Fast, certified and "tuning-free" two-field reduced basis method for the meta-modelling of parametrised elasticity problems

Khac Chi Hoang[1,*],
Pierre Kerfriden[1], Stéphane Bordas[1,2]

[1] Advanced Materials and Computational Mechanics Group, School of Engineering, Cardiff University, UK

[2] Faculté des Sciences, de la Technologie et de la Communication, University of Luxembourg, LU

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2. Projection-based reduced order models
3. Error estimation
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   - Goal-oriented error bounds
4. Sampling strategies
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Parametrised problems of linear elasticity

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- Parametrised principle of virtual work

$$\int_{\Omega} \sigma^{\mathrm{h}}(\mu) : \epsilon(v)\, d\Omega = \int_{\Omega} b(\mu)\, v\, d\Omega + \int_{\partial\Omega^{\mathrm{t}}} t(\mu)\, v\, d\Gamma, \;\; \forall v \in \mathcal{U}^{\mathrm{h},0}(\Omega), \mu \in \mathcal{D}$$

$$a\left(u^{\mathrm{h}}(\mu), v; \mu\right) = f\left(v; \mu\right), \;\; \forall v \in \mathcal{U}^{\mathrm{h},0}(\Omega), \mu \in \mathcal{D}$$

- Constitutive relation

$$\sigma^{\mathrm{h}}(\mu) = D(\mu) : \epsilon(u^{\mathrm{h}}(\mu))$$

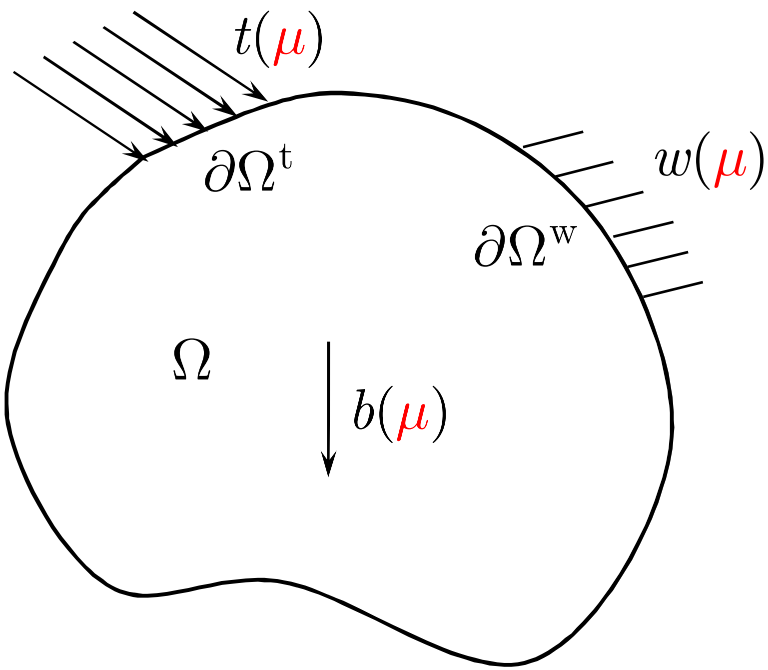
$$\epsilon\left(u^{\mathrm{h}}(\mu)\right) = \frac{1}{2}\left(\nabla u^{\mathrm{h}}(\mu) + \nabla u^{\mathrm{h}}(\mu)^{T}\right)$$

- Nonhomogeneous Dirichlet BC

$$u^{\mathrm{h}}(\mu) = w(x, \mu), \;\; x \in \partial\Omega^{\mathrm{w}}$$

- Outputs (Quantity of Interest)

$$Q_i\left(u^{\mathrm{h}}(\mu)\right) = \ell_i\left(u^{\mathrm{h}}(\mu)\right), \;\; 1 \le i \le n_{\mathrm{Q}}$$



Affine decomposition assumption

- Parametrised data are given in the forms of separate variables

$$D(\mu, x) = \sum_{i=1}^{n_{\mathrm{d}}} \gamma_i^{\mathrm{d}}(\mu) \bar{D}_i(x), \qquad \forall \mu \in \mathcal{D}, \forall x \in \Omega$$

$$t(\mu, x) = \sum_{i=1}^{n_{\mathrm{t}}} \gamma_i^{\mathrm{t}}(\mu) \bar{t}_i(x), \qquad \forall \mu \in \mathcal{D}, \forall x \in \partial\Omega^{\mathrm{t}}$$

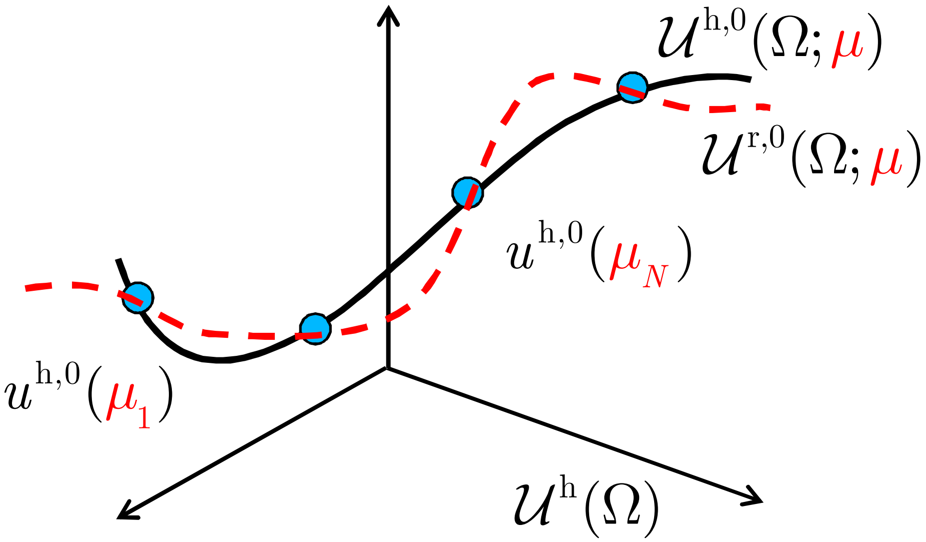
$$b(\mu, x) = \sum_{i=1}^{n_{\mathrm{b}}} \gamma_i^{\mathrm{b}}(\mu) \bar{b}_i(x), \qquad \forall \mu \in \mathcal{D}, \forall x \in \Omega$$

$$w(\mu, x) = \sum_{i=1}^{n_{\mathrm{w}}} \gamma_i^{\mathrm{w}}(\mu) \bar{w}_i(x), \qquad \forall \mu \in \mathcal{D}, \forall x \in \partial\Omega^{\mathrm{w}}$$

- Energy norms

$$\left\| u^{\star} \right\|_{D(\mu)} = \left(\int_{\Omega} \epsilon(u^{\star}) : D(\mu) : \epsilon(u^{\star}) d\Omega \right)^{1/2} ; \quad \left\| \sigma^{\star} \right\|_{D(\mu)^{-1}} = \left(\int_{\Omega} \sigma^{\star} : D(\mu)^{-1} : \sigma^{\star} \, d\Omega \right)^{1/2}$$

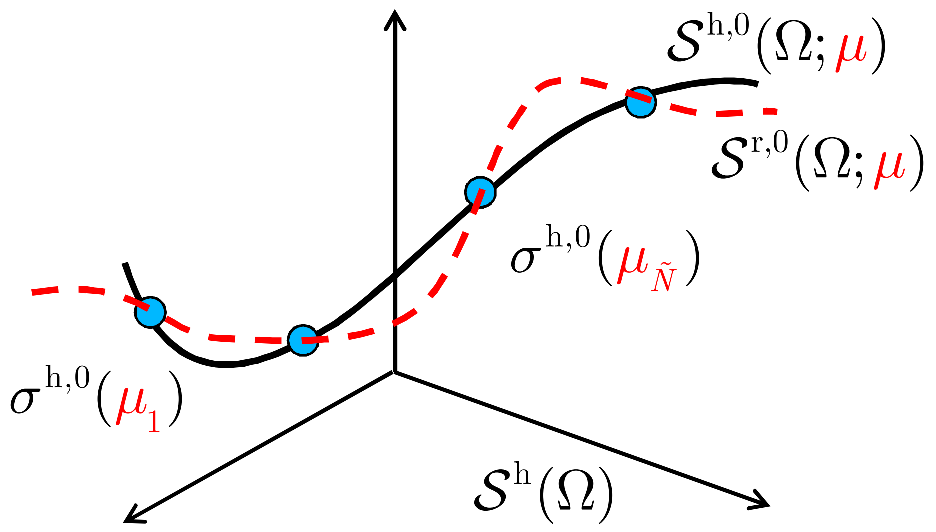
ROM: Parametrised settings



Displacement field

- Opportunities & collaborations
  - *Smooth* and *low-dimensional* parametrically induced manifold $\mathcal{U}^{\mathrm{h},0}(\Omega;\mu)$
  - Parametric setting -> decouple computational tasks to 2 stages: *Offline* (once, expensive) and *Online* (numerous, cheap) stages thanks to the affine decomposition

ROM: Parametrised settings



Stress field

- Opportunities & collaborations
  - *Smooth* and *low-dimensional* parametrically induced manifold $\mathcal{S}^{\mathrm{h},0}(\Omega;\mu)$
  - Parametric setting -> decouple computational tasks to 2 stages: *Offline* (once, expensive) and *Online* (numerous, cheap) stages thanks to the affine decomposition

- Separation of variables

Greedy sampling

$$u^{\mathrm{h}}(\mu) \approx u^{\mathrm{r}}(\mu) := \sum_{n=1}^{N} \alpha_n(\mu)\, \phi_n + u^{\mathrm{h,p}}(\mu), \quad \forall \mu$$

$$\mathcal{Z}_N = \{\phi_n, 1 \leq n \leq N\}$$

- Optimal generalised coordinates

$$(\alpha_n)_{1\leq n\leq N} = \underset{u^{\star}(\mu)=\sum_{n=1}^{N}\alpha_n(\mu)\phi_n + u^{\mathrm{h,p}}(\mu)}{\arg\min} \left(\| u^{\mathrm{h}}(\mu) - u^{\star}(\mu) \|_{D(\mu)} \right)$$

$$N \ll \mathcal{N}$$

Projection-based reduced order models

- Separation of variables

Greedy sampling

$$\underbrace{u^{\mathrm{h}}(\mu) \approx u^{\mathrm{r}}(\mu) := \sum_{n=1}^{N} \alpha_n(\mu)\,\phi_n + u^{\mathrm{h,p}}(\mu), \quad \forall \mu}$$

$$\mathcal{Z}_N = \{\phi_n, 1 \le n \le N\}$$

$$\sigma^{\mathrm{h}}(\mu) \approx \hat{\sigma}(\mu) := \sum_{m=1}^{\tilde{N}} \tilde{\alpha}_m(\mu)\,\tilde{\phi}_m + \sigma^{\mathrm{h,p}}(\mu), \quad \forall \mu$$

$$\tilde{\mathcal{Z}}_{\tilde{N}} = \{\tilde{\phi}_m, 1 \le m \le \tilde{N}\}$$

Greedy sampling

- Optimal generalised coordinates

$$(\alpha_n)_{1\le n\le N} = \underset{u^\star(\mu)=\sum_{n=1}^{N}\alpha_n(\mu)\phi_n + u^{\mathrm{h,p}}(\mu)}{\arg\min} \left(\| u^{\mathrm{h}}(\mu) - u^\star(\mu) \|_{D(\mu)} \right)$$

$$(\tilde{\alpha}_m)_{1\le m\le \tilde{N}} = \underset{\sigma^\star(\mu)=\sum_{m=1}^{\tilde{N}}\tilde{\alpha}_m \tilde{\phi}_m(\mu) + \sigma^{\mathrm{h,p}}(\mu)}{\arg\min} \left(\| \sigma^{\mathrm{h}}(\mu) - \sigma^\star(\mu) \|_{D(\mu)^{-1}} \right)$$

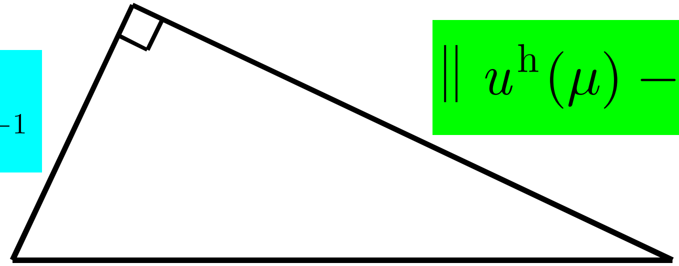
$$N, \tilde{N} \ll \mathcal{N}$$

Error estimation (CRE)

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

$$\sigma^{\mathrm{h}}(\mu) = D(\mu) : \epsilon(u^{\mathrm{h}}(\mu))$$

$$\| \sigma^{\mathrm{h}}(\mu) - \hat{\sigma}(\mu) \|_{D(\mu)^{-1}}$$



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

$$\hat{\sigma}(\mu) \qquad \Delta^{\mathrm{CRE}}(\mu) \qquad \sigma^{\mathrm{r}}(\mu) = D(\mu) : \epsilon(u^{\mathrm{r}}(\mu))$$

$$\Delta^{\mathrm{CRE}}(\mu)^2 = \| \sigma^{\mathrm{r}}(\mu) - \hat{\sigma}(\mu) \|^2_{D(\mu)^{-1}} = \| u^{\mathrm{h}}(\mu) - u^{\mathrm{r}}(\mu) \|^2_{D(\mu)} + \| \sigma^{\mathrm{h}}(\mu) - \hat{\sigma}(\mu) \|^2_{D(\mu)^{-1}}$$

$$\boxed{\Delta^{\mathrm{CRE}}(\mu) \equiv \| \sigma^{\mathrm{r}}(\mu) - \hat{\sigma}(\mu) \|_{D(\mu)^{-1}} \geq \| u^{\mathrm{h}}(\mu) - u^{\mathrm{r}}(\mu) \|_{D(\mu)}}$$

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

Goal-oriented error bounds

- Using duality argument [Rozza *et al.* ‘08][Oden *et al.* ‘01]: for noncompliant output, $1 \le i \le n_{\mathrm{Q}}$

$$Q_i^{\mathrm{r}}(\mu) + R\left(z_i^{\mathrm{r},0}(\mu)\right) - \Delta^{\mathrm{CRE}}(\mu)\Delta_{z,i}^{\mathrm{CRE}}(\mu) \le Q_i^{\mathrm{h}}(\mu) \le Q_i^{\mathrm{r}}(\mu) + R\left(z_i^{\mathrm{r},0}(\mu)\right) + \Delta^{\mathrm{CRE}}(\mu)\Delta_{z,i}^{\mathrm{CRE}}(\mu)$$

Primal residual of dual/adjoint solution

CRE energy upper error bound

CRE upper error bound for dual/adjoint problem

- Special case: compliant output

$$Q^{\mathrm{r}}(\mu) \le Q^{\mathrm{h}}(\mu) \le Q^{\mathrm{r}}(\mu) + \Delta^{\mathrm{CRE}}(\mu)^2$$

$$\boxed{Q_i^{r,-}(\mu) \le Q_i^{\mathrm{h}}(\mu) \le Q_i^{r,+}(\mu)}$$

Goal-oriented error bounds (cont.)

- Quantities of Interest (QoI) relative gaps:

$$\boxed{\mathtt{gap}_i(\mu) = \frac{\mid Q_i^{\mathrm{r},+}(\mu) - Q_i^{\mathrm{r},-}(\mu) \mid}{1 / 2\left(\mid Q_i^{\mathrm{r},+}(\mu) \mid + \mid Q_i^{\mathrm{r},-}(\mu) \mid\right)}}$$

$$\Delta^{\mathrm{CRE}}(\mu)\Delta_{z,i}^{\mathrm{CRE}}(\mu) \qquad Q_i^{\mathrm{r}}(\mu) + R\left(z_i^{\mathrm{r},0}(\mu)\right) \qquad \Delta^{\mathrm{CRE}}(\mu)\Delta_{z,i}^{\mathrm{CRE}}(\mu)$$

"Uncertainty interval" for $Q_i\left(u^{\mathrm{h}}(\mu)\right)$

Two-field Greedy sampling strategy

- Initialize the two reduced spaces: $\mathcal{Z}_1 = \{\phi(\mu_1)\}$
  $\tilde{\mathcal{Z}}_1 = \{\tilde{\phi}(\mu_1)\}$
- **While** $\Delta^{\mathrm{CRE,max}} > \varepsilon^{\mathrm{tol}}$
  - Compute $\Delta^{\mathrm{CRE}}(\mu), \forall \mu \in \Xi_{\mathrm{train}}$ to find:

$$\mu^\star = \arg \max_{\mu \in \Xi_{\mathrm{train}}} \Delta^{\mathrm{CRE}}(\mu)$$

  - Test 1: $\mathcal{Z}_{N+1}^{\mathrm{test}} = \mathcal{Z}_N \cup \phi(\mu^\star)$, recompute $\Delta_1^{\mathrm{CRE}}(\mu^\star)$
  - Test 2: $\tilde{\mathcal{Z}}_{\tilde{N}+1}^{\mathrm{test}} = \tilde{\mathcal{Z}}_{\tilde{N}} \cup \tilde{\phi}(\mu^\star)$, recompute $\Delta_2^{\mathrm{CRE}}(\mu^\star)$

  - Actual enrichment depending on which “testing” set decreases $\Delta^{\mathrm{CRE}}(\mu^\star)$ the most
- **end**

Goal-oriented Greedy sampling strategy

- Initialize the four reduced spaces: primal displacement, primal stress, dual displacement and dual stress sets
- **While** $\mathtt{gap}^{\max} > \varepsilon_{\mathrm{gap}}^{\mathrm{tol}}$
  - Compute $\mathtt{gap}_i(\mu), \ \forall \mu \in \Xi_{\mathrm{train}}, 1 \leq i \leq n_{\mathrm{Q}}$ to find:

$$\left(\mu^\star, i_{\max}\right) = \arg \max_{\mu \in \Xi_{\mathrm{train}}, 1 \leq i \leq n_{\mathrm{Q}}} \mathtt{gap}_i(\mu)$$

  - Test 1: enrich RB primal displacement set, recompute $\mathtt{gap}_{i_{\max}}^1(\mu^\star)$
  - Test 2: enrich RB primal stress set, recompute $\mathtt{gap}_{i_{\max}}^2(\mu^\star)$
  - Test 3: enrich RB dual displacement set, recompute $\mathtt{gap}_{i_{\max}}^3(\mu^\star)$
  - Test 4: enrich RB dual stress set, recompute $\mathtt{gap}_{i_{\max}}^4(\mu^\star)$
  - Actual enrichment depending on which “testing” set decreases $\mathtt{gap}_{i_{\max}}^j(\mu^\star), 1 \leq j \leq 4$ the most
- **end**

Numerical Example: Material Homogenisation

- Dirichlet localisation problem

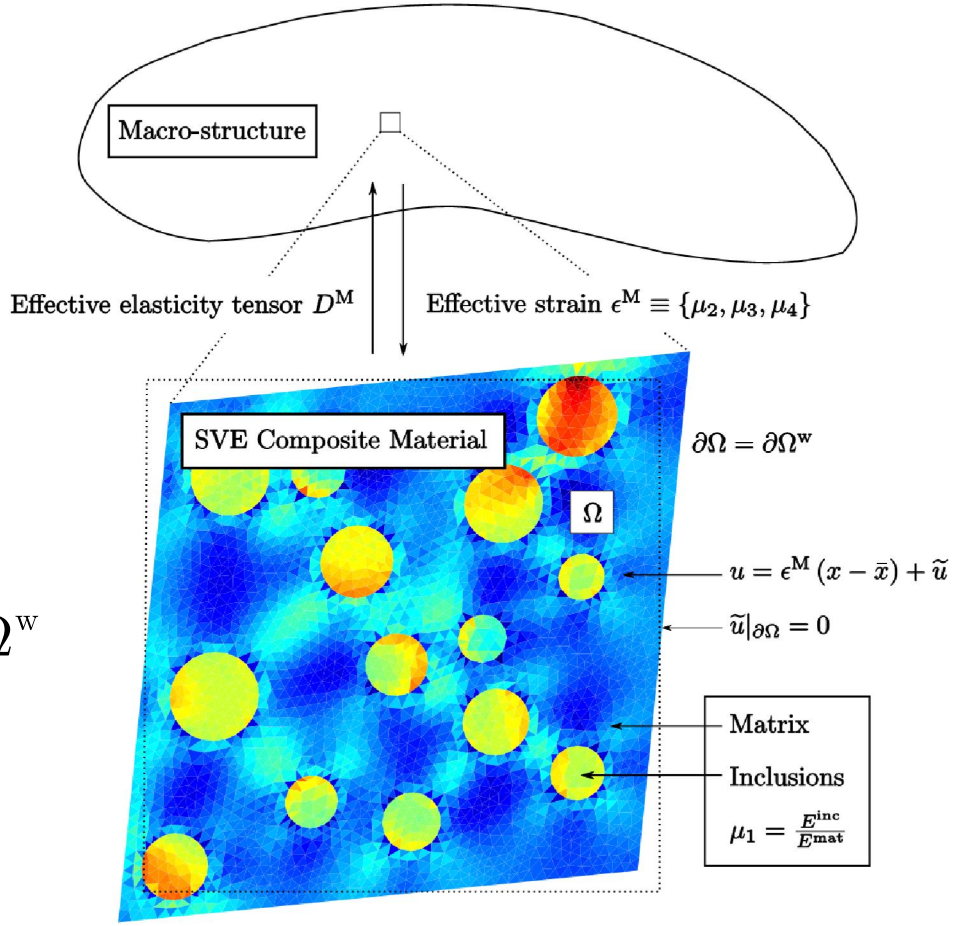
$$\mathrm{div}\ \sigma^{\mathrm{h}}(\mu) = 0$$

$$\sigma^{\mathrm{h}}(\mu) = D(\mu_1) : \epsilon(u^{\mathrm{h}}(\mu))$$

$\uparrow$

Parametrised tensor field (affine)

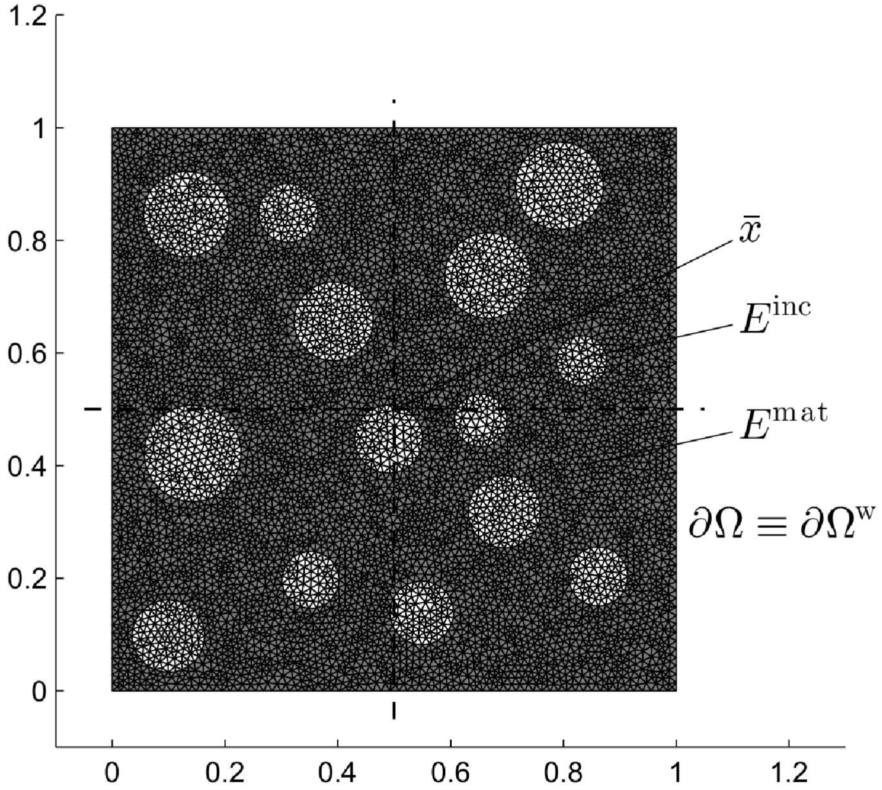
$$w(x,\mu) = \begin{pmatrix} \mu_2 & \mu_4 \\ \mu_4 & \mu_3 \end{pmatrix} . (x - \overline{x}), \quad x \in \partial\Omega^{\mathrm{w}}$$



- Outputs (Quantity of Interest)

$$Q_{(i)}(u^{\mathrm{h}}(\mu)) = \Sigma_{(i)} : \left(\frac{1}{|\,\Omega\,|} \int_{\Omega} D(\mu) : \epsilon(u^{\mathrm{h}}(\mu))\, d\Omega \right), \qquad 1 \le i \le n_{\mathrm{Q}}$$

Numerical results



FEM mesh: 7728 nodes, 15184 linear triangular elements $\mathcal{N} = 14196$

$$\mu \equiv \mu^G = \left(\mu_1, 0, 0, \frac{1}{2}\right); \ \Sigma_G = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}$$

$$\mu \equiv \mu^\lambda = \left(\mu_1, 1, 0, \frac{1}{\sqrt{2}}\right); \ \Sigma_\lambda = \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

$$\mu_1 = \frac{E^{\text{inc}}}{E^{\text{mat}}} \in \mathcal{D} \equiv [0.1, 10]$$

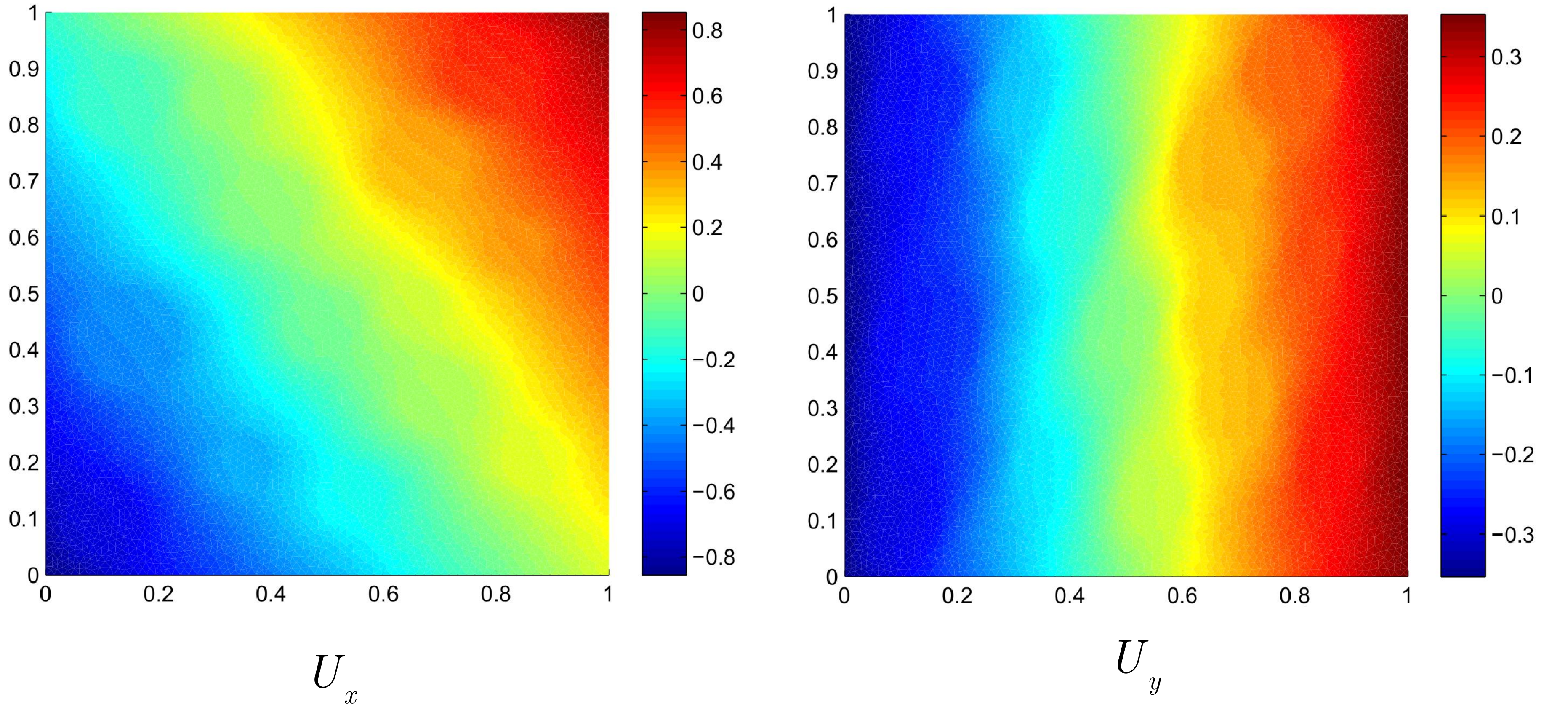
$$\int_\Omega \epsilon\left(u^{\text{h},0}(\mu)\right) : D(\mu) : \epsilon(v) d\Omega = -\int_\Omega \epsilon\left(u^{\text{h,p}}(\mu)\right) : D(\mu) : \epsilon(v) d\Omega, \quad \forall v \in \mathcal{U}^{\text{h},0}(\Omega)$$

$$G^{\text{h}}(\mu) = \ell^G\left(u^{\text{h}}(\mu)\right) = \frac{1}{|\Omega|}\int_\Omega \Sigma_G : D(\mu) : \epsilon(u^{\text{h}}(\mu)) d\Omega$$ Compliant output

$$\lambda^{\text{h}}(\mu) = \ell^\lambda\left(u^{\text{h}}(\mu)\right) = \frac{1}{|\Omega|}\int_\Omega \Sigma_\lambda : D(\mu) : \epsilon(u^{\text{h}}(\mu)) d\Omega$$ Noncompliant output

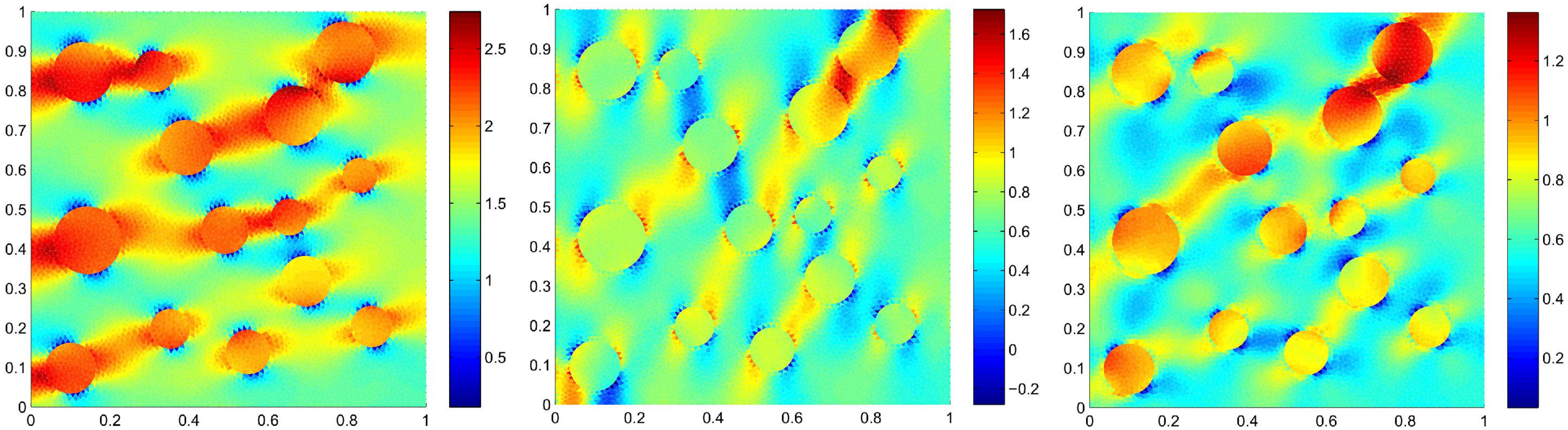
Numerical results

- FE displacement field with $\mu^{\text{test}} \equiv \mu^{\lambda} = \left(5, 1, 0, \dfrac{1}{\sqrt{2}}\right)$



Numerical results

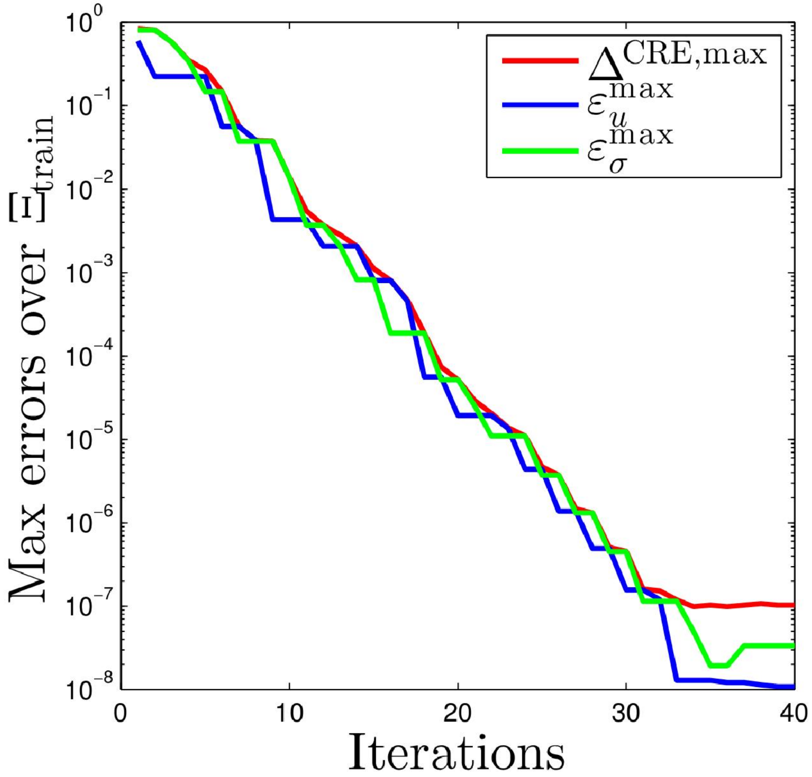
- FE stress field with $\mu^{\text{test}} \equiv \mu^{\lambda} = \left(5, 1, 0, \frac{1}{\sqrt{2}}\right)$

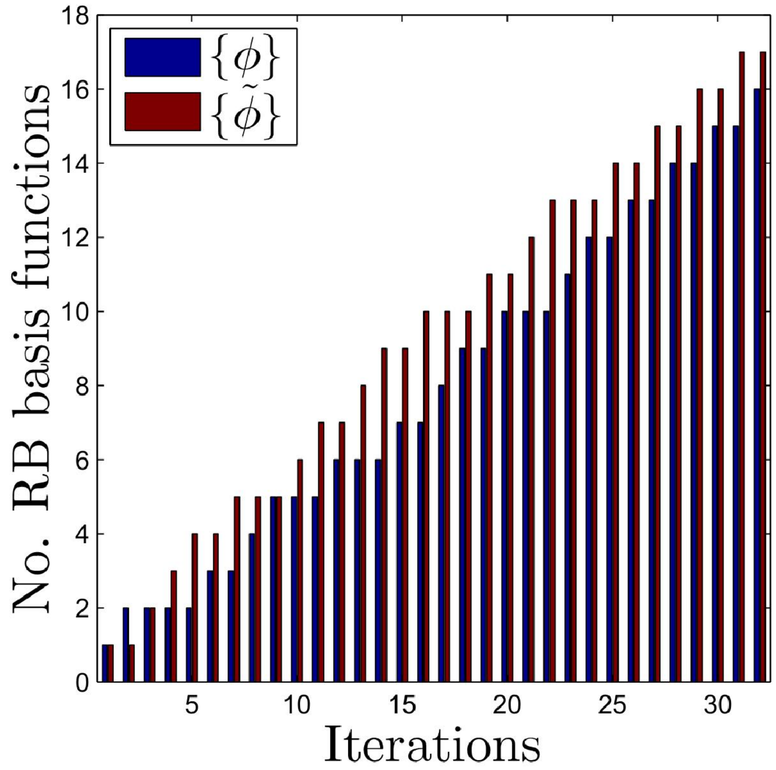


σ_{xx} σ_{yy} σ_{xy}

Numerical results

- Two-field Greedy sampling algorithm





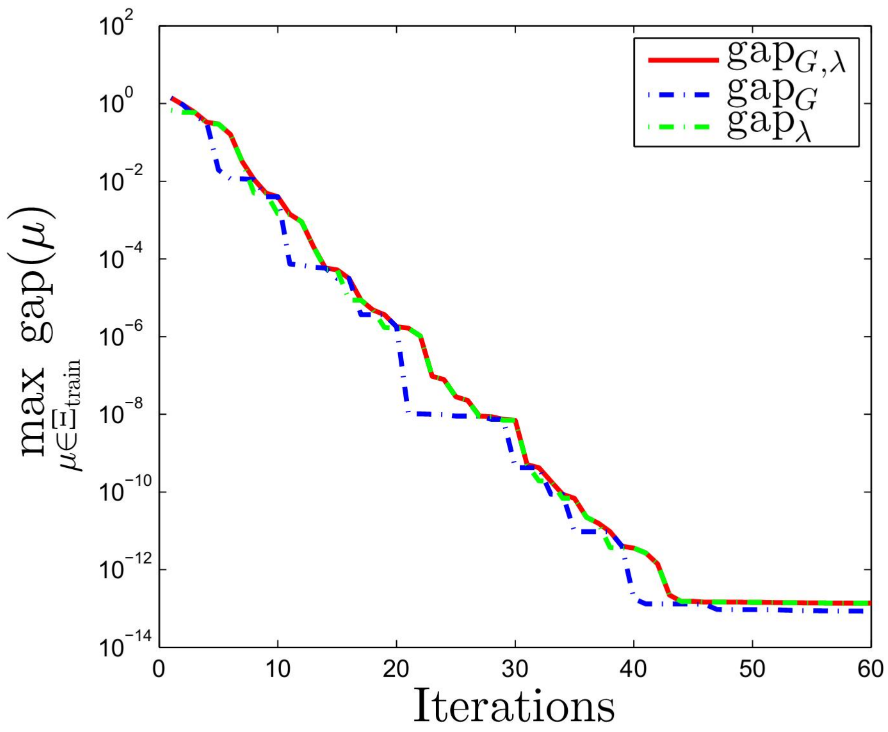
$$\Delta^{\text{CRE,max}} = \max_{\mu \in \Xi_{\text{train}}} \Delta^{\text{CRE}}(\mu)$$

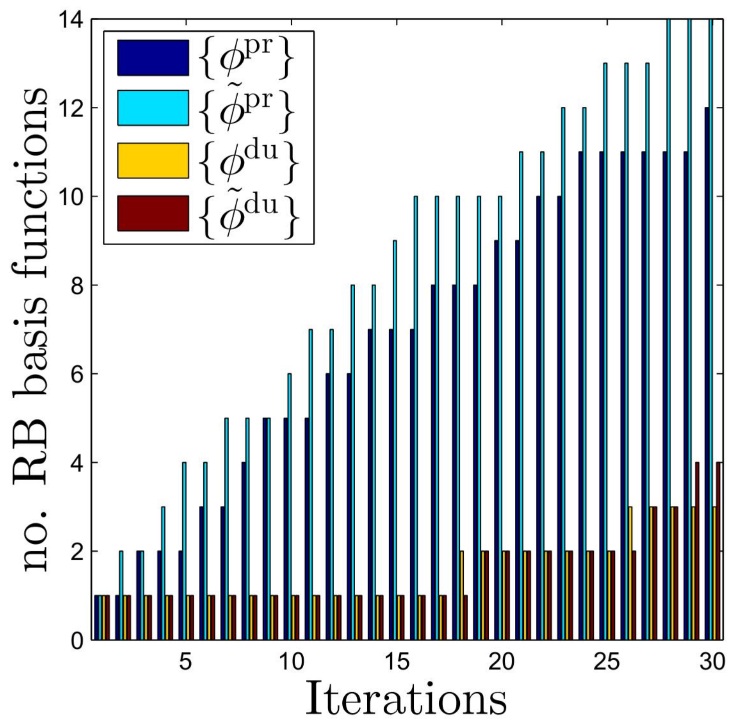
$$\varepsilon_u^{\max} = \max_{\mu \in \Xi_{\text{train}}} \| u^{\text{h}}(\mu) - u^{\text{r}}(\mu) \|_{D(\mu)}$$

$$\varepsilon_\sigma^{\max} = \max_{\mu \in \Xi_{\text{train}}} \| \sigma^{\text{h}}(\mu) - \hat{\sigma}(\mu) \|_{D(\mu)^{-1}}$$

Numerical results

- Goal-oriented Greedy sampling algorithm





$$\text{gap}_G^{\max} = \max_{\mu^G\in\Xi_{\text{train}}} \text{gap}_G$$

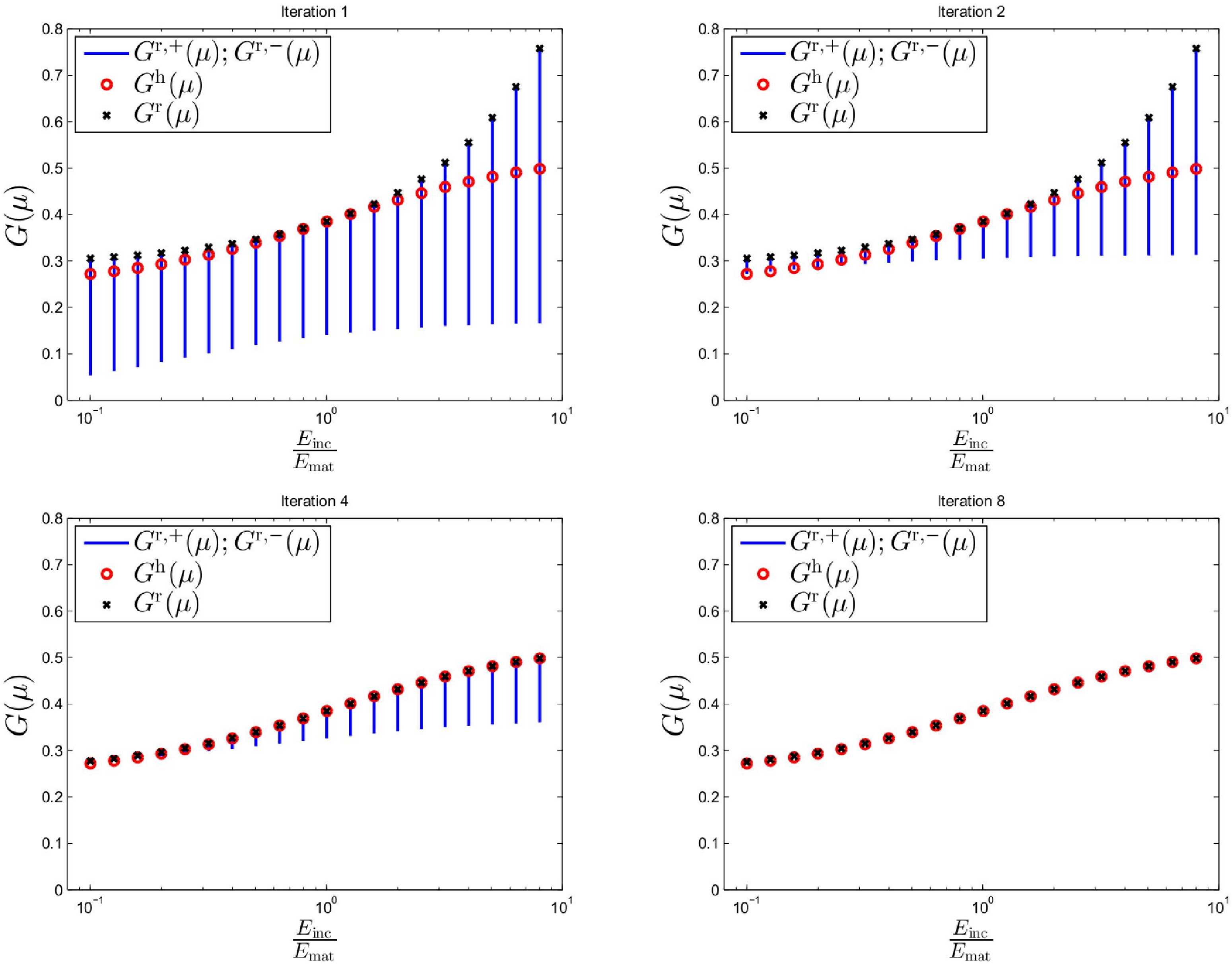
$$\text{gap}_\lambda^{\max} = \max_{\mu^\lambda\in\Xi_{\text{train}}} \text{gap}_\lambda$$

$$\text{gap}_{G,\lambda}^{\max} = \max_{\mu\in\Xi_{\text{train}}} \left\{\text{gap}_G, \text{gap}_\lambda\right\}$$

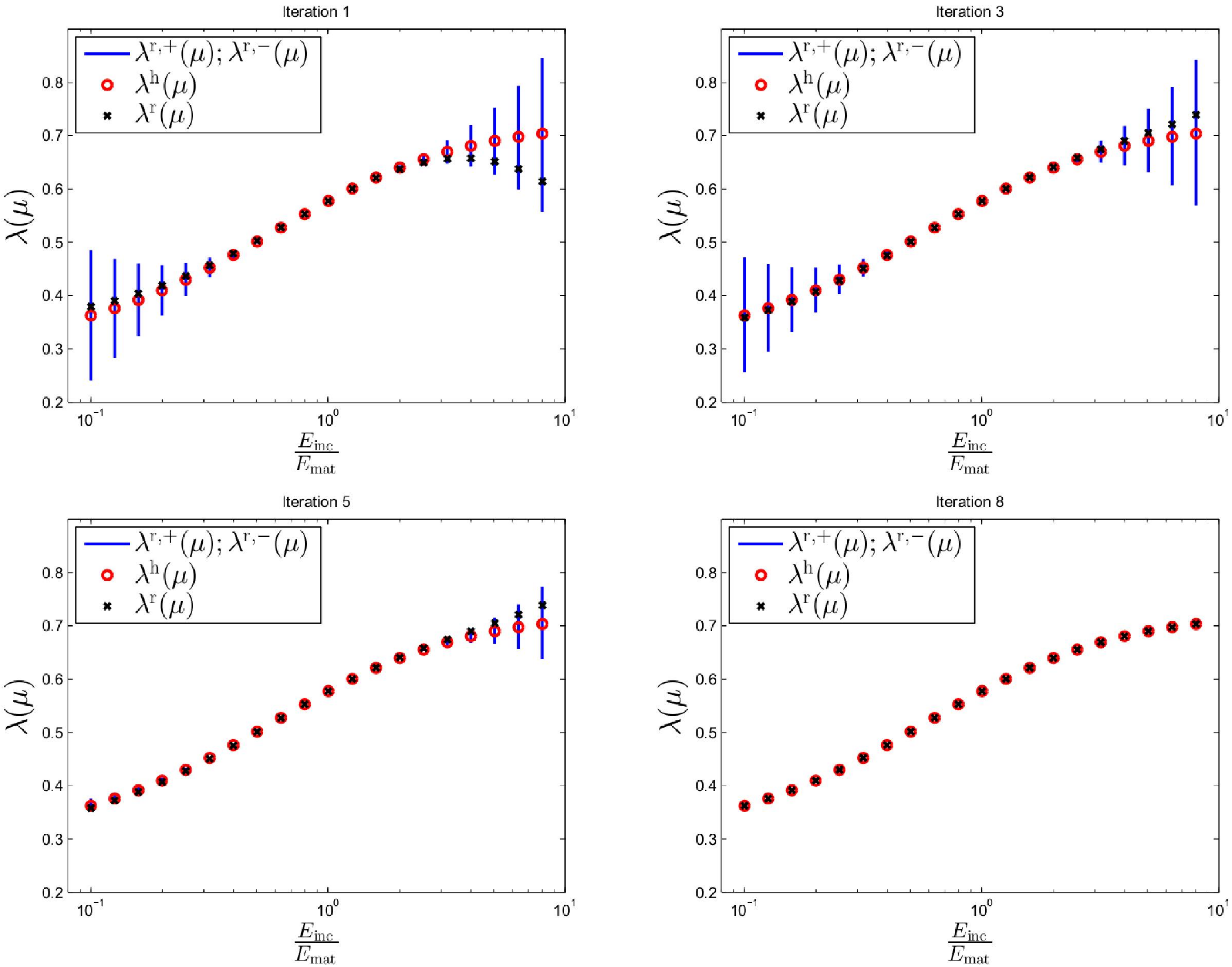
$$\text{gap}_G \equiv \text{gap}(\mu^G) = \frac{2\left|G^{\text{r},+}(\mu^G) - G^{\text{r},-}(\mu^G)\right|}{\left|G^{\text{r},+}(\mu^G)\right| + \left|G^{\text{r},-}(\mu^G)\right|}$$

$$\text{gap}_\lambda \equiv \text{gap}(\mu^\lambda) = \frac{2\left|\lambda^{\text{r},+}(\mu^\lambda) - \lambda^{\text{r},-}(\mu^\lambda)\right|}{\left|\lambda^{\text{r},+}(\mu^\lambda)\right| + \left|\lambda^{\text{r},-}(\mu^\lambda)\right|}$$

Numerical results

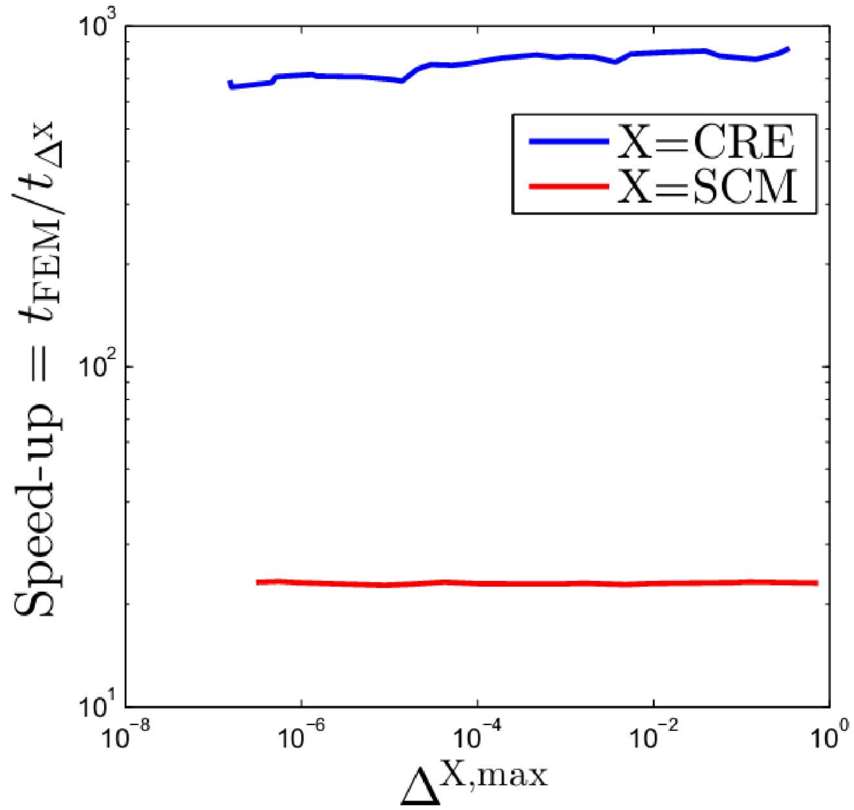


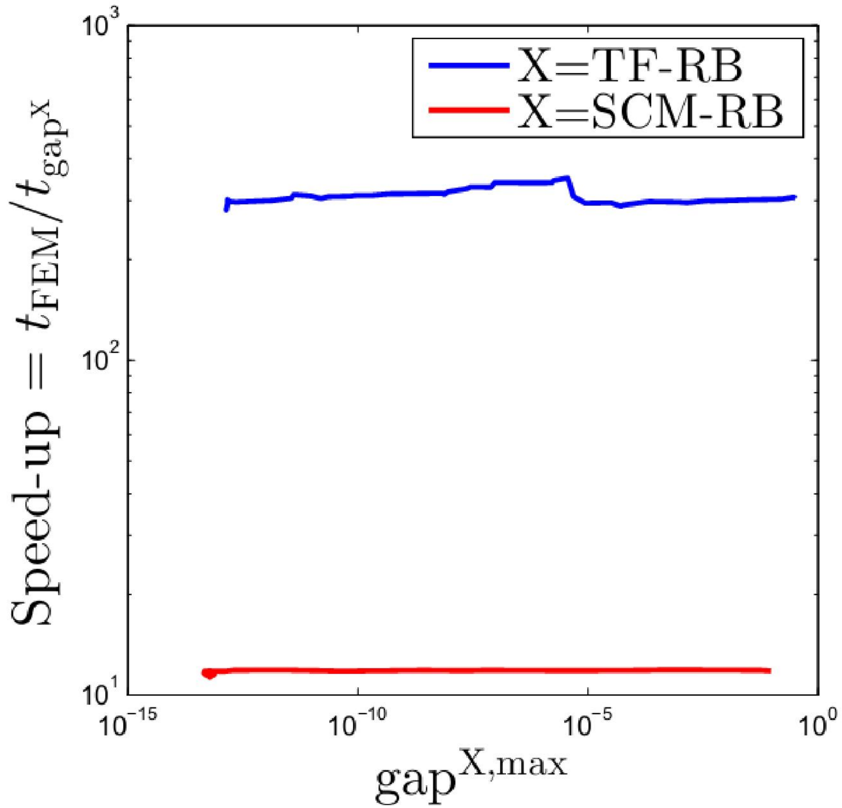
Numerical results



Numerical results

- Speed-up?





Conclusions

- A truly goal-oriented Greedy algorithm was proposed
- Faster online computations but looser bound compared with SCM approach [Rozza *et al.* ‘08]
- Extend to time-dependent problems: linear parabolic PDEs

Sponsors

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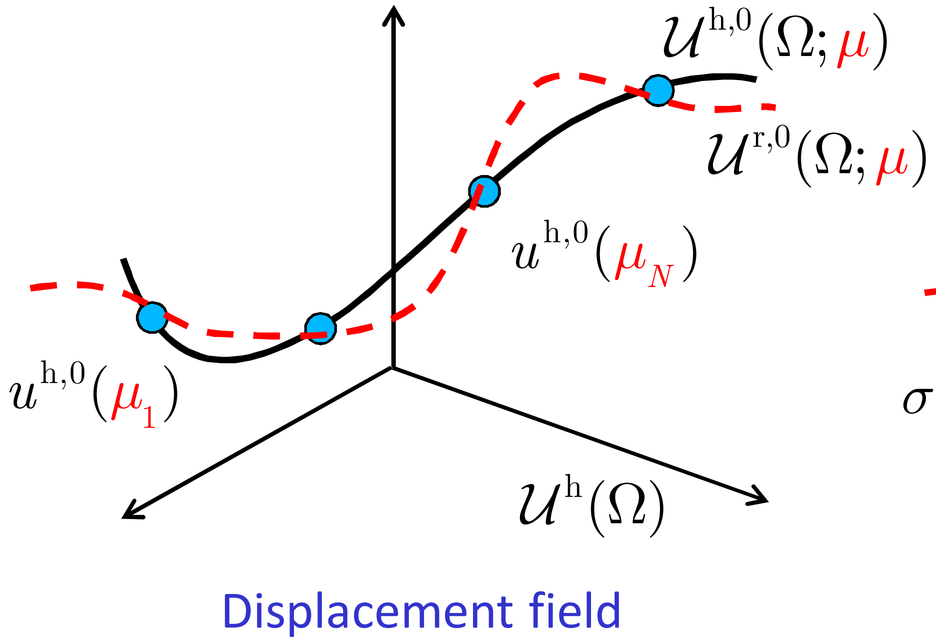
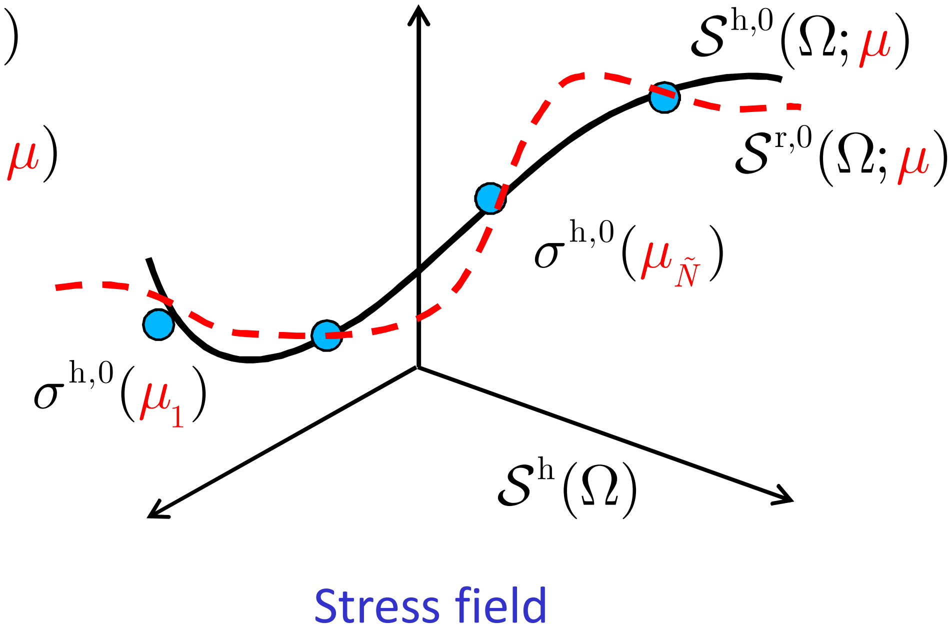
Thank you for your attention!

Questions?





- Opportunities & collaborations
  - *Smooth* and *low-dimensional* parametrically induced manifold $\mathcal{M}^{\mathrm{h},0}(\Omega;\mu)$
  - Parametric setting -> decouple computational tasks to 2 stages: *Offline* (once, expensive) and *Online* (numerous, cheap) stages thanks to the affine decomposition