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Statistical modeling of ROM Errors on the solution of parametrized PDEs by the ROMES method

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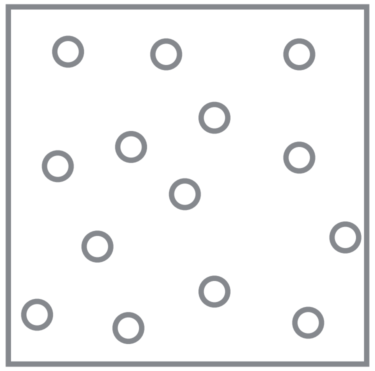
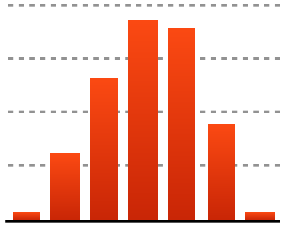
Outline

- We develop a statistical model of the state error introduced by a reduced-order model (ROM) for parameterized stationary problems.
- This technique extends the reduced-order model error surrogate method.
- The statistical model enables the error in any state-dependent quantity of interest to be quantified a posteriori.
- Impact in many-query scenarios: forward and inverse uncertainty quantification.

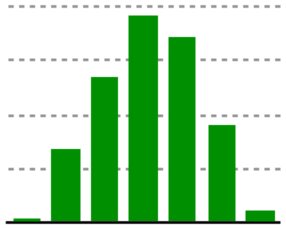


$$\boldsymbol{\mu} \longrightarrow \mathbf{u}_h(\boldsymbol{\mu}) \longrightarrow \mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu}))$$



input | forward PDE model | output

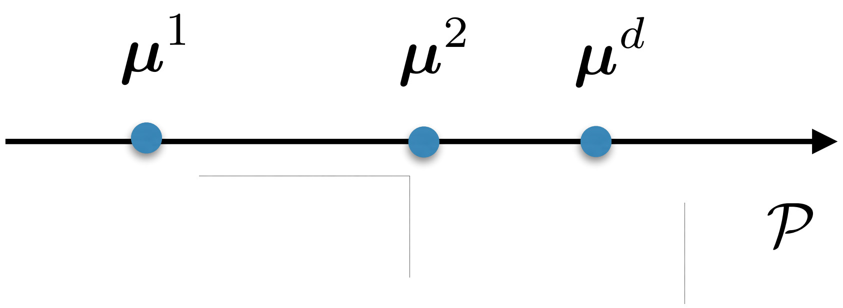
$$\boldsymbol{\mu} \longrightarrow \tilde{\mathbf{u}}_h(\boldsymbol{\mu}) \longrightarrow \mathcal{Q}(\tilde{\mathbf{u}}_h(\boldsymbol{\mu}))$$

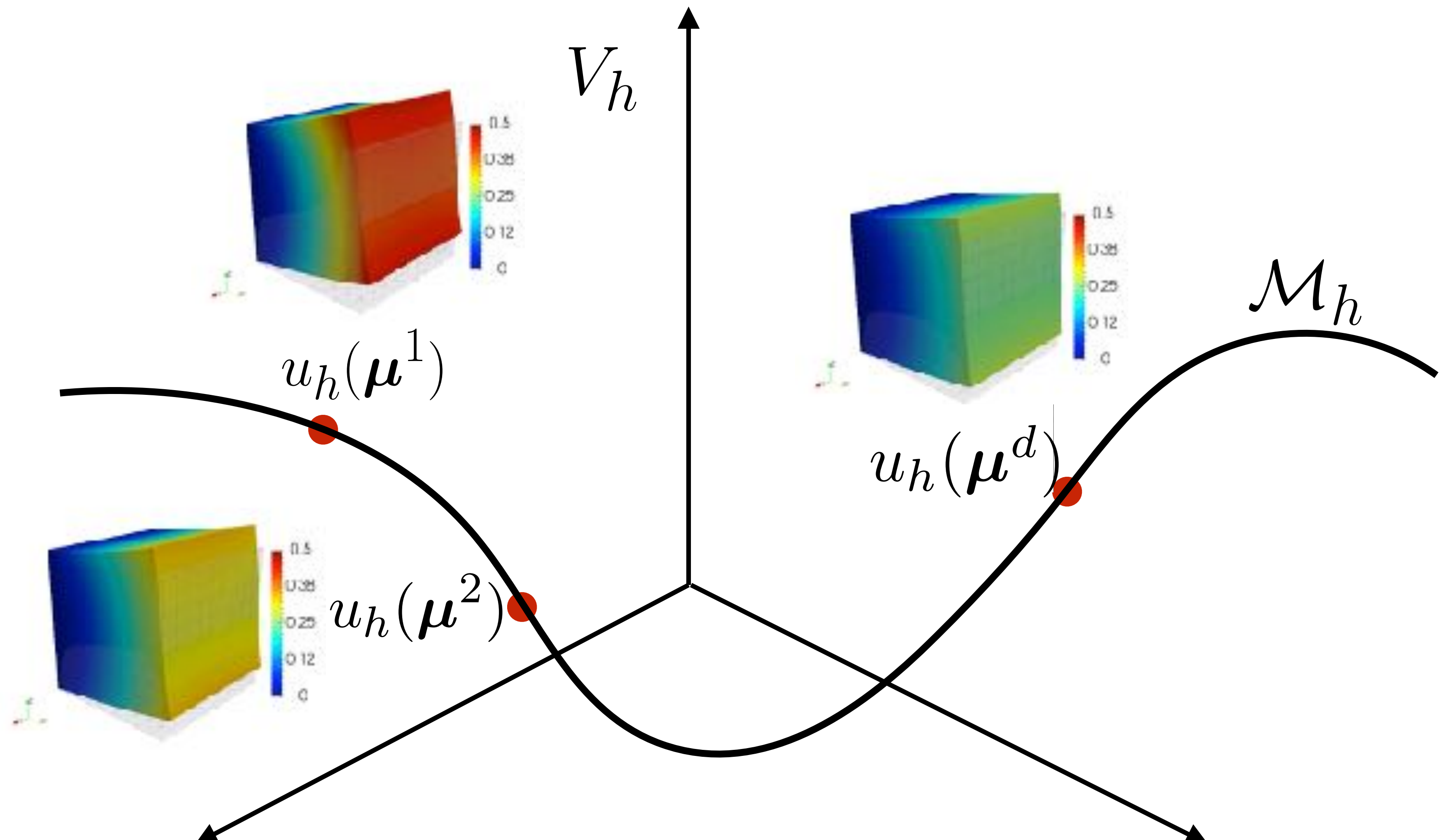


$$\tilde{\mathbf{u}}_h(\boldsymbol{\mu}) = \mathbb{V}(\mathbf{u}_n(\boldsymbol{\mu}) + \boldsymbol{\delta}_{V_n}(\boldsymbol{\mu})) + \mathbb{V}^{\perp}\boldsymbol{\delta}_{V_n^{\perp}}(\boldsymbol{\mu})$$

Projection-based ROM in a nutshell

<u>Goal</u>: compute efficiently the solution of a problem when a set of parameters vary





- parameter-dependent PDEs
- (un)steady (non)linear PDEs
- physical/geometrical parameters
  - ✓ material coefficients
  - ✓ initial/boundary data
  - ✓ geometrical configuration …

Nonlinear steady case:

- **Snapshots computed offline**

$$\boxed{\mathbf{J}_h} \; \boxed{\delta \mathbf{u}_h} = \boxed{-\mathbf{r}_h}$$

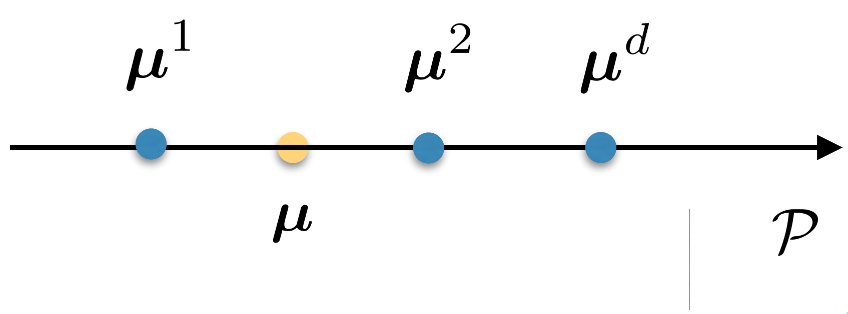
$\mathbf{J}_h$ Jacobian

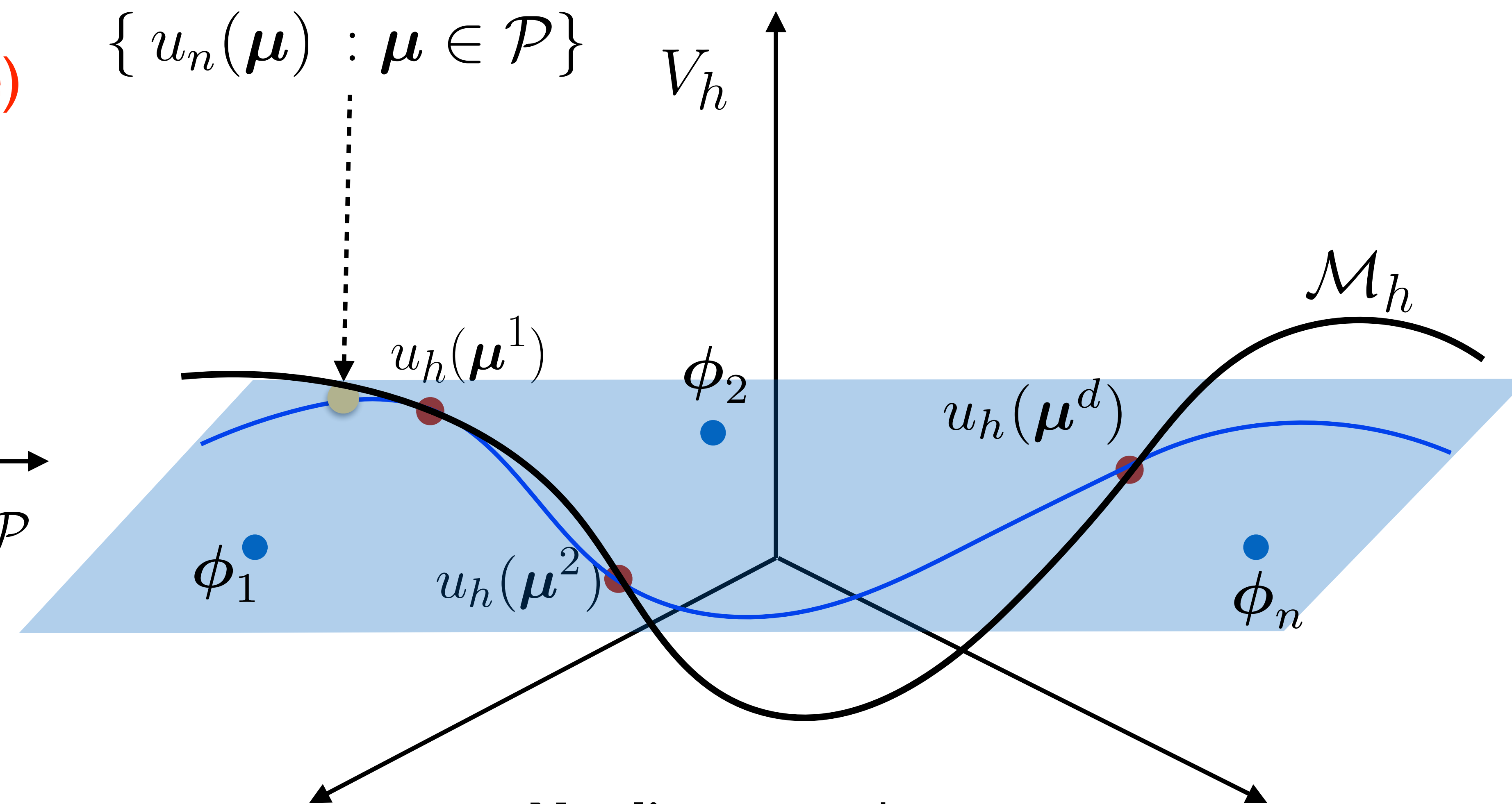
$\mathbf{r}_h$ residual

```
while err < tol
    u_h^(k+1) = u_h^(k) + δu_h
end
```

Projection-based ROM in a nutshell

ROM Approximation
(new parameter value)





Overall computational efficiency ensured by the (discrete) empirical interpolation method.

Nonlinear steady case:

- **Snapshots computed offline**
- **RB space:** $V_n = span\{\phi_1, \dots, \phi_n\}$
- **RB problem** $P_n(\mu)$ solved **online**

$$\boxed{\mathbf{J}_n}\,\boxed{\delta\mathbf{u}_n} = \boxed{\text{-}\mathbf{r}_n}$$

while $err < tol$

$$\mathbf{u}_n^{(k+1)} = \mathbf{u}_n^{(k)} + \delta\mathbf{u}_n$$

end

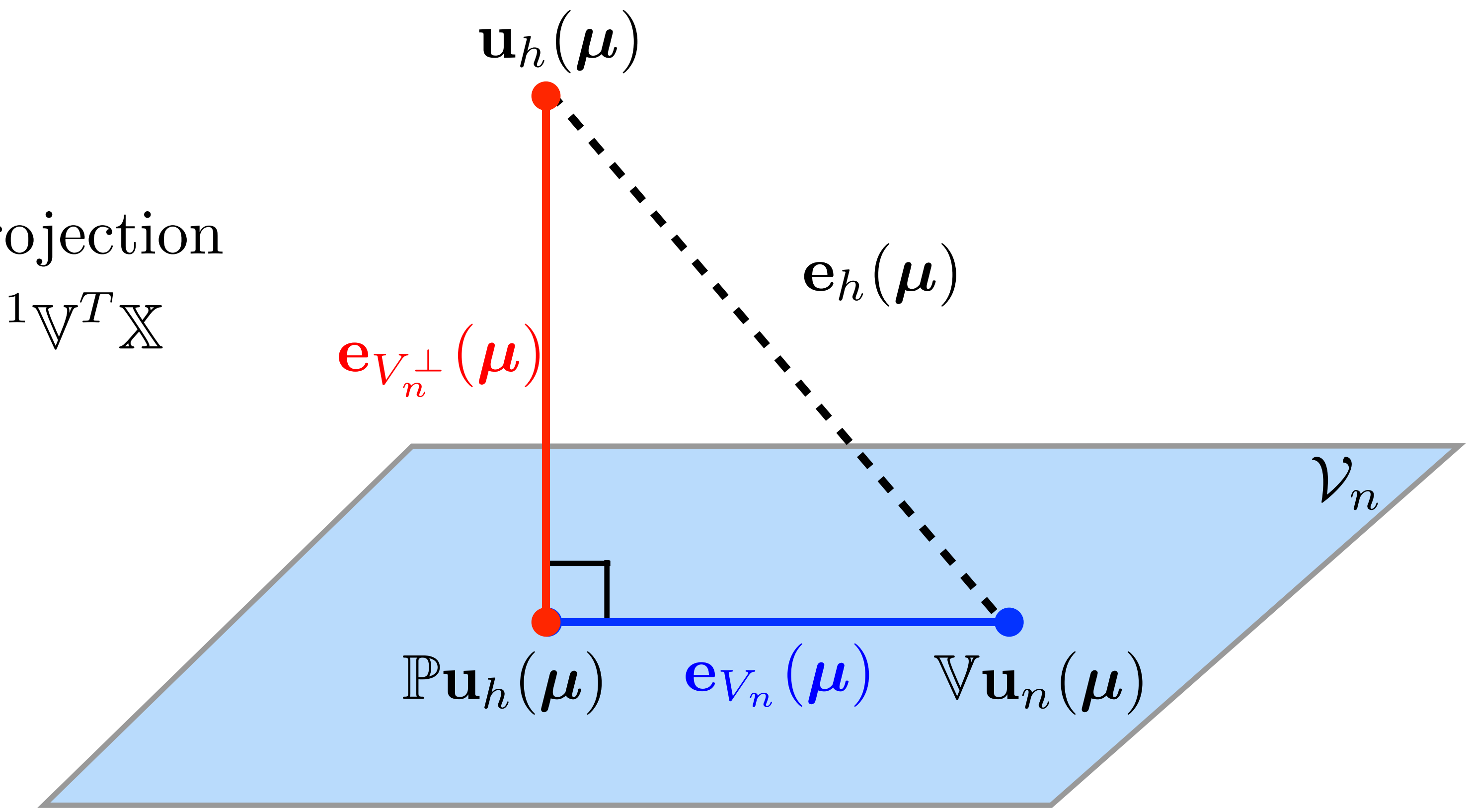
State error

The state error $\mathbf{e}_h = \mathbf{u}_h - \mathbb{V}\mathbf{u}_n$ can be additively split into

$$\begin{aligned}\mathbf{e}_h(\boldsymbol{\mu}) &= (\mathbf{u}_h(\boldsymbol{\mu}) - \mathbb{P}\mathbf{u}_h(\boldsymbol{\mu})) + (\mathbb{P}\mathbf{u}_h(\boldsymbol{\mu}) - \mathbb{V}\mathbf{u}_n(\boldsymbol{\mu})) \\ &= (\mathbb{I}_{N_h} - \mathbb{P})\mathbf{u}_h(\boldsymbol{\mu}) + \mathbb{V}((\mathbb{V}^T\mathbb{X}\mathbb{V})^{-1}\mathbb{V}^T\mathbf{u}_h(\boldsymbol{\mu}) - \mathbf{u}_n(\boldsymbol{\mu})) \\ &= \mathbf{e}_{V_n^\perp}(\boldsymbol{\mu}) + \mathbf{e}_{V_n}(\boldsymbol{\mu}).\end{aligned}$$

$\mathbb{X}$ − orthogonal projection

$$\mathbb{P} = \mathbb{V}(\mathbb{V}^T\mathbb{X}\mathbb{V})^{-1}\mathbb{V}^T\mathbb{X}$$



$$\mathbb{V} = [\phi_1, \ldots, \phi_n]$$

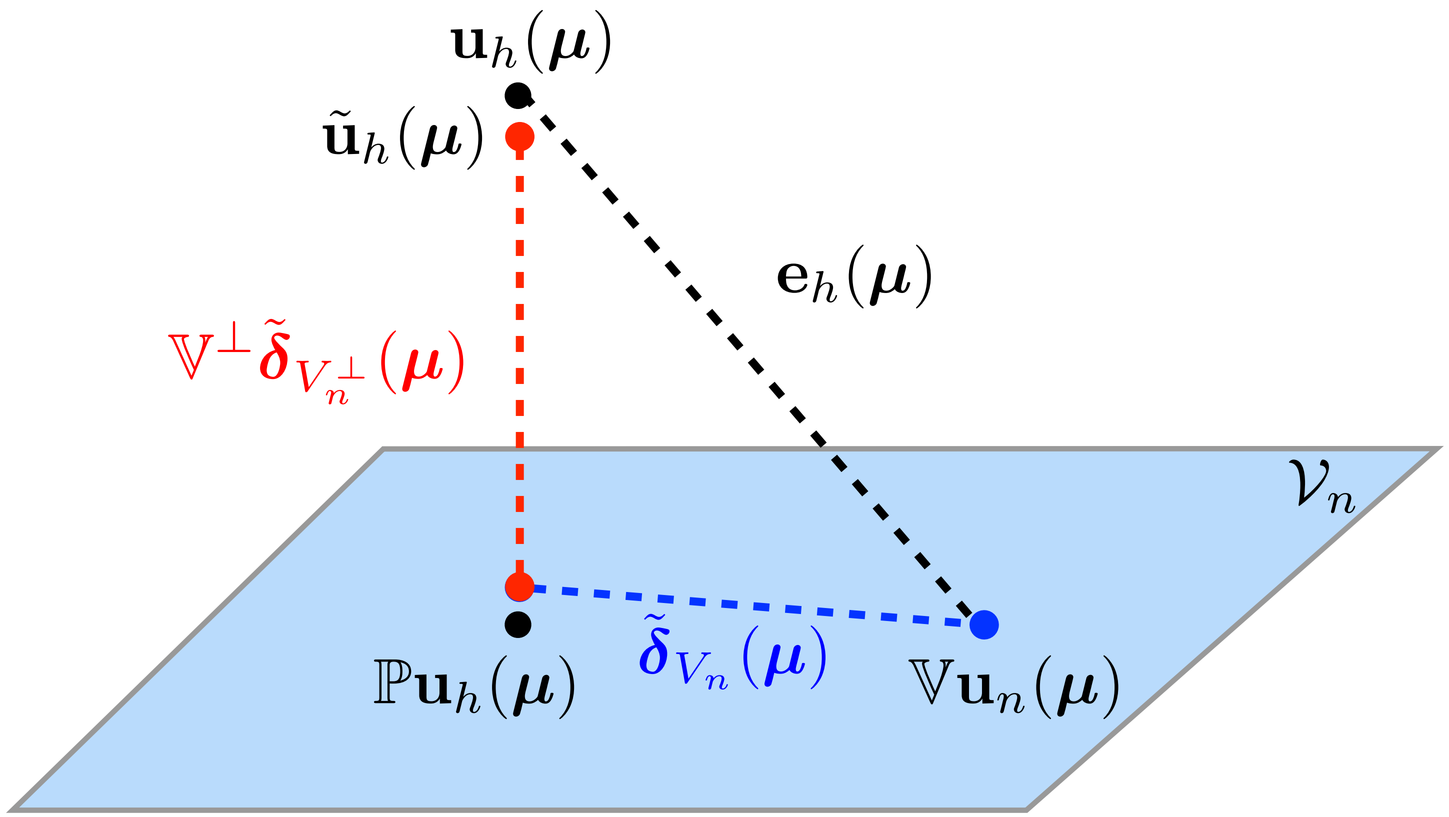
- $\mathbf{e}_{V_n^\perp}(\boldsymbol{\mu})$ lies in the full-order space (*out-of-plane state error*);
- $\mathbf{e}_{V_n}(\boldsymbol{\mu})$ lies in the reduced-order space (*in-plane state error*).

We assume that

$$\mathbf{e}_{V_n}(\boldsymbol{\mu}) = \mathbb{V}\boldsymbol{\delta}_{V_n}(\boldsymbol{\mu}) \quad \mathbf{e}_{V_n^\perp}(\boldsymbol{\mu}) \approx \mathbb{V}^\perp \boldsymbol{\delta}_{V_n^\perp}(\boldsymbol{\mu}),$$

where $\mathbb{V} \in \mathbb{R}^{N_h \times n}$ and $\mathbb{V}^\perp \in \mathbb{R}^{N_h \times n^\perp}$ and $\boldsymbol{\delta}_{V_n}(\boldsymbol{\mu}) \in \mathbb{R}^n$, $\boldsymbol{\delta}_{V_n^\perp}(\boldsymbol{\mu}) \in \mathbb{R}^{n^\perp}$, for any $\boldsymbol{\mu} \in \mathcal{P}$.

ROMES models $\tilde{\boldsymbol{\delta}}_{V_n}(\boldsymbol{\mu})$ and $\tilde{\boldsymbol{\delta}}_{V_n^\perp}(\boldsymbol{\mu})$ are built for each element of $\boldsymbol{\delta}_{V_n}(\boldsymbol{\mu})$ and $\boldsymbol{\delta}_{V_n^\perp}(\boldsymbol{\mu})$.



$$\mathbf{u}_h(\boldsymbol{\mu}) \approx \underbrace{\mathbb{V}\mathbf{u}_n(\boldsymbol{\mu})}_{\text{ROM (deterministic)}} + \underbrace{\mathbb{V}\tilde{\boldsymbol{\delta}}_{V_n}(\boldsymbol{\mu}) + \mathbb{V}^\perp \tilde{\boldsymbol{\delta}}_{V_n^\perp}(\boldsymbol{\mu})}_{\text{ROMES (statistical)}} := \tilde{\mathbf{u}}_h(\boldsymbol{\mu});$$

ROM error surrogate

We assume that

$$\mathbf{e}_{V_n}(\boldsymbol{\mu}) = \mathbb{V}\boldsymbol{\delta}_{V_n}(\boldsymbol{\mu}) \quad \mathbf{e}_{V_n^\perp}(\boldsymbol{\mu}) \approx \mathbb{V}^\perp \boldsymbol{\delta}_{V_n^\perp}(\boldsymbol{\mu}),$$

where $\mathbb{V} \in \mathbb{R}^{N_h \times n}$ and $\mathbb{V}^\perp \in \mathbb{R}^{N_h \times n^\perp}$ and $\boldsymbol{\delta}_{V_n}(\boldsymbol{\mu}) \in \mathbb{R}^n$, $\boldsymbol{\delta}_{V_n^\perp}(\boldsymbol{\mu}) \in \mathbb{R}^{n^\perp}$, for any $\boldsymbol{\mu} \in \mathcal{P}$.

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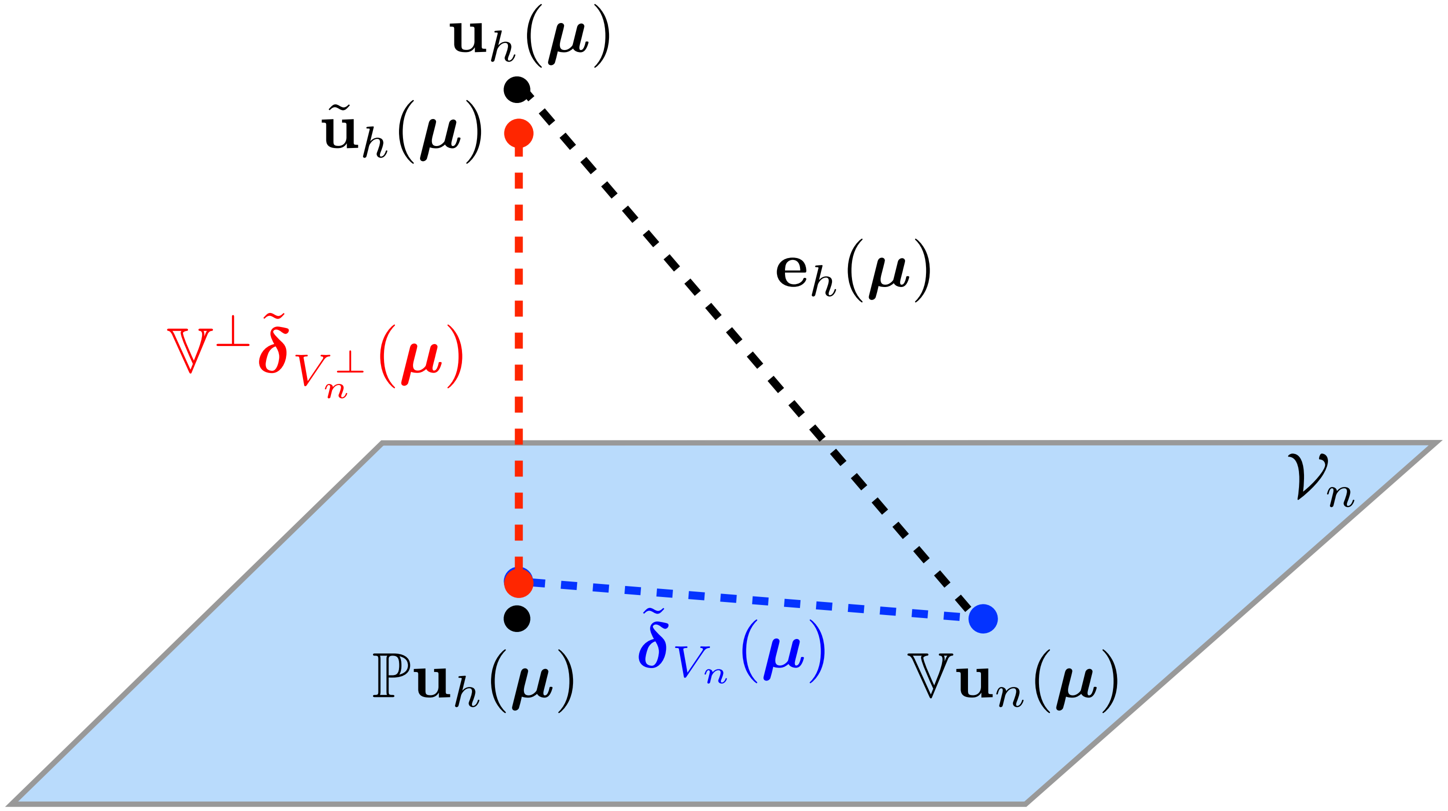
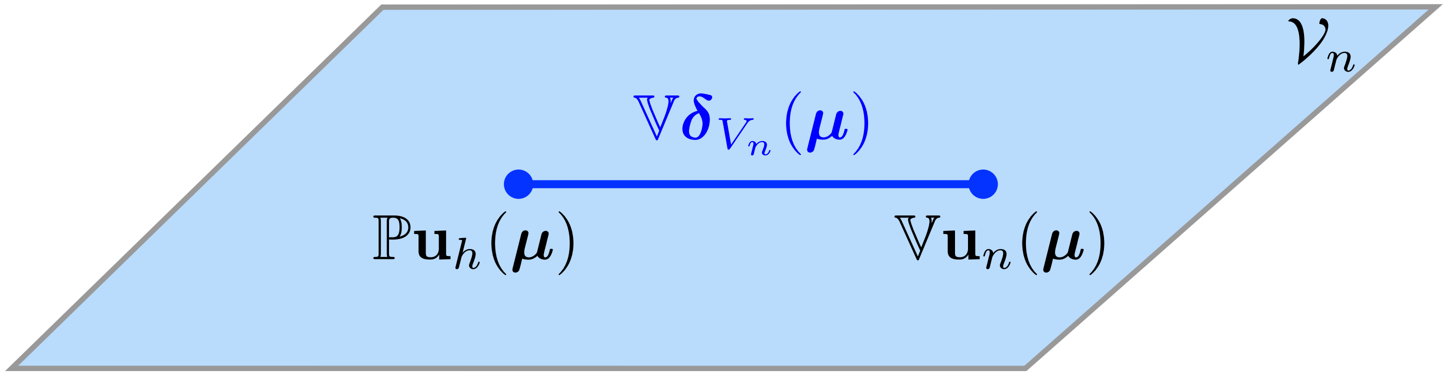


GOAL $\quad \|\mathbf{u}_h(\boldsymbol{\mu}) - \tilde{\mathbf{u}}_h(\boldsymbol{\mu})\|_{\mathbb{X}} \ll \|\mathbf{u}_h(\boldsymbol{\mu}) - \mathbb{V}\mathbf{u}_n(\boldsymbol{\mu})\|_{\mathbb{X}}$

In-plane state error case



1. each component $i = 1, \ldots, n$ of the *in-plane* state error is given by

$$(\delta_{V_n})_i = (\mathbb{V}^T \mathbb{X} \mathbb{V})^{-1} \mathbb{V}^T \mathbb{X} (\mathbf{u}_h - \mathbb{V}\mathbf{u}_n)_i; \qquad \text{(a)}$$

2. we can approximate the residual $\mathbf{r}$ of the problem as

$$\mathbf{0} = \mathbf{r}(\mathbf{u}_h) = \mathbf{r}(\mathbb{V}\mathbf{u}_n) + \frac{\partial \mathbf{r}}{\partial u}(\mathbb{V}\mathbf{u}_n)(\mathbf{u}_h - \mathbb{V}\mathbf{u}_n) + \mathcal{O}((\mathbf{u}_h - \mathbb{V}\mathbf{u}_n)^2); \qquad \text{(b)}$$

3. by combining (a) with (b), we have that

$$(\delta_{V_n})_i \approx -(\mathbb{V}^T \mathbb{X} \mathbb{V})^{-1} \mathbb{V}^T \mathbb{X} \left[\frac{\partial \mathbf{r}}{\partial u}(\mathbb{V}\mathbf{u}_n) \right]^{-1} \mathbf{r}(\mathbb{V}\mathbf{u}_n).$$

= for linear problem

ROMES derivation

By introducing $\mathbf{p}_h^i \in V_h$, $i = 1, \dots, n$, such that:

$$(\mathbf{p}_h^i)^T = (\mathbb{V}^T \mathbb{X} \mathbb{V})^{-1} \mathbb{V}^T \mathbb{X} \left[\frac{\partial \mathbf{r}}{\partial u}(\mathbb{V}\mathbf{u}_n) \right]^{-1},$$

solution of the following dual problem

$$\left[\frac{\partial \mathbf{r}}{\partial u}(\mathbb{V}\mathbf{u}_n) \right]^T (\mathbf{p}_h^i) = -((\mathbb{V}^T \mathbb{X} \mathbb{V})^{-1} \mathbb{V}^T \mathbb{X})_i^T. \qquad \text{(c)}$$

Full-order ROM *in-plane* state error correction

$$(\delta_{V_n})_i \underset{\uparrow}{\approx} -(\mathbf{p}_h^i)^T \mathbf{r}(\mathbb{V}\mathbf{u}_n).$$

= for linear problem

Instead of solving (c) for each $i = 1, \dots, n$, we compute the reduced-order dual solution $\mathbf{p}_n^i = \mathbb{V}_p \mathbf{p}_h^i$ where:

$$\mathbb{V}_p^T \left[\frac{\partial \mathbf{r}}{\partial u}(\mathbb{V}\mathbf{u}_n) \right]^T \mathbb{V}_p \mathbf{p}_n^i(\boldsymbol{\mu}) = -\mathbb{V}_p^T ((\mathbb{V}^T \mathbb{X} \mathbb{V})^{-1} \mathbb{V}^T \mathbb{X})_i^T$$

using a unique transformation matrix $\mathbb{V}_p$ for all $i = 1, \dots, n$.

ROMES derivation

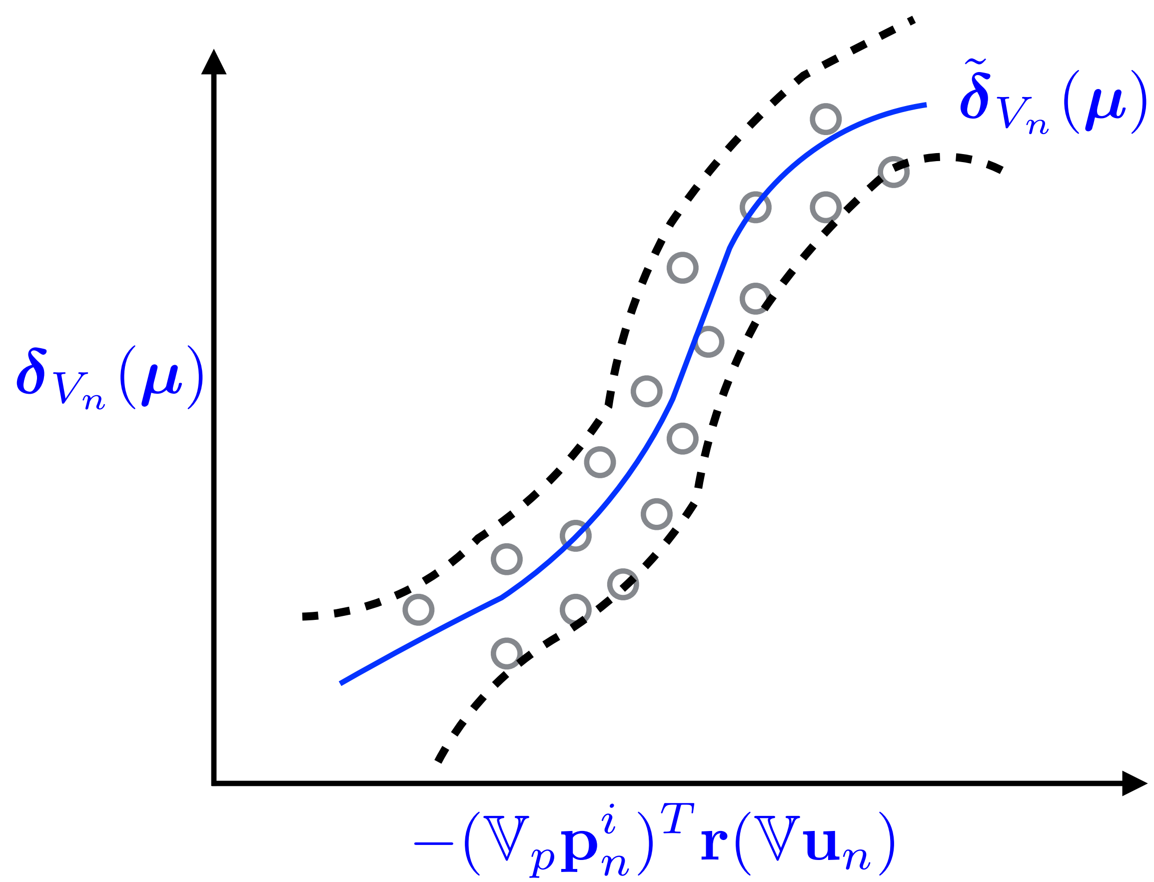
Final reduced-order ROM *in-plane* state error correction:

$$(\delta_{V_n})_i \approx -(\mathbb{V}_p \mathbf{p}_n^i)^T \mathbf{r}(\mathbb{V}\mathbf{u}_n).$$

Final reduced-order ROM *out-of-plane* state error correction:

$$(\delta_{V_n^\perp})_i \approx -(\mathbb{V}_p^\perp (\mathbf{p}_n^\perp))^T \mathbf{r}(\mathbb{V}\mathbf{u}_n).$$

Statistical ROMES: regression (Gaussian Process) model $\tilde{\boldsymbol{\delta}}_{V_n}(\boldsymbol{\mu})$ and $\tilde{\boldsymbol{\delta}}_{V_n^\perp}(\boldsymbol{\mu})$.



Summary: nonlinear problem

Standard ROM method

```
while err < tol
```

$$\boxed{\mathbf{J}_n}\,\boxed{\delta\mathbf{u}_n} = \boxed{-\mathbf{r}_n}$$

```
end
```

ROMES enhanced method (in-plane)

```
while err < tol
```

$$\boxed{\mathbf{J}_n}\,\boxed{\delta\mathbf{u}_n} = \boxed{-\mathbf{r}_n}$$

```
end
```

$$\boxed{\mathbf{J}_n^d}\,\boxed{\mathbf{p}_n^i} = -\,\boxed{\mathbf{D}}$$

$$\mathbf{J}_n^d = \mathbf{V}_d^T \left[\frac{\delta \mathbf{r}}{\delta u}(\mathbb{V}\mathbf{u}_n)\right]^T \mathbf{V}_d$$

$$\mathbf{D} = ((\mathbb{V}^T \mathbb{X} \mathbb{V})^{-1} \mathbb{V}^T \mathbb{X})^T$$

$$\|\mathbf{u}_h - \mathbb{V}\mathbf{u}_n(\boldsymbol{\mu})\|_{\mathbb{X}} \quad > \quad \|\mathbf{u}_h - \mathbb{V}(\mathbf{u}_n(\boldsymbol{\mu}) + \boldsymbol{\delta}_{V_n}(\boldsymbol{\mu}))\|_{\mathbb{X}}$$

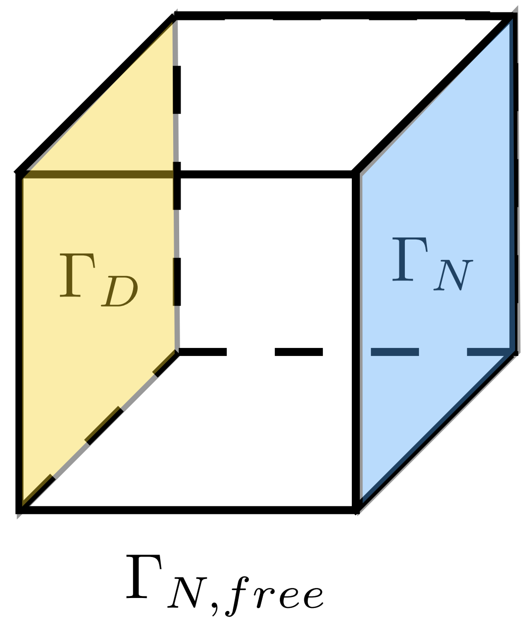
\# operations: $\mathcal{O}\left(n_{it}\frac{2}{3}n^3\right)$ $<$ # operations: $\mathcal{O}\left(n_{it}\frac{2}{3}n^3 + \frac{2}{3}n_d^3 + 2nn_d^2\right)$

In the steady nonlinear case the additional relative cost is smaller.

Numerical example: mechanical steady problem

We consider the following shear test on the domain $\Omega_0 = [0,1]^3$: find $\mathbf{u} = \mathbf{u}(\mathbf{x};\mu)$ s.t.

$$\begin{cases} div(\mathbf{P}(\mathbf{u};\mu)) = \mathbf{0} & \mathbf{x} \in \Omega_0 \\ \mathbf{P}(\mathbf{u};\mu)\mathbf{n}(\mathbf{x}) = \mu_3 \mathbf{n}_z & \mathbf{x} \in \Gamma_N \\ \mathbf{P}(\mathbf{u};\mu)\mathbf{n}(\mathbf{x}) = 0 & \mathbf{x} \in \Gamma_{N,free} \\ \mathbf{u} = 0 & \mathbf{x} \in \Gamma_D \end{cases}$$



where the parameter vector μ is composed by:

- the Young modulus $\mu_1 \in [6 \cdot 10^4, 7 \cdot 10^4]$;
- the Poisson coefficient $\mu_2 \in [0.3, 0.4]$;
- the external load $\mu_3 \in [10^3, 2 \cdot 10^3]$.

$\boldsymbol{\mu} = [6.98 \cdot 10^4, 0.3144, 1.64 \cdot 10^3]$ $\boldsymbol{\mu} = [6.22 \cdot 10^4, 0.39, 1.99 \cdot 10^3]$ $\boldsymbol{\mu} = [6.43 \cdot 10^4, 0.34, 1.22 \cdot 10^3]$

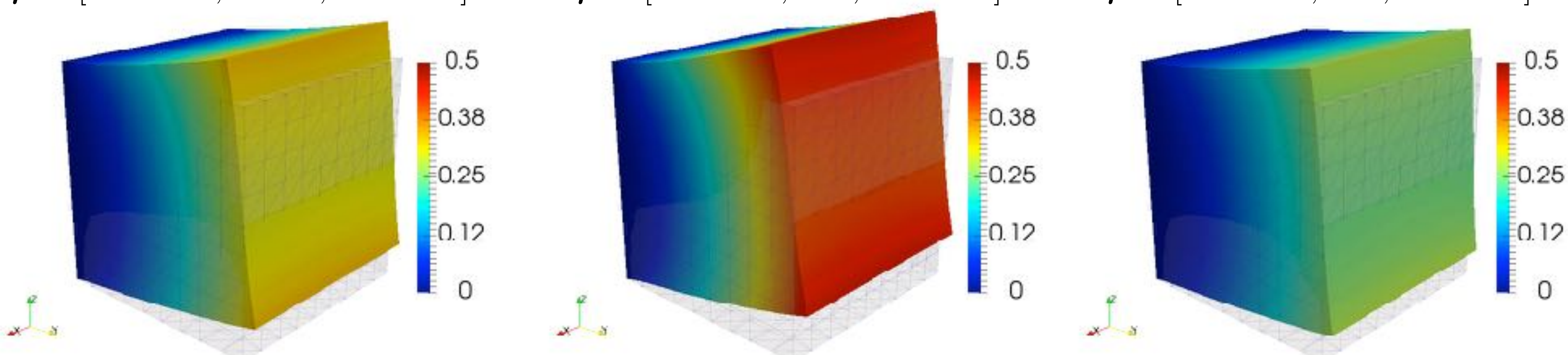


Fig: FOM displacement approximation for different values of the parameter vector

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Full-order model

Finite element model:

- number of parameters: 3
- degrees of freedom: 2700
- number of elements: 4374
- average computational time: 1.3860 [*sec*.]
- average number of Newton iterations: 4 (tolerance 10^{-5}).

$\boldsymbol{\mu} = [6.1 \cdot 10^4, 0.393, 1.59 \cdot 10^3]$ $\boldsymbol{\mu} = [6.86 \cdot 10^4, 0.37, 1.26 \cdot 10^3]$ $\boldsymbol{\mu} = [6.43 \cdot 10^4, 0.306, 1.91 \cdot 10^3]$

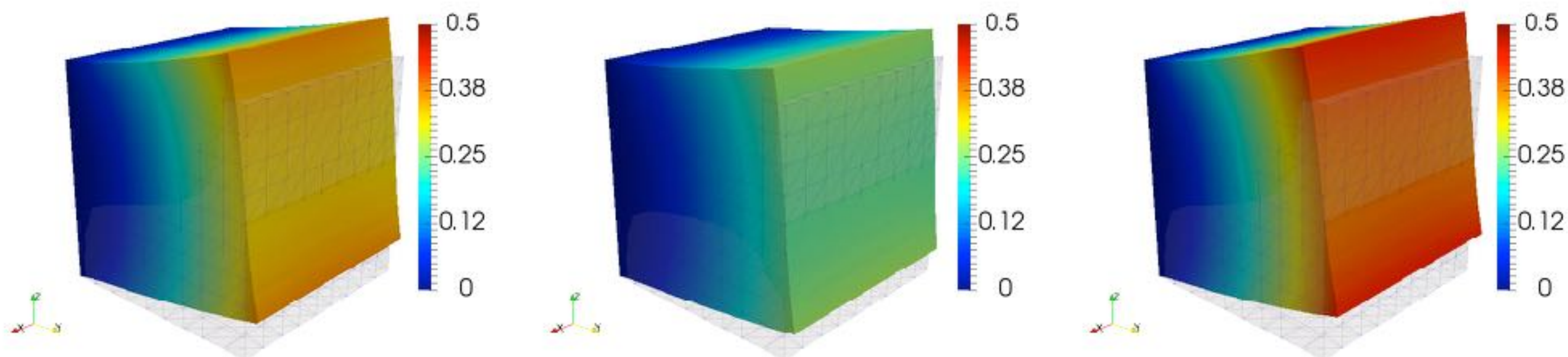


Fig: FOM displacement approximation for different values of the parameter vector

Reduced-order model

POD-DEIM reduced basis model:

- number of parameters: 3
- number of basis functions: 5
- number of basis functions for the DEIM approximation: 41
- average computational time: 0.1346 [*sec.*]
- average number of Newton iterations: 4 (tolerance 10^{-5}).

$\boldsymbol{\mu} = [6.1 \cdot 10^4, 0.393, 1.59 \cdot 10^3]$ $\boldsymbol{\mu} = [6.86 \cdot 10^4, 0.37, 1.26 \cdot 10^3]$ $\boldsymbol{\mu} = [6.43 \cdot 10^4, 0.306, 1.91 \cdot 10^3]$

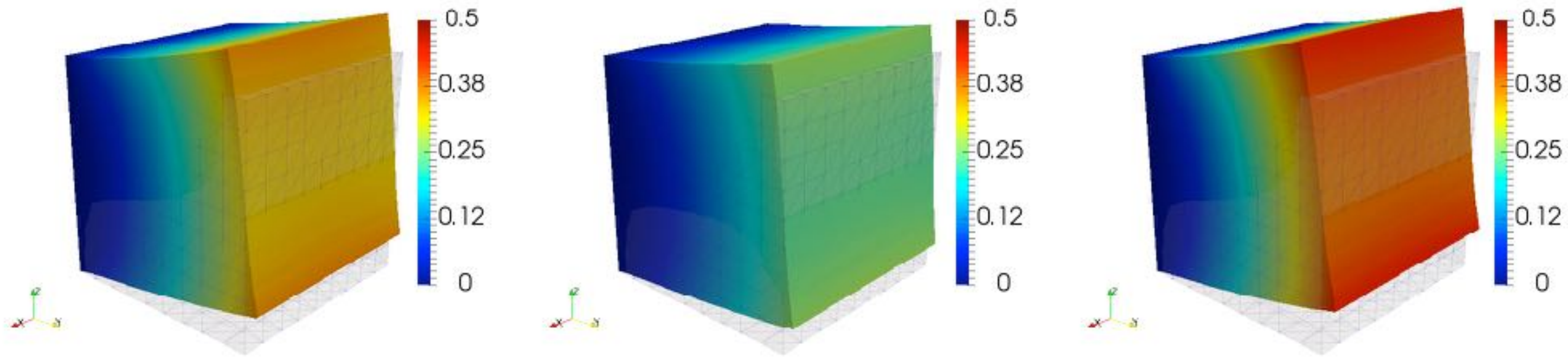


Fig: ROM displacement approximation for different values of the parameter vector

Error analysis

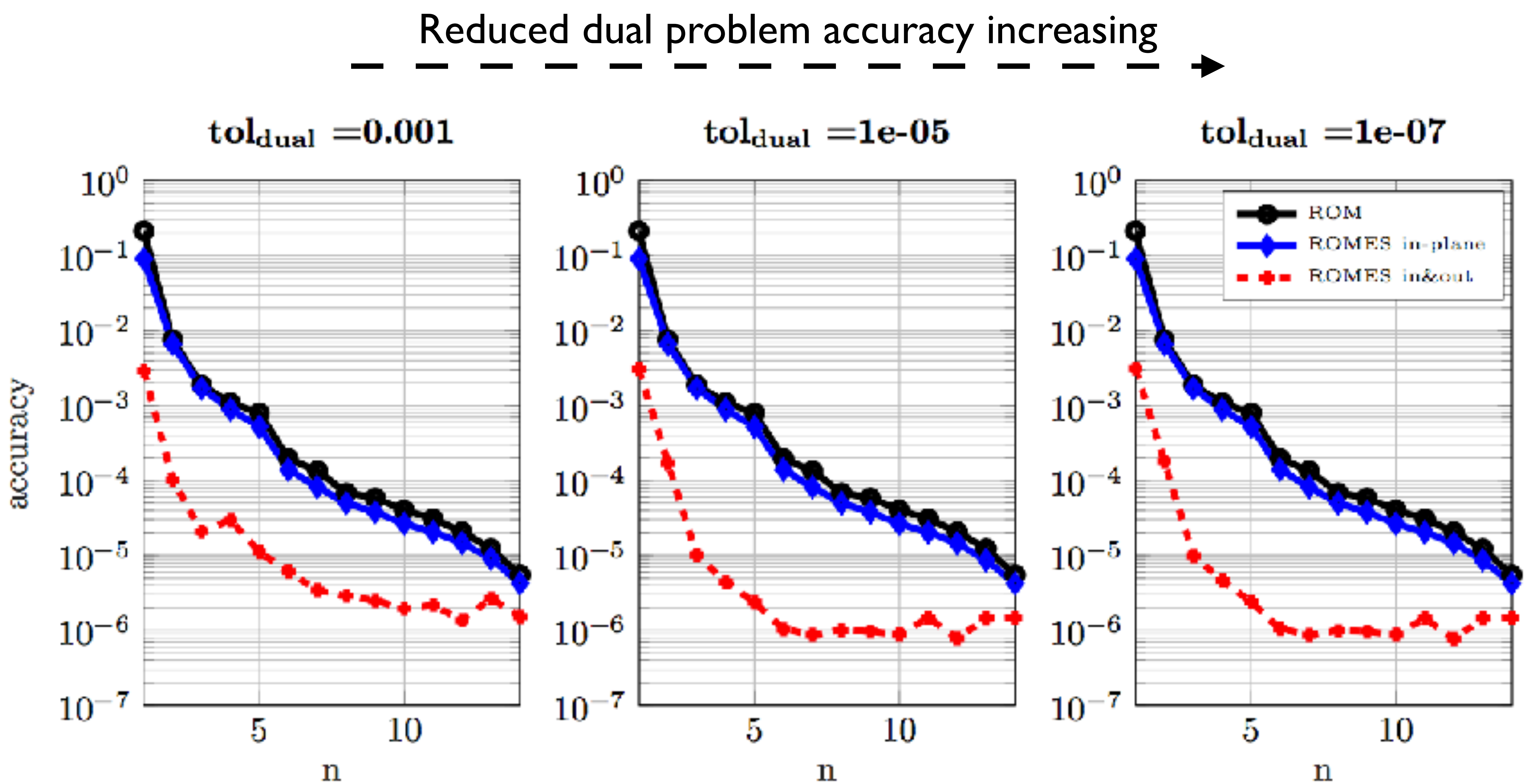


Fig: approximation error vs number of basis functions

- ROMES decreases by two order of magnitude the mean state error;
- by increasing the POD tolerance tol_{dual}, CPU times might become more relavant.

Performance

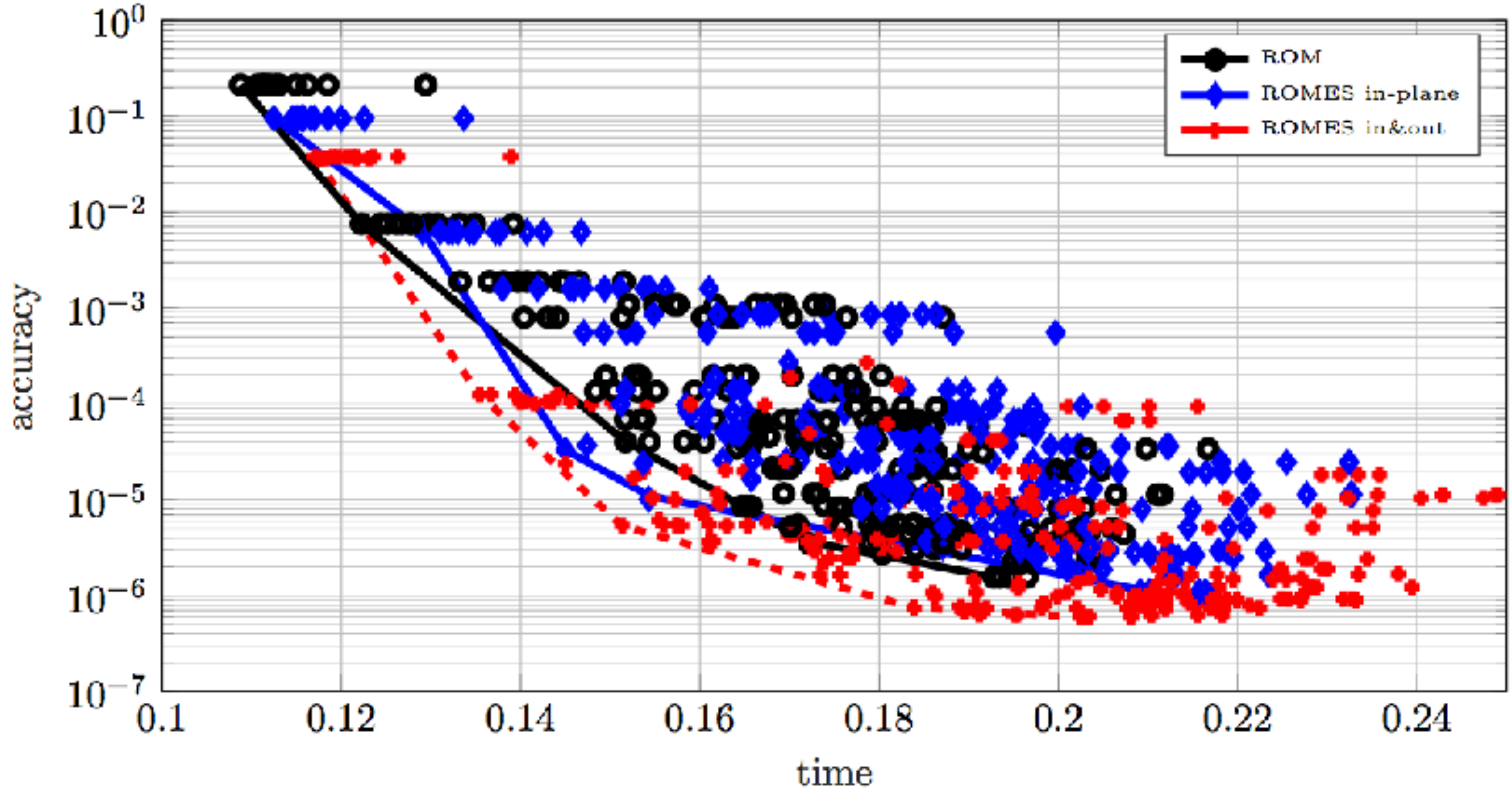


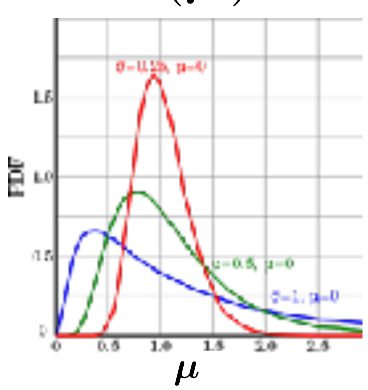
Fig: average online relative error over the test sample vs the CPU time [s]

- ROMES of the *in- and out-of-plane* state error leads to the best performance;

Forward uncertainty quantification

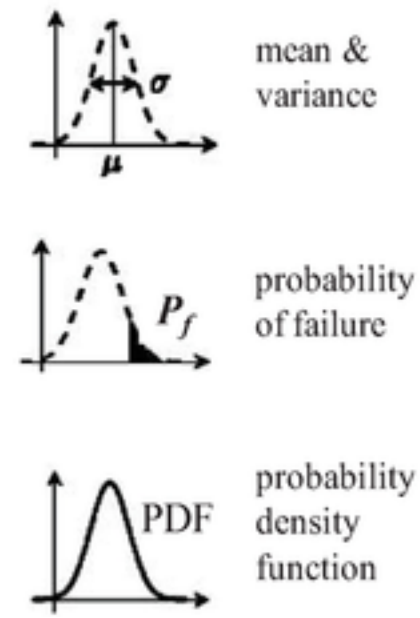
How does uncertainty in model parameters propagate to the outputs of interest?

$\pi(\boldsymbol{\mu})$



PDE model

$\mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu}))$



The goal is e.g. to estimate the expected value:

$$\mathbb{E}[Q] = \int_\Theta \mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu}))\pi(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu}_q)),$$

and/or its variance

$$\mathrm{Var}(Q) = \int_\Theta (\mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu})) - \mathbb{E}[Q])^2 \pi(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \left(\mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu}_q)) - \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \mathcal{Q}(\mathbf{u}_h(\boldsymbol{\mu}_q)) \right)^2.$$

Forward uncertainty quantification

SPEED-UP: reduced-order expected value

$$\mathbb{E}[Q_n] = \int_{\Theta} \mathcal{Q}(\mathbb{V}\mathbf{u}_n(\boldsymbol{\mu}))\pi(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \mathcal{Q}(\mathbb{V}\mathbf{u}_n(\boldsymbol{\mu}_q)).$$

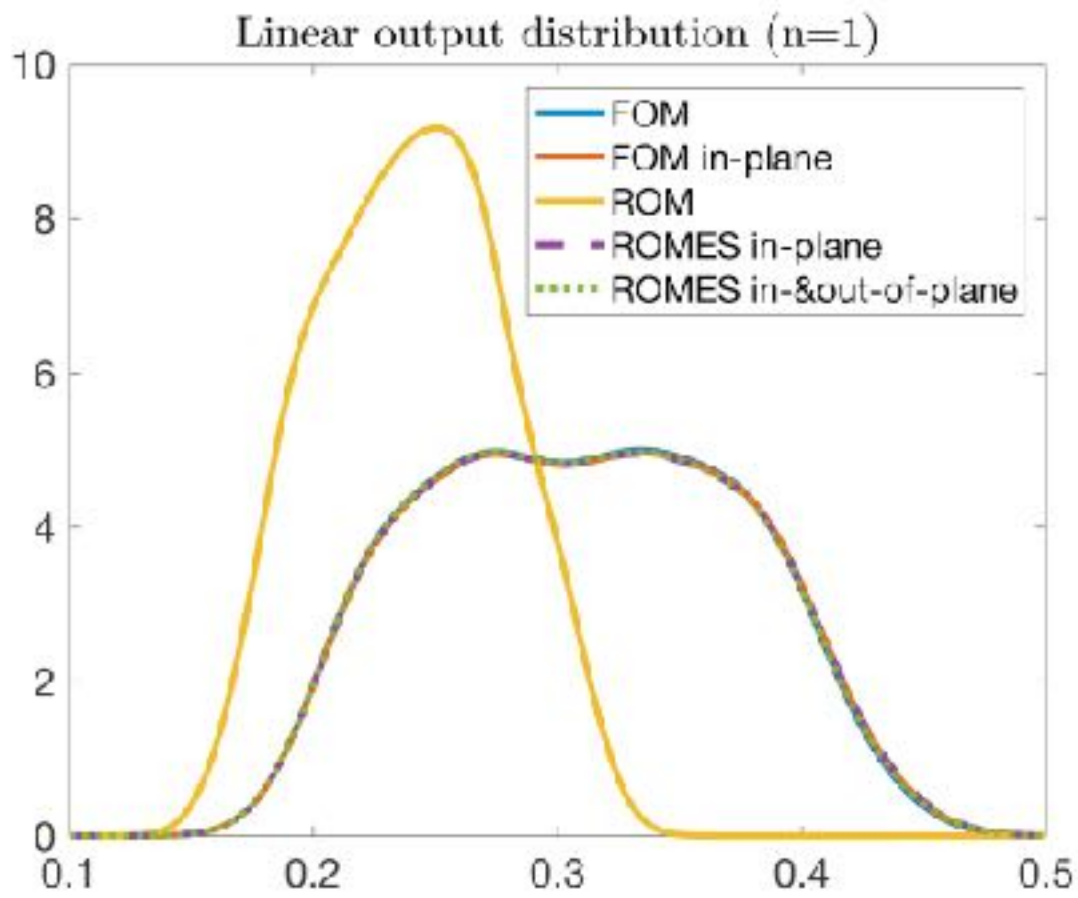
The effect of the state error can be outlined by decomposing the error

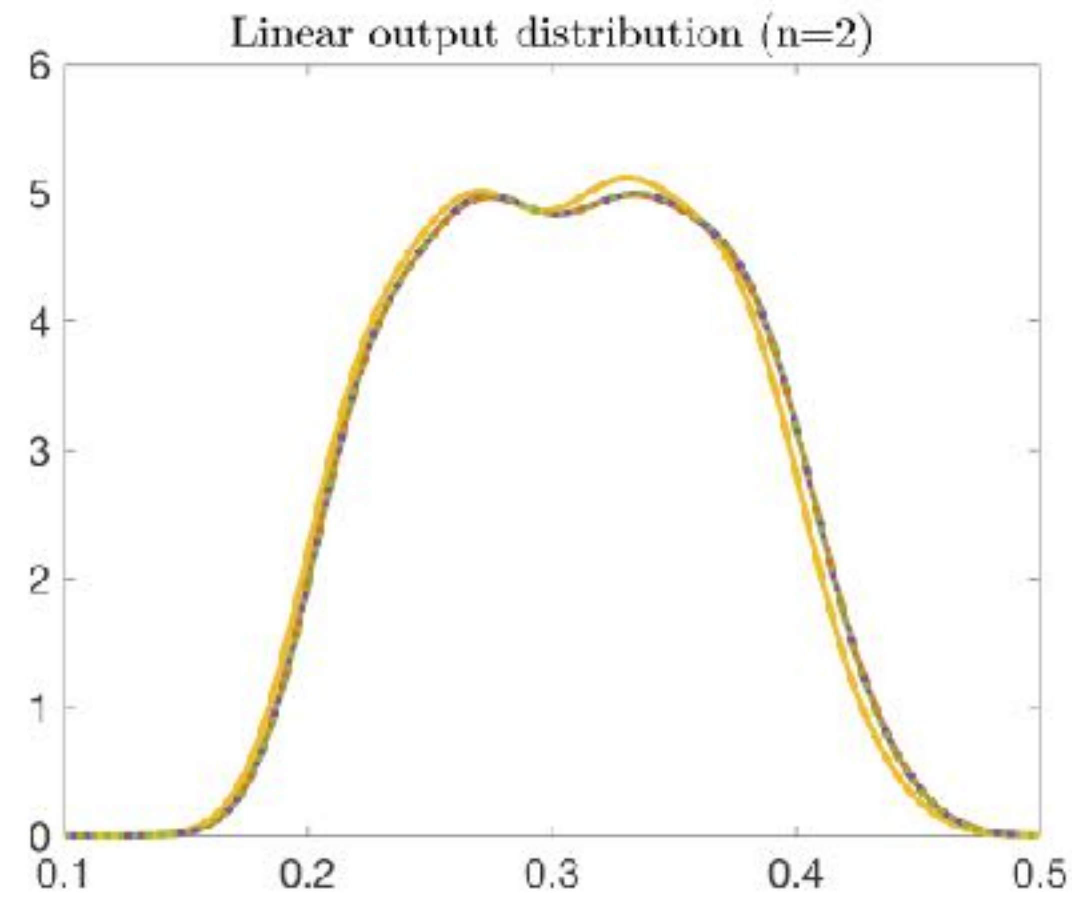
$$\mathbb{E}[Q] - \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \mathcal{Q}(\mathbb{V}\mathbf{u}_n(\boldsymbol{\mu}_q)) = \underbrace{\mathbb{E}[Q - Q_n]}_{\text{approx. error}} + \underbrace{\mathbb{E}[Q_n] - \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \mathcal{Q}(\mathbb{V}\mathbf{u}_n(\boldsymbol{\mu}_q))}_{\text{statistical error}}.$$

ROMES enables to minimize $\mathbb{E}[Q - Q_n]$ without changing the ROM:

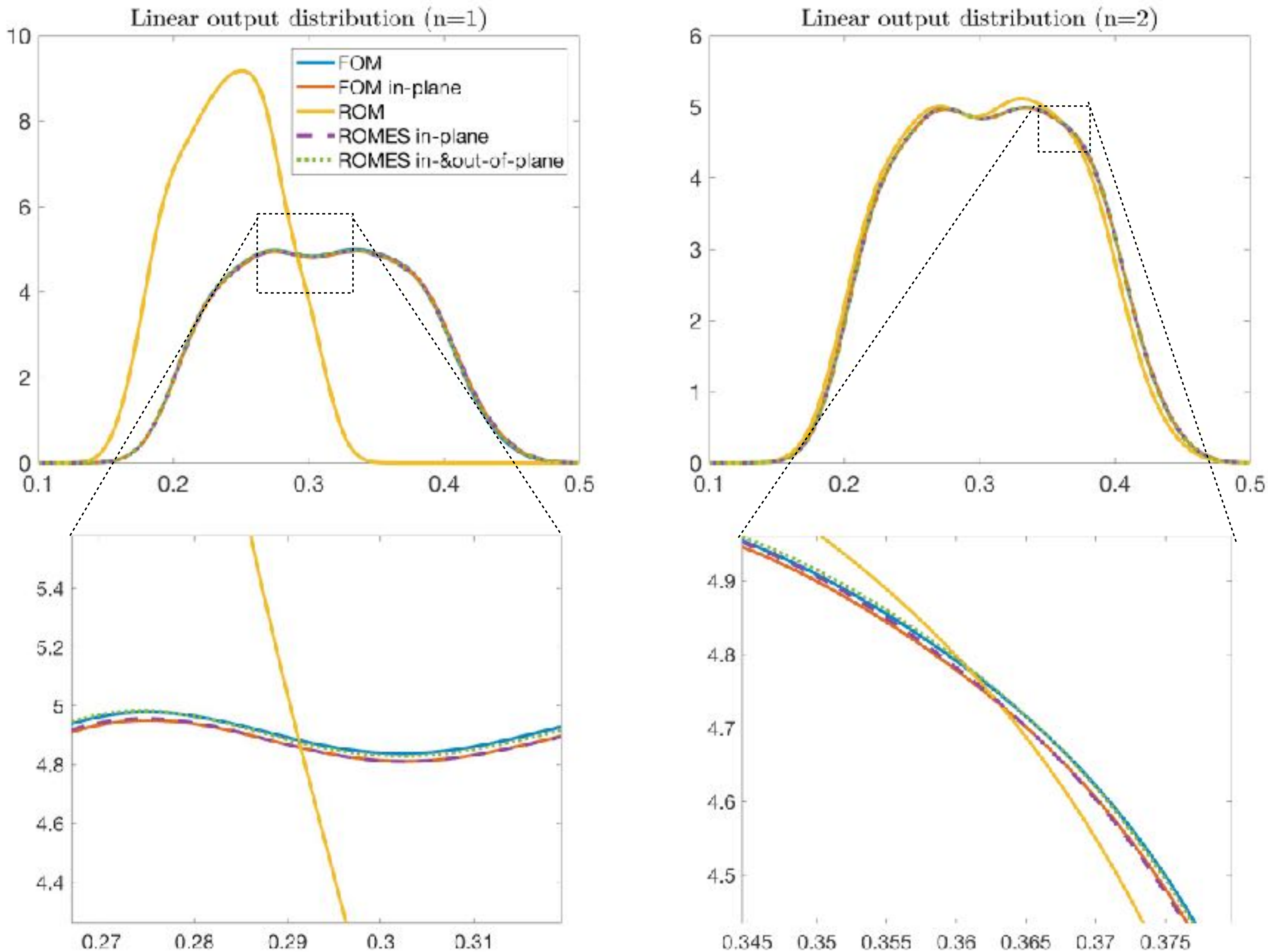
$$\mathbb{E}[\tilde{Q}_n] \approx \frac{1}{N_{mc}} \sum_{q=1}^{N_{mc}} \mathcal{Q}(\mathbb{V}\mathbf{u}_n(\boldsymbol{\mu}_q) + \mathbb{V}\tilde{\boldsymbol{\delta}}_{V_n}(\boldsymbol{\mu}_q) + \mathbb{V}^{\perp}\tilde{\boldsymbol{\delta}}_{V_n^{\perp}}(\boldsymbol{\mu}_q)).$$

Forward UQ: linear scalar output





Forward UQ: linear scalar output



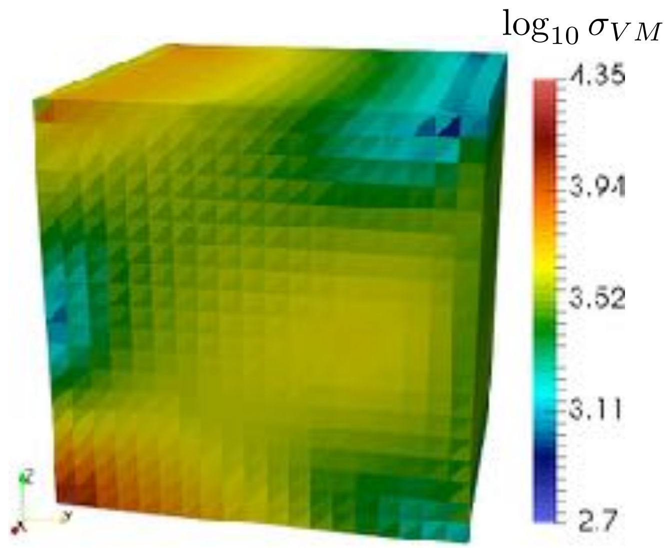
Forward UQ: Von Miss stress

Quantity of interest: Von Mises stress field

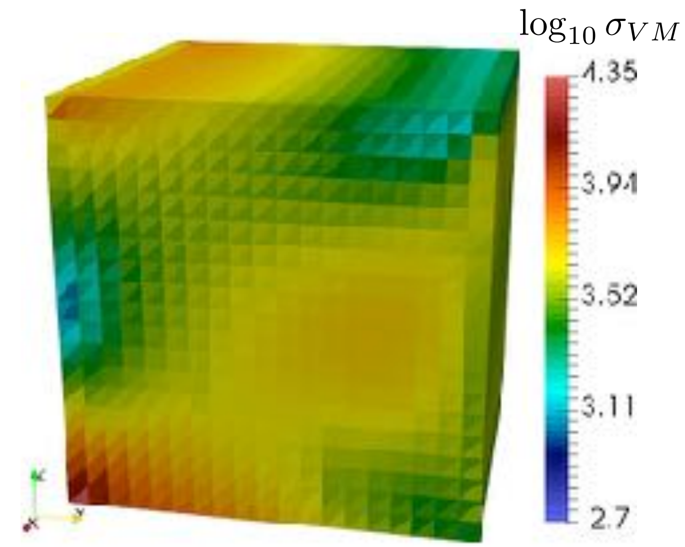
$$\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbf{u}) = \sqrt{0.5((\sigma_{11}-\sigma_{22})^2 + (\sigma_{22}-\sigma_{33})^2 + (\sigma_{33}-\sigma_{11})^2 + 6*(\sigma_{12}^2+\sigma_{23}^2+\sigma_{31}^2))},$$

where $\sigma_{ij} = (\mathbf{P}(\mathbf{u})(\mathbf{I}+\nabla\mathbf{u})^T)_{ij},\ i,j=1,2,3.$

$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbf{u}_h)]$

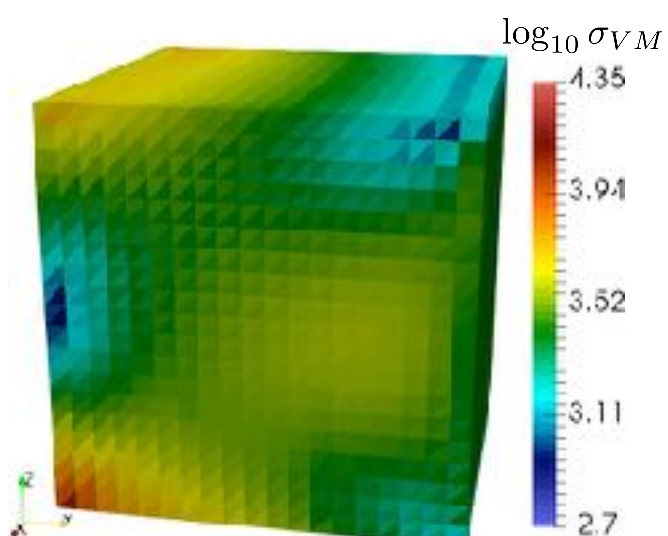


$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbb{V}(\mathbf{u}_n+\tilde{\boldsymbol{\delta}}_{V_n}))]$

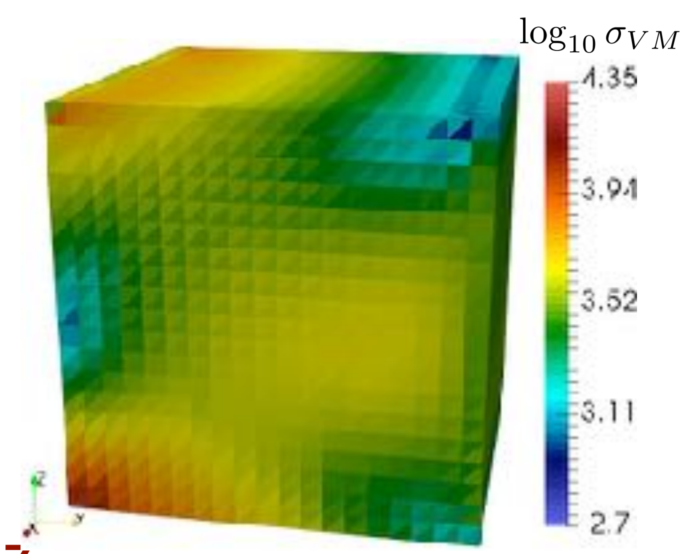


$n=1$

$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbb{V}\mathbf{u}_n)]$



$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbb{V}(\mathbf{u}_n+\tilde{\boldsymbol{\delta}}_{V_n})+\mathbb{V}^{\perp}\tilde{\boldsymbol{\delta}}_{V_n^{\perp}})]$ $\quad n^{\perp}=13$

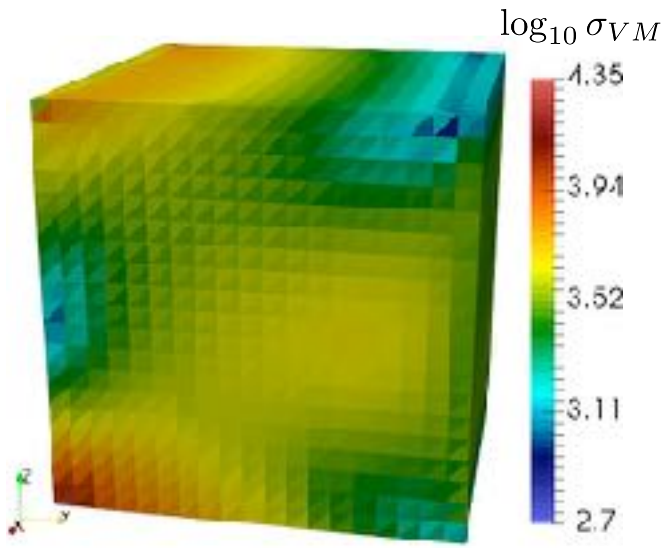


Quantity of interest: Von Mises stress field

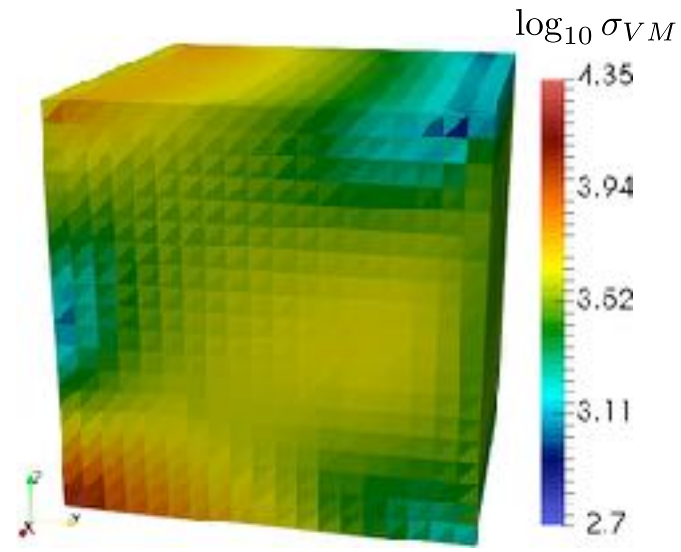
$$\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbf{u}) = \sqrt{0.5((\sigma_{11}-\sigma_{22})^2+(\sigma_{22}-\sigma_{33})^2+(\sigma_{33}-\sigma_{11})^2+6*(\sigma_{12}^2+\sigma_{23}^2+\sigma_{31}^2))},$$

where $\sigma_{ij} = (\mathbf{P}(\mathbf{u})(\mathbf{I}+\nabla\mathbf{u})^T)_{ij},\ i,j = 1,2,3.$

$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbf{u}_h)]$

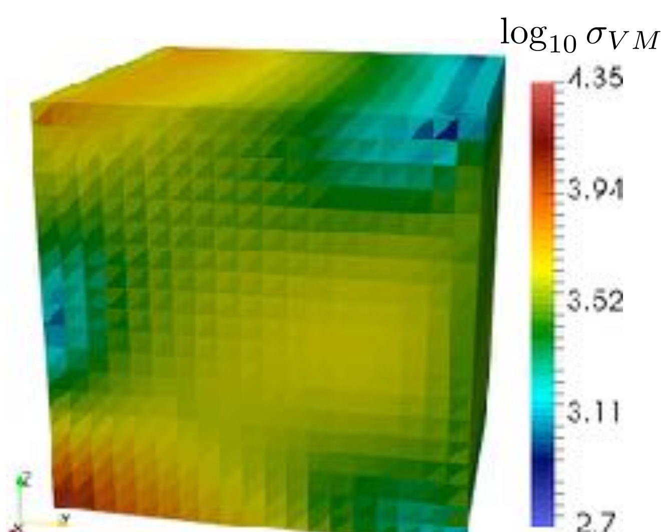


$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbb{V}(\mathbf{u}_n+\tilde{\boldsymbol{\delta}}_{V_n}))]$

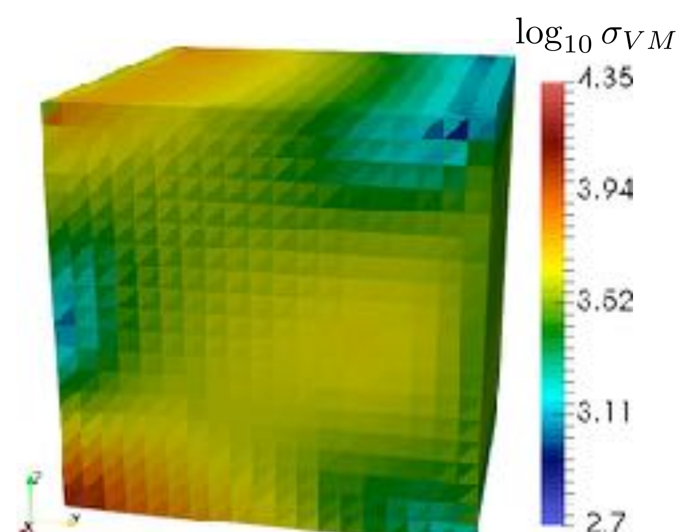


$n = 2$

$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbb{V}\mathbf{u}_n)]$



$\mathbb{E}[\boldsymbol{\sigma}_{VM}(\mathbf{x};\mathbb{V}(\mathbf{u}_n+\tilde{\boldsymbol{\delta}}_{V_n})+\mathbb{V}^{\perp}\tilde{\boldsymbol{\delta}}_{V_n^{\perp}})]$ $n^{\perp} = 12$



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Thank you!

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