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& Advanced Materials

A Model Order Reduction approach to construct efficient and reliable virtual charts in computational homogenisation

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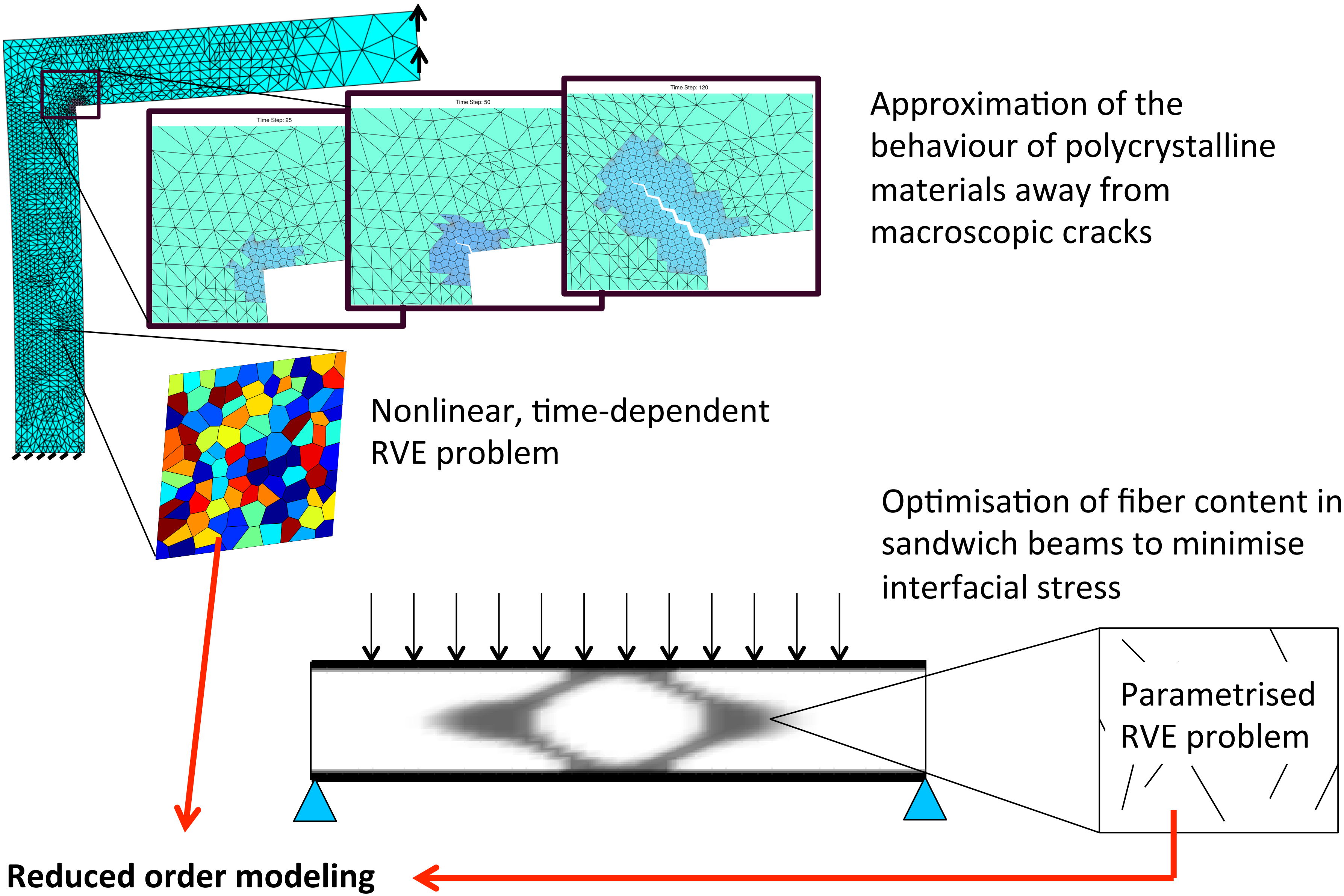
Multiscale modelling



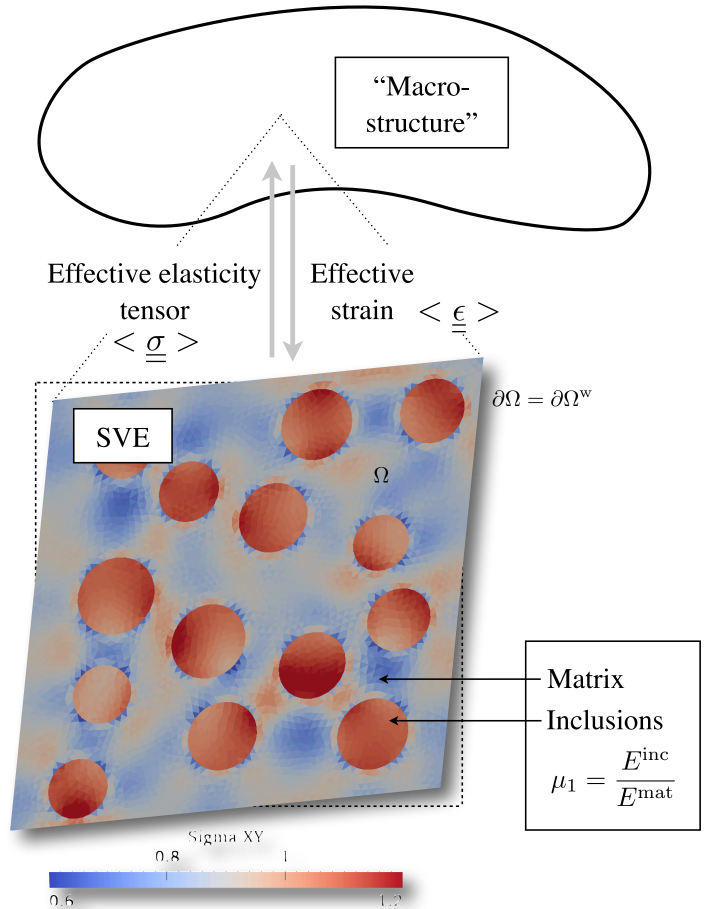
- Introduction

- CRE-driven reduced basis method (for the computational homogenisation of elastic material properties)

- Automatic snapshot selection in nonlinear computational homogenisation

Parametrised homogenisation in lin. elasticity

- Dirichlet localisation problem
  - $\mathrm{div}\ \underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) = 0$
  - $\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) = \underset{\sim}{D}(\mu_1) : \underline{\underline{\epsilon}}(\underline{u}^{\mathrm{h}}(\underline{\mu}))$
    Parametrised tensor field (affine)
  - Boundary conditions:
    $$\underline{u}^{\mathrm{h}}(\underline{\mu}) = \begin{pmatrix} \mu_2 & \mu_4 \\ \mu_4 & \mu_3 \end{pmatrix} \cdot \underline{x}$$



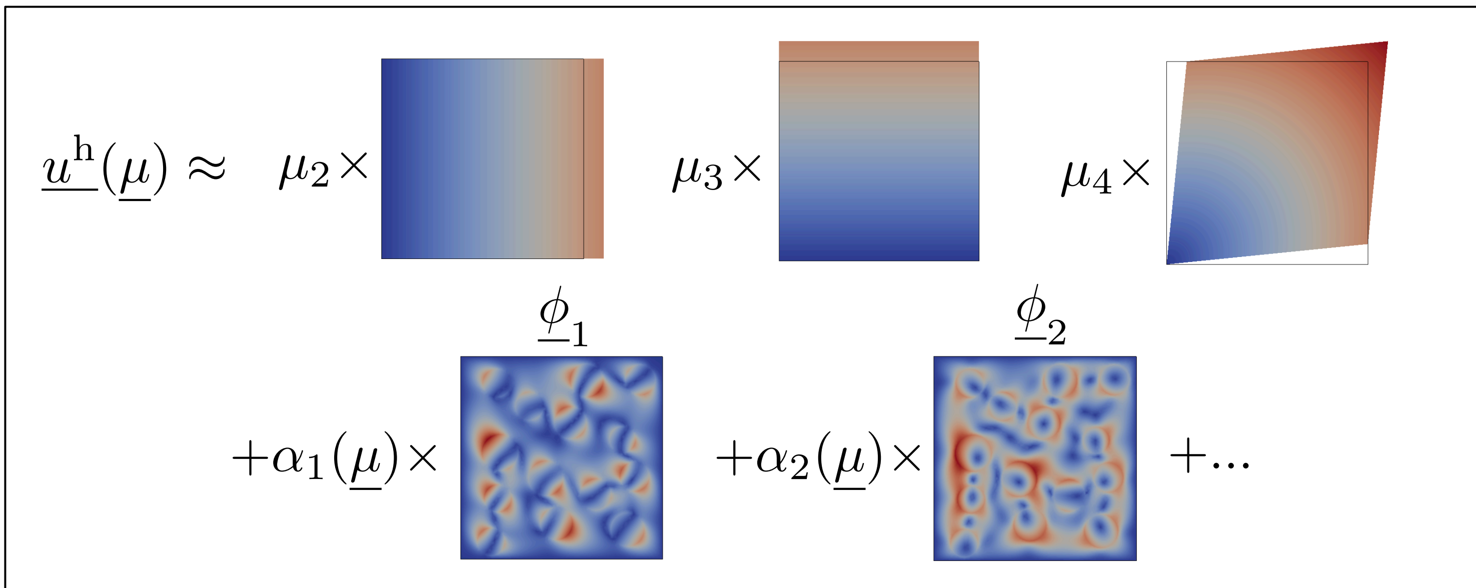
- Outputs:

$$\widetilde{Q}^{(i)}(\underline{u}^{\mathrm{h}}(\underline{\mu})) = \underline{\underline{\Sigma}}^{(i)} : \left(\frac{1}{|\Omega|} \int_{\Omega} \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^{\mathrm{h}}(\underline{\mu}))\, d\Omega \right)$$

ROM-based Virtual charts

- **Interpolate the fluctuation field** over parameter domain

  → For any applied macroscopic field, and **any elastic contrast**



"Macro field"

"Micro fluctuation"

Projection-based reduced order model

- Separation of variables:

“Micro fluctuation” “Macro field”

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

- Optimal generalised coordinates:

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

Projection-based reduced order model

- Separation of variables:

"Micro fluctuation"

"Macro field"

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

$$\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) \approx \widehat{\underline{\underline{\sigma}}}(\underline{\mu}) := \sum_{i=1}^{\tilde{n}_\phi} \widetilde{\underline{\underline{\phi}}}_i \, \widetilde{\alpha}_i(\underline{\mu})$$

"equilibrated"

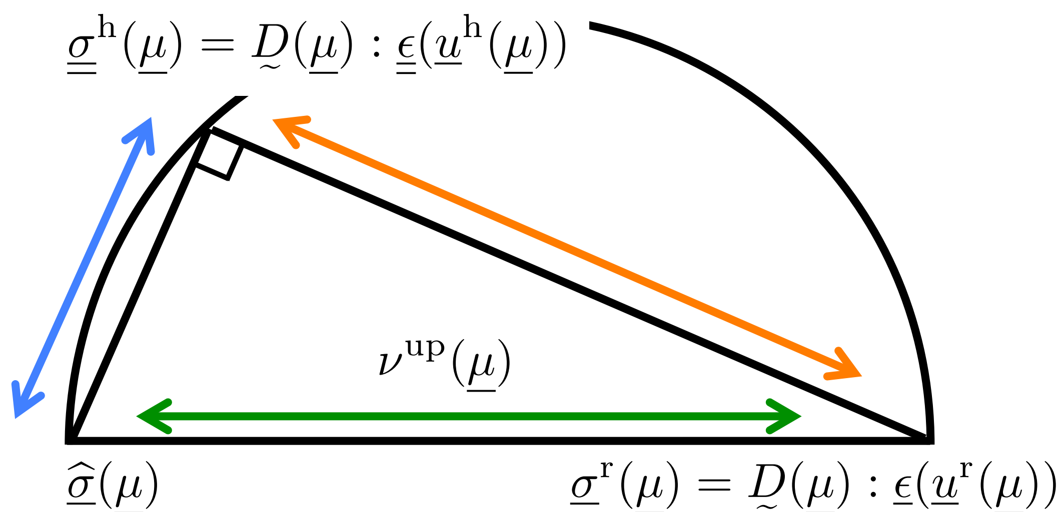
- Optimal generalised coordinates:

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

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

Error bounding by duality (CRE)

- Upper bound in energy norm: Error in the constitutive relation [Prager-Synge '47][Ladevèze '85]

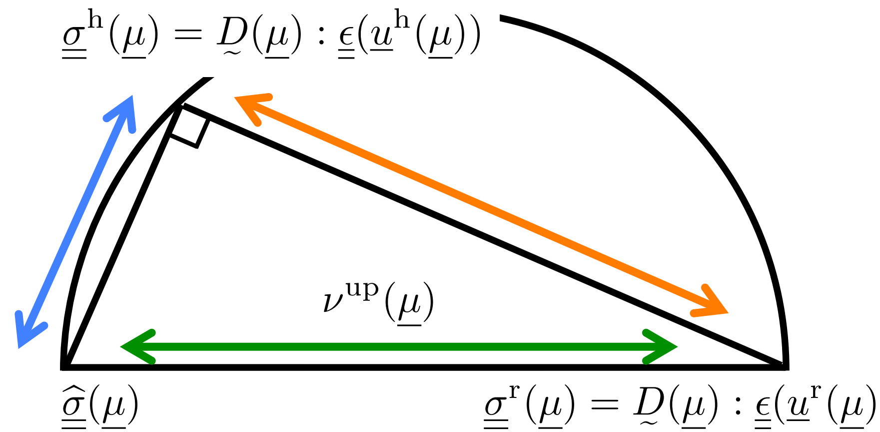


$$\nu^{\mathrm{up}}(\underline{\mu}) := \|\widehat{\underline{\underline{\sigma}}}(\underline{\mu}) - \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^{\mathrm{r}}(\underline{\mu}))\|^2_{\underset{\sim}{D}(\underline{\mu})^{-1}} = \|\underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}^{\mathrm{r}}(\underline{\mu})\|^2_{\underset{\sim}{D}(\underline{\mu})} + \|\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|^2_{\underset{\sim}{D}(\underline{\mu})^{-1}}$$

Related work in the context of PGD in [Ladevèze *et al.* '11]

CRE-driven reduced basis

- Initialise the two reduced spaces



- Greedy iterations
  - Detect the max of ν^{up} over the parameter domain
    - → Stop greedy if small enough
  - Evaluate the exact errors in stress and displacements by computing the reference solution

$$\|\underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}^{\mathrm{r}}(\underline{\mu})\|^2_{\underset{\sim}{D}(\underline{\mu})}$$

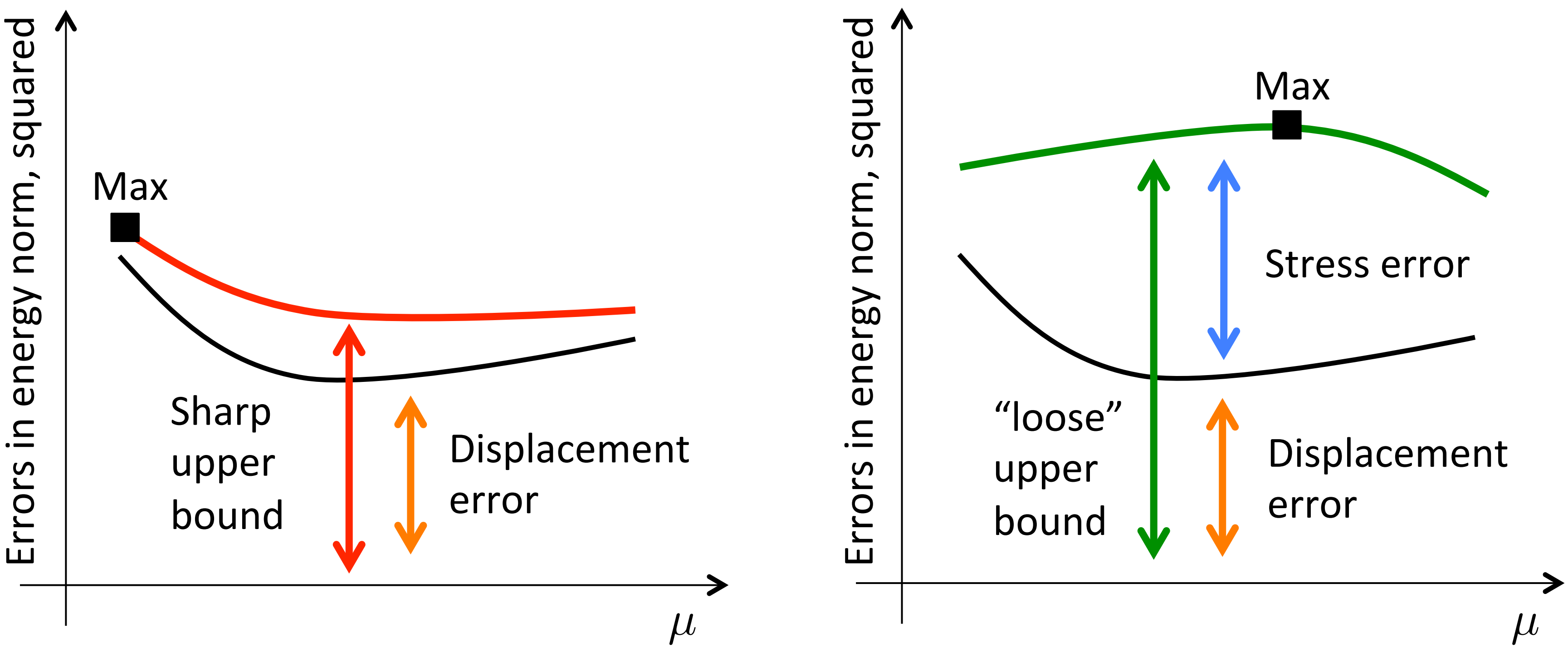
$$\|\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|^2_{\underset{\sim}{D}(\underline{\mu})^{-1}}$$

  - Depending on which of these error measures is the largest, enrich the displacement or stress ROM

Displacement-biased interpretation

RBM (with SCM bound)

CRE-driven RBM

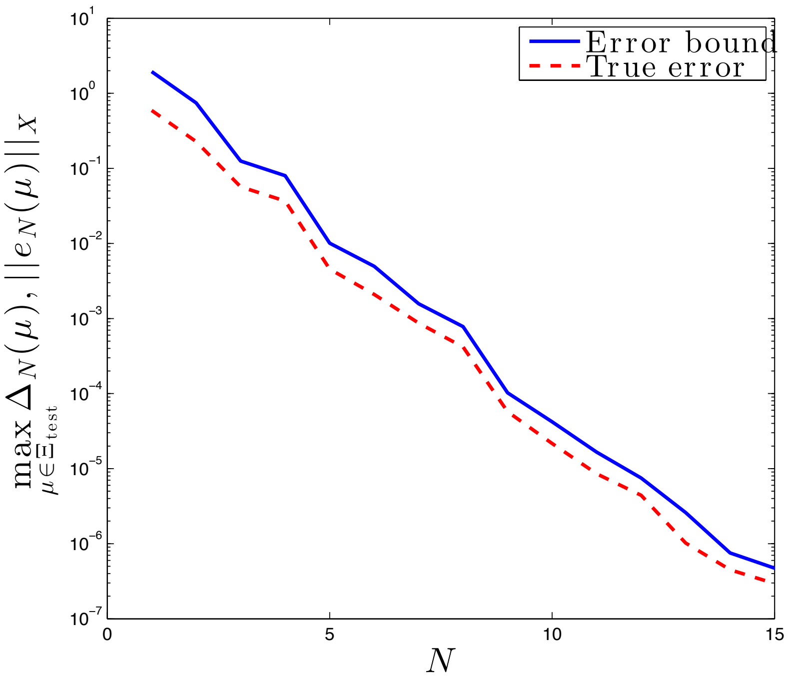


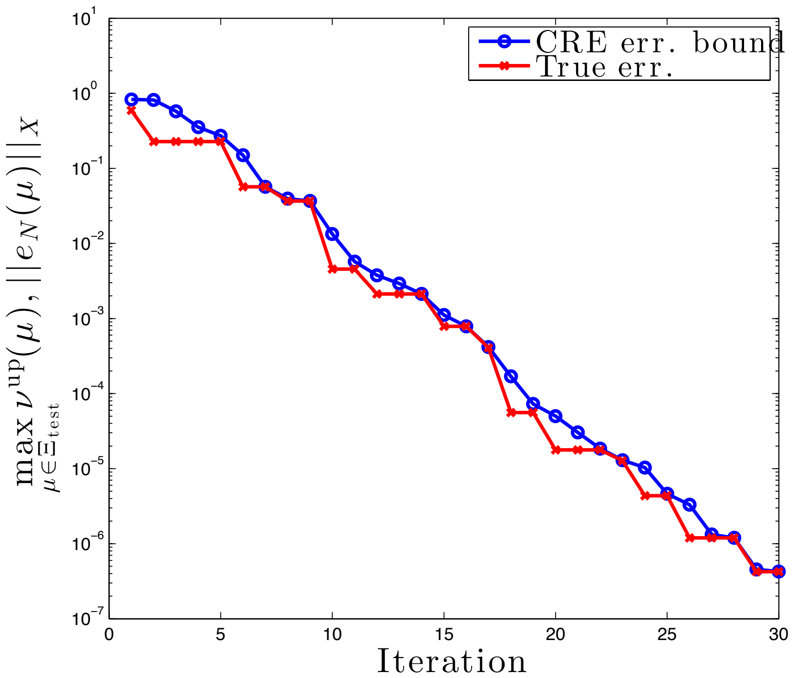
RBM: [Prud'homme *et al.* '02], SCM: [Huynh *et al.* '07]

Convergence results

RBM (with SCM bound)

CRE-driven RBM





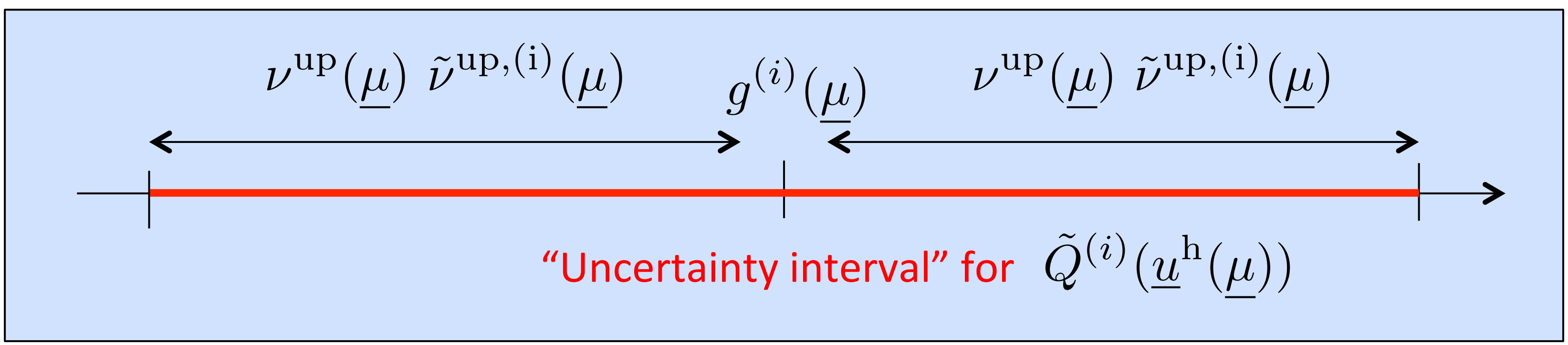
Goal-oriented variation

- Using standard duality arguments,

$$-\,\nu^{\mathrm{up}}(\underline{\mu})\;\tilde{\nu}^{\mathrm{up},(\mathrm{i})}(\underline{\mu}) + g^{(i)}(\underline{\mu}) \leq \tilde{Q}^{(i)}(\underline{u}^{\mathrm{h}}(\underline{\mu})) \leq \nu^{\mathrm{up}}(\underline{\mu})\;\tilde{\nu}^{\mathrm{up},(\mathrm{i})}(\underline{\mu}) + g^{(i)}(\underline{\mu})$$

CRE energy bound for adjoint problem I (solve with CRE-driven RBM)

CRE energy bound

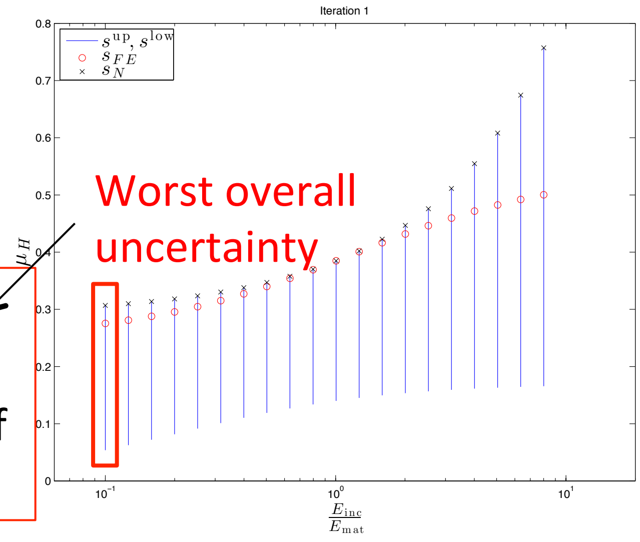


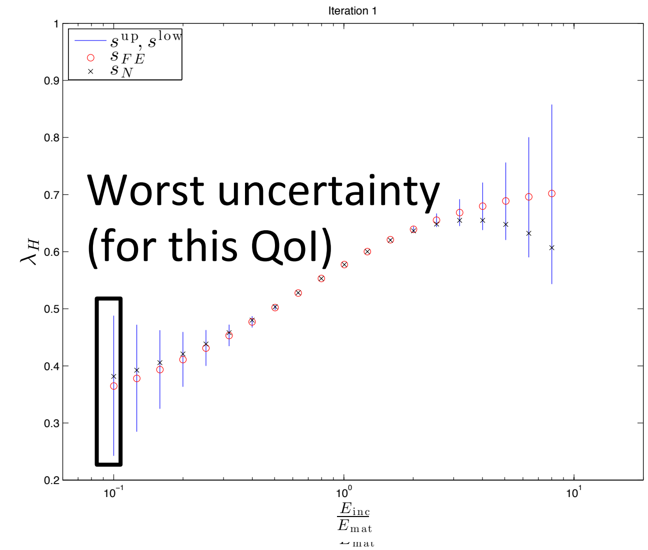
Goal-oriented variation

QoI 1 (overall bulk modulus)

QoI 2 (overall shear modulus)

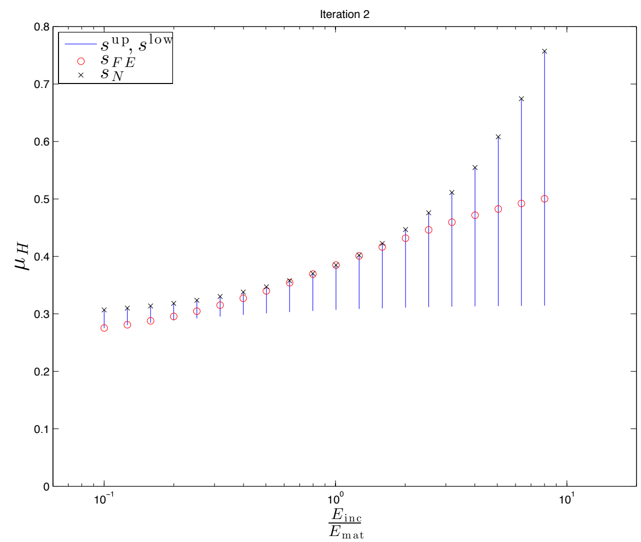
Iteration 1

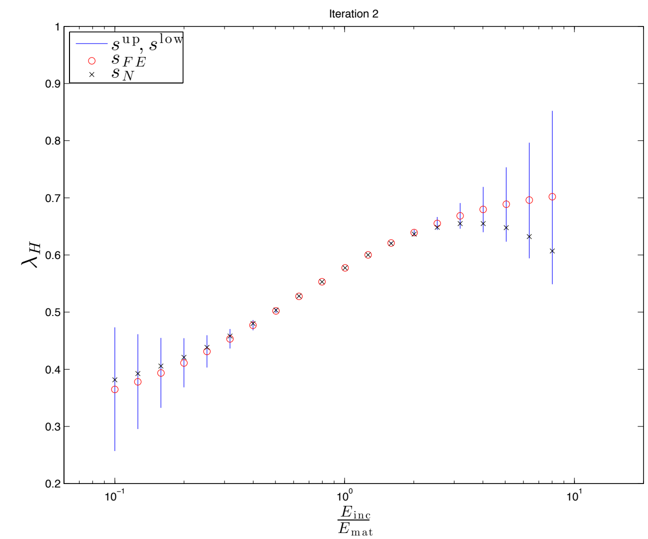




Best reduced by enriching displacement RB of adjoint problem

Iteration 2





Goal-oriented variation

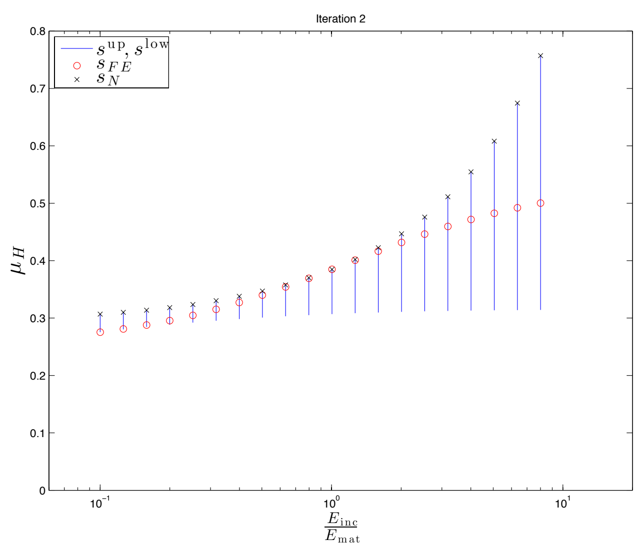
QoI 1 (overall bulk mudulus)

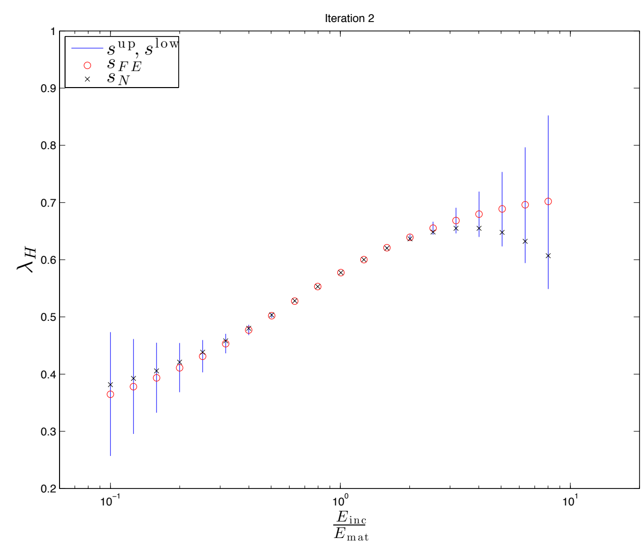
QoI 2 (overall shear modulus)

Iteration 1

Best reduced by enriching displacement of adjoint problem

Iteration 2





Goal-oriented variation

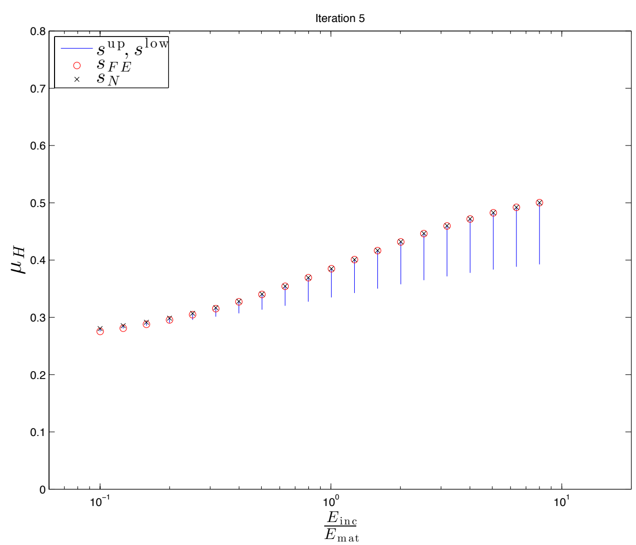
QoI 1 (overall bulk mudulus)

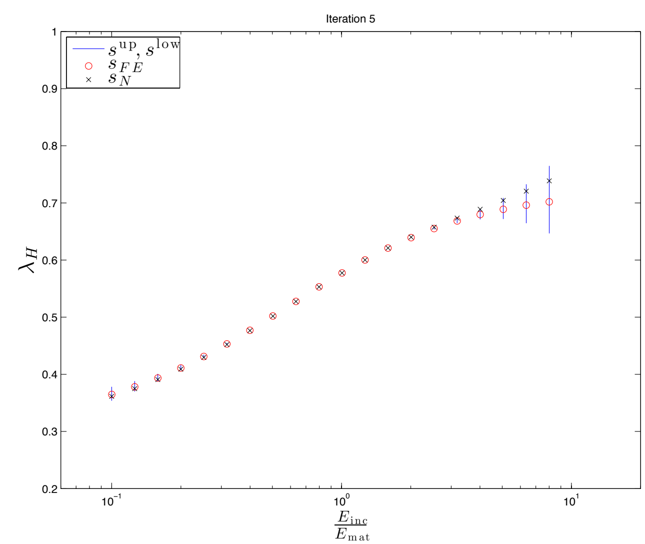
QoI 2 (overall shear modulus)

Iteration 1

Best reduced by enriching displacement of adjoint problem

Iteration 5





Goal-oriented variation

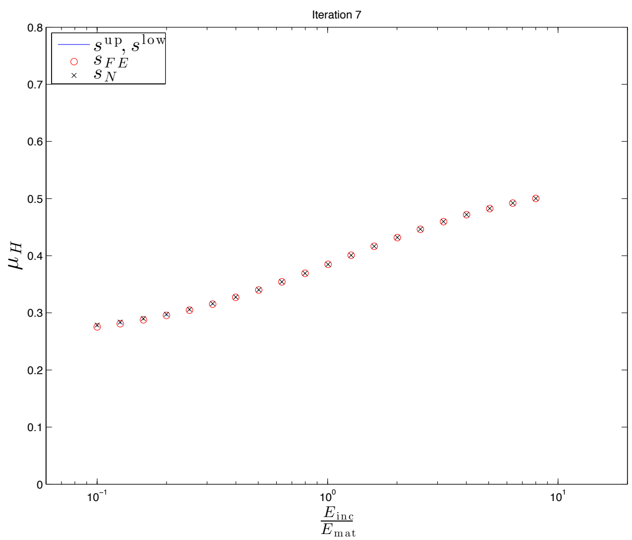
QoI 1 (overall bulk mudulus)

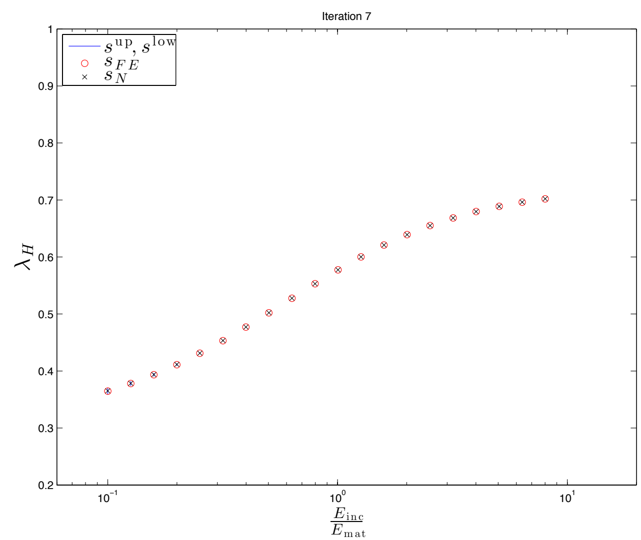
QoI 2 (overall shear modulus)

Iteration 1

Best reduced by enriching displacement of adjoint problem

Iteration 7





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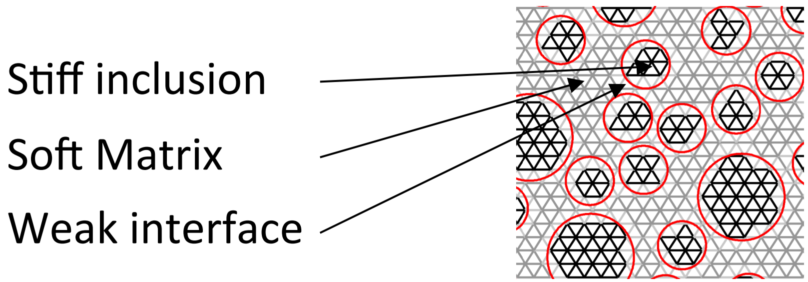
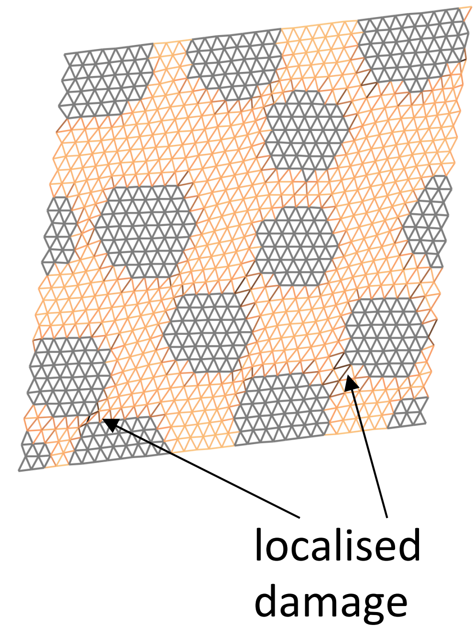
Damageable elastic material





- Modelled by a network of Euler-Bernouilli beams

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

"d_x": damage variable representing the extent of subscale networks of cracks

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

Parametrised Dirichlet localisation problem

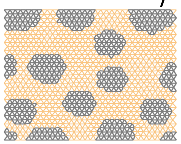
- Uniform Dirichlet BC:

$$\underline{\mathbf{U}}(t) = \underline{\bar{\mathbf{U}}}(t) + \underline{\widetilde{\mathbf{U}}}(t)$$

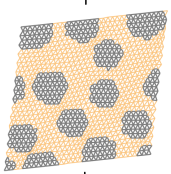
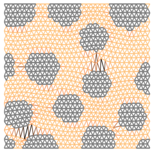
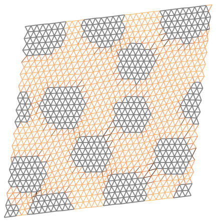
such that:

$$\underline{\underline{N}}(\underline{x})\,\underline{\bar{\mathbf{U}}}(t) = \begin{pmatrix} \epsilon_{11}^{\mathrm{M}}(t) & \epsilon_{12}^{\mathrm{M}}(t) \\ \epsilon_{12}^{\mathrm{M}}(t) & \epsilon_{22}^{\mathrm{M}}(t) \end{pmatrix} \cdot \underline{x}$$

Parameters (" Dimension 3 times number of time steps ")

$\epsilon_{11}^{\mathrm{M}}(t)\times$ 

$+$

$\epsilon_{12}^{\mathrm{M}}(t)\times$  +  = 

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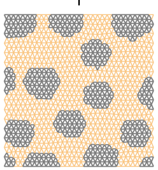
$\epsilon_{22}^{\mathrm{M}}(t)\times$ 

prescribed

Fluctuation, **vanishes on boundary**

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

- Fluctuation governed by equilibrium (discrete), for any load history:

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

Galerkin-ROM

- Surrogate for the displacement vector:

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

Macro displacment vector (known)

Generalised coordinates

Basis functions for fluctuation

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

- Hyper-reduction with Gappy-POD: $\boxed{\forall i \quad \underline{\boldsymbol{\phi}}_i^T \, \underline{\underline{\mathbf{P}}} \, \underline{\mathbf{F}}_{\mathrm{int}} \left(\underline{\boldsymbol{\alpha}}(t); \left(\underline{\bar{\mathbf{U}}}(\tau)\right)_{\tau \leq t} \right) = 0}$

Closely related work: **EIM, DEIM and GNAT** [Barrault *et al.* '04] [Chaturantabut *et al.* '10] [Carlberg *et al.* '11], **hyper-reduction** [Ryckelynck '05][Kerfriden *et al.* '10], **MPE** [Astrid *et al.* '08]

Snapshot: QR proportional loadings

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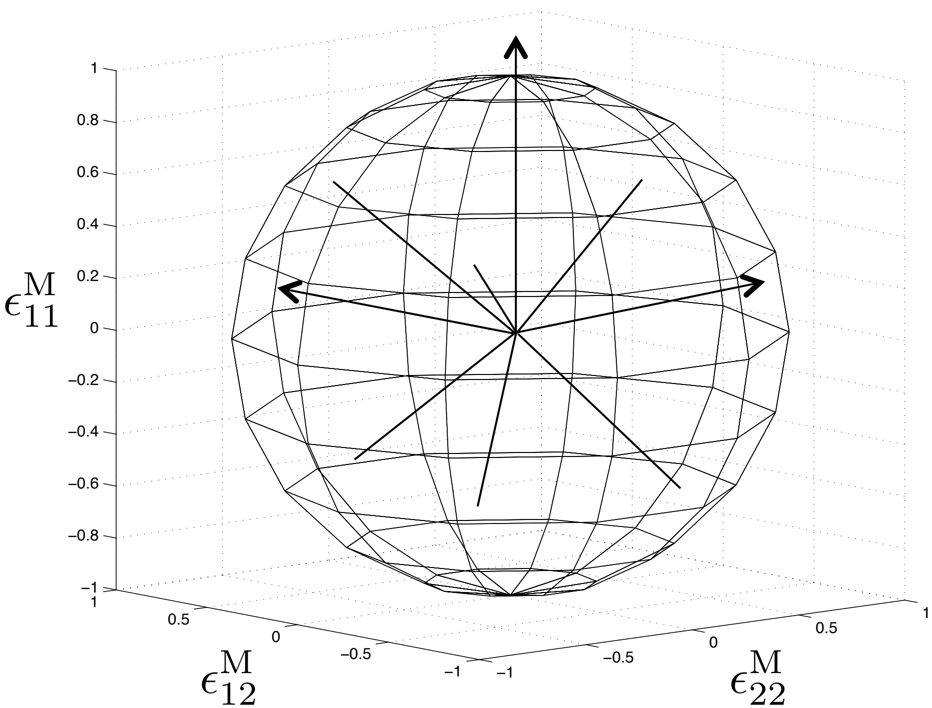


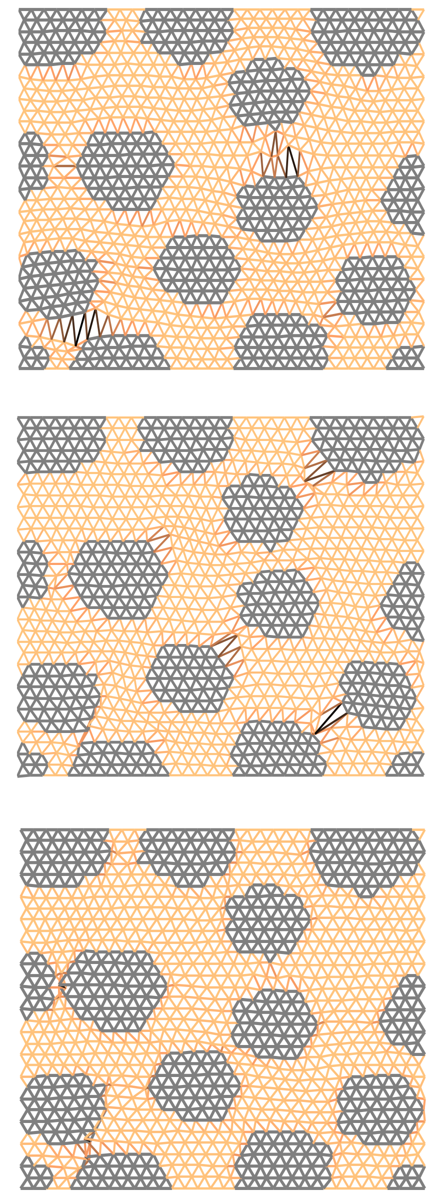
100 QR sampling in the macro strain space

SVD

$\underline{\phi}_1$

$\underline{\phi}_2$

$\underline{\phi}_3$



Reliable selection of non-proportional loadings

- Initialise snapshot $S^0 \equiv \left(\epsilon^{\mathrm{M},(0)}(t) \,|\, t \in [\![0, t_{n_t}]\!]\right)$ and TSVD of order M^0

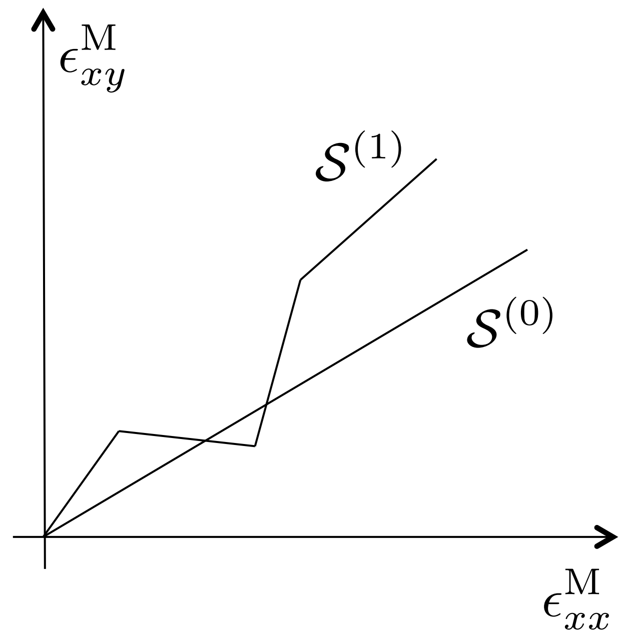
- POD-Greedy iterations

  - Look for the load of worst prediction $\tilde{S}^{(i)} \equiv \left(\epsilon^{\mathrm{M},(\mathrm{i})}(t) \,|\, t \in [\![0, t_{n_t}]\!]\right)$

    → Out if error small enough

    and TSVD of order M^i

  - TSVD order N^i ($N^{i-1} < N^i <= N^{i-1} + M^i$) on all available RB functions to avoid duplicated info



Related methods: **POD-Greedy** [Haasdonk et al. ‘08], **optimisation-based Greedy** [Bui-Thanh *et al.* ‘08] **optimal snaphot location** [Kunisch *et al*. ‘10]

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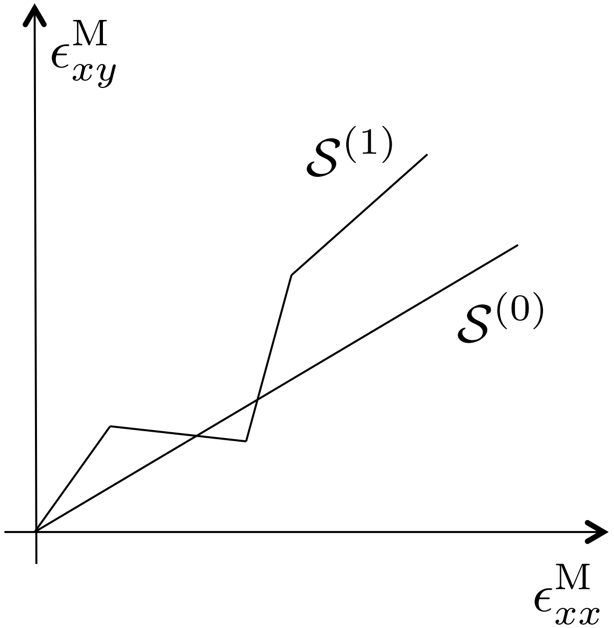

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Reliable selection of non-proportional loadings

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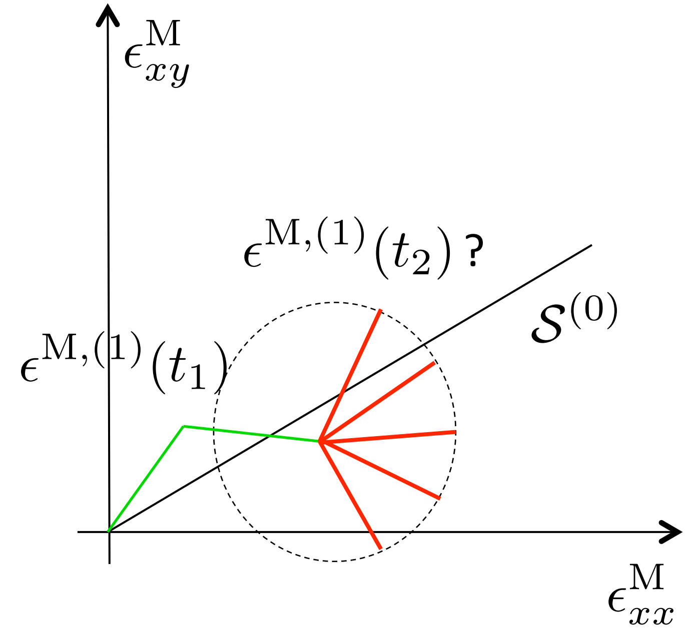
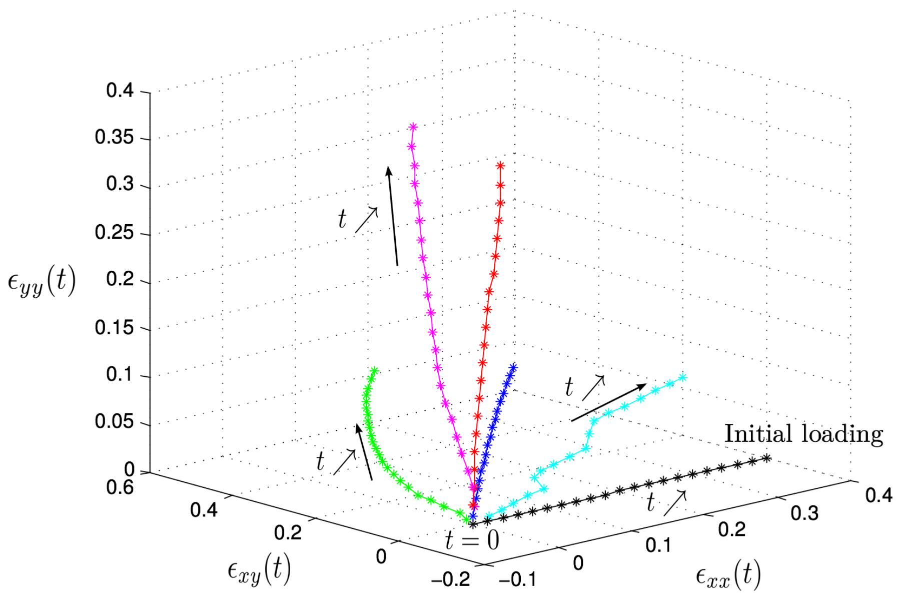
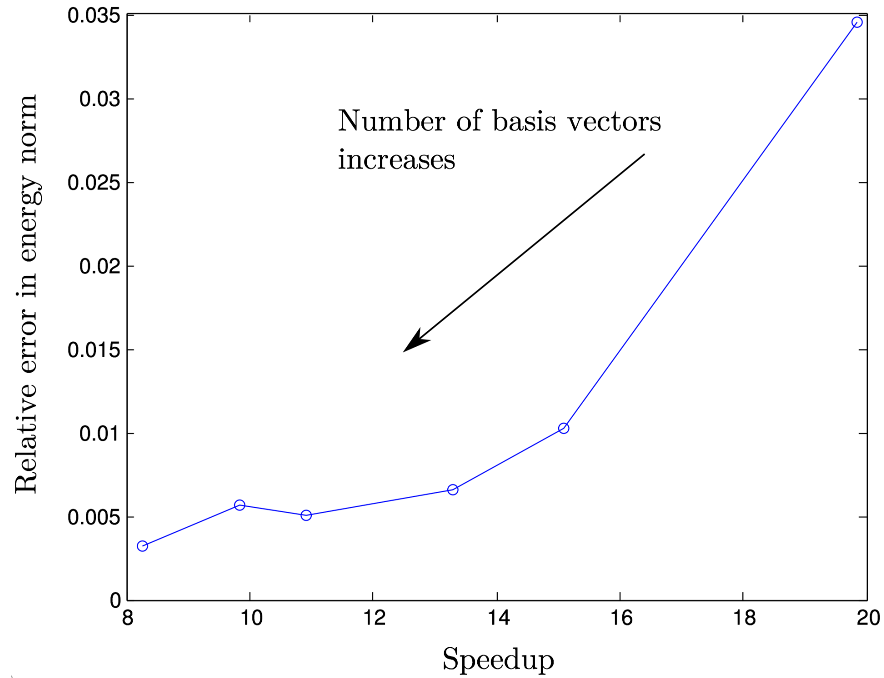


Time-sequence of indendent 3D optimisation problems: gradient descent with numerical perturbation and bissection-type line search

Some (qualitative) results





Conclusions

- RBM is ideal to build virtual charts and reduced models in computational homogenisation: significant reduction of the costs associated with RVEs with control of errors
  - → Next step: integration in FE^2
- New parameter-free RBM for elliptic problems, should be applicable to parabolic problems
  - → Next step: parametrised geometry of inclusions
- Efficient snapshot selection procedure for time-dependent parameters
  - → Extension to stability control?