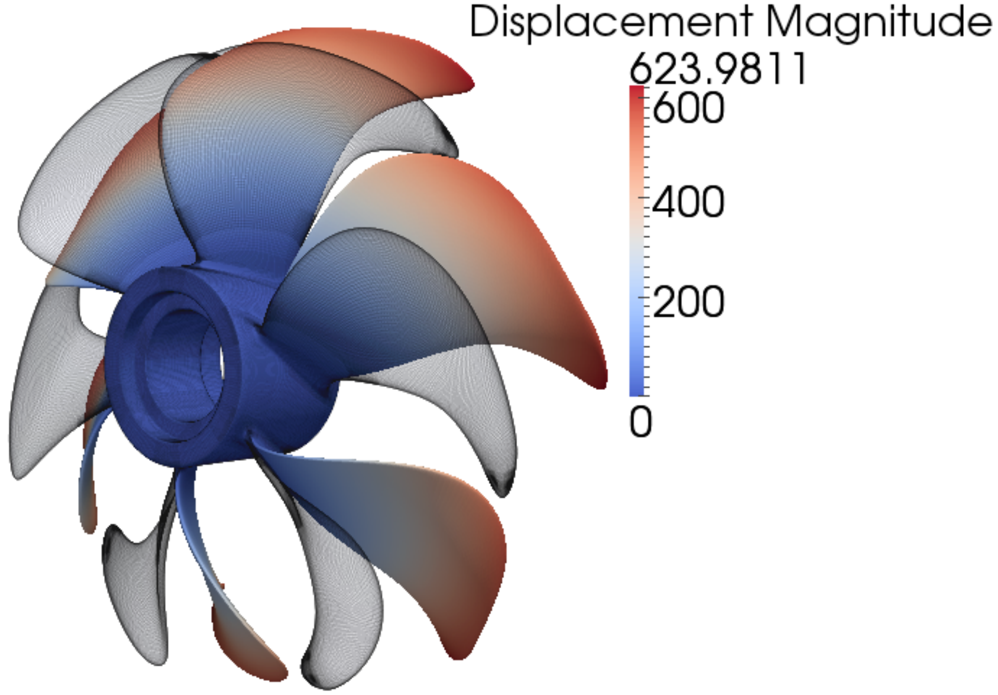
Approximate the unknown fields with the same basis functions (NURBS, T-splines …) as that used to generate the CAD model

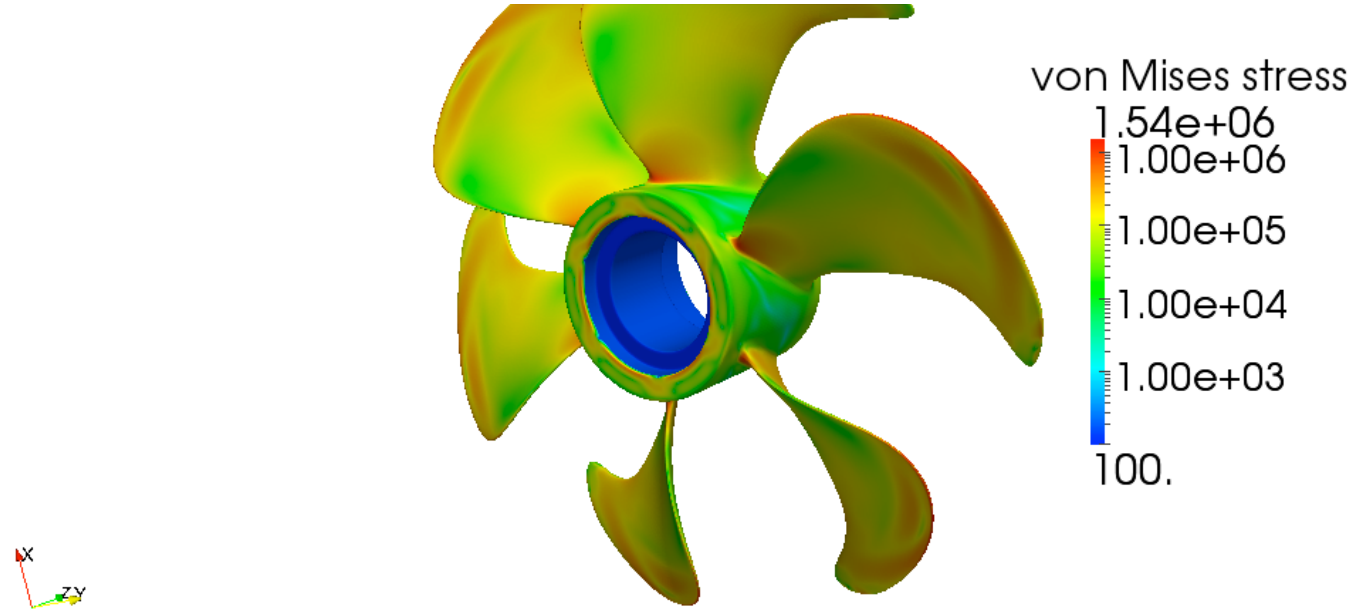


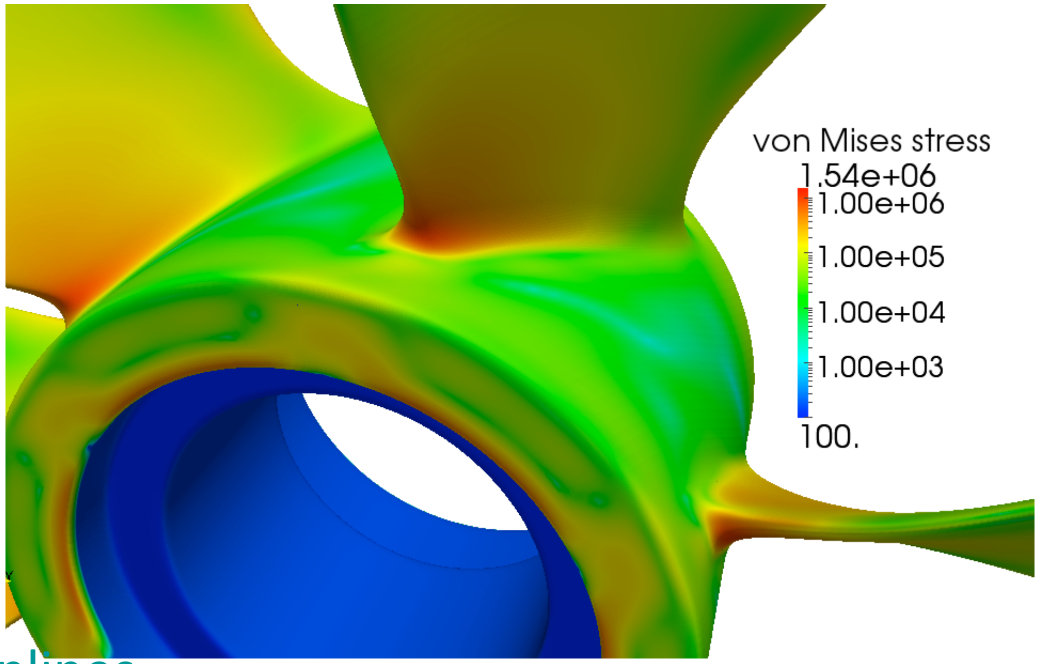
- Exact geometry.
- High order continuity.
- *hpk*-refinement

Propeller: NURBS would require several patches - single patch T-splines









Isogeometric boundary element analysis using unstructured T-splines
MA Scott, RN Simpson, JA Evans, S Lipton, SPA Bordas, TJR Hughes, TW Sederberg
CMAME, 2013. http://orbilu.uni.lu/handle/10993/11850

Shape and topology optimisation

Challenges for "conventional methods"

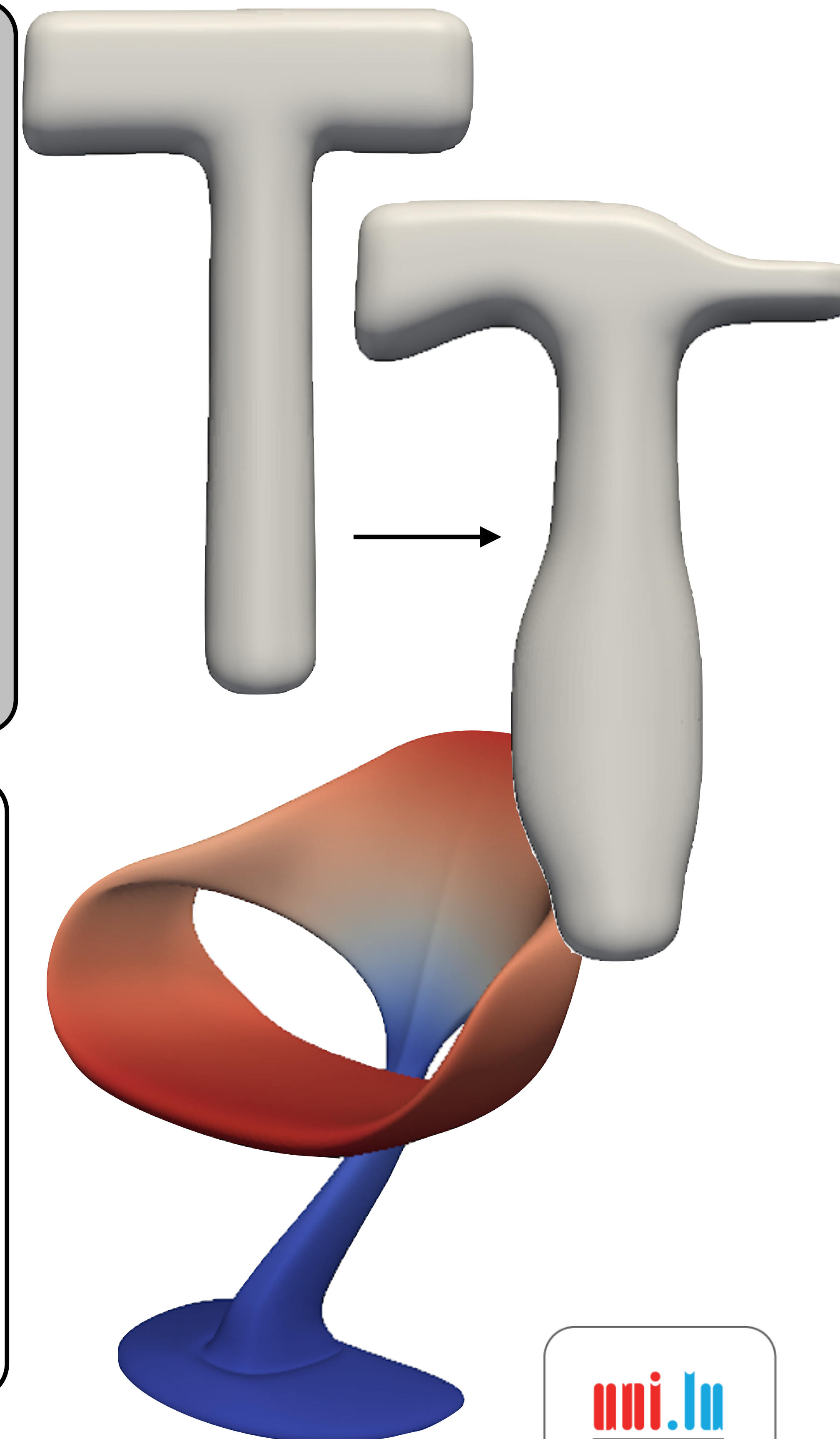
- Inverse problem - ill posed
- Choice of the approximation space for the boundary and the field approximation
- Evolving boundary (shape)
- Manual Redesign of the Topology: Smoothing of the "optimised" shape

Methods

- Isogeometric
- Boundary Elements
- Geometry-independent field approximation

Results

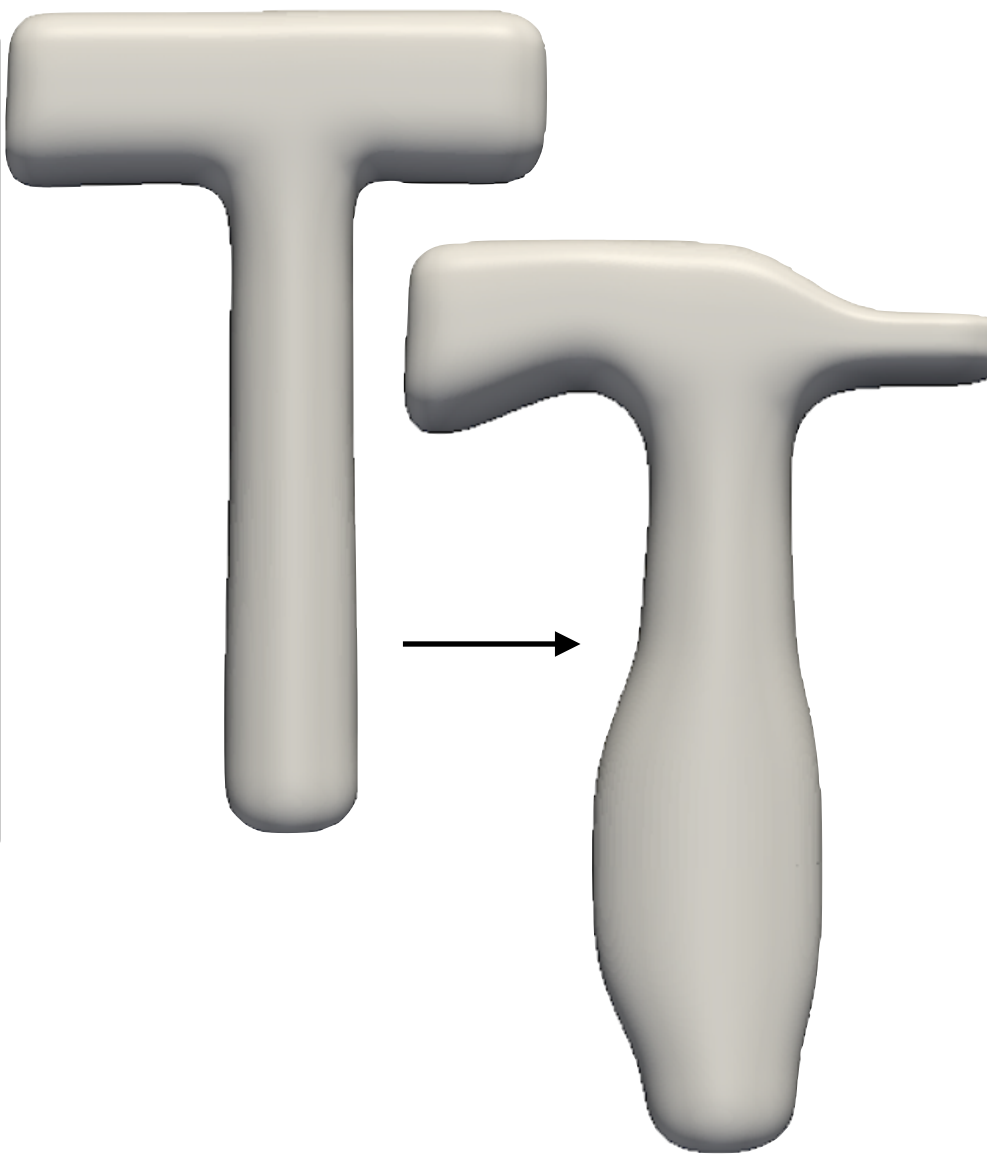
- Shape optimisation without meshing

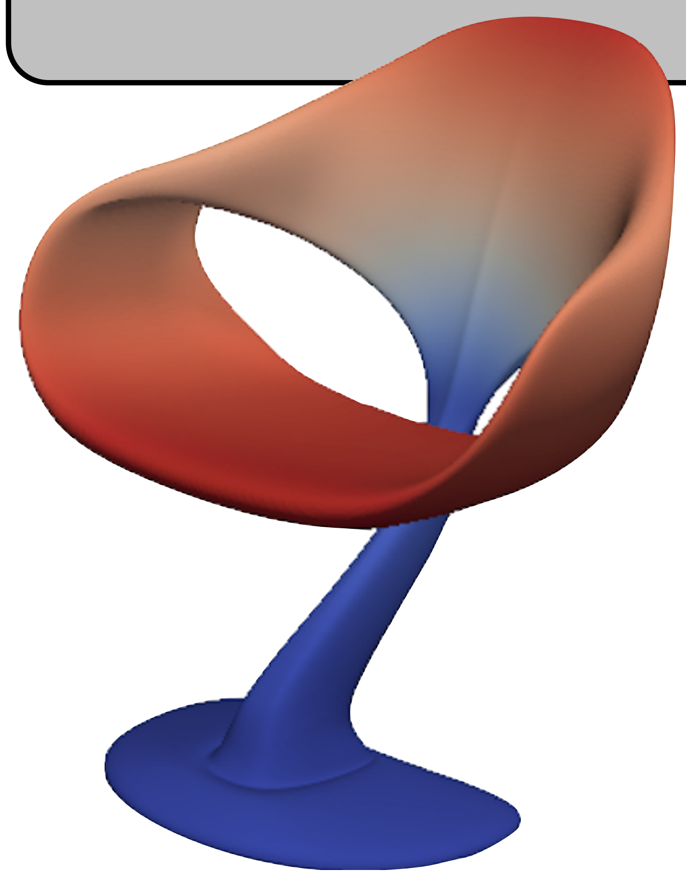


Shape and topology optimisation

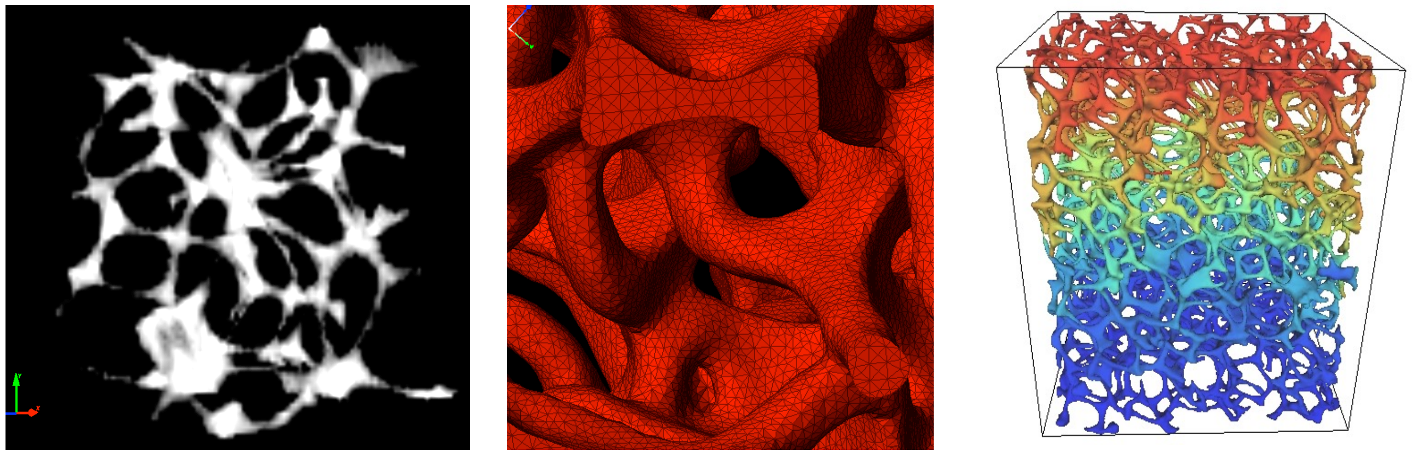
Possible new approach

- start from an initial CAD
- use IGA to represent the surface
- optimise
- the CAD is still available and the piece can be displayed and reworked if necessary (no mesh).

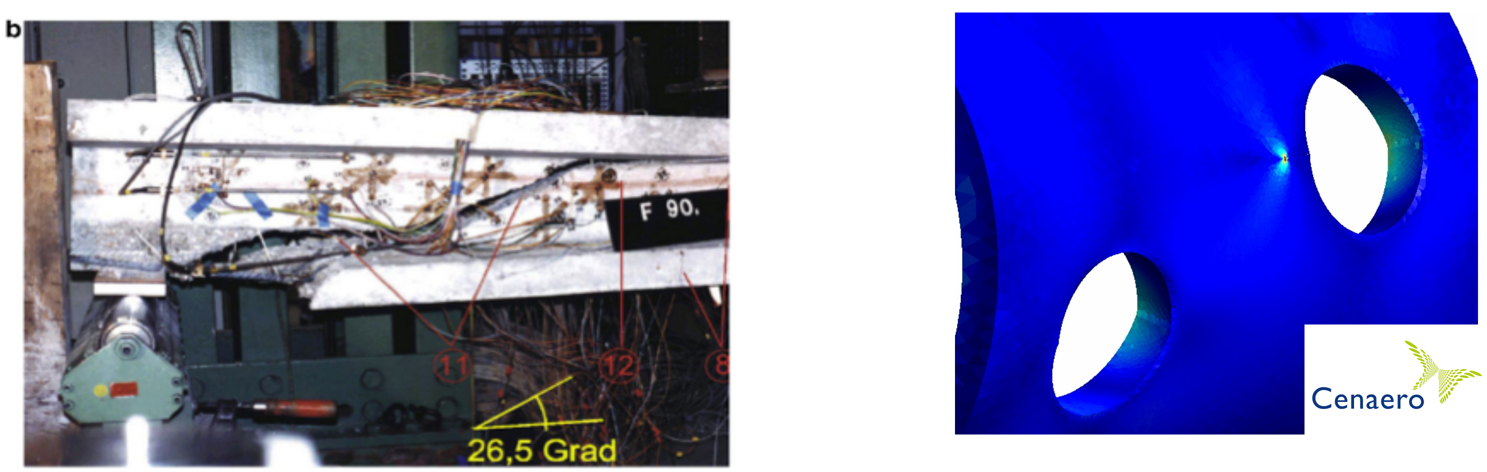




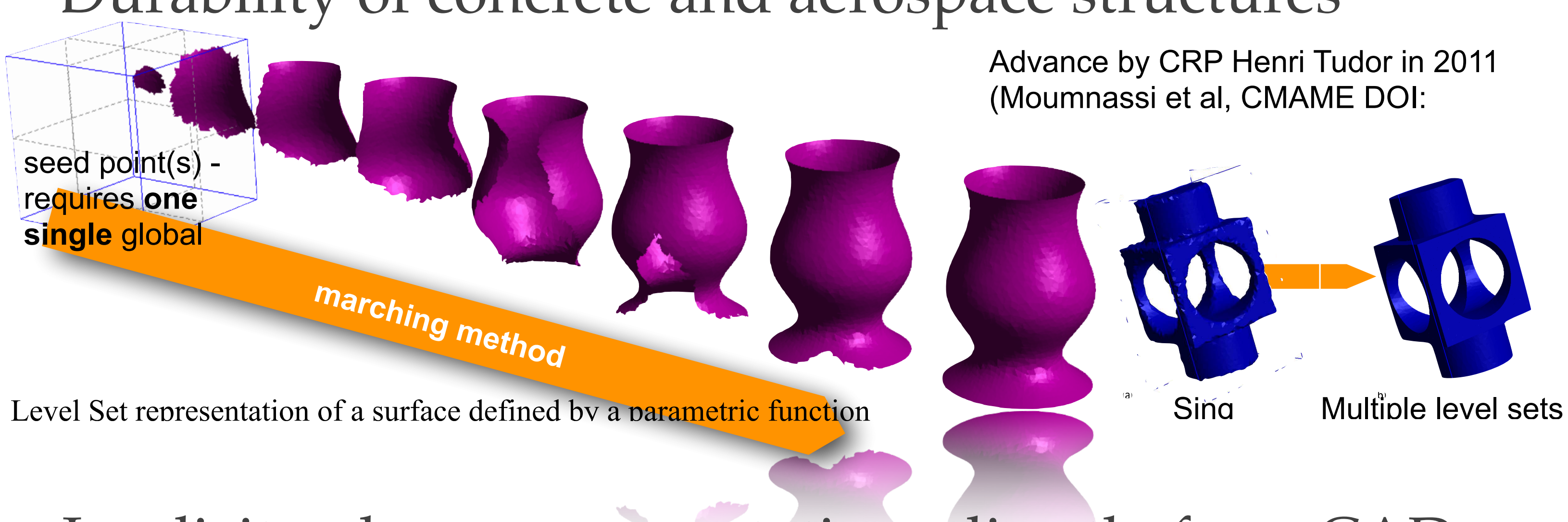
Other applications



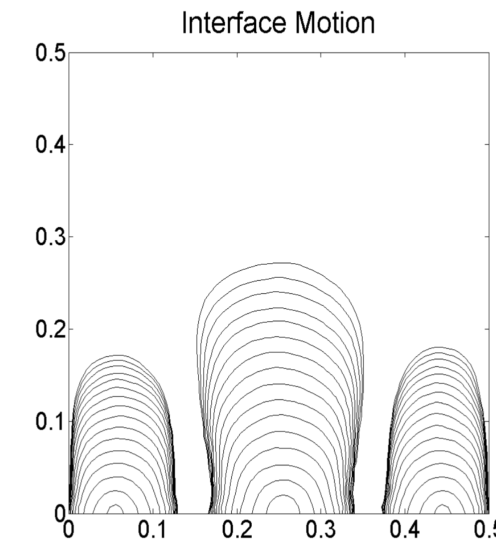
Microstructurally faithful material modeling

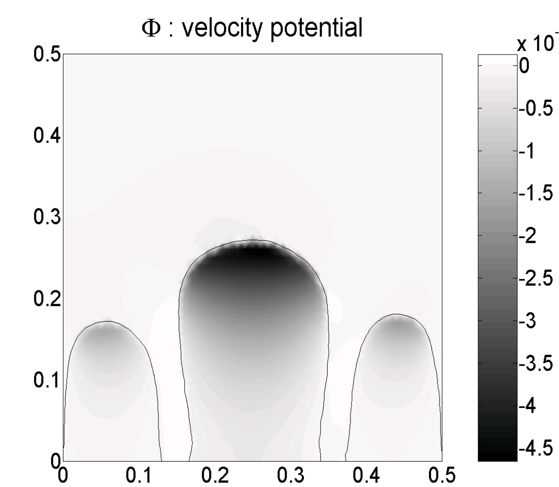


Durability of concrete and aerospace structures



Implicit volume representations directly from CAD

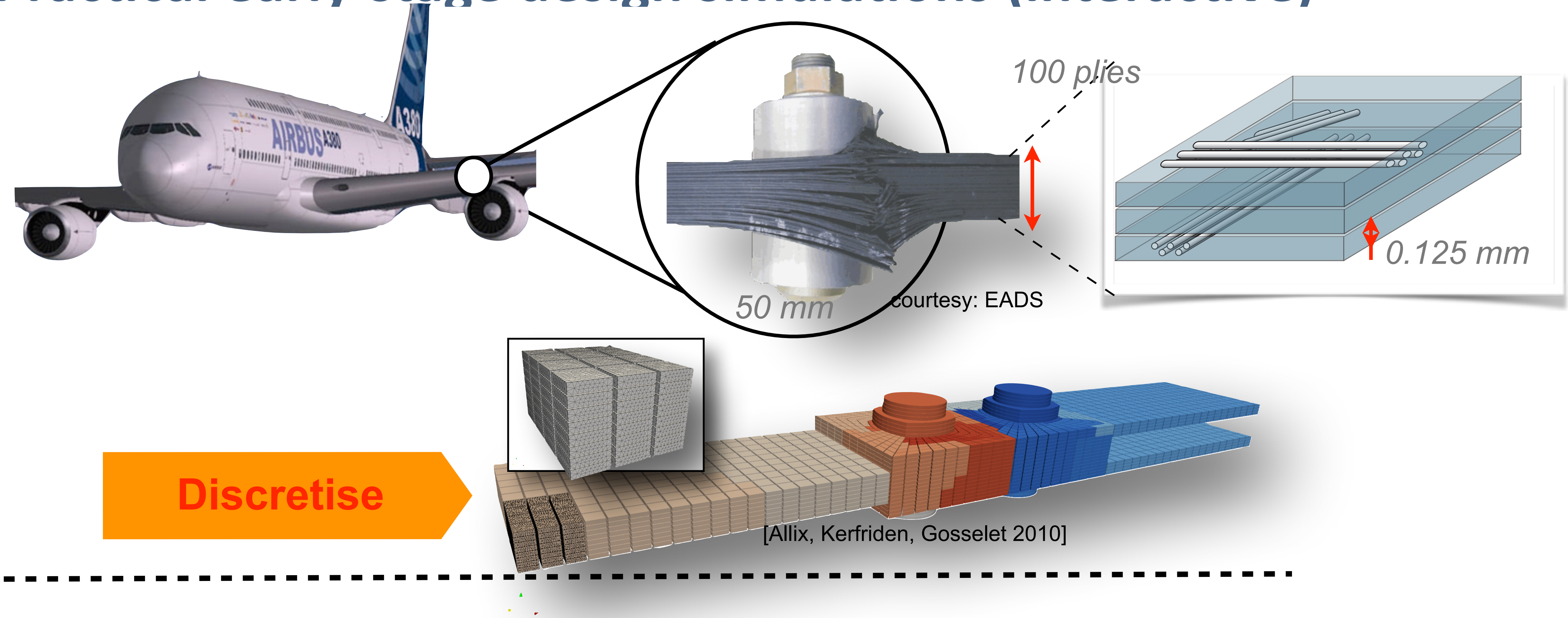




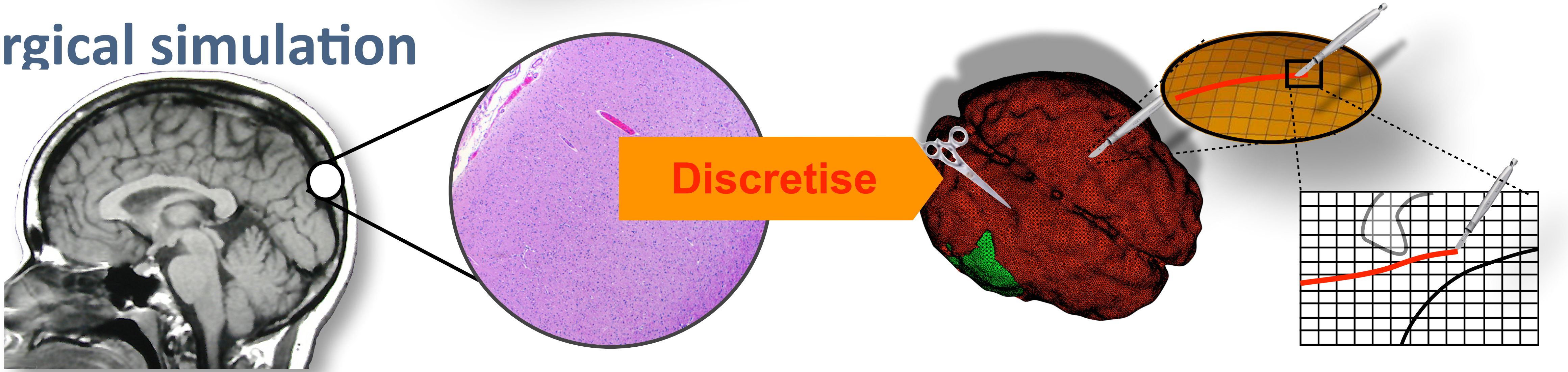
Biofilm growth

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

Surgical simulation

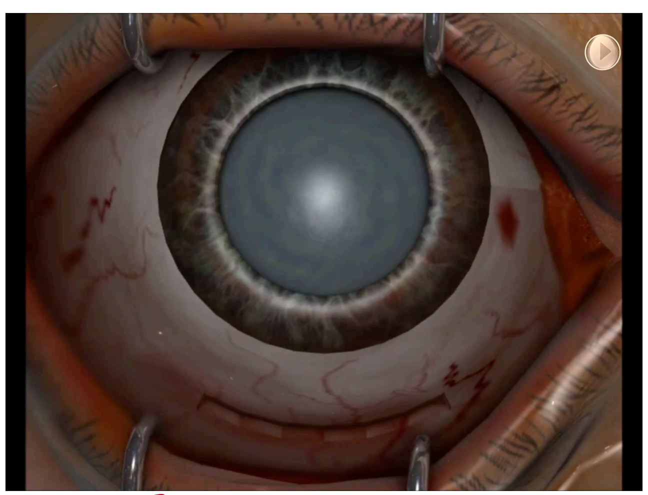
RealTcut

erc

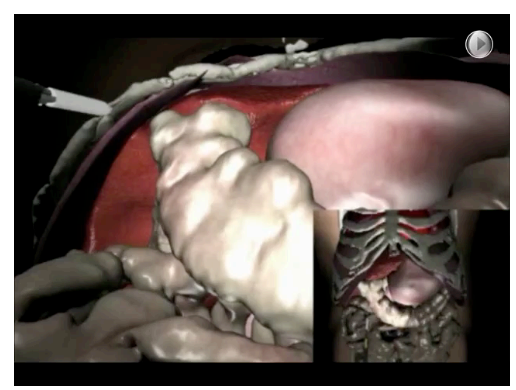
Precision

Learning → Planning → Assistance

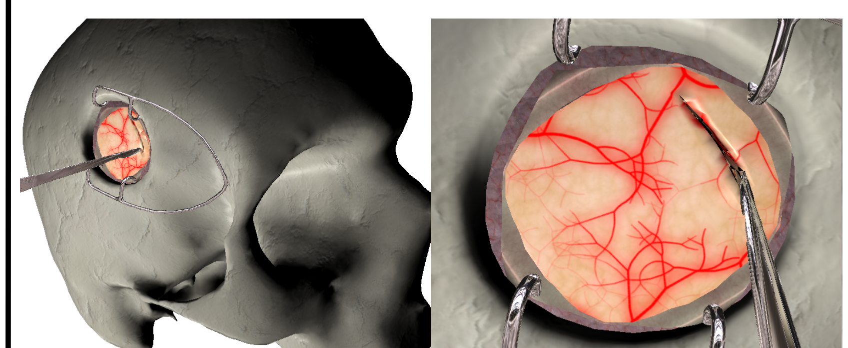
Cataract Surgery



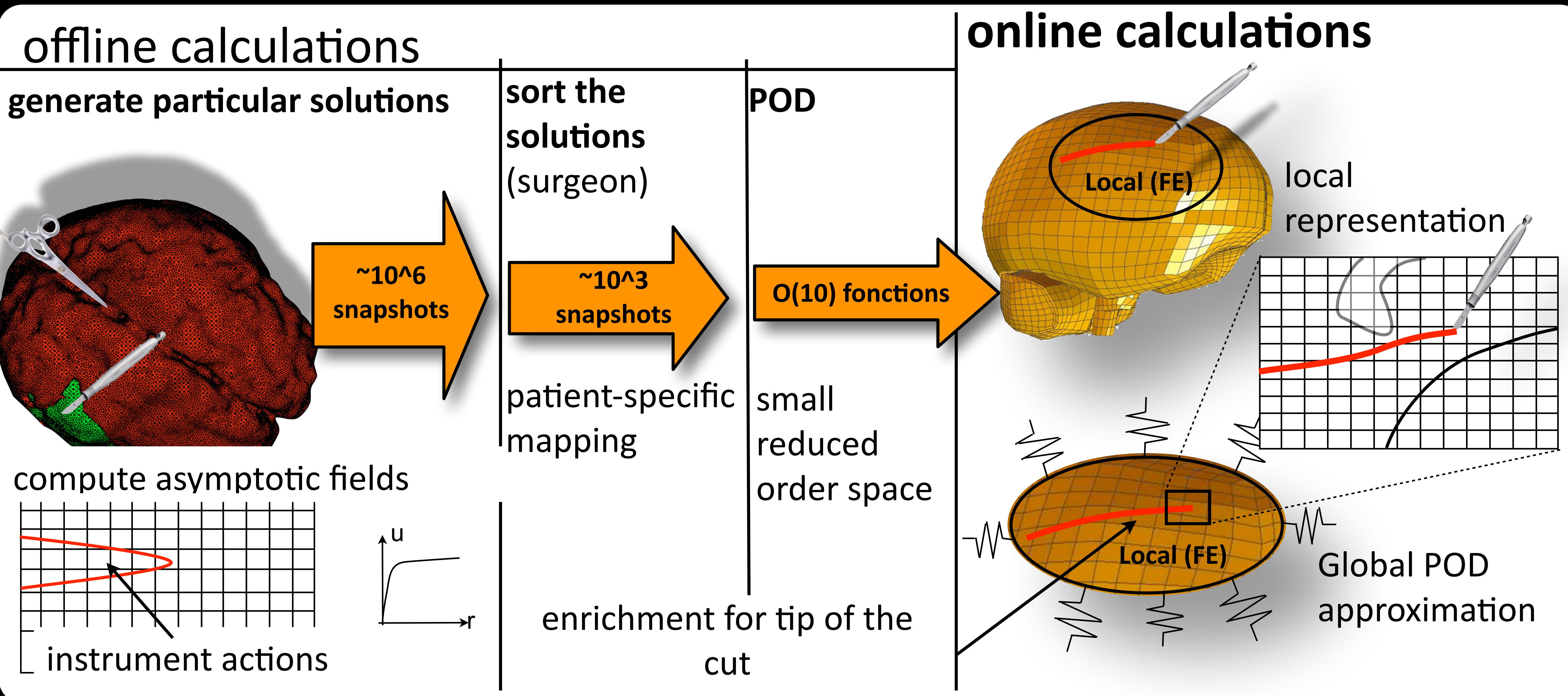
Abdominal minimally invasive surgery simulation (Inria, Shacra)



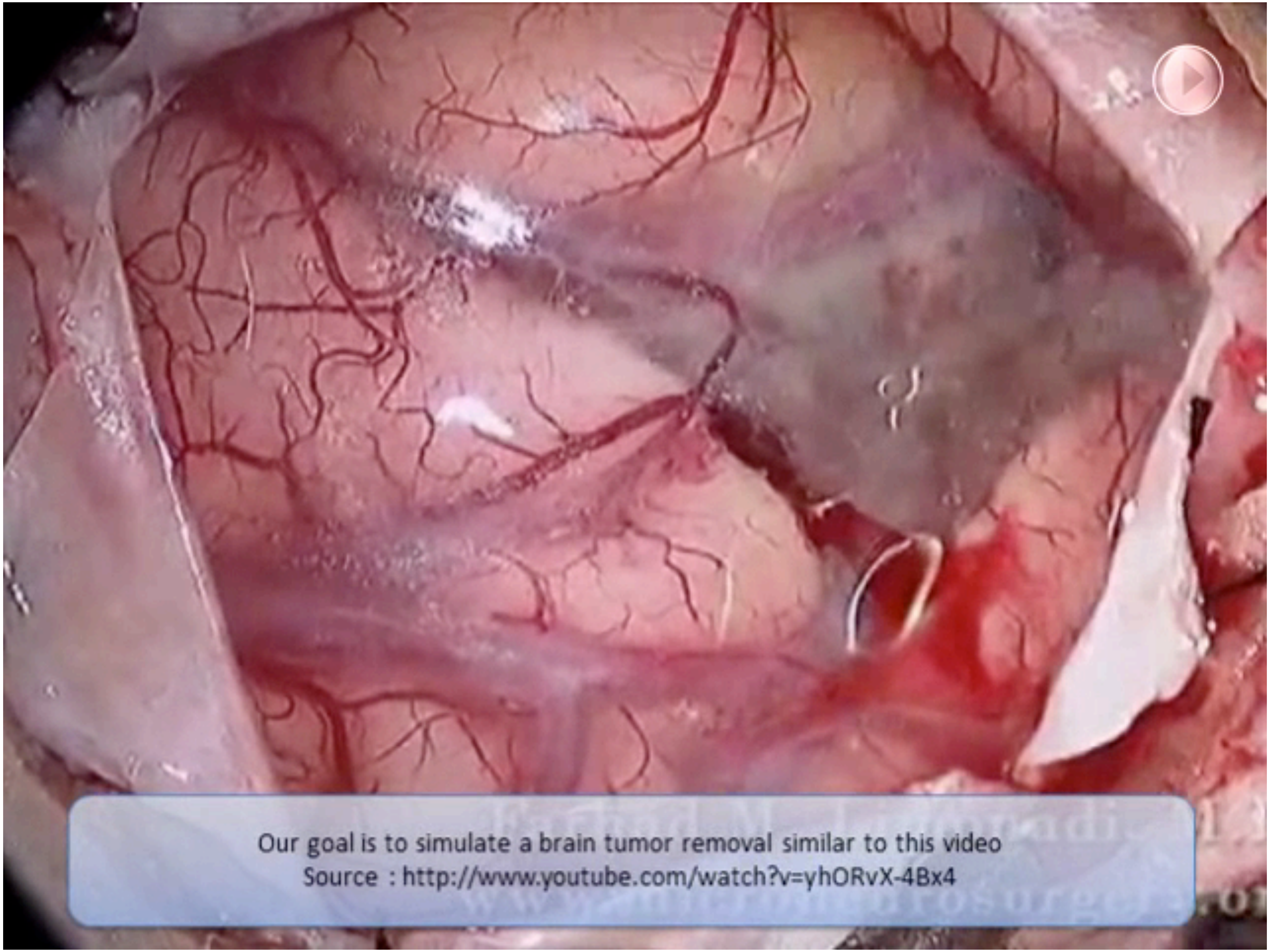
First implicit, interactive method for cutting with contact



[Courtecuisse et al., MICCAI, 2013 and Medical Image Analysis, 2014]


offline calculations
online calculations
generate particular solutions
sort the solutions (surgeon)
POD
~10^6 snapshots
~10^3 snapshots
O(10) fonctions
Local (FE)
local representation
patient-specific mapping
small reduced order space
compute asymptotic fields
u
r
instrument actions
enrichment for tip of the cut
Local (FE)
Global POD approximation

… not exactly brain surgery



Courtecuisse, Kerfriden, Bordas… Medical Image Analysis 2014

Outlook

- **Understanding and optimisation of fracture of heterogeneous materials - including human tissue :)**
  - multi-scale methods are being developed
  - these methods are expensive
  - model selection remains an open problem
  - variability of the material properties exacerbate these difficulties
  - taking into account realistic situations remains elusive
  - coupling with sensing systems may be the future

... twinning

real-time simulations could help engineers gain insight into complex non-intuitive phenomena by allowing to probe, quickly, the parameter space and design space

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merci de votre attention

Partners and Funding

Gracias por su atención

Merci de votre attention

Thank you for your attention

Danke für Ihre Aufmerksamkeit

Gracie per la vostra attenzione

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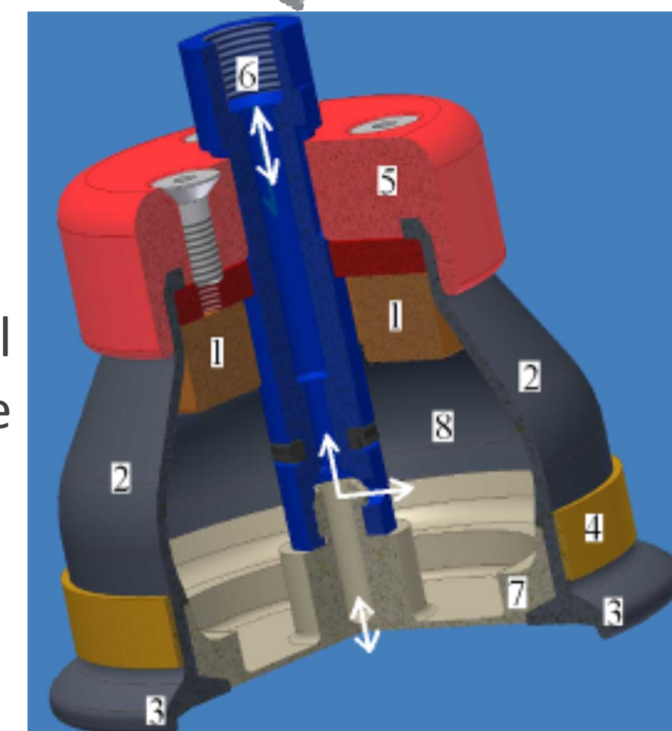
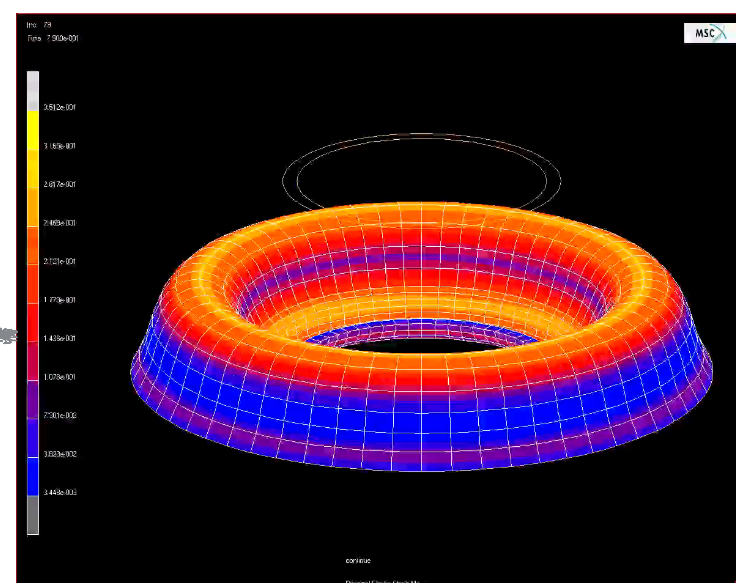
product-specific

Increase product durability?

Virtual model
of the device



Virtual testing & Simulation



Analysis
of the results

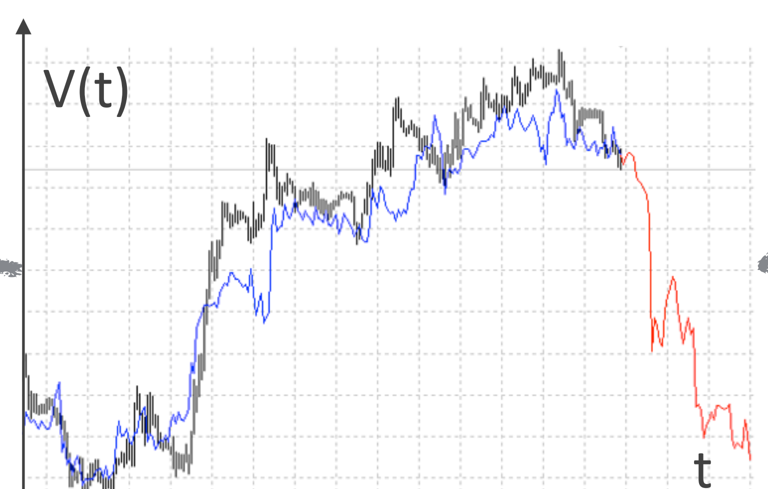
market-specific

Buy or sell?

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

Mathematical model + initial conditions

Real-time future option pricing



Identify behaviour

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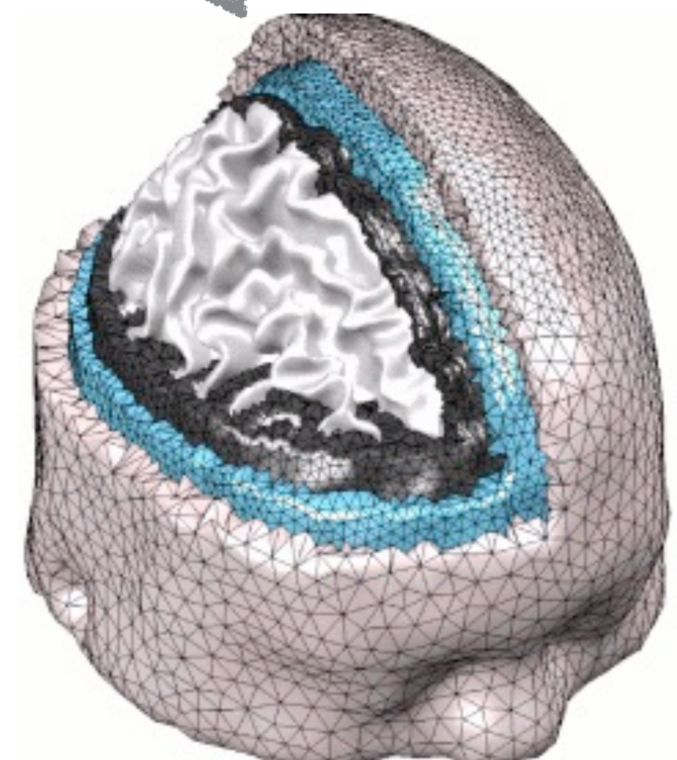
PRIFYSGOL CAERDYDD

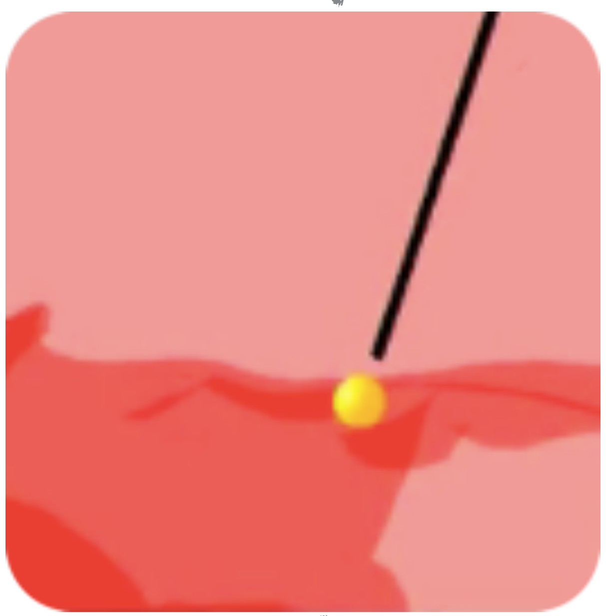
patient-specific

Devise effective deep brain stimulation

- reach the target area
- maintain contact with the electrode

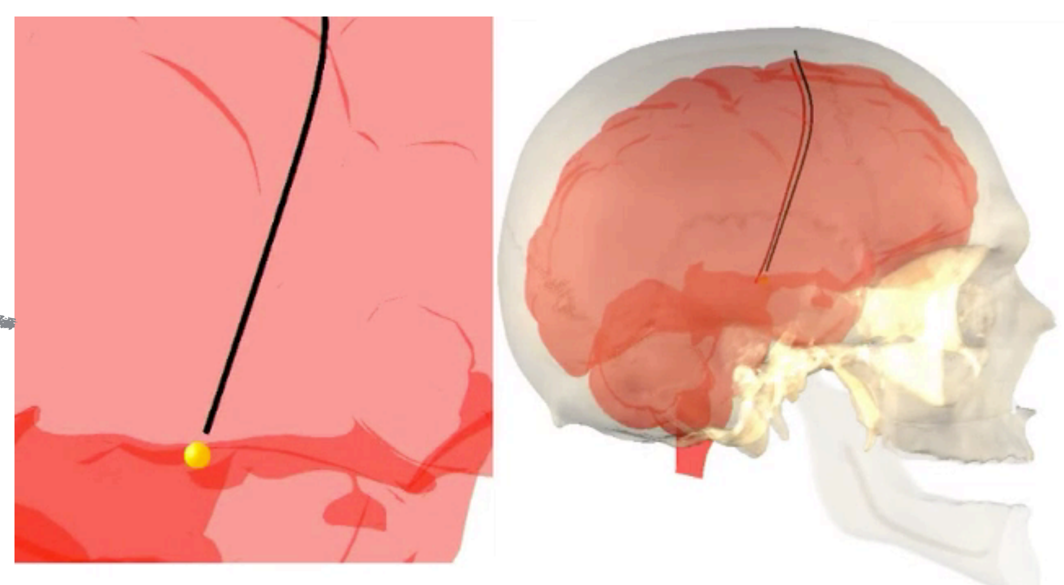


Model of the brain material



Electrode separates from target

Predict electrode behaviour



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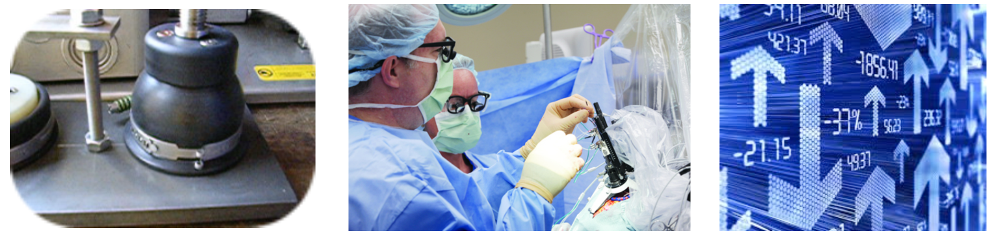

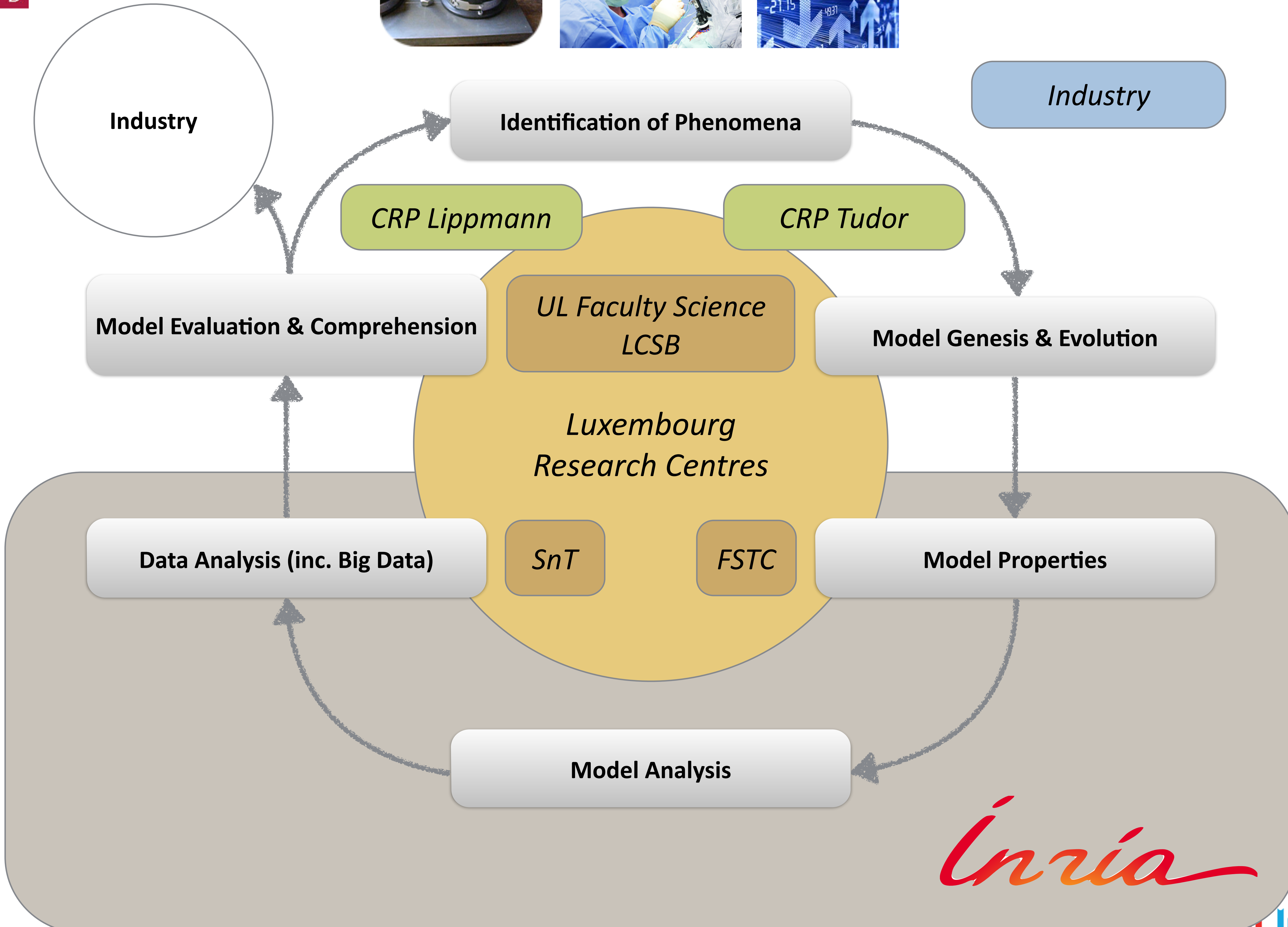
Industry
Identification of Phenomena
Industry
CRP Lippmann
CRP Tudor
Model Evaluation & Comprehension
UL Faculty Science
LCSB
Model Genesis & Evolution
Luxembourg
Research Centres
Data Analysis (inc. Big Data)
SnT
FSTC
Model Properties
Model Analysis

Links to relevant publications

Acknowledgements

- The isogeometric BEM results were produced by Robert Simpson in collaboration with ICES in Texas, whose contribution is gratefully acknowledged.