Reduced order modelling: towards tractable computational homogenisation schemes

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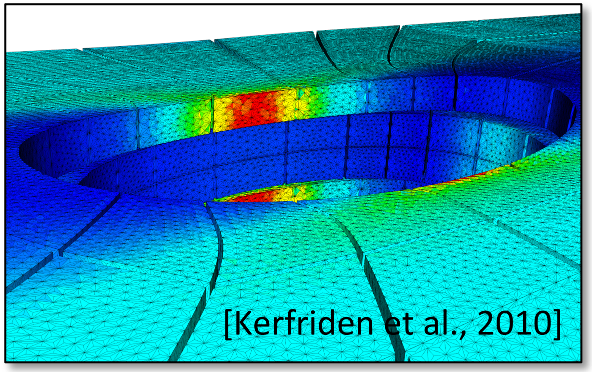
Team in Cardiff: main research topics

- Efficient numerical prediction of material and structural failure

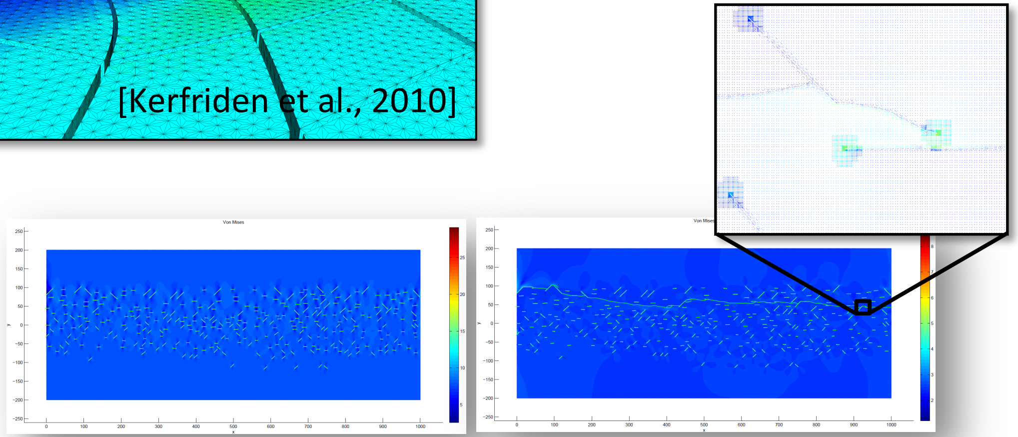
L. Beex

S.P.-A. Bordas

P. Kerfriden



[Kerfriden et al., 2010]

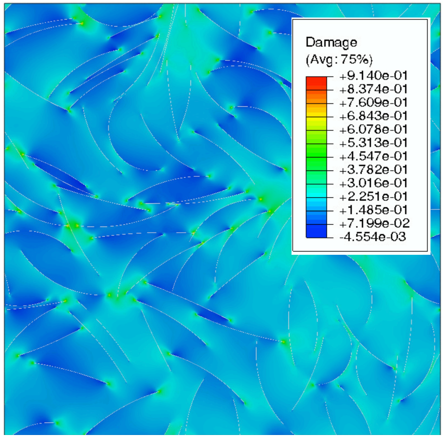


Initial crack distribution

Final fracture

[Sutula et al., 2013]

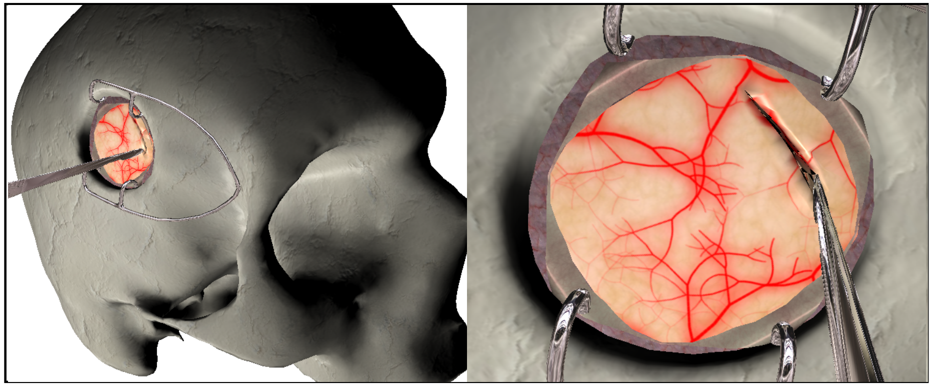
- Characterisation and optimisation of composites



[Silani et al., 2013]

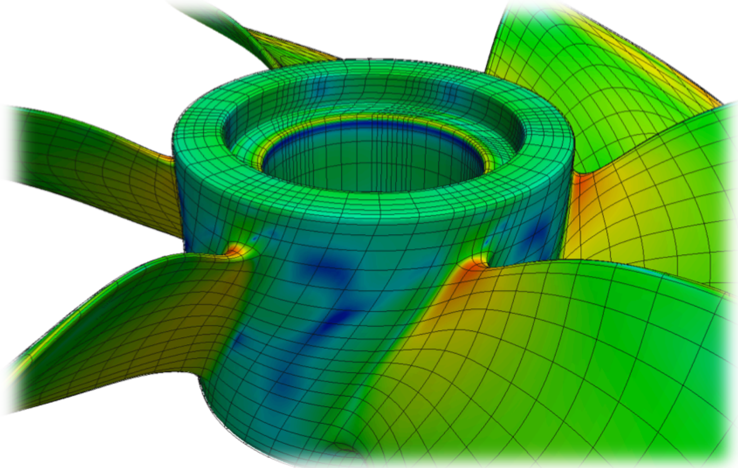
Team in Cardiff: main research topics

- Interactive simulations of biological structures

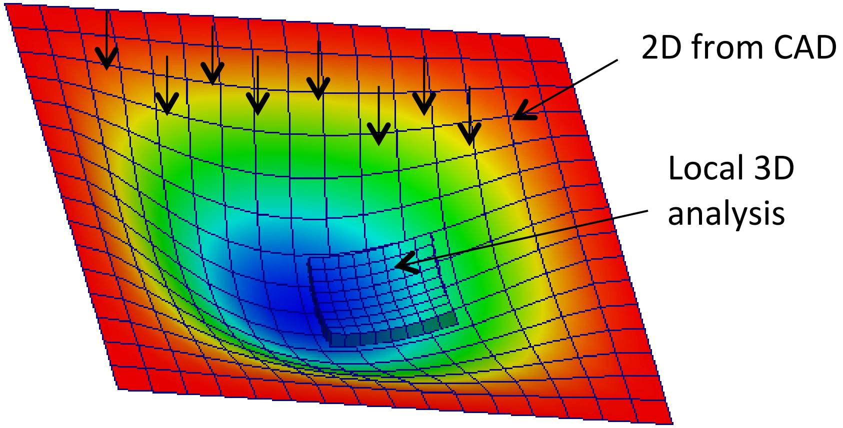


[Courtecuisse et al., 2013]

- Simplified Link between CAD/CT scans and analysis



[Scott et al., 2013]

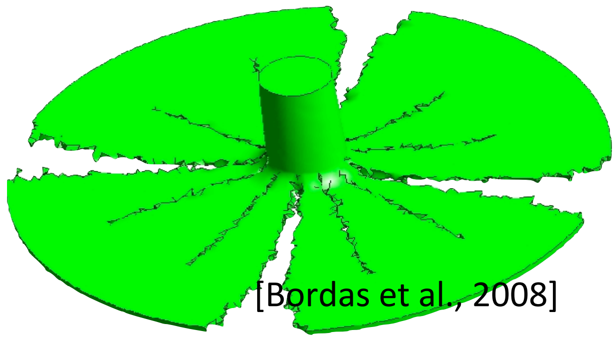


[Nguyen et al., 2013]

Toolkit 1: advanced discretisation methods

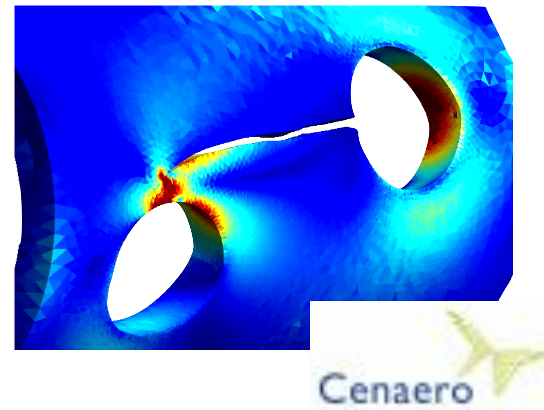
- Advanced discretization techniques for complex PDEs

  - XFEM/meshfree



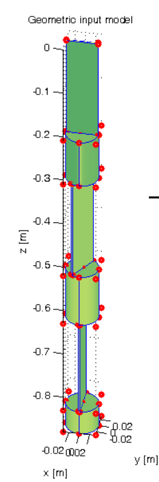
[Bordas et al., 2008]

Taylor bar problem
(dynamic fragmentation)

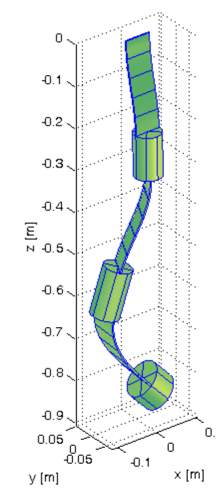


  - Isogemetric analysis

Model simplification (CAD)



IGA

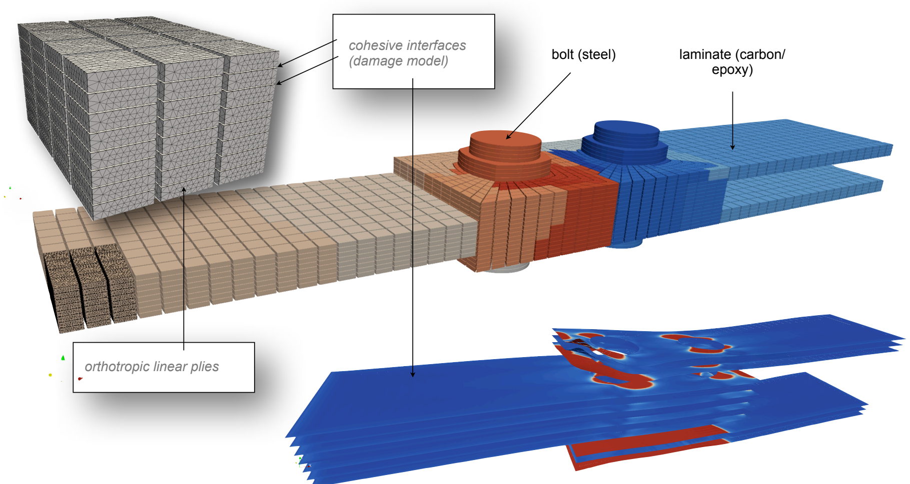


[Tornincasa et al., 2013]

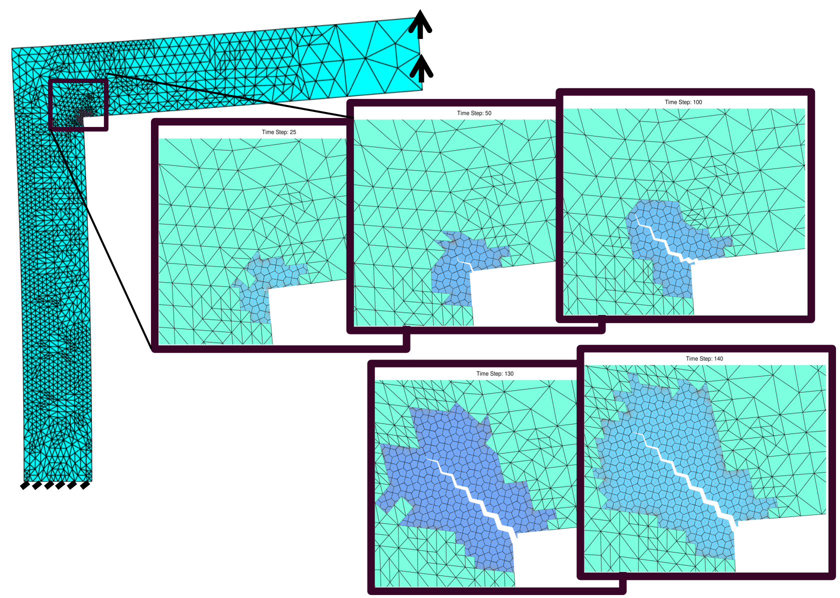
Toolkit 2: multilevel methods

- 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



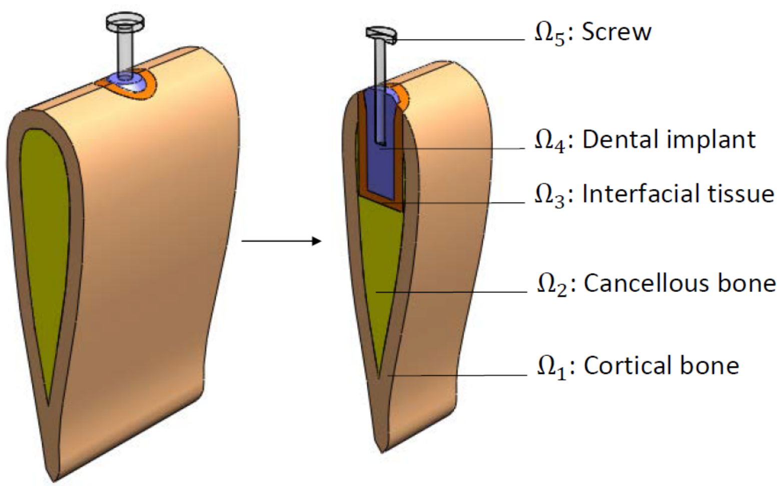
[Kerfriden et al., 2010]



[Akbari et al., 2013]

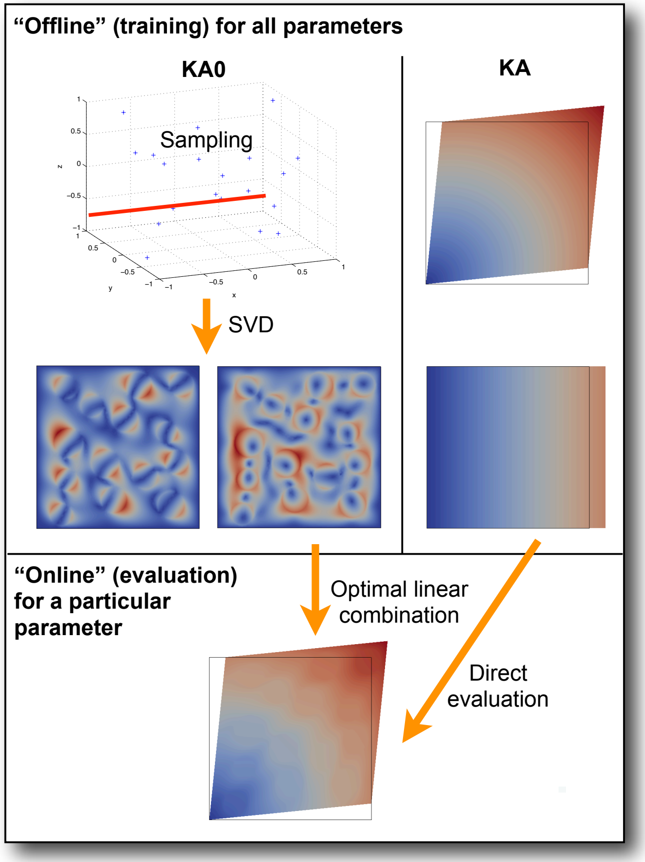
Toolkit 2: multilevel methods

- 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



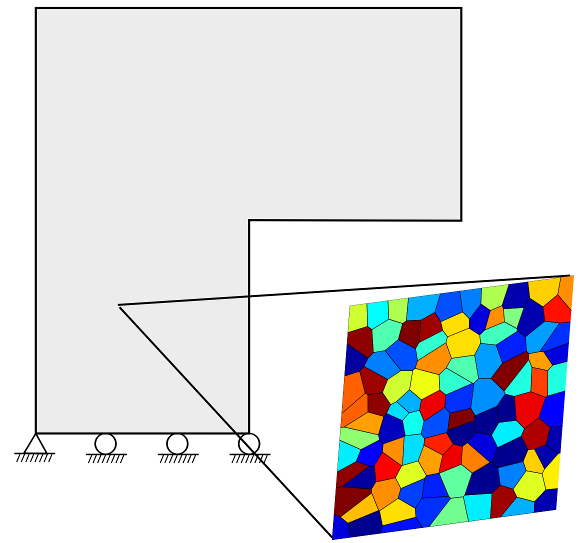
[Kerfriden et al., 2013]

- Introduction: computational homogenisation
- Virtual charts for parametrised homogenisation in linear elasticity
- Reduced order modelling in nonlinear homogenisation

Multiscale modelling

- Bottom-up view: **replace heterogeneous subscale model by an equivalent**, smoother, **model** at the scale where predictions are required (i.e. macroscopic scale)

- When is scale-bridging necessary?
  - Derive predictive macroscopic models that are difficult to obtain using phenomenological approaches
  - Optimise subscale properties to obtain better overall characteristics
  - Observations at microscale but approximations required away from region of interest to remain tractable



[Chen et al. 2011]

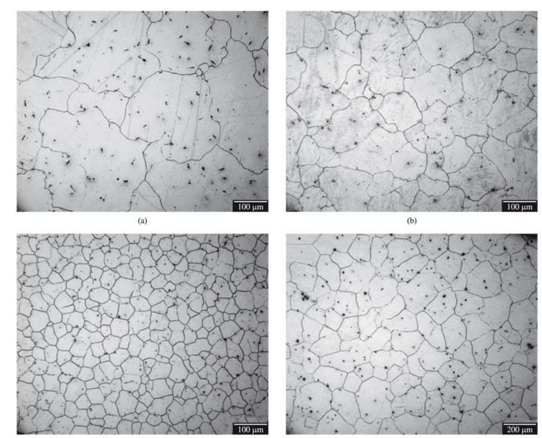
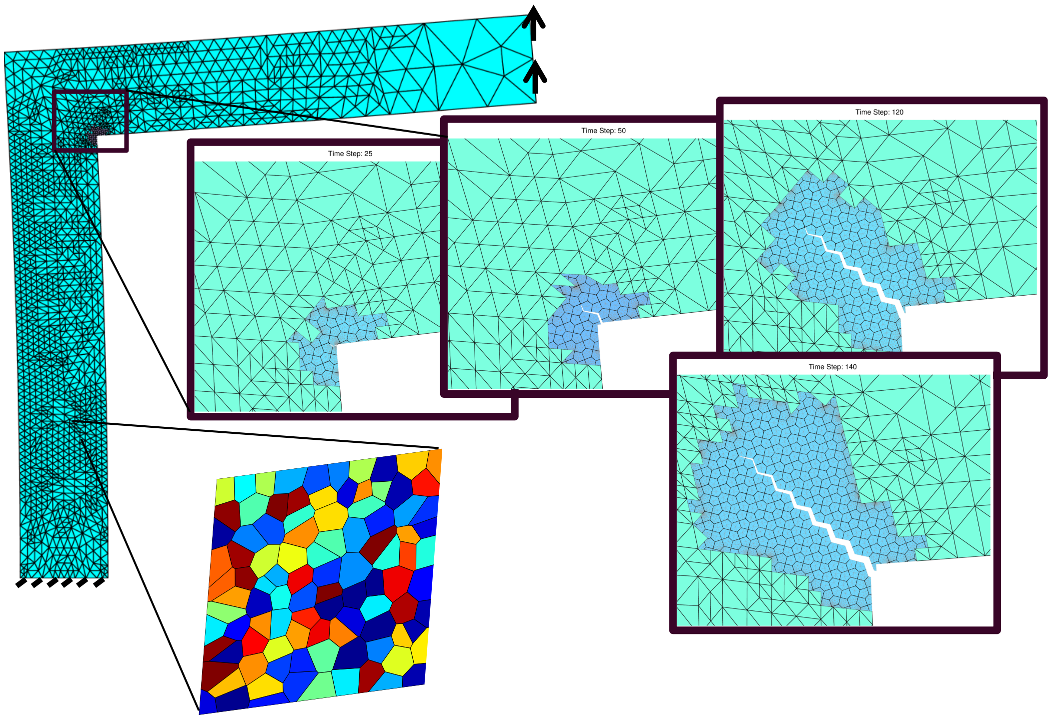


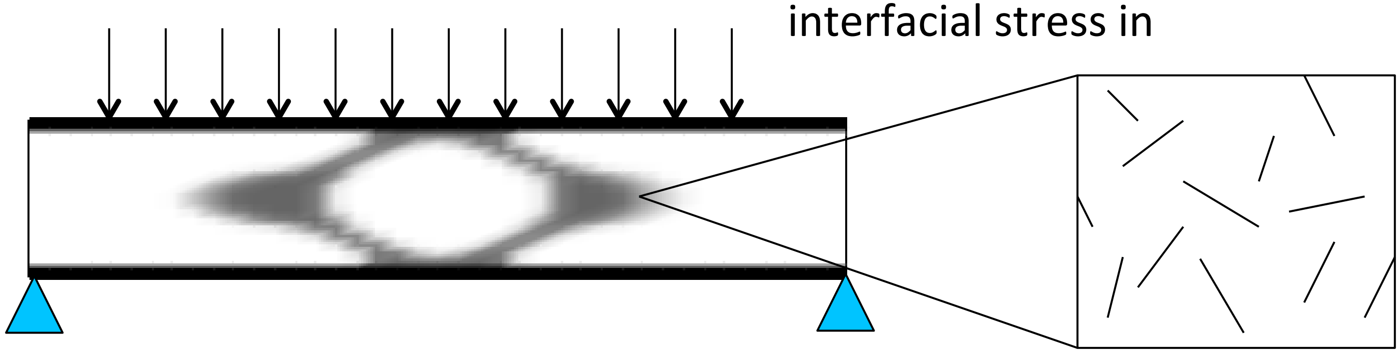
Figure 2. Microstructures of the AZ91D alloys shown in Figure 1 after being solution-treated at 420 °C for 8 hours.

Examples



Approximation of the behaviour of polycrystalline materials away from macroscopic cracks

Optimisation of fiber content in sandwich beams to minimise interfacial stress in



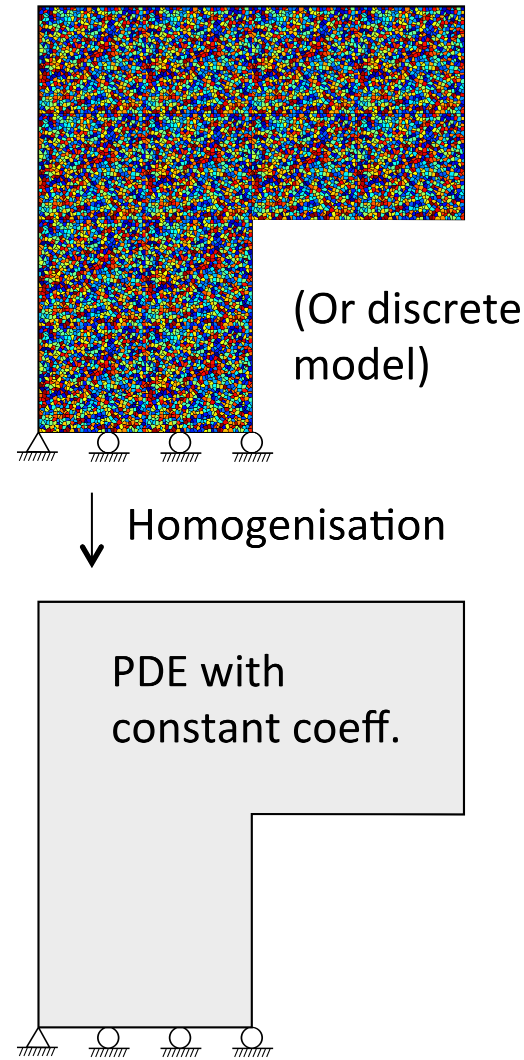
Mathematical formulation

- Knowing the governing equations at the microscale, can we find homogeneous governing equations at the macroscale s. t.:
  - The solution of the macroscale problem converges to the solution of the microscale problem when the scale ratio tends to zero

- Hopefully: the solution of the macroscale problem is a good approximation of the solution of the microscale problem (in some sense) even **when the scale ratio is not very small.**

Error in QoI macroscopic < Tolerance
Cost of solving macromodel << subscale model

Heterog. continuum



Classical homogenisation in linearised elasticity

- Heterogeneous microstructure undergoing moderate deformations, observations at macroscale, slow loading, scale separability

- Macroscale candidate model: lin. elasticity
  - Equilibrium

    $$\operatorname{div} \underline{\underline{\sigma}}^{\mathrm{M}} + \underline{f} = \underline{0} \qquad \text{in } \Omega$$

    $$\underline{\underline{\sigma}}^{\mathrm{M}} \cdot \underline{n} = \underline{0} \qquad \text{in } \partial\Omega_{\mathrm{f}}$$

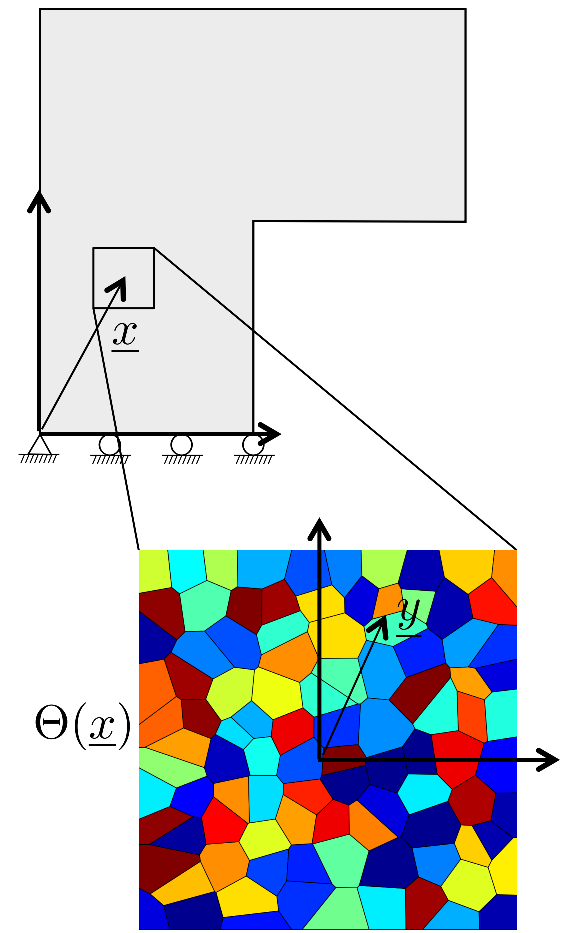
  - Kinematic equations

    $$\underline{u}^{\mathrm{M}} = \underline{U}_{\mathrm{d}} \qquad \text{in } \partial\Omega_{\mathrm{u}}$$

    $$\underline{\underline{\epsilon}}^{\mathrm{M}} = \frac{1}{2}\left(\underline{\operatorname{grad}}\, \underline{u}^{\mathrm{M}} + \underline{\operatorname{grad}}\, \underline{u}^{\mathrm{M}\,T}\right) \qquad \text{in } \Omega$$

  - Constitutive relation by classical micromechanics

    $$\underline{\underline{\sigma}}^{\mathrm{M}} = \mathcal{S}^{\mathrm{M}}\left(\underline{\underline{\epsilon}}(\underline{u}^{\mathrm{M}})\right) \qquad \text{in } \Omega$$



Classical homogenisation in linearised elasticity

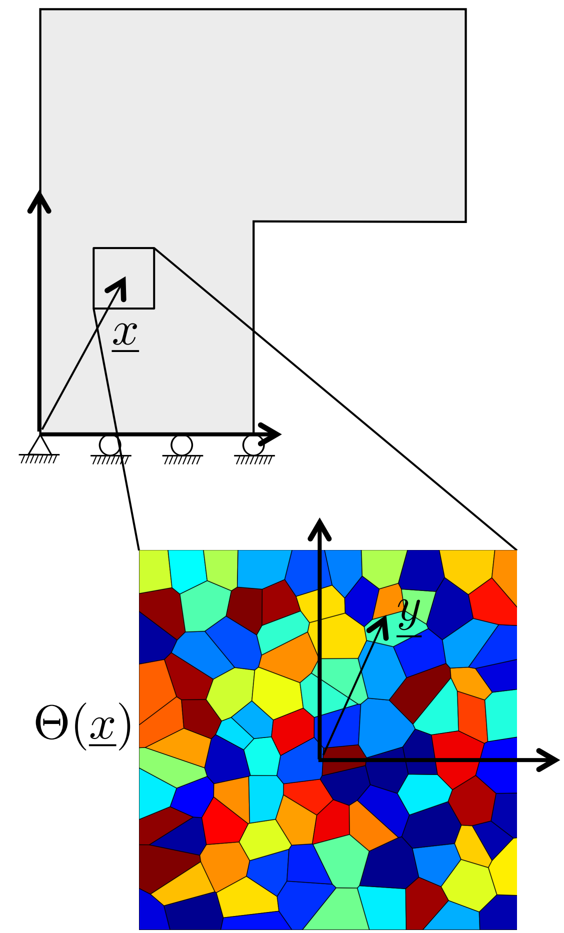
- Attach a representative volume element to the material point: volume of material large enough to represent the statistics of the distribution of material properties (unit cell in periodic case)

  $\underline{\underline{\sigma}}^{\mathrm{m}} = \underset{\sim}{D}(\underline{y}) : \underline{\underline{\epsilon}}^{\mathrm{m}}$

- Suppose that the RVE is mechanically equilibrated: $\underline{\mathrm{div}}\, \underline{\underline{\sigma}}^{\mathrm{m}} = \underline{0}$

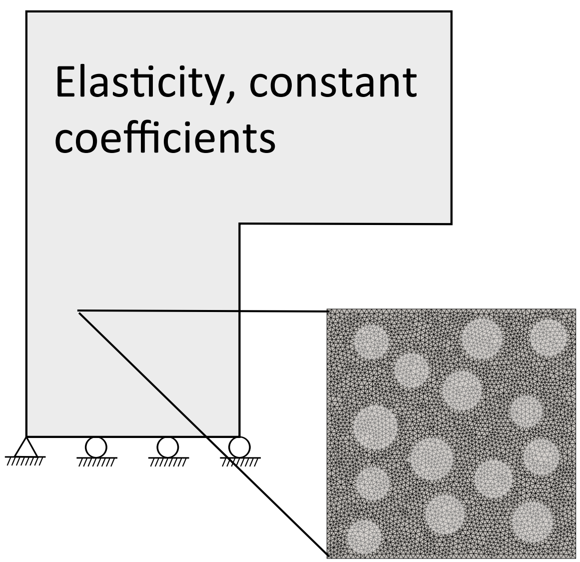
- The effective constitutive law the/a relationship between average stress and average strain

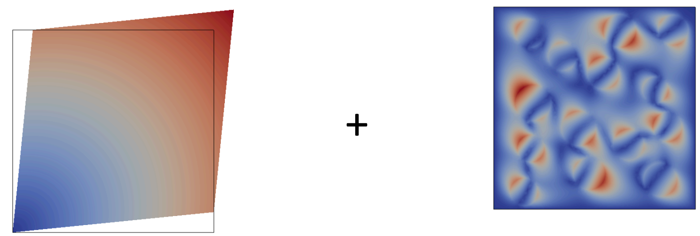
  $< \underline{\underline{\sigma}}^{\mathrm{m}} >= \mathcal{S}^{\mathrm{M}} \left(< \underline{\underline{\epsilon}}^{\mathrm{m}} > \right)$



Computational homogenisation

- Obtain $< \underline{\underline{\sigma}}^{\mathrm{m}} >= \mathcal{S}^{\mathrm{M}}\left(< \underline{\underline{\epsilon}}^{\mathrm{m}} >\right)$ by solving RVE problem numerically





Homogeneous strain (macroscopic part)

"micro" fluctuation

$$\underline{\bar{u}}(\underline{y}) = \underline{\underline{\epsilon}}^{\mathrm{M}} \cdot \underline{y} + \underline{\tilde{u}}(\underline{y})$$

- Ill-posed, requires BC for fluctuation compatible with $< \underline{\underline{\epsilon}}(\underline{\tilde{u}}(\underline{y})) >$
- One possibility: Dirichlet problem, fluctuation vanishes on boundary

→ Very expensive too solve

- Introduction

- Virtual charts for parametrised homogenisation in linear elasticity

- Reduced order modelling in nonlinear homogenisation

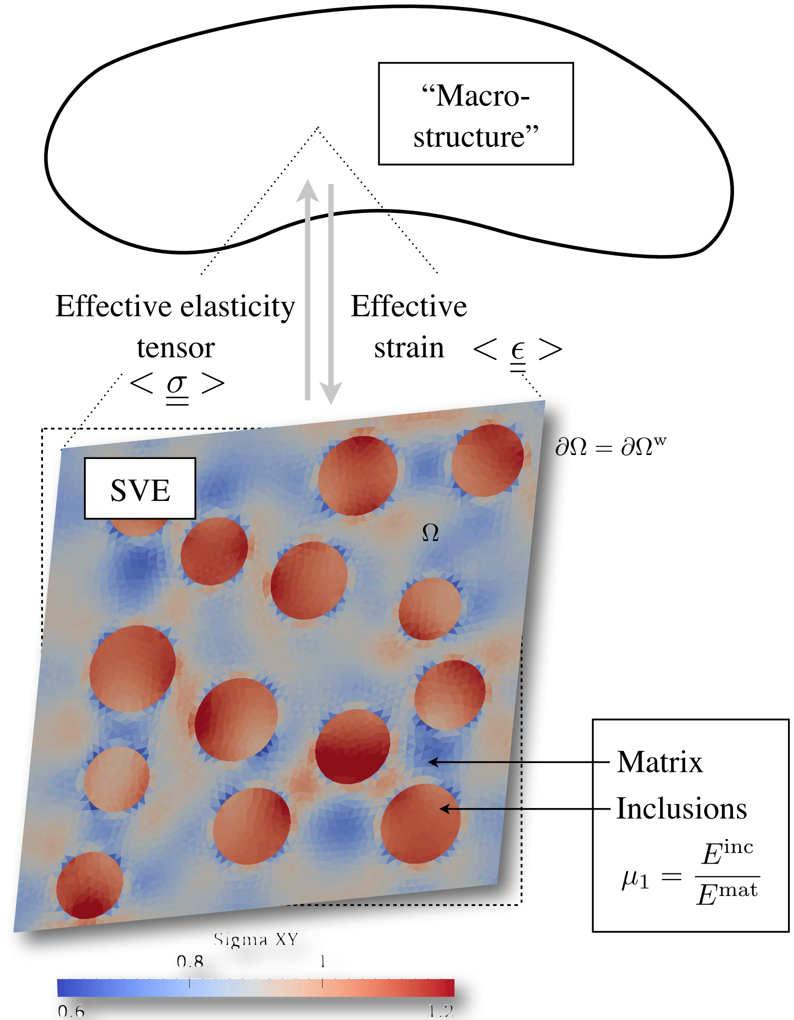
Parametrised homogenisation

- Homogenisation

$$< \underline{\underline{\sigma}}(\underline{\mu}) >= \underset{\sim}{D}^{\star}(\underline{\mu}) :< \underline{\underline{\epsilon}}(\underline{u}(\underline{\mu})) >$$

- Dirichlet localisation problem
  - $\underline{\underline{\sigma}}(\underline{\mu}) = \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}(\underline{\mu}))$

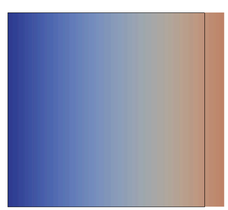
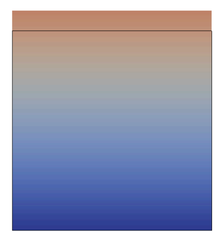
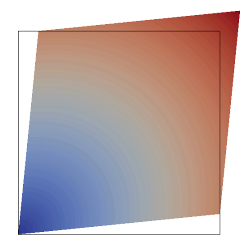
    Parametrised tensor field
  - $\text{div } \underline{\underline{\sigma}}(\underline{\mu}) = 0$
  - Boundary conditions: $\underline{u}(\underline{\mu}) = < \underline{\underline{\epsilon}}(\underline{u}(\underline{\mu})) > \cdot \underline{x}$



- Homogenised Hooke tensor (assuming major and minor symmetries)

$$< \underline{\sigma}(\underline{\mu}) > = \underset{\sim}{D}^{\star}(\underline{\mu}) :< \underline{\epsilon}(\underline{u}(\underline{\mu})) >$$

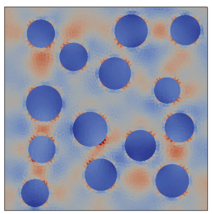
$$\begin{pmatrix} \langle \sigma_{11} \rangle \\ \langle \sigma_{22} \rangle \\ \langle \sigma_{12} \rangle \end{pmatrix} = \begin{pmatrix} D^{\star}_{1111} & D^{\star}_{1122} & D^{\star}_{1112} \\ - & D^{\star}_{2222} & D^{\star}_{2212} \\ - & - & D^{\star}_{1212} \end{pmatrix} \begin{pmatrix} \langle \epsilon_{11} \rangle \\ \langle \epsilon_{22} \rangle \\ 2 \; \langle \epsilon_{12} \rangle \end{pmatrix}$$

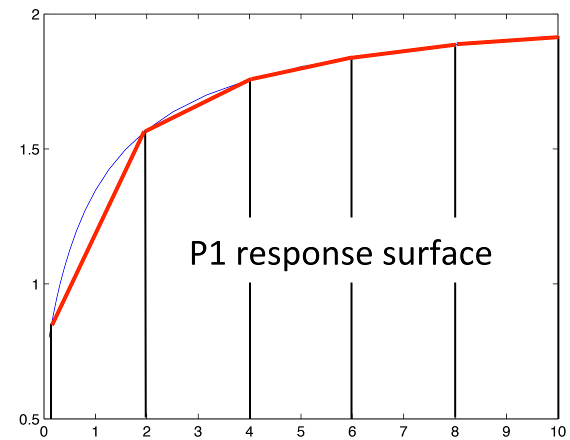
Effective strain by DBC	 $\underline{u}(\underline{\mu}) = (e_1 \otimes e_1) \cdot \underline{x}$ $\leftarrow \; < \epsilon >$		 $\underline{u}(\underline{\mu}) = \frac{1}{2}(e_1 \otimes e_2 + e_2 \otimes e_1) \cdot \underline{x}$
Effective stress from FE calculation	$< \underline{\sigma}(\underline{\mu}) > = \begin{pmatrix} D^{\star}_{1111} \\ D^{\star}_{1122} \\ D^{\star}_{1112} \end{pmatrix}$		$< \underline{\sigma}(\underline{\mu}) > = \begin{pmatrix} D^{\star}_{1112} \\ D^{\star}_{2212} \\ D^{\star}_{1212} \end{pmatrix}$

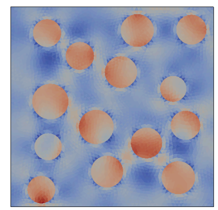
Virtual charts

- Response surface method: interpolate the quantities of interest

$\underset{\sim}{D}^{\star}_{1111}$

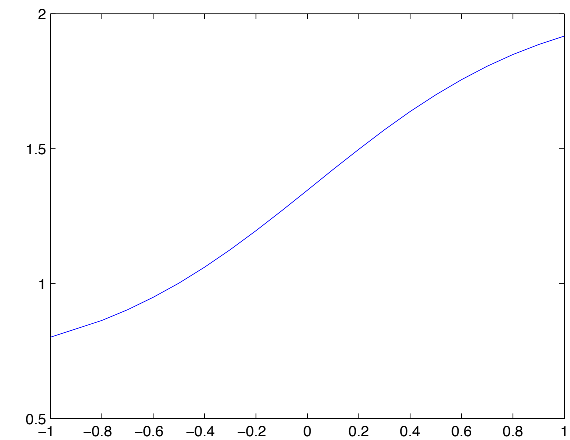






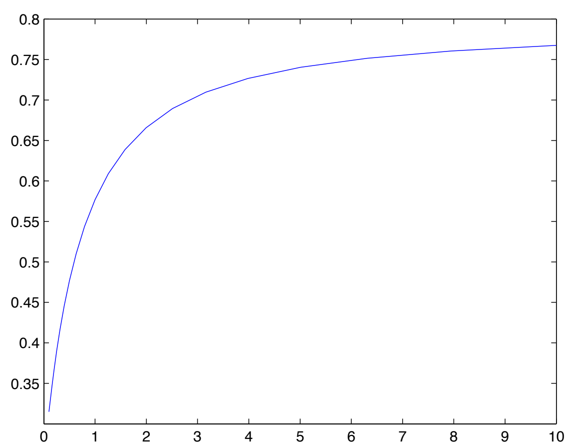
Elastic contrast

$\underset{\sim}{D}^{\star}_{1111}$



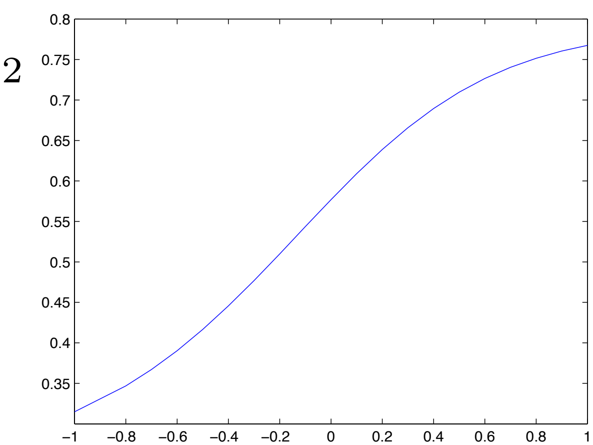
Elastic contrast (log)

$\underset{\sim}{D}^{\star}_{1122}$



Elastic contrast

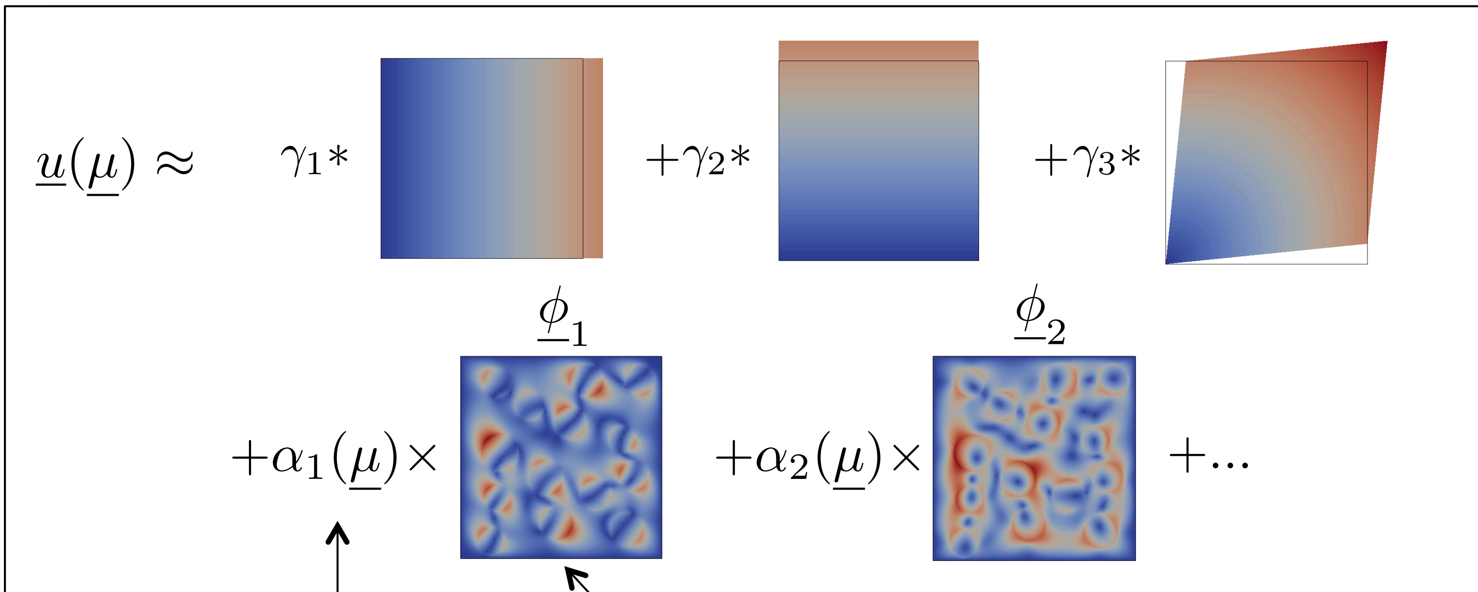
$\underset{\sim}{D}^{\star}_{1122}$



Elastic contrast (log)

ROM-based Virtual charts

- **Interpolate the state variables** instead: reduced order model
  - For any applied macroscopic field, and **any elastic contrast**



“Macro field”

“Micro fluctuation”

global displacement mode (pre-computed)

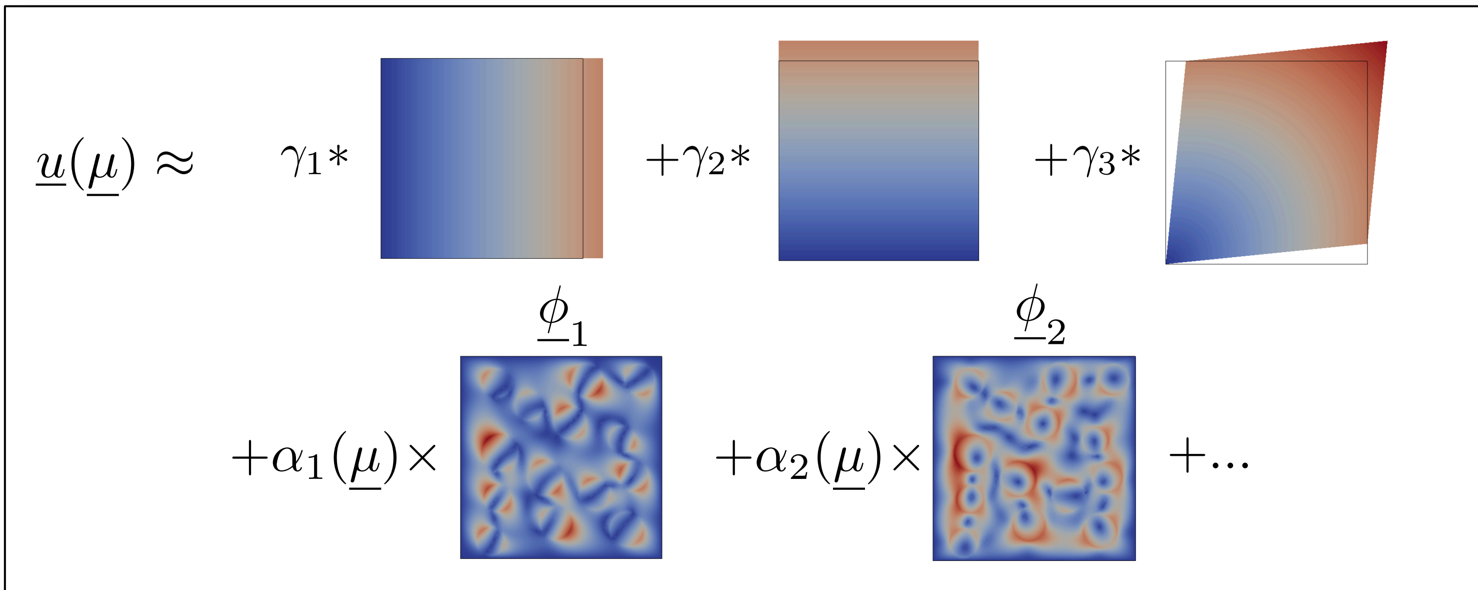
Generalised coordinate: minimise an error measure (Galerkin)

$$\underline{\underline{\mathbf{K}}}(\underline{\mu})\,\underline{\mathbf{U}}(\underline{\mu}) = \underline{\mathbf{F}}(\underline{\mu}) \longrightarrow \underline{\underline{\mathbf{K}}}^{\mathrm{r}}(\underline{\mu})\,\underline{\boldsymbol{\alpha}}(\underline{\mu}) = \underline{\mathbf{F}}^{\mathrm{r}}(\underline{\mu})$$

Reduced stiffness $\mathbf{K}^{\mathrm{r}}_{ij}(\underline{\mu}) = \underline{\phi}_i^T\,\underline{\underline{\mathbf{K}}}(\underline{\mu})\,\underline{\phi}_j$

ROM-based Virtual charts

- **Interpolate the state variables** instead: reduced order model
  - For any applied macroscopic field, and **any elastic contrast**



"Macro field"

"Micro fluctuation"

→ Often, state variables belong to a low-dimensional vector space

- **Then, post-process the quantities of interest**

→ (Sub-) optimal surrogates can be constructed

→ Error estimates available

Reduced order model

- Separation of variables:

$$\underline{u}^{\mathrm{h}}(\underline{\mu}) \approx \underline{u}^{\mathrm{r}}(\underline{\mu}) := \sum_{i=1}^{n_\phi} \underline{\phi}_i \, \alpha_i(\underline{\mu}) + \underline{u}^{\mathrm{h,p}}(\underline{\mu})$$

- Example of optimal decomposition: POD

$$(\underline{\phi}_i, \alpha_i)_{i \in [\![1, n_\phi]\!]} = \arg\min \left(\frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \left\| \underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}^{\mathrm{r}}(\underline{\mu}) \right\|_X \, d\underline{\mu} \right)$$

  - Not computable without approximation
    - → Galerkin Empirical POD
    - → Reduced Basis method
    - → PGD

Galerkin-POD with QRandom sampling

- Suboptimal surrogate in two steps:

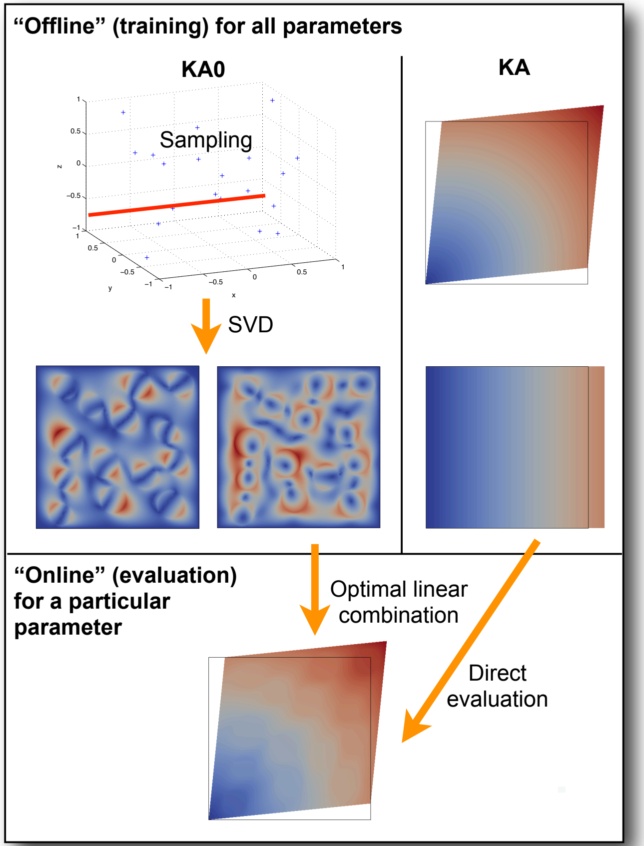
  - **Empirical POD "offline"**:
    - Compute sampling (Snapshot):
      $$\Xi^0 = \{\underline{u}^{\mathrm{h},0}(\underline{\mu}) := \underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}^{\mathrm{h,p}}(\underline{\mu}) \mid \underline{\mu} \in \tilde{\mathcal{P}}\}$$
    - Spectral analysis (SVD)

$$(\underline{\phi}_i)_{i\in[\![1,n_\phi]\!]} = \underset{(\underline{\phi}_i^\star)_{i\in[\![1,n_\phi]\!]},\ \left\langle \underline{\phi}_i^\star, \underline{\phi}_j^\star \right\rangle_X = \delta_{ij}}{\operatorname{argmin}} J\left((\underline{\phi}_i^\star)_{i\in[\![1,n_\phi]\!]}\right)$$

$$J\left((\underline{\phi}_i^\star)_{i\in[\![1,n_\phi]\!]}\right) = \sum_{\underline{\mu}\in\tilde{\mathcal{P}}} \left\| \underline{u}^{\mathrm{h},0}(\underline{\mu}) - \sum_{i=1}^{n_\phi} \left\langle \underline{u}^{\mathrm{h},0}(\underline{\mu}), \underline{\phi}_i^\star \right\rangle_X \underline{\phi}_i^\star \right\|_X$$

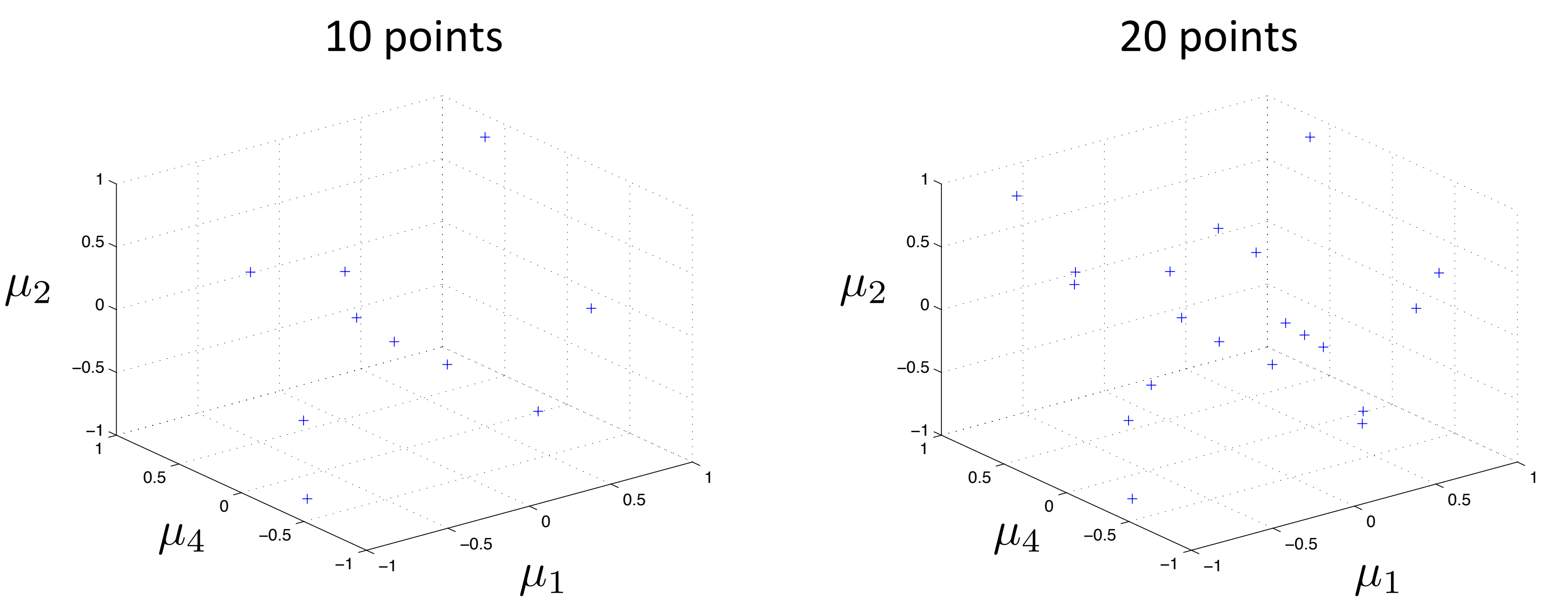
  - **"Online" optimal coordinates** by Galerkin

$$(\alpha_i)_{i\in[\![1,n_\phi]\!]} = \underset{\underline{u}^\star(\underline{\mu}) = \sum_{i=1}^{n_\phi} \underline{\phi}_i \alpha_i(\underline{\mu}) + \underline{u}^{\mathrm{h,p}}(\underline{\mu})}{\operatorname{argmin}} \left(\| \underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}^\star(\underline{\mu}) \|_{\underset{\sim}{D}(\underline{\mu})} \right)$$



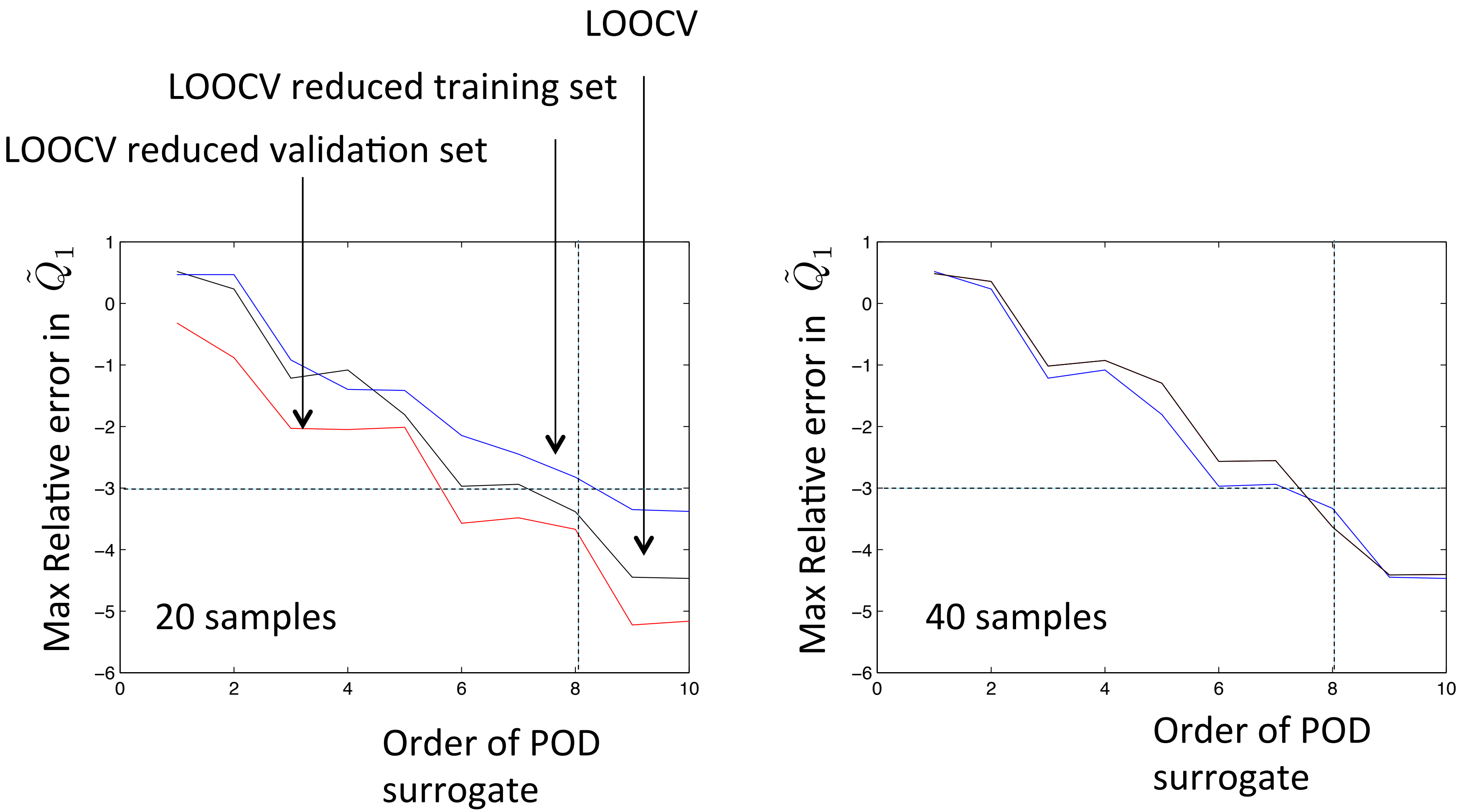
Key issue 1: choice of samples

- Key issue 1: Empirical POD
  - Hierarchical sampling too expensive (curse of dimensionality)
    - → Quasi-random sampling



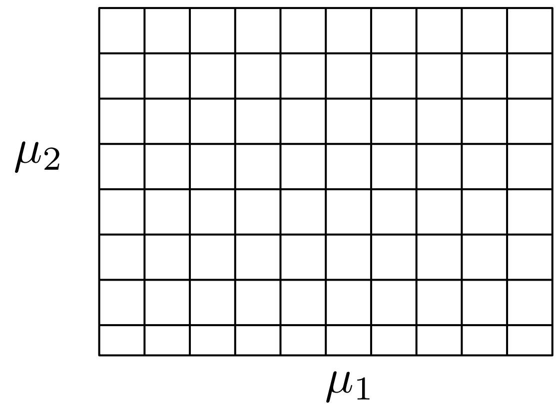
→ Error evaluated by cross-validation estimates and stagnation criteria

Convergence estimate

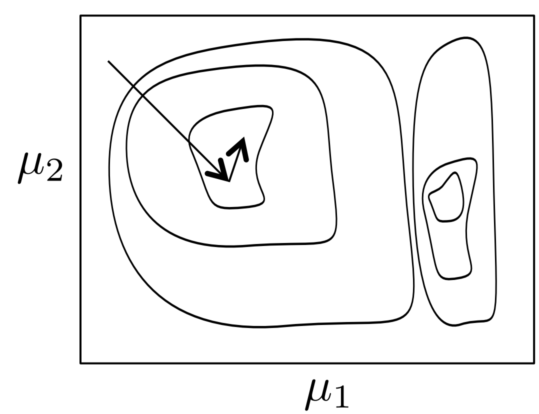


Alternative methods for snapshot selection

- Greedy sampling (RBM) (see the work of Maday, Patera, …)
  - Evaluate the error of a Galerkin-surrogate of order N on a fine grid of the parameter domain
  - Add to the basis the sample for which the prediction error (in QoI) is the largest
    - → Efficient when sharp estimate available
    - → But limited to small number of parameters



- QRandom-based Greedy-sampling (see [Rozza *et al*. 2011])
- Optimisation-based Greedy sampling (work of Volkwein, Willcox, …)
  - Look for a new sample to add to a basis N such that the error of the surrogate of order N+1 is minimised
    - → Localisation of local minima is difficult



Key issue 2: efficient assembly of ROM

- "online" cost:

$$(\alpha_i)_{i\in[\![1,n_\phi]\!]} = \underset{\underline{u}^\star(\underline{\mu})=\sum_{i=1}^{n_\phi}\underline{\phi}_i\,\alpha_i(\underline{\mu})+\underline{u}^{\mathrm{h,p}}(\underline{\mu})}{\operatorname{argmin}} \left(\|\underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}^\star(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})} \right)$$

$$\rightarrow \quad \underline{\underline{\mathbf{K}}}^{\mathrm{r}}(\underline{\mu})\,\underline{\boldsymbol{\alpha}}(\underline{\mu}) = \underline{\mathbf{F}}^{\mathrm{r}}(\underline{\mu})$$

$$\underline{\underline{\mathbf{K}}}^{\mathrm{r}}(\underline{\mu}) = \underline{\underline{\phi}}^T\,\underline{\underline{\mathbf{K}}}(\underline{\mu})\,\underline{\underline{\phi}}$$

But assembly cost needs to be small!

- OK if data is separable: $\forall\,\underline{\mu},\quad \underline{\underline{\mathbf{K}}}(\underline{\mu}) = \sum_{i=1}^{n_{\mathrm{K}}} \underline{\underline{\bar{\mathbf{K}}}}_i\,\gamma_i(\underline{\mu})$

$$\rightarrow \quad \forall\,\underline{\mu},\quad \underline{\underline{\mathbf{K}}}^{\mathrm{r}}(\underline{\mu}) = \sum_{i=1}^{n_{\mathrm{K}}} \left(\underline{\underline{\phi}}^T\,\underline{\underline{\bar{\mathbf{K}}}}_i\,\underline{\underline{\phi}} \right) \gamma_i(\underline{\mu})$$

Pre-computed "offline"

→ **Otherwise, one needs further approximations** (force data separation)

Goal-oriented error estimation

- Aim: Bound $\tilde{Q}_i(\underline{e}^{\mathrm{r}}(\underline{\mu})) = \tilde{Q}_i(\underline{u}^{\mathrm{h}}(\underline{\mu})) - \tilde{Q}_i(\underline{u}^{\mathrm{r}}(\underline{\mu}))$ from above and below

- Adjoint problem for each QoI: $a(\underline{u}^{\star}, \underline{z}^{(\mathrm{i}),\mathrm{h}}(\underline{\mu}); \underline{\mu}) = \tilde{Q}_i(\underline{u}^{\star})$

  → Galerkin-POD: $\underline{z}^{(\mathrm{i}),\mathrm{r}}(\underline{\mu}) \approx \underline{z}^{(\mathrm{i}),\mathrm{h}}(\underline{\mu})$

$$-\|\underline{e}^{\mathrm{r}}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})} \|\underline{\tilde{e}}^{(i)}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})} + r^{(i)} \le \tilde{Q}_i(\underline{e}^{\mathrm{r}}(\underline{\mu})) \le \|\underline{e}^{\mathrm{r}}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})} \|\underline{\tilde{e}}^{(i)}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})} + r^{(i)}$$

  - $r^{(i)}$ is minus the residual of the forward problem in $\underline{z}^{(\mathrm{i}),\mathrm{r}}(\underline{\mu})$ (computable)
  - $\underline{\tilde{e}}^{(i)}$ is the error in the i$^{\mathrm{th}}$ adjoint problem

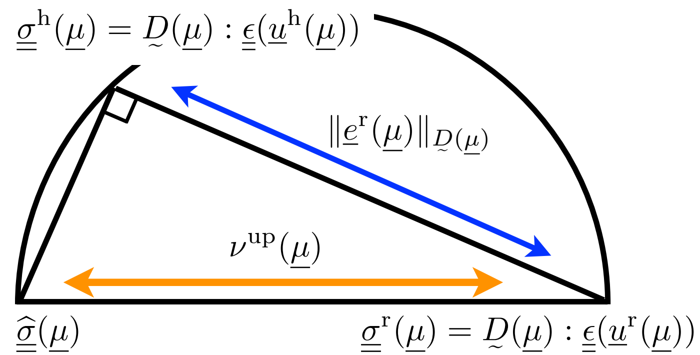
- Special case: compliant problem (adjoint and forward solutions i are collinear)

  → $\tilde{Q}_i(\underline{e}^{\mathrm{r}}(\underline{\mu})) = \beta \, \|\underline{e}^{\mathrm{r}}(\underline{\mu})\|^2_{\underset{\sim}{D}(\underline{\mu})}$

Error bounding by duality

- Upper bound in energy norm: Error in the constitutive relation [Ladevèze '85][Ladevèze and Chamoin '11]

$$\nu^{\mathrm{up}}(\underline{\mu}) := \|\underline{\underline{\widehat{\sigma}}}(\underline{\mu}) - \underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})^{-1}} \geq \|\underline{e}^{\mathrm{r}}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})}$$



  - The recovered stress must be statically admissible in the FE sense

$$\forall\, \underline{u}^{\star} \in \mathcal{U}^{\mathrm{h},0}(\Omega), \quad \int_{\Omega} \underline{\underline{\widehat{\sigma}}}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^{\star})\, d\Omega = 0$$

→ More effective as the recovered stress approaches the FE stress

Local error estimation

- Construction of the statistically admissible stress: POD-surrogate: SVD from stress snapshot:

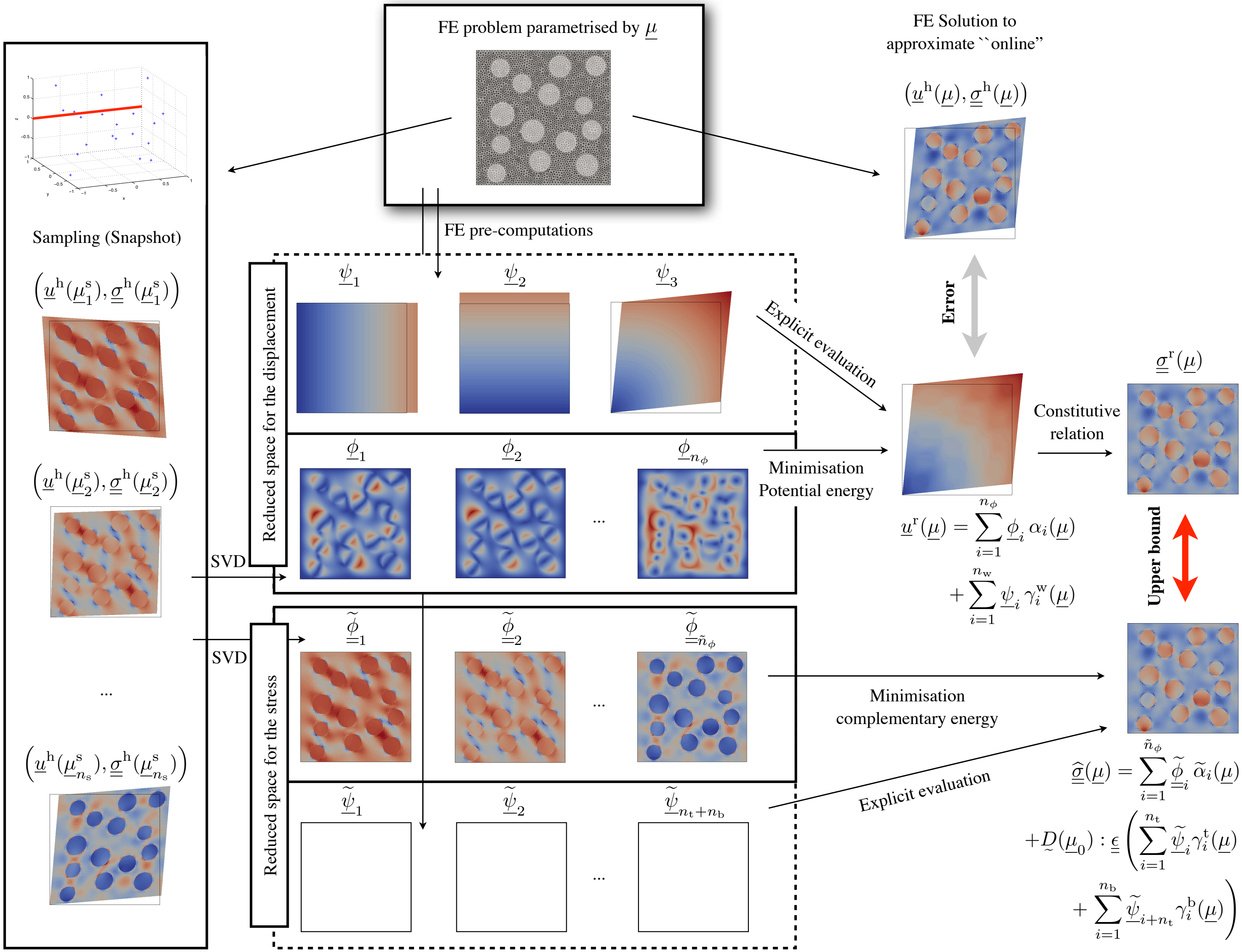
$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{\underline{\widehat{\sigma}}}(\underline{\mu}) = \sum_{i=1}^{\tilde{n}_\phi} \underline{\underline{\widetilde{\phi}}}_i \, \widetilde{\alpha}_i(\underline{\mu})$$

  - "Offline:" Empirical POD on stress samples
    → Basis $(\underline{\underline{\widetilde{\phi}}}_i)$ such that average projection error over snapshots is minimised.

  - "Online:" Minimisation of CRE upper bound:

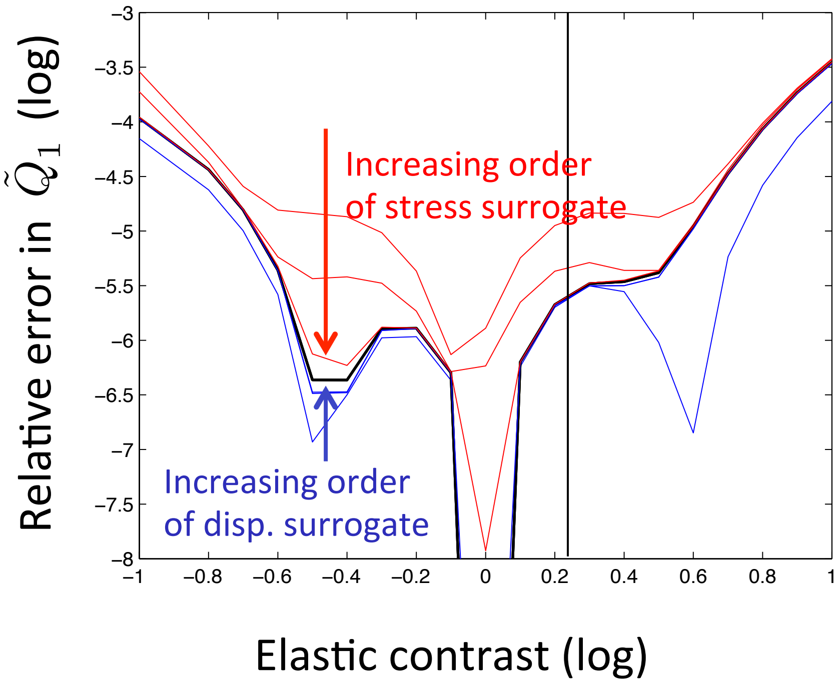
$$(\widetilde{\alpha}_i)_{i \in [\![1, \tilde{n}_\phi]\!]} = \underset{\underline{\underline{\sigma}}^\star(\underline{\mu}) = \sum_{i=1}^{\tilde{n}_\phi} \underline{\underline{\widetilde{\phi}}}_i \, \widetilde{\alpha}_i(\underline{\mu})}{\operatorname{argmin}} \left(\| \underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \underline{\underline{\sigma}}^\star(\underline{\mu}) \|_{\underset{\sim}{D}(\underline{\mu})^{-1}} \right)$$

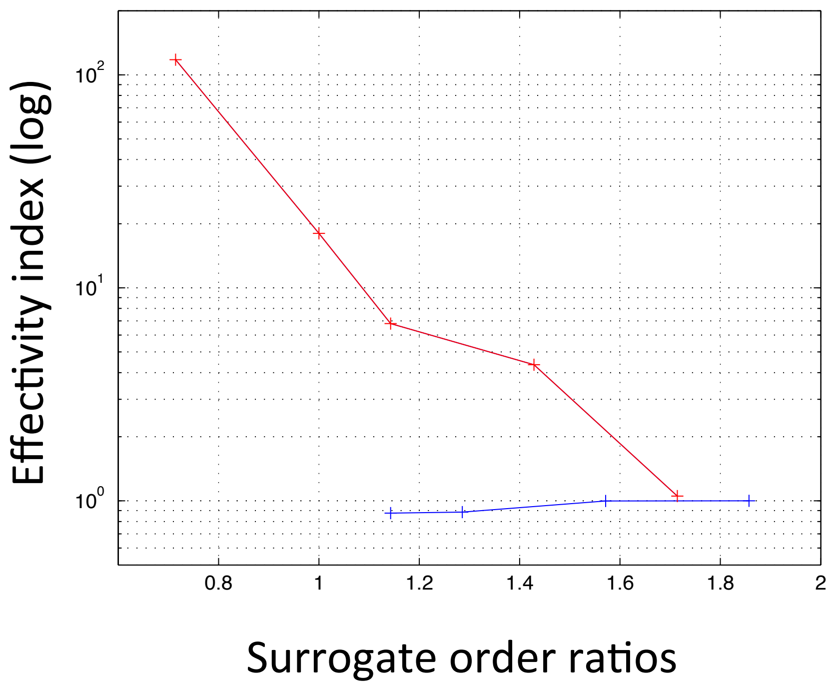
Schematic of duality-based ROM



Results

- Illustration for $\underline{\underline{\epsilon}}^{M} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $\tilde{Q}_1 \equiv \underset{\sim}{D}^{\star}_{1111}$ (compliant problem)





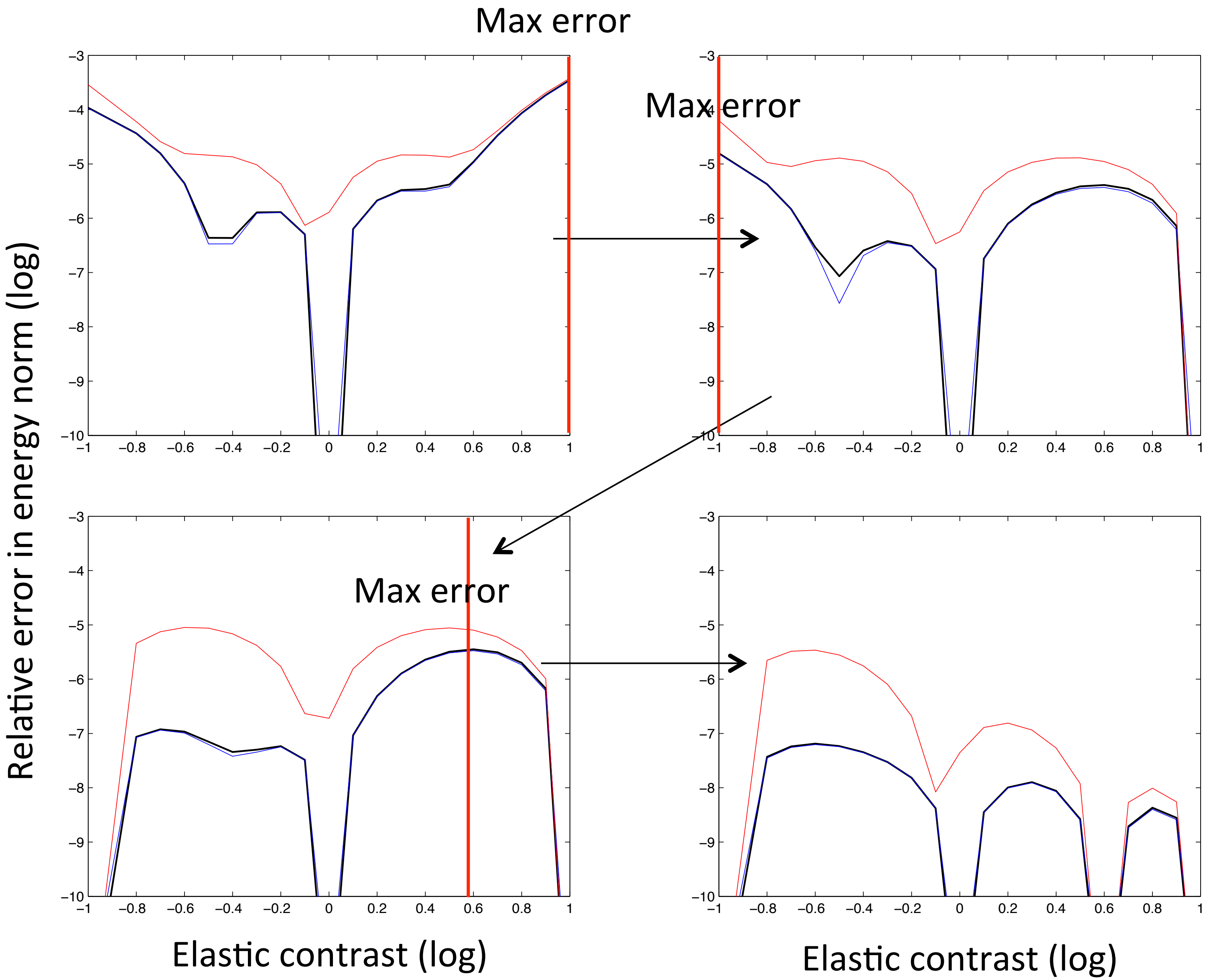
→ Lower bound necessary to control the sharpness of the upper bound as no a priori convergence estimate available

Partial conclusions

- (Sub-) optimal virtual charts for parametrised homogenisation problems, based on Galerkin-POD
- **No a priori assumption on fluctuation fields**: smooth transition between approximate RVE problem and fully resolved (FEM), by just enriching the reduced basis
- Guaranteed accuracy
- We are working on optimal sampling of displacement versus stress surrogates to reach the desired level of accuracy on QoI

  → Goal-oriented, hybrid reduced basis strategy

Reduced basis sampling technique

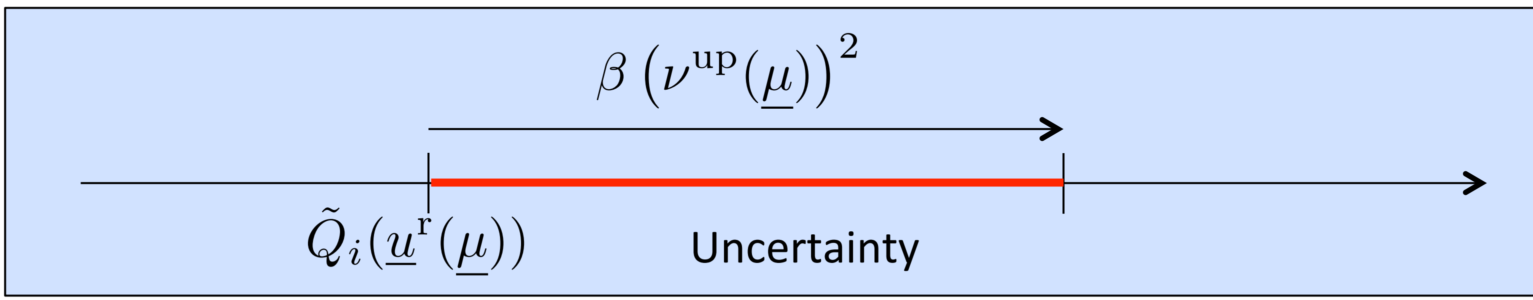


GO hybrid reduced basis approach

- Interpretation of error bound as uncertainty on QoI

- Illustration for a compliant problem (if $\beta > 0$):

$$\tilde{Q}_i(\underline{u}^{\mathrm{r}}(\underline{\mu})) \leq \tilde{Q}_i(\underline{u}^{\mathrm{h}}(\underline{\mu})) \leq \tilde{Q}_i(\underline{u}^{\mathrm{r}}(\underline{\mu})) + \beta \left(\nu^{\mathrm{up}}(\underline{\mu})\right)^2$$



→ uncertainty reduced by error reduction (increase displacement accuracy) or increase in bound effectivity (increase accuracy of stress)

→ **Hybrid reduced basis**

GO hybrid reduced basis approach

- Start with one random sample at μ_0 and initialise the surrogates
  - KA Displacement: $\forall \underline{\mu} \in \mathcal{P}, \quad \underline{u}^{\mathrm{r}}(\underline{\mu}) = \underline{\phi}_1 \, \alpha_1(\underline{\mu}) + \underline{u}^{\mathrm{h,p}}(\underline{\mu})$

    fluctuation at μ_0
  - Equilibrated stress: $\forall \underline{\mu} \in \mathcal{P}, \quad \underline{\underline{\widehat{\sigma}}}(\underline{\mu}) = \underline{\underline{\widetilde{\phi}}}_1 \, \widetilde{\alpha}_1(\underline{\mu})$

    stress at μ_0

- **Max uncertainty** over parameter domain detected at μ_1
  - Check which of the enrichments create maximum reduction in uncertainty

$$\underline{u}^{\mathrm{r}}(\underline{\mu}) = \sum_{i=1}^{2} \underline{\phi}_i \, \alpha_i(\underline{\mu}) + \underline{u}^{\mathrm{h,p}}(\underline{\mu}) \quad \text{or} \quad \underline{\underline{\widehat{\sigma}}}(\underline{\mu}) = \sum_{i=1}^{2} \underline{\underline{\widetilde{\phi}}}_i \, \widetilde{\alpha}_i(\underline{\mu})$$

fluctuations at μ_0 and μ_1

stresses at μ_0 and μ_1

  - Proceed until max uncertainty is small enough

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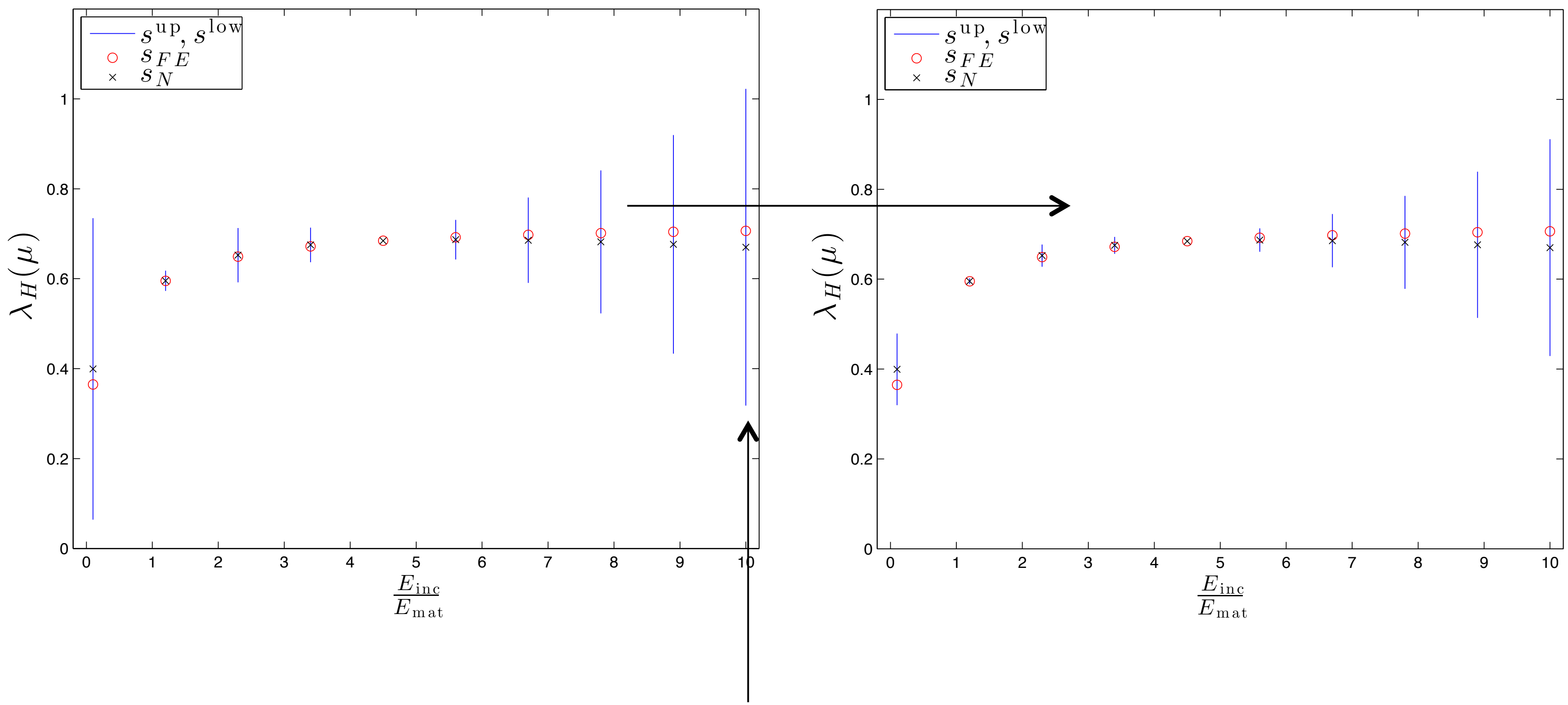
Illustration for compliant problem

Iteration 1 Iteration 2



Worst uncertainty, best reduced by enriching stress surrogate

limitations / questions

- Guaranteed accuracy limited to elliptic and parabolic (e.g. viscoelasticity) problems, with a priori separation of variables (problems with parametrised geometry or nonlinearities rarely respect this condition)

- Open questions / remarks
  - Error bounds can be obtained for "smooth" problems, in which case empirical, more general estimates seem to give reliable results.
  - How to choose the QoI in imbricated problems (chains of approximations)?

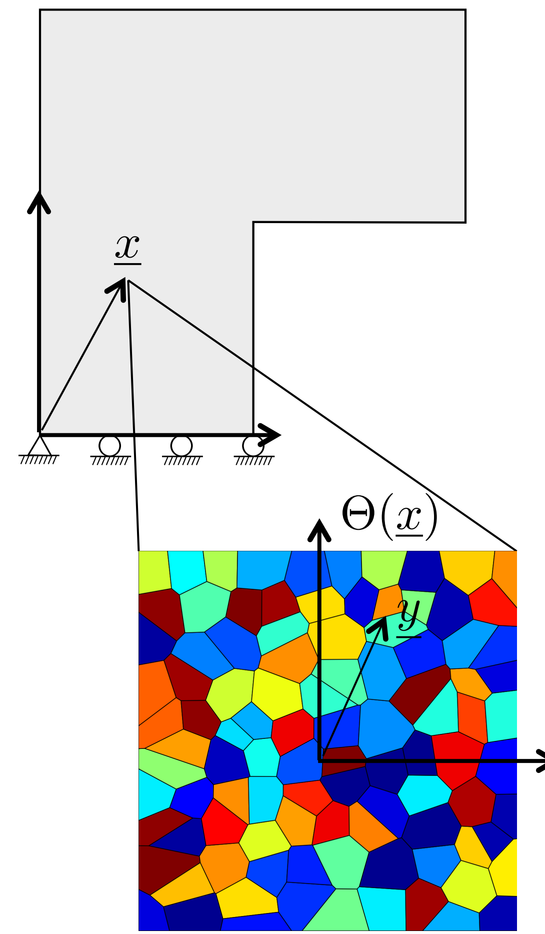
- Introduction

- Virtual charts for parametrised homogenisation in linear elasticity

- Reduced order modelling in nonlinear homogenisation

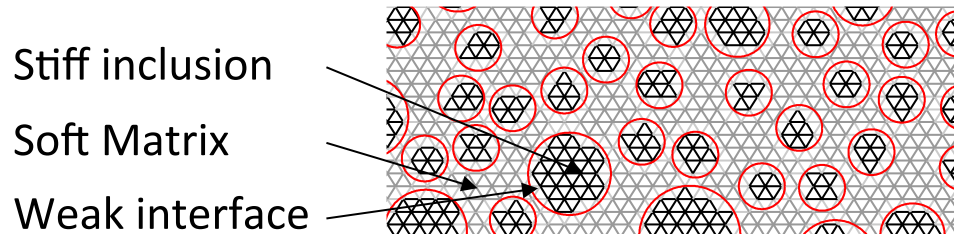
Nonlinear comput. homogenisation by FE^2

- Implicitly defined nonlinear homogenised constitutive relations
- Macro problem:
  - Equilibrium: $\int_{\Omega} \underline{\underline{\sigma}}^{\mathrm{M}} : \underline{\underline{\epsilon}}(\delta \underline{u})\, d\Omega = \int_{\Omega} \underline{f} \cdot \delta \underline{u}\, d\Omega + \int_{\partial\Omega_{\mathrm{N}}} \underline{F} \cdot \delta \underline{u}\, d\Gamma$
  - CR: $\underline{\underline{\sigma}}^{\mathrm{M}} = \mathcal{S}^{\mathrm{M}}\left(\underline{\underline{\epsilon}}(\underline{u}^{\mathrm{M}})\right)$ **(not specified explicitly)**
- Micro problem:
  - Equilibrium: $\int_{\Theta} \underline{\underline{\sigma}}^{\mathrm{m}} : \underline{\underline{\epsilon}}(\delta \underline{u})\, d\Omega = \int_{\partial\Theta} \left(\underline{\underline{\sigma}}^{\mathrm{m}} \cdot \underline{n}\right) \cdot \delta \underline{u}\, d\Gamma$
  - CR: $\underline{\underline{\sigma}}^{\mathrm{m}} = \mathcal{S}^{\mathrm{m}}\left(\underline{\underline{\epsilon}}^{\mathrm{m}}\right)$ (known, non-linear)
- Scale linking
  - DBC $\underline{u}^{\mathrm{m}} = \underline{\underline{\epsilon}}^{\mathrm{M}} \cdot \underline{y}$
  - Stress average: $\underline{\underline{\sigma}}^{\mathrm{M}} = \int_{\Theta} (\sigma^{\mathrm{m}} \cdot \underline{n}) \otimes \underline{y}\, d\Omega$



Damageable RVE

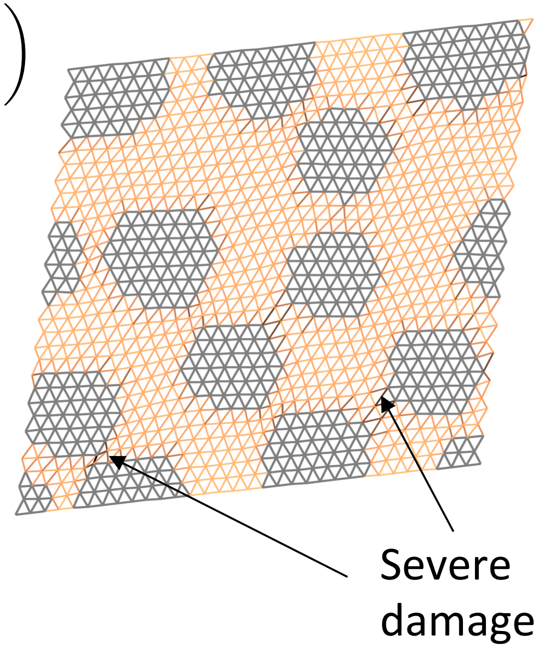
- Damageable elastic heterogeneous



- Modelled by a network of Euler-Bernouilli beams with CR:

$$\begin{pmatrix} N \\ M \end{pmatrix} = \frac{\partial \psi}{\partial \underline{\bar{\epsilon}}} = \begin{pmatrix} E^{(b)} S^{(b)} (1 - d_n) \frac{< v_{,\xi} >_+}{v_{,\xi}} & 0 \\ 0 & E^{(b)} I^{(b)} (1 - d_t) \end{pmatrix} \begin{pmatrix} v_{,\xi} \\ \theta_{,\xi} \end{pmatrix}$$

"d" Damage variable represents the extent of subscale networks of cracks



- Properties of resulting problem:
  - Damage depends on deformation -> Nonlinear
  - Irreversibility of damage -> pseudo-time dependent

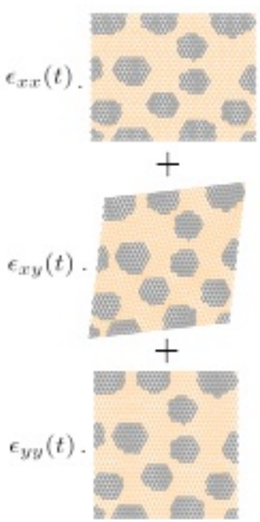
Parametrised RVE problem

- Homogenisation using Dirichlet localisation on RVE:
  - Fully discrete equilibrium, for any load history:

$$\forall t \in \{t_1, t_2, \ldots, t_N\}, \quad \underline{\mathbf{U}}^{\star\,T}\, \underline{\mathbf{F}}_{\mathrm{int}} \left(\underline{\widetilde{\mathbf{U}}}(t); \left(\underline{\bar{\mathbf{U}}}(\tau)\right)_{\tau \leq t} \right) = \underline{\mathbf{0}}$$

  - Uniform displacement boundary conditions

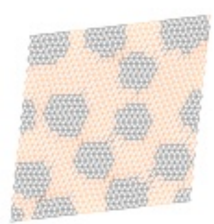
$$\underline{\mathbf{U}}(t) = \underline{\bar{\mathbf{U}}}(t) + \underline{\widetilde{\mathbf{U}}}(t) \quad \text{Such that} \quad \underline{\underline{N}}(\underline{x})\, \underline{\bar{\mathbf{U}}}(t) = \begin{pmatrix} \epsilon^{\mathrm{M}}_{11}(t) & \epsilon^{\mathrm{M}}_{12}(t) \\ \epsilon^{\mathrm{M}}_{12}(t) & \epsilon^{\mathrm{M}}_{22}(t) \end{pmatrix} \cdot (\underline{x} - \underline{x}_{\mathrm{c}})$$



+

Fluctuation **vanishes on boundary**

=



Full micro solution, used to **extract average stress**

Parameters
(“ Dimension 3N ”)

Galerkin-ROM

- Approximation for the fluctuation field for any load history

$$\underline{\mathbf{U}}(t) \approx \underline{\mathbf{U}}^{\mathrm{r}}(t) := \sum_{i=1}^{n_\phi} \underline{\boldsymbol{\phi}}_i \, \alpha_i(t) + \bar{\underline{\mathbf{U}}}(t)$$

Modal coordinates associated with POD basis vectors

Global basis functions for fluctuation field (obtained by Snapshot POD)

- Galerkin: $\forall i \quad \underline{\boldsymbol{\phi}}_i^T \, \underline{\mathbf{F}}_{\mathrm{int}} \left(\underline{\boldsymbol{\alpha}}(t); \left(\bar{\underline{\mathbf{U}}}(\tau)\right)_{\tau \le t} \right) = 0$

- Solution by Newton: $\underline{\underline{\mathbf{K}}}^{\mathrm{r},(k)} \, \boldsymbol{\Delta} \underline{\boldsymbol{\alpha}}^{(k+1)} = -\bar{\mathbf{R}}^{(k)}$

BUT: $\bar{\mathbf{R}}_i^{(k)} = \underline{\boldsymbol{\phi}}_i^T \, \underline{\mathbf{F}}_{\mathrm{int}} \left(\underline{\boldsymbol{\alpha}}^{(k)}(t); \left(\bar{\underline{\mathbf{U}}}(\tau)\right)_{\tau \le t} \right)$

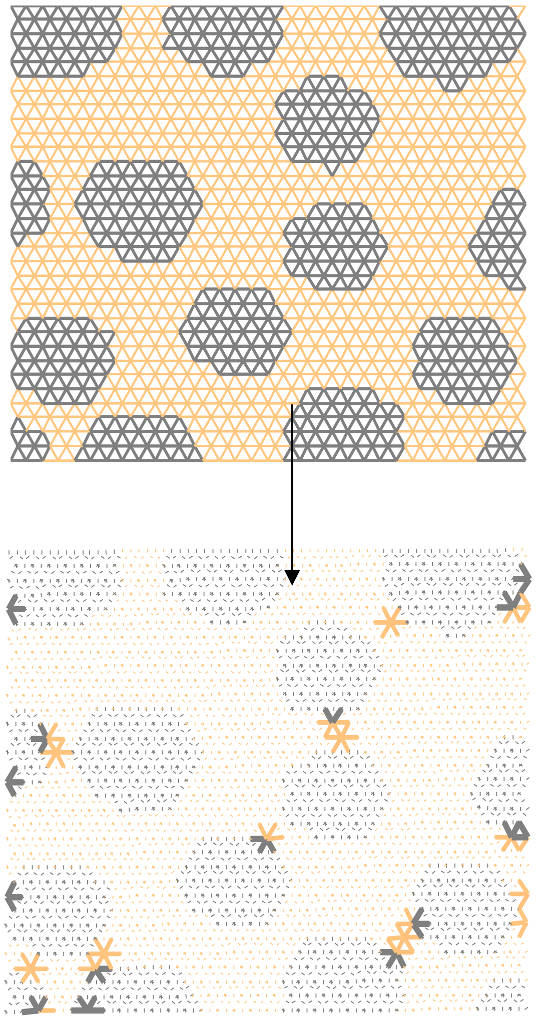
Requires integration, complexity depends on the underlying discretisation

Gappy approximation of nonlinear term

- Affine approximate of the nonlinear force vector

$$\underline{\mathbf{F}}_{\text{int}}\left(\underline{\boldsymbol{\alpha}}(t)+\delta\underline{\boldsymbol{\alpha}}\right)\approx\underline{\widetilde{\mathbf{F}}}_{\text{int}}=\sum_{i=1}^{\tilde{n}_{\phi}}\underline{\widetilde{\phi}}_{i}\beta_{i}=\underline{\underline{\tilde{\boldsymbol{\Phi}}}}\,\underline{\boldsymbol{\beta}}$$

Any variation around the Galerkin solution



- Coefficients of the expansion obtained optimally w.r.t. to sample points:

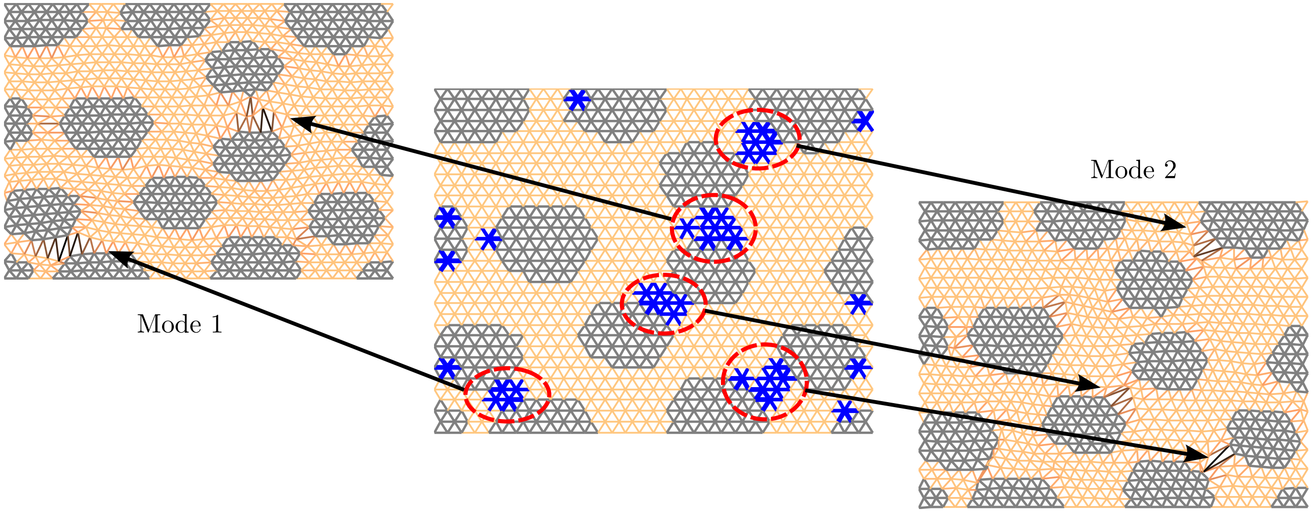
$$\underline{\boldsymbol{\beta}}=\arg\min\|\underline{\mathbf{F}}_{\text{int}}-\underline{\underline{\tilde{\boldsymbol{\Phi}}}}\,\underline{\boldsymbol{\beta}}\|_{\underline{\underline{\mathbf{X}}}}$$

$$\underline{\widetilde{\mathbf{F}}}_{\text{int}}=\underline{\underline{\mathbf{P}}}\,\underline{\mathbf{F}}_{\text{int}}=\left(\underline{\underline{\tilde{\boldsymbol{\Phi}}}}\left(\underline{\underline{\tilde{\boldsymbol{\Phi}}}}^{T}\underline{\underline{\mathbf{X}}}\,\underline{\underline{\tilde{\boldsymbol{\Phi}}}}\right)^{-1}\underline{\underline{\tilde{\boldsymbol{\Phi}}}}^{T}\underline{\underline{\mathbf{X}}}\right)\underline{\mathbf{F}}_{\text{int}}$$

Only the contributions of sample points are required

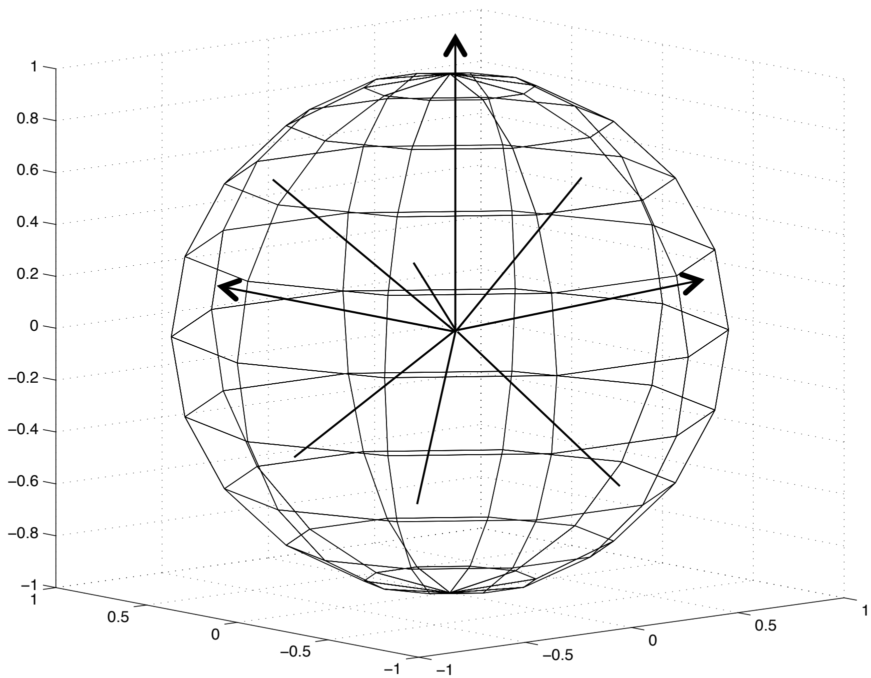
Choosing the parameters of the Gappy approx

- Basis functions: consistent approach $\underline{\mathbf{F}}_{\text{int}}\left(\underline{\boldsymbol{\alpha}}(t)+\delta\underline{\boldsymbol{\alpha}}\right)$
  - Basis obtained by standard empirical POD for
    - → In practice, solve the snapshots a second time using standard Galerkin-POD and use the residuals of the Newton solver
  - Truncate the POD expansion at an order such that displacement and stress errors are of the same order of magnitude
- Interpolation points minimise reconstruction error (EIM [Barrault '04], MPE [Astrid '08])



Test case

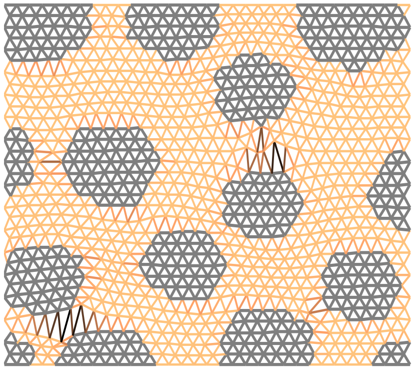
- Snapshot:



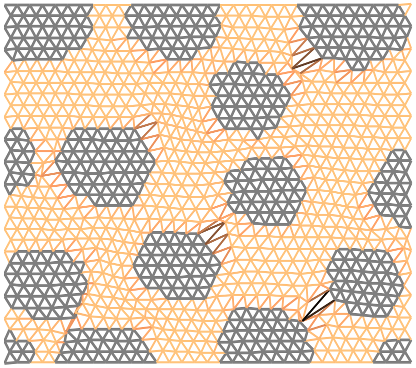
100 QR sampling in the macro strain space

SVD →

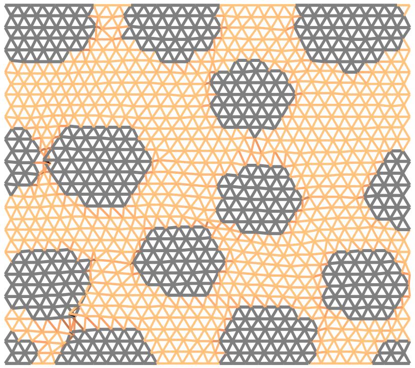
$\underline{\phi}_1$



$\underline{\phi}_2$



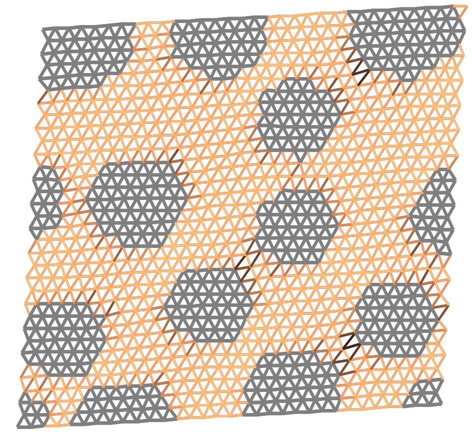
$\underline{\phi}_3$

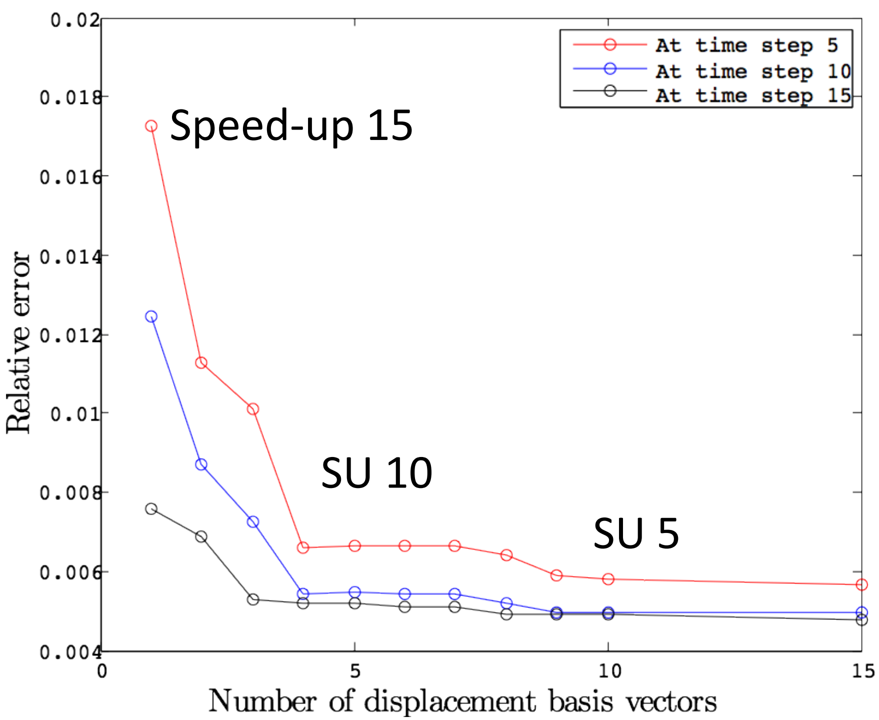


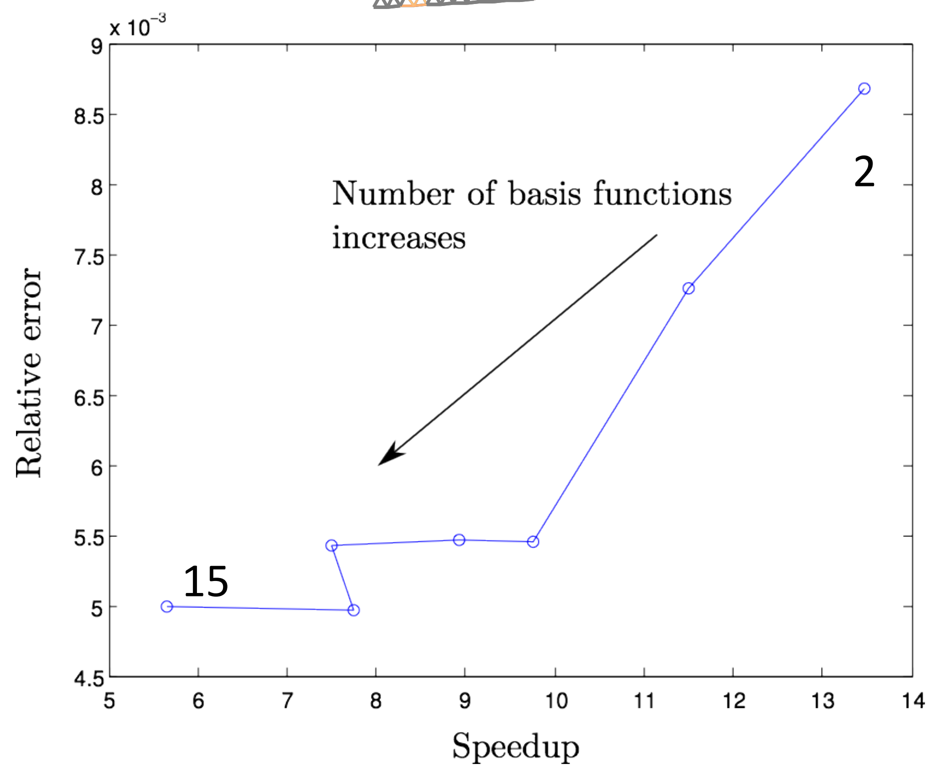
Speed-up

- Validation for one particular loading

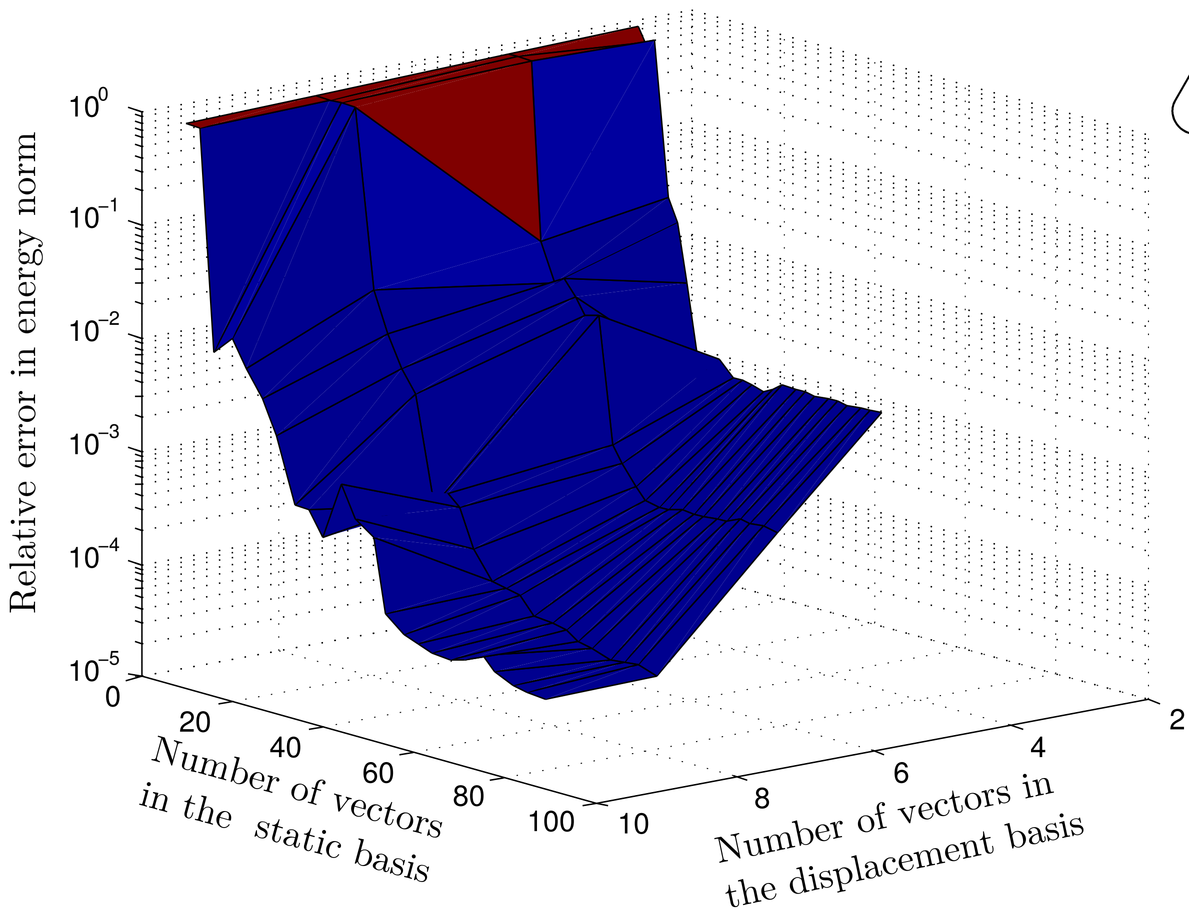
Last time step before localisation:



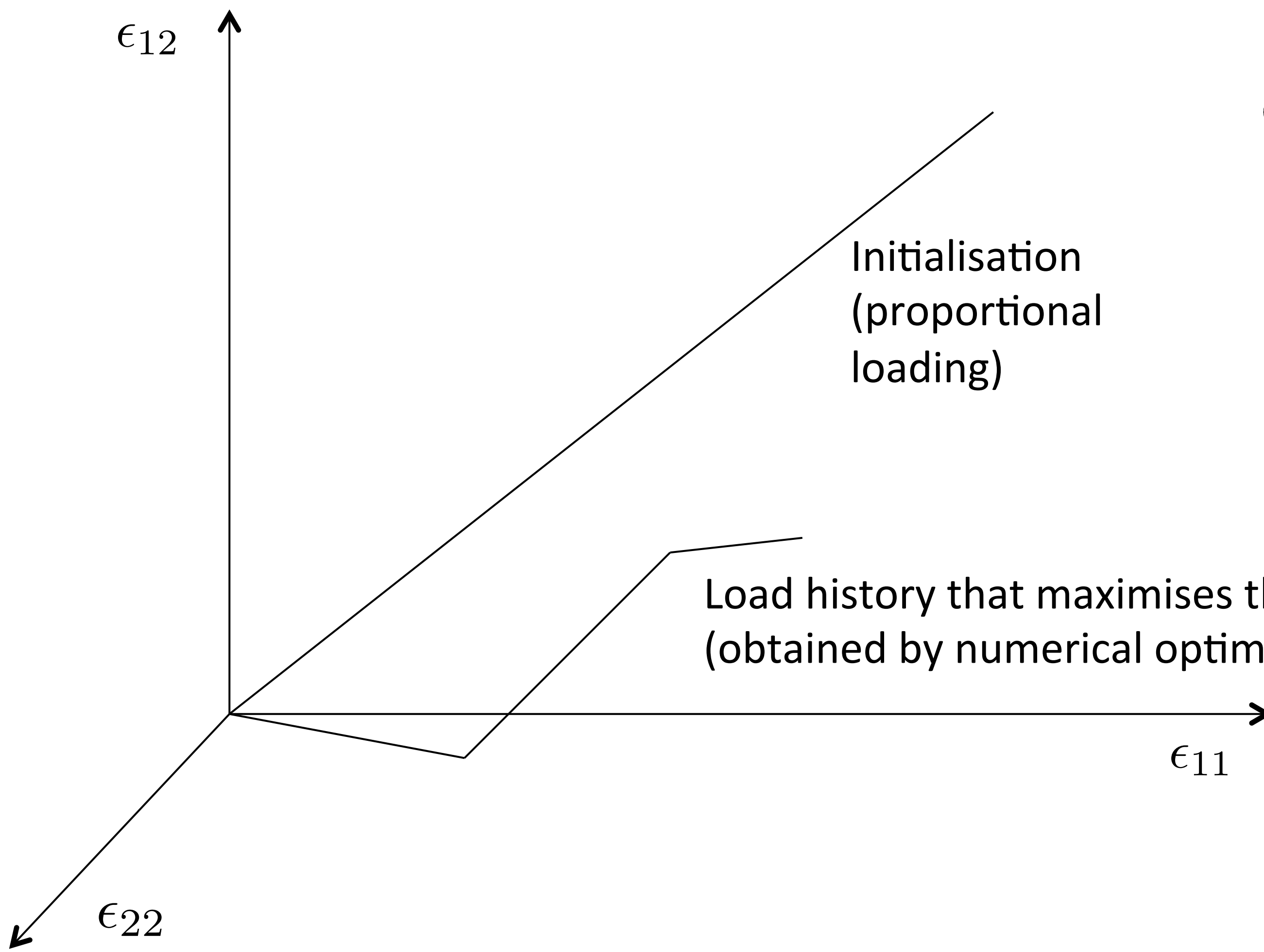




Optimal static vs kinematic surrogate sizes



Automatised snapshot selection



Conclusions

- Numerical solution of RVE problems avoids assumptions on microscale fields, but too expensive
- Reduced order modelling permits to alleviate this problem, but providing error-controlled approximations that seamlessly span from full-FE solution to highly-reduced RVE problems
- Open-question: multiscale modelling and reduced order modelling do the same thing: look for and use invariances in solution sets. Is there a more formal way to couple them?