# Modeling and controlling reduced-order-model uncertainty in data assimilation

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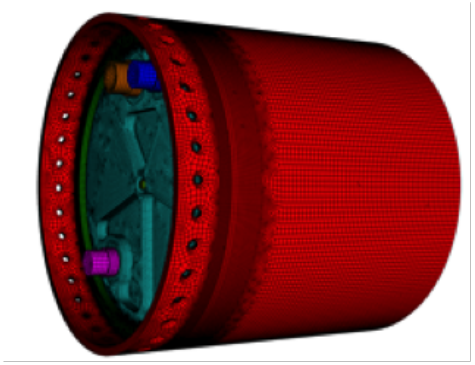
*Modeling and simulation*

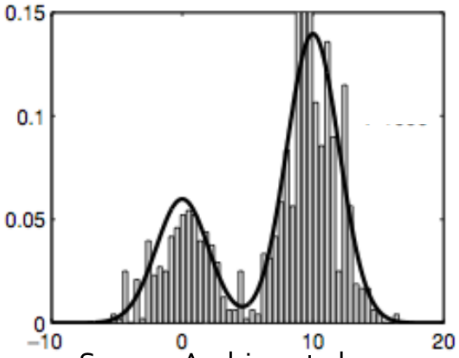
+ Indispensible tool
- Only a few simulations possible



## Barrier

*Time-critical applications*

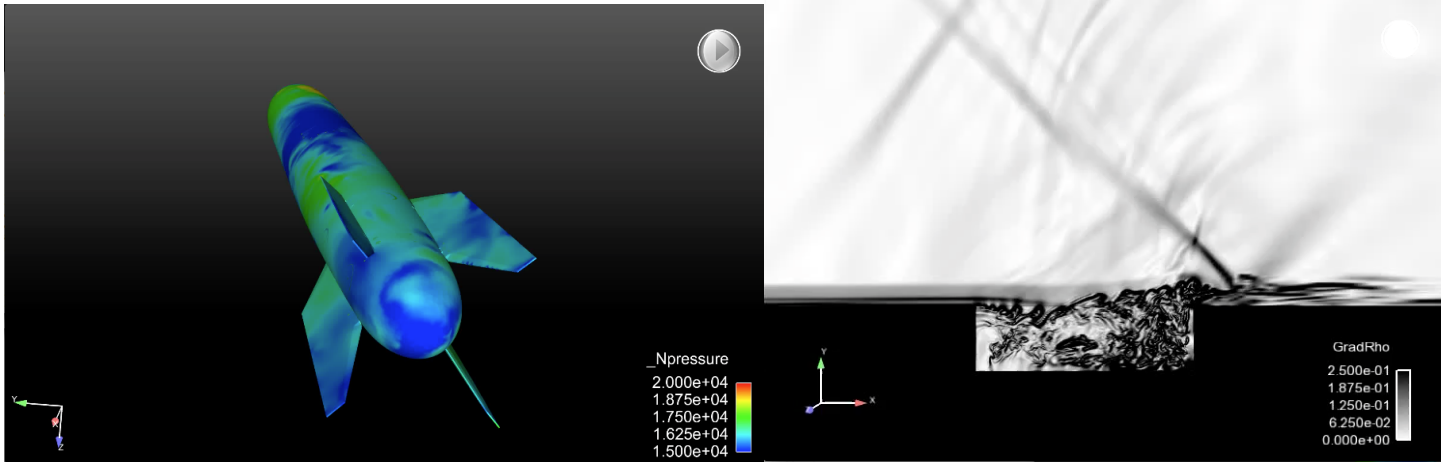
- Many query
- Real time



Source: Andrieu et al., 2003

**Objective: break barrier**

# At Sandia




- Full-order model
  - 100 million cells
  - 200,000 time steps
- High simulation costs
  - 6 weeks
  - 5000 cores
  - 6 runs maxes out Cielo

## Barrier

- Design engineers require faster simulations
- Uncertainty quantification (UQ)

# Data assimilation

source: Holger Speckmann, Airbus

*Given sensor data, what is the updated knowledge of material properties?*

- Bayesian inference problem

# Bayesian inference

$$\text{inputs } \boldsymbol{\mu} \rightarrow \boxed{\text{full-order model (FOM)}} \rightarrow \text{outputs } \mathbf{z}$$

$$P(\boldsymbol{\mu}|\bar{\mathbf{z}}) \propto P(\bar{\mathbf{z}}|\boldsymbol{\mu})P(\boldsymbol{\mu})$$

**Given**:

- Prior: $P(\boldsymbol{\mu})$
- Measurements: $\bar{\mathbf{z}}$
- Measurements/FOM relationship: $\bar{\mathbf{z}} = \mathbf{z}(\boldsymbol{\mu}^\star) + \boldsymbol{\varepsilon}$
  - Sensor noise: $\boldsymbol{\varepsilon} \sim \mathcal{N}(0, \sigma^2\mathbf{I})$
  - Likelihood: $P(\bar{\mathbf{z}}|\boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{z}(\boldsymbol{\mu}), \sigma^2\mathbf{I})$

**Compute**:

- Samples of the posterior $P(\boldsymbol{\mu}|\bar{\mathbf{z}})$

- Expensive: Likelihood samples requires FOM evaluations

# Bayesian inference with *reduced-order models*

$$\text{inputs } \boldsymbol{\mu} \rightarrow \boxed{\text{reduced-order model (ROM)}} \rightarrow \text{outputs } \mathbf{z}_{\text{red}}$$

$$P(\boldsymbol{\mu}|\bar{\mathbf{z}}) \propto P(\bar{\mathbf{z}}|\boldsymbol{\mu})P(\boldsymbol{\mu})$$

**Given**:

- Prior: $P(\boldsymbol{\mu})$
- Measurements: $\bar{\mathbf{z}}$
- Measurements/ROM relationship: $\bar{\mathbf{z}} = \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \boldsymbol{\varepsilon}$
  - Sensor noise: $\boldsymbol{\varepsilon} \sim \mathcal{N}(0, \sigma^2\mathbf{I})$
  - Likelihood: $P(\bar{\mathbf{z}}|\boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{z}_{\text{red}}(\boldsymbol{\mu}), \sigma^2\mathbf{I})$

**Compute**:

- Samples of the posterior $P(\boldsymbol{\mu}|\bar{\mathbf{z}})$

\+ Cheap: Likelihood samples requires ROM evaluations

\- Neglects ROM errors:

$$\begin{aligned}\bar{\mathbf{z}} &= \mathbf{z}(\boldsymbol{\mu}^\star) + \boldsymbol{\varepsilon} \\ &= \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \boxed{\delta_{\mathbf{z}}(\boldsymbol{\mu}^\star)} + \boldsymbol{\varepsilon}\end{aligned}$$

# Reduced-order modeling: modeling and controlling error

$$\bar{\mathbf{z}} = \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \boxed{\delta_{\mathbf{z}}(\boldsymbol{\mu}^\star)} + \varepsilon$$

*"An interesting future research direction is the inclusion of estimates of reduced model error as an additional source of uncertainty in the Bayesian formulation."*

*[Galbally et al., 2009]*

**Our goals**:

1. construct a statistical model of this error
2. control this error

# Error control

$$\bar{\mathbf{z}} = \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \boxed{\delta_{\mathbf{z}}(\boldsymbol{\mu}^\star)} + \varepsilon$$

*"An interesting future research direction is the inclusion of estimates of reduced model error as an additional source of uncertainty in the Bayesian formulation."*

*[Galbally et al., 2009]*

**Our goals**:

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2. control this error

# Reduced-order modeling: accuracy limitation

- FOM: parameterized sequence of systems of equations

$$\mathbf{r}^k(\mathbf{x}^k; \boldsymbol{\mu}) = 0, \quad k = 1, \ldots, t$$

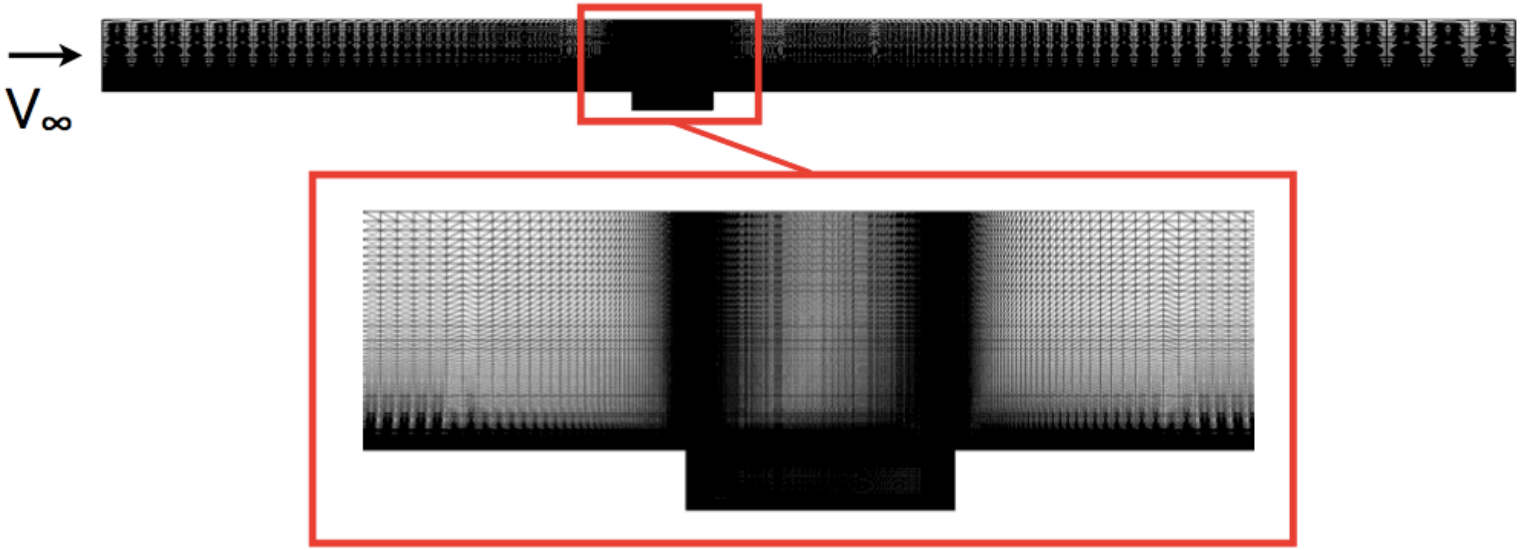
  with state $\mathbf{x} \in \mathbb{R}^n$, and residual $\mathbf{r}$.
- ROM
  1. *Offline*: construct low-dimensional basis $\mathbf{V} \in \mathbb{R}^{n \times p}$ with $p \ll n$
  2. *Online*: approximate $\mathbf{x}^k \approx \mathbf{V}\hat{\mathbf{x}}^k$ and solve

$$\mathbf{V}^T \mathbf{r}^k(\mathbf{V}\hat{\mathbf{x}}^k; \boldsymbol{\mu}) = 0, \quad k = 1, \ldots, t$$

  Additional approximations needed if $\mathbf{r}$ nonlinear or nonaffine

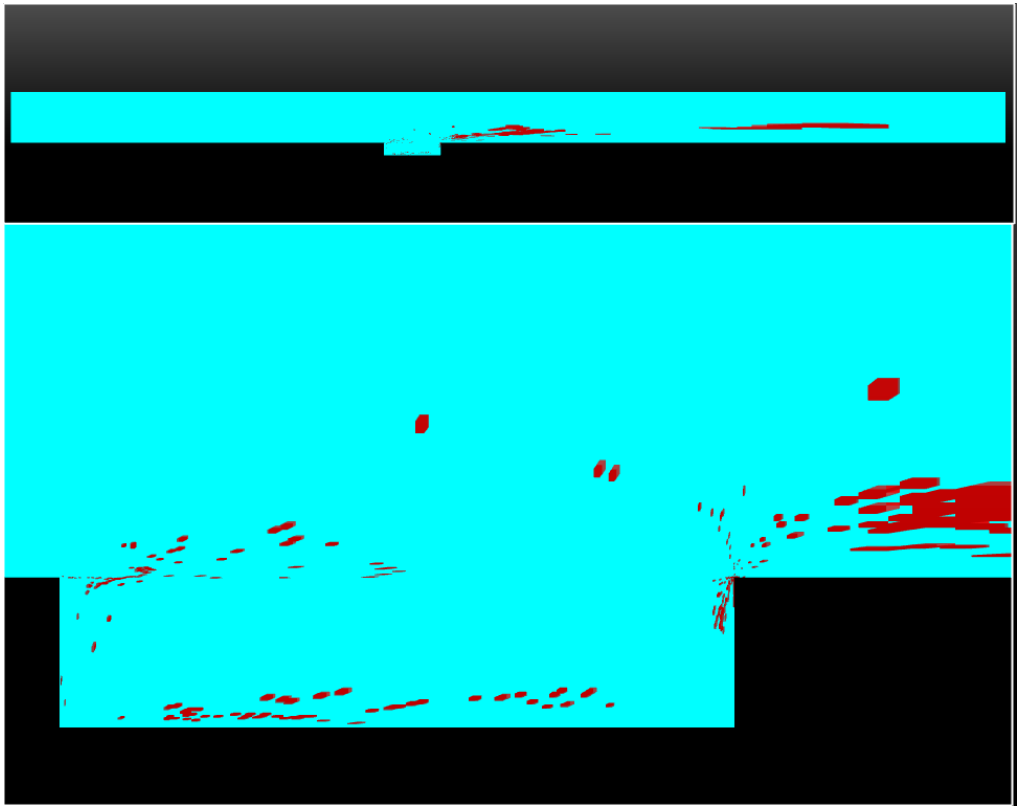
\+ ROMs are almost always *fast* ($p \ll n$).

# Example: Cavity-flow problem (collaborators: M Barone, S Arunajatesan)




- FOM: Compressible Navier–Stokes (AERO-F)
  - Nonlinear dynamical system
  - $\mathrm{Re} = 6.3 \times 10^6$
  - $M_\infty = 0.6$
  - DES turbulence model
  - 3 point BDF integrator
  - 1.2 million degrees of freedom
- ROM: GNAT [Carlberg et al., 2013]
  - 179 degrees of freedom

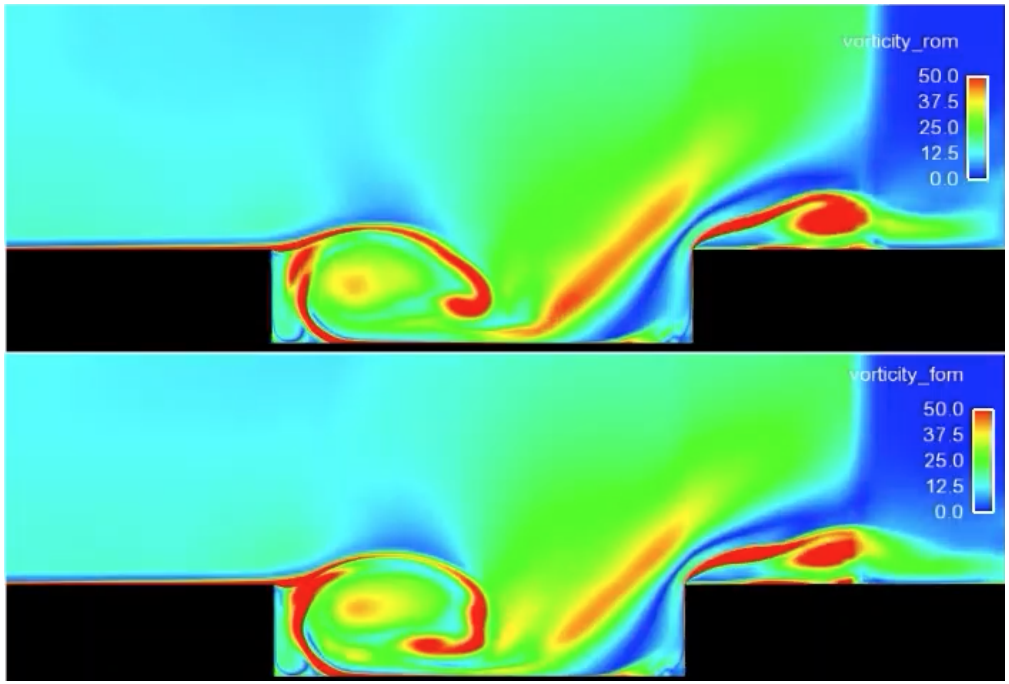
# Example: Cavity-flow problem (collaborators: M Barone, S Arunajatesan)



- sample mesh: 4% of original mesh

+ enables the ROM to run on far fewer cores

# When a ROM works




- FOM: 48 cpu x 5 hours
- ROM: 2 cpu x 31 min = 229X cpu savings
- However, ROMs are not guaranteed to be *accurate*.

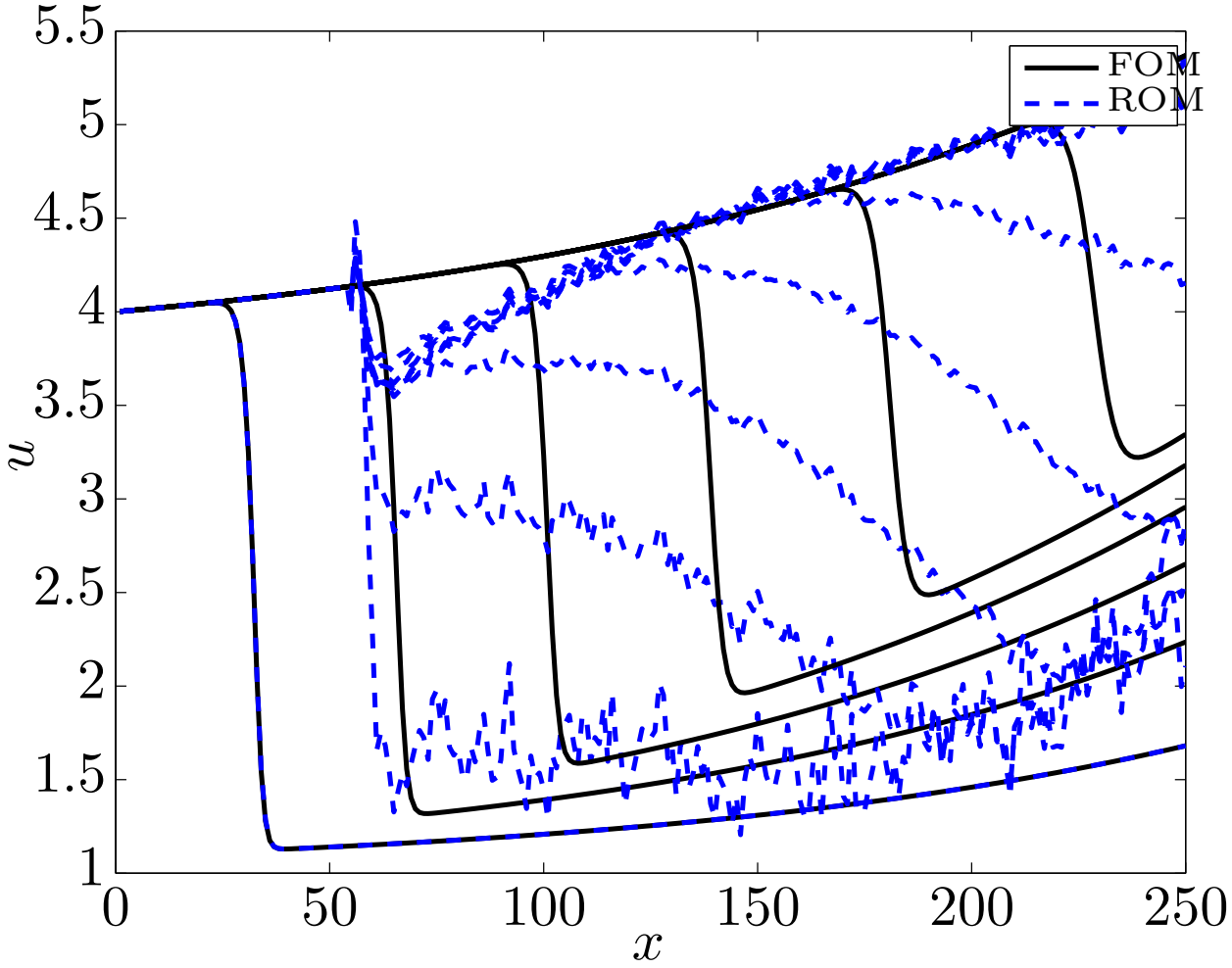
*ROM accuracy is limited by the information in* $\mathbf{V}$.

# Example: inviscid Burgers equation [Rewienski, 2003]

$$\frac{\partial u(x,\tau)}{\partial \tau} + \frac{1}{2}\frac{\partial\left(u^2(x,\tau)\right)}{\partial x} = 0.02e^{0.02x}$$
$$u(0,\tau) = 3,\ \forall \tau > 0$$
$$u(x,0) = 1,\ \forall x \in [0,\ 100]\,,$$

- Discretization: Godunov's scheme
- Simulate $\tau \in [0, 50]$
- FOM: 250 degrees of freedom
- ROM: 150 degrees of freedom
- **V** constructed via POD using snapshots in $\tau_{\text{train}} \in [0, 2.5]$

# ROM accuracy limited by relevance of training data




- ROM inaccurate when outside predictive domain of **V**

# Existing ROM adaptation methods

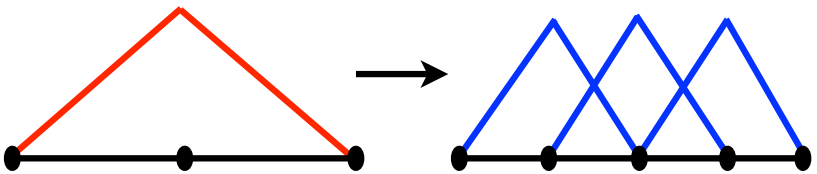
- *A priori* adaptation: unique ROM for separate regions of the
  - input space [Amsallem and Farhat, 2008, Amsallem et al., 2009, Eftang et al., 2010, Eftang et al., 2011, Haasdonk et al., 2011, Drohmann et al., 2011, Peherstorfer et al., 2014]
  - time domain [Drohmann et al., 2011, Dihlmann et al., ]
  - state space [Amsallem et al., 2012, Washabaugh et al., 2012, Peherstorfer et al., 2014].
  - \+ Reduces the dimension of the ROM
  - \- No mechanism to improve the ROM *a posteriori*
- *A posteriori* adaptation
  - Revert to the FOM, solve it, and add solution to the basis [Eldred et al., 2009, Arian et al., 2000, Ryckelynck, 2005]
  - Use ROM as a preconditioner for the FOM iterative solver [Carlberg and Farhat, 2009]
  - \+ Improves the ROM *a posteriori*
  - \- Incurs large-scale operations

**Goal**: *Cheap, a posteriori improvement of the ROM*

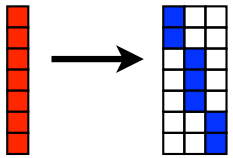
# Main idea

*ROM analog to mesh-adaptive h-refinement*

- 'Split' basis vectors

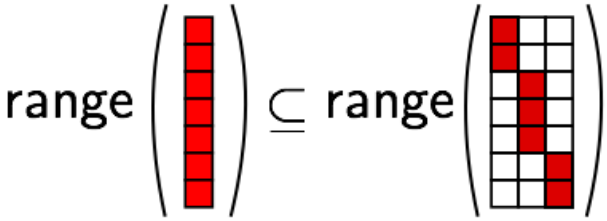


*finite element h-refinement*

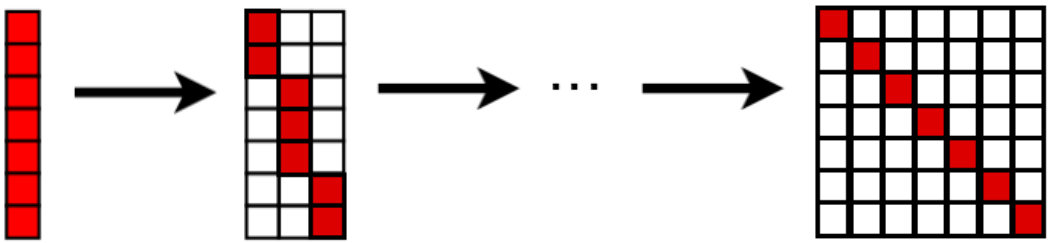


*ROM h-refinement*

- Generate hierarchical subspaces

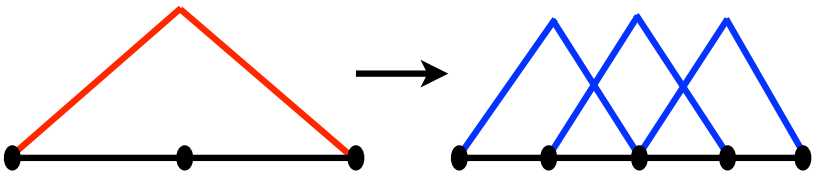


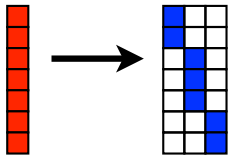

- ROM converges to the FOM



# *h*-refinement ingredients

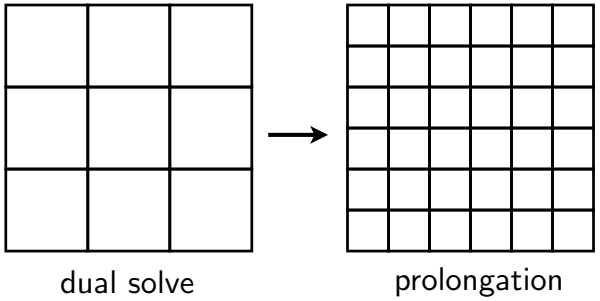
1. *Refinement*: split into basis vectors with different support

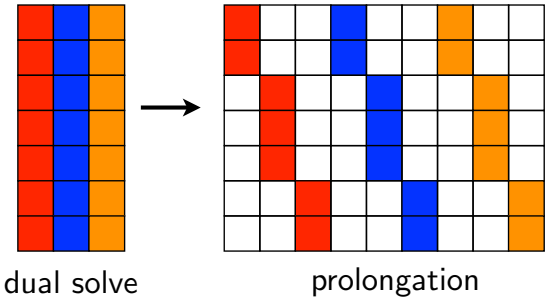




*finite element h-refinement* *ROM h-refinement*

2. *Error indicators*: a) dual solve (coarse), b) prolongation (fine)



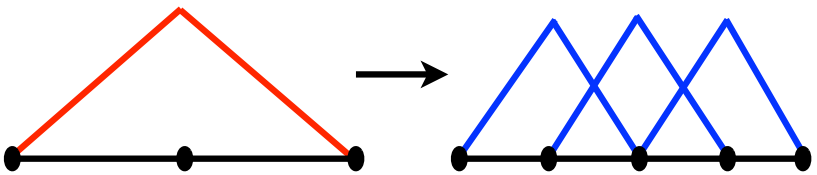




*finite element h-refinement* *ROM h-refinement*

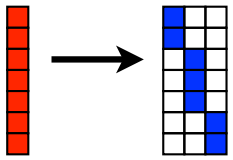
3. *Adaptive algorithm*: refine vectors with large error indicators

# Ingredient 1: Refinement

1. *Refinement*: split into basis vectors with different support



*finite element h-refinement*



*ROM h-refinement*

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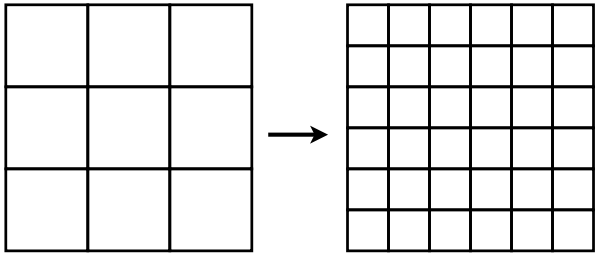
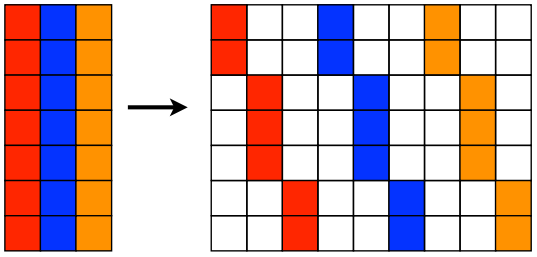


dual solve prolongation

*finite element h-refinement*

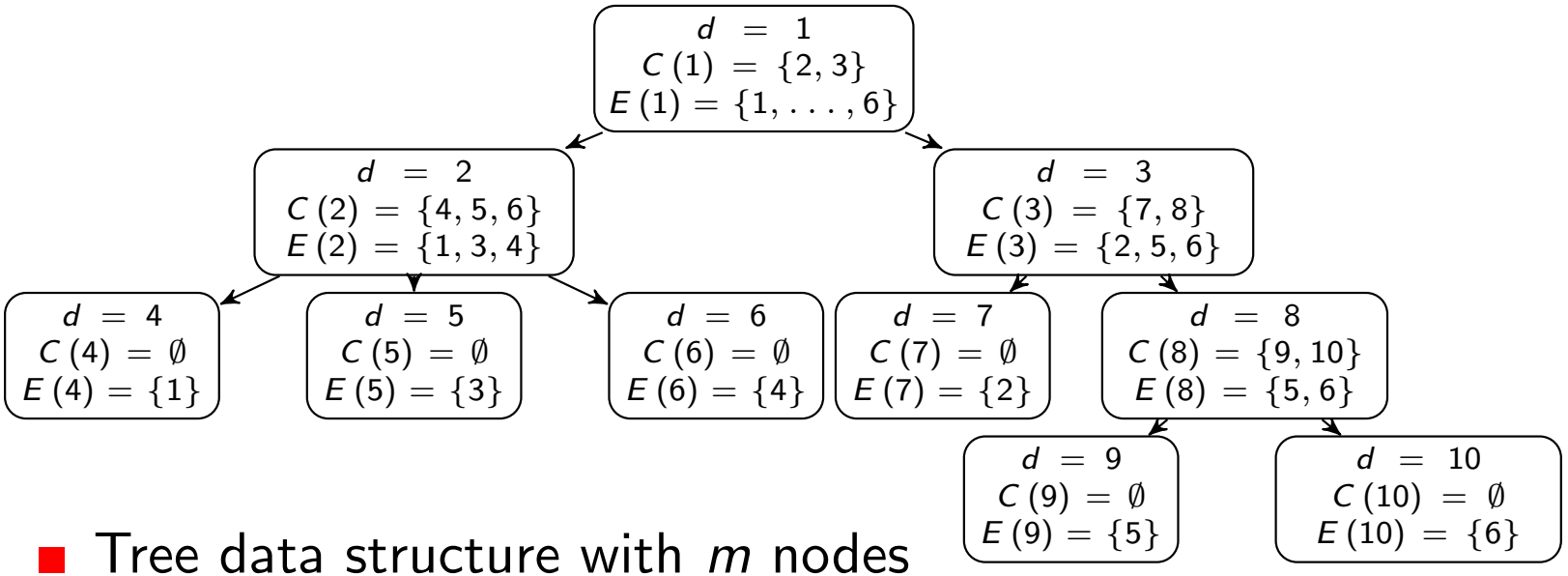


dual solve prolongation

*ROM h-refinement*

3. *Adaptive algorithm*: refine basis vecs with large error indicators

# Tree data structure

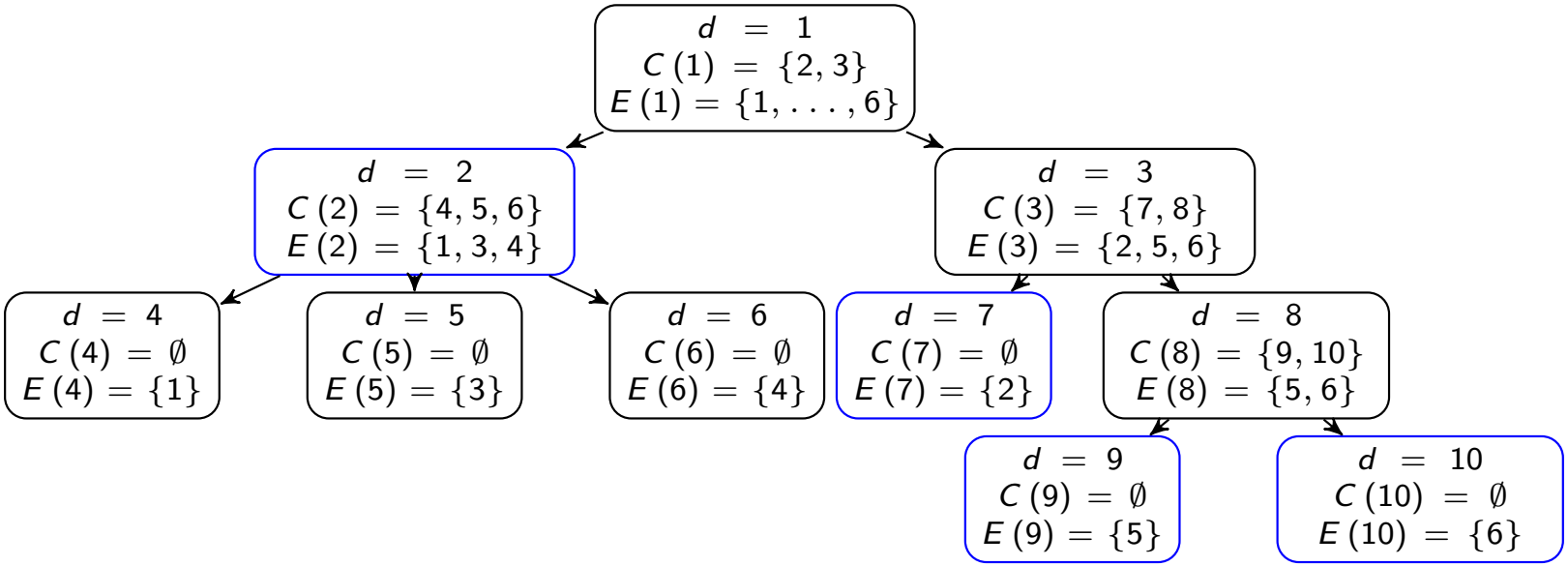



- Tree data structure with $m$ nodes
  - *child* function $C : \mathbb{N}(m) \to \mathcal{P}(\mathbb{N}(m))$
  - *element* function $E : \mathbb{N}(m) \to \mathcal{P}(\mathbb{N}(n))$
- Requirements
  1. Root node includes all elements $E(1)$
  2. Each element has a single leaf node
  3. Disjoint support of children $E(j) \cap E(k) = \emptyset, \ \forall j \neq k \in C(i)$
  4. $\cup_{j \in C(i)} E(j) = E(i)$

  \+ 1–2 ensure the ROM converges to the FOM

  \+ 4 ensures hierarchical refined subspaces

# Tree example: $n = 6$

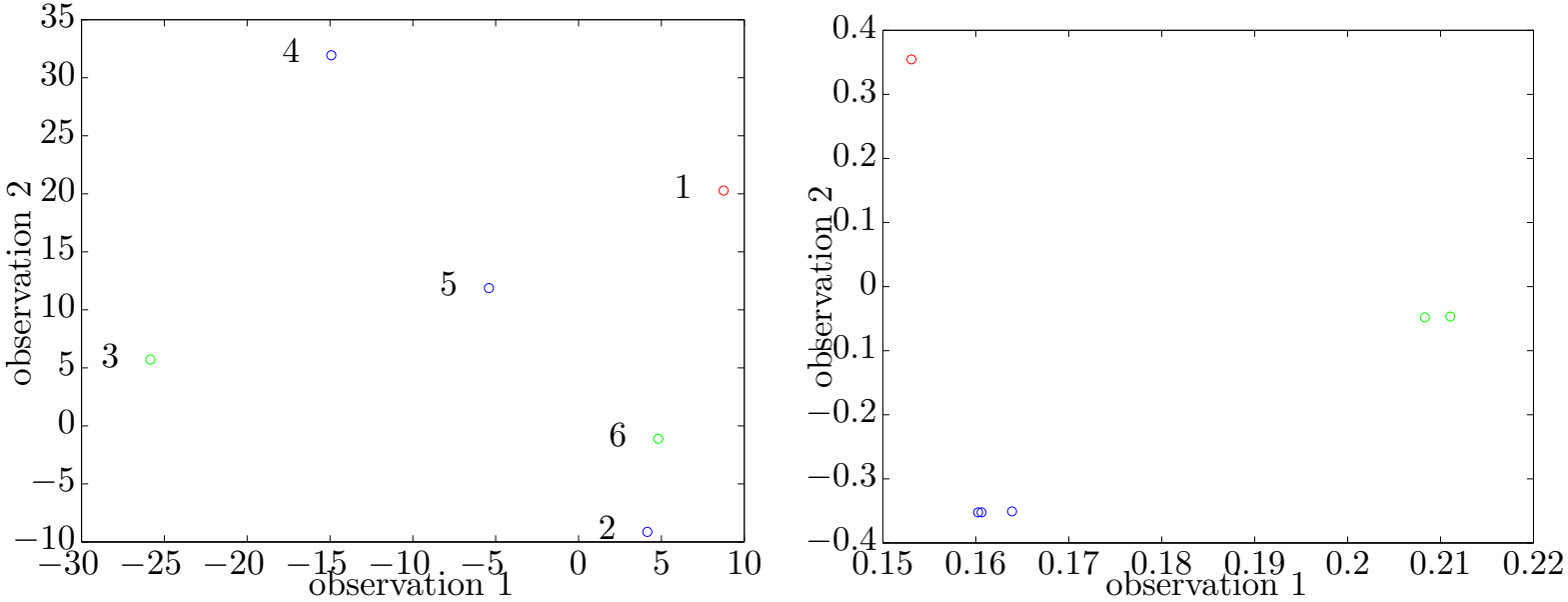



$$\mathbf{v}^{(0)} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{bmatrix} \quad \rightarrow \quad \mathbf{V} = \begin{bmatrix} v_1 & 0 & 0 & 0 \\ 0 & v_2 & 0 & 0 \\ v_3 & 0 & 0 & 0 \\ v_4 & 0 & 0 & 0 \\ 0 & 0 & v_5 & 0 \\ 0 & 0 & 0 & v_6 \end{bmatrix}.$$

# Tree construction

*State variables that are strongly* **correlated** *or* **anticorrelated** *should reside in the same tree node.*

1. Normalize state-variable observation history
2. If first observation is negative, flip over origin
3. Recursively apply **k-means clustering**

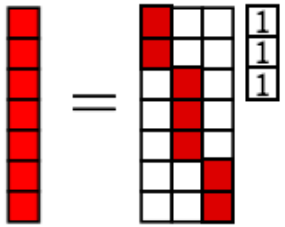



(a) before modification (b) after modification

Figure : State-variable observation history (variable index labeled).

# Refinement machinery

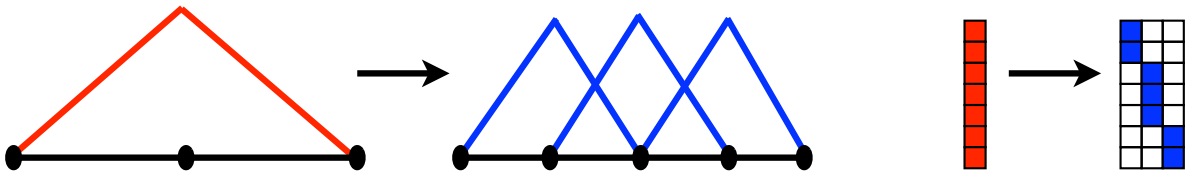
$$\mathbf{V}^H = \mathbf{V}^h \mathbf{I}_H^h$$




- coarse basis $\mathbf{V}^H \in \mathbb{R}^{n \times p}$ $\mathbf{V}^{(0)}$)
- fine basis $\mathbf{V}^h \in \mathbb{R}^{n \times q}$ with $q = \sum_{i=1}^{p} \text{card}\left(C\left(d_i\right)\right)$
- prolongation operator $\mathbf{I}_H^h \in \{0, 1\}^{q \times p}$
- prolongated generalized coordinates $\hat{\mathbf{x}}_H^h = \mathbf{I}_H^h \hat{\mathbf{x}}^H$
- restriction operator $\mathbf{I}_h^H = \left(\mathbf{I}_H^h\right)^+$

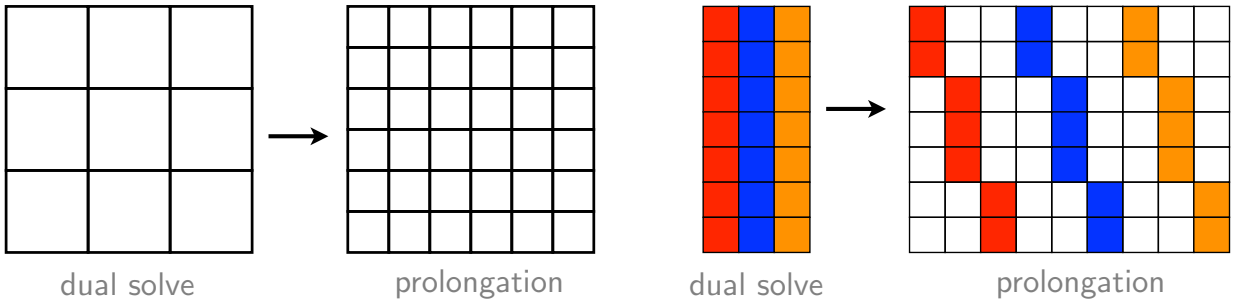
# Ingredient 2: Error indicators

- **Main idea**: ROM analog to mesh-adaptive *h*-refinement
  1. *Refinement*: split into basis vectors with different support



*finite element h-refinement* *ROM h-refinement*

  2. *Error indicators*: a) dual solve (coarse), b) prolongation (fine)




*finite element h-refinement* *ROM h-refinement*

  3. *Adaptive algorithm*: refine basis vecs with large error indicators

# Dual-weighted residual error indicators

- **Goal-oriented**: reduce the error in output $z(\mathbf{x})$
- Analogous to duality-based error control for
  - differential equations [Estep, 1995, Pierce and Giles, 2000]
  - finite elements [Babuška and Miller, 1984, Becker and Rannacher, 1996, Rannacher, 1999, Bangerth and Rannacher, 1999, Becker and Rannacher, 2001, Bangerth and Rannacher, 2003],
  - finite volumes [Venditti and Darmofal, 2000, Venditti and Darmofal, 2002, Park, 2004, Nemec and Aftosmis, 2007]
  - discontinuous Galerkin methods [Lu, 2005, Fidkowski, 2007]

# Dual-weighted residual error indicators

- Approximate fine output:

$$z(\mathbf{V}^h\hat{\mathbf{x}}^h) \approx z(\mathbf{V}^H\hat{\mathbf{x}}^H) + \frac{\partial z}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)\mathbf{V}^h(\hat{\mathbf{x}}^h - \mathbf{I}_H^h\hat{\mathbf{x}}^H) \qquad (1)$$

- Approximate the fine residual:

$$0 = (\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^h\hat{\mathbf{x}}^h) \approx (\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H) + (\mathbf{V}^h)^T\frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)\mathbf{V}^h(\hat{\mathbf{x}}^h - \mathbf{I}_H^h\hat{\mathbf{x}}^H)$$

- Solve for the error:

$$(\hat{\mathbf{x}}^h - \mathbf{I}_H^h\hat{\mathbf{x}}^H) \approx -[(\mathbf{V}^h)^T\frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)\mathbf{V}^h]^{-1}(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H) \qquad (2)$$

- Substitute (2) in (1):

$$\boxed{z(\mathbf{V}^h\hat{\mathbf{x}}^h) - z(\mathbf{V}^H\hat{\mathbf{x}}^H) \approx -(\hat{\mathbf{y}}^h)^T(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H)},$$

with the fine adjoint solution $\hat{\mathbf{y}}^h \in \mathbb{R}^q$ satisfying

$$\boxed{(\mathbf{V}^{h\,T}\frac{\partial \mathbf{r}^k}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T\mathbf{V}^h\hat{\mathbf{y}}^h = \mathbf{V}^{h\,T}\frac{\partial z}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T}.$$

# Dual-weighted residual error indicators

$$\boxed{z(\mathbf{V}^h\hat{\mathbf{x}}^h) - z(\mathbf{V}^H\hat{\mathbf{x}}^H) \approx -(\hat{\mathbf{y}}^h)^T(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H)} \tag{3}$$

$$\boxed{(\mathbf{V}^h)^T\frac{\partial \mathbf{r}^k}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T\mathbf{V}^h\hat{\mathbf{y}}^h = (\mathbf{V}^h)^T\frac{\partial z}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T} \tag{4}$$

- We want to avoid fine solve (4), so approximate $\hat{\mathbf{y}}^h$ as

$$\hat{\mathbf{y}}^h_H = \mathbf{I}^h_H\hat{\mathbf{y}}^H,$$

  where $\hat{\mathbf{y}}^H$ is the coarse adjoint solution to

$$(\mathbf{V}^H)^T\frac{\partial \mathbf{r}^k}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T\mathbf{V}^H\hat{\mathbf{y}}^H = (\mathbf{V}^H)^T\frac{\partial z}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T.$$

- Substituting $\hat{\mathbf{y}}^h_H$ for $\hat{\mathbf{y}}^h$ in (3) yields cheaply computable

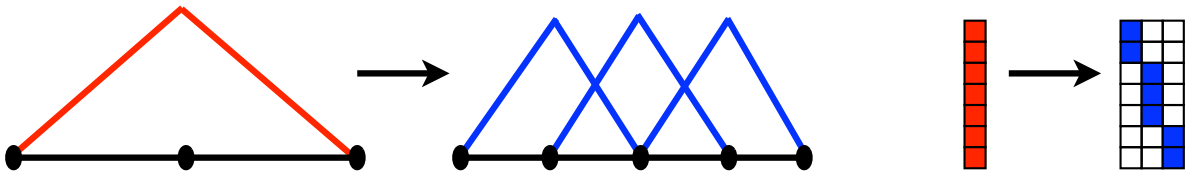
$$z(\mathbf{V}^h\hat{\mathbf{x}}^h) - z(\mathbf{V}^H\hat{\mathbf{x}}^H) \approx -(\hat{\mathbf{y}}^h_H)^T(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H).$$

- The RHS can be bounded by cheaply computable error indicators

$$|(\hat{\mathbf{y}}^h_H)^T(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H)| \leq \sum_{i=1}^{q}\boldsymbol{\Delta}^h_i, \quad \boxed{\boldsymbol{\Delta}^h_i = |\left[\hat{y}^h_H\right]_i\left(\mathbf{v}^h_i\right)^T\mathbf{r}\left(\mathbf{V}^H\hat{\mathbf{x}}^H\right)|.}$$

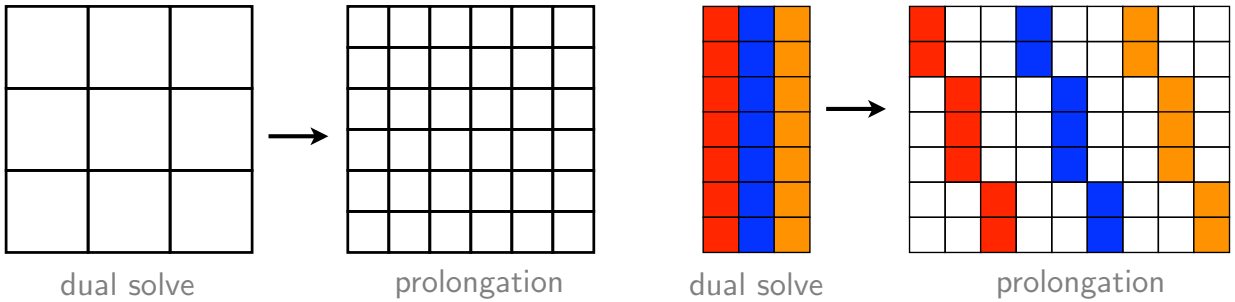
# Ingredient 3: Adaptive algorithm

- **Main idea**: ROM analog to mesh-adaptive *h*-refinement
  1. *Refinement*: split into basis vectors with different support



*finite element h-refinement* *ROM h-refinement*

  2. *Error indicators*: a) dual solve (coarse), b) prolongation (fine)




*finite element h-refinement* *ROM h-refinement*

  3. *Adaptive algorithm*: refine basis vecs with large error indicators

# Adaptive algorithm

**Algorithm 1** Outer loop

**Input:** timestep $k$, basis $\mathbf{V}$
**Output:** updated basis $\mathbf{V}$, generalized state $\hat{\mathbf{x}}^k$

1: Compute ROM solution $\hat{\mathbf{x}}^k$ satisfying $\mathbf{V}^T\mathbf{r}^k(\mathbf{V}\hat{\mathbf{x}}^k;\boldsymbol{\mu}) = 0$.
2: **if** estimate of output error $\delta_{\mathbf{z}}$ is 'too large' **then**
3: Refine basis via Algorithm 2: $\mathbf{V} \leftarrow \text{Refine}\left(\mathbf{V}, \hat{\mathbf{x}}^k\right)$.
4: Return to Step 1.
5: **end if**
6: **if** $\text{mod}\left(k, n_{\text{reset}}\right) = 0$ **then**
7: Reset basis $\mathbf{V} \leftarrow \mathbf{V}^{(0)}$.
8: **end if**

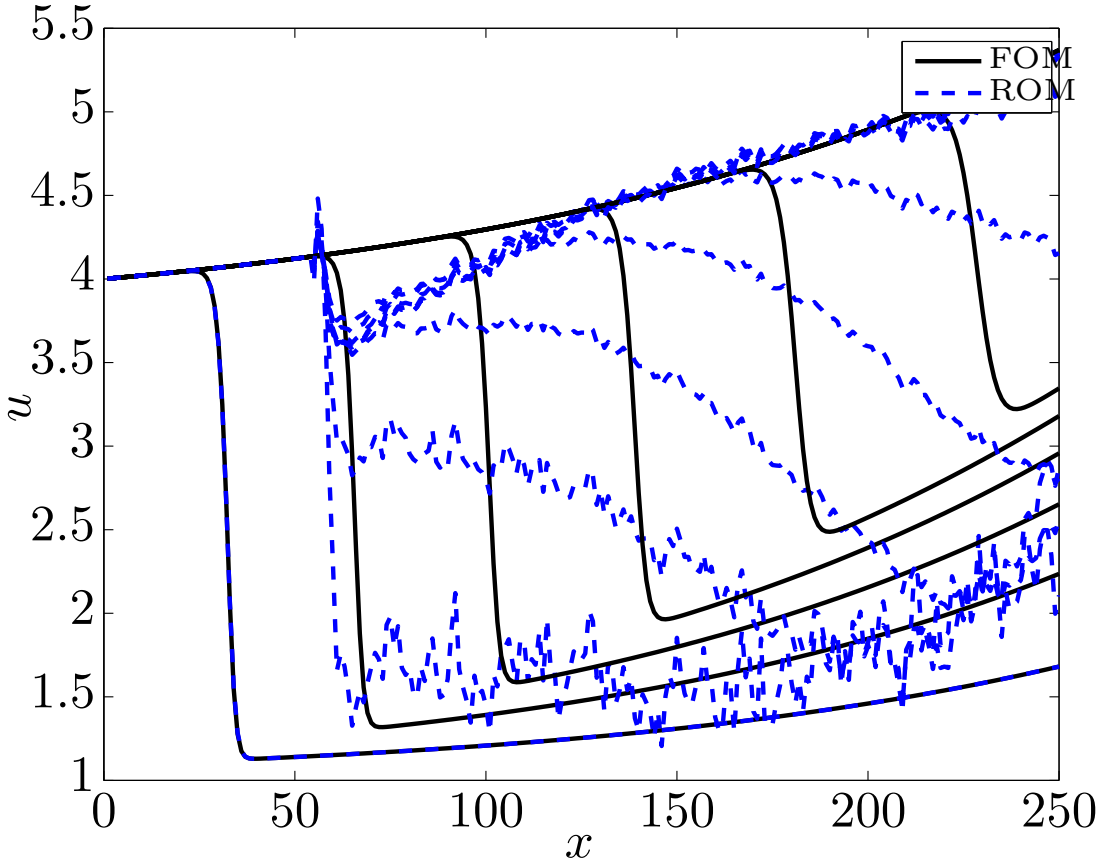
# Adaptive algorithm

**Algorithm 2** Refine

**Input:** initial basis $\mathbf{V}$, reduced solution $\hat{\mathbf{x}}$
**Output:** refined basis $\mathbf{V}$

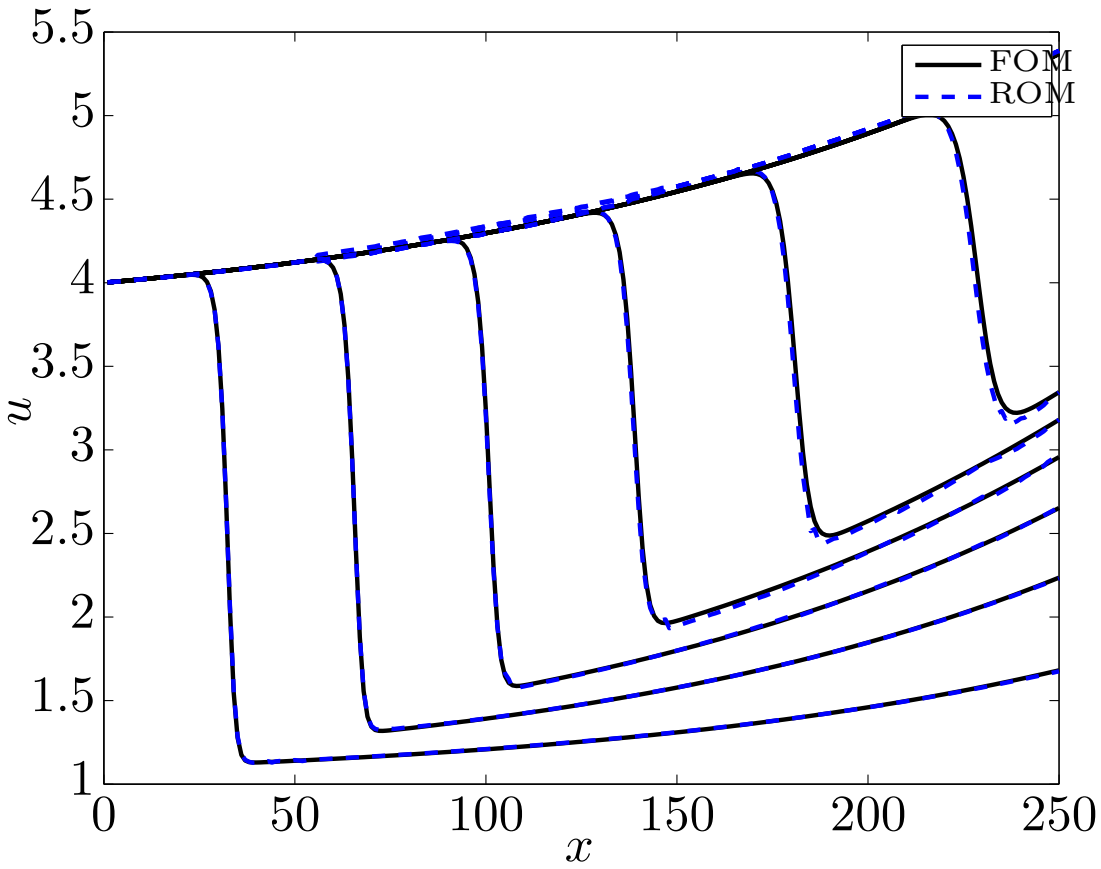
1: Compute prolongation operator $\mathbf{I}_H^h$ and fine basis $\mathbf{V}^h$
2: Solve: Compute coarse adjoint solution $\hat{\mathbf{y}}^H$ and prolongation $\hat{\mathbf{y}}_H^h$
3: Estimate: Compute fine error indicators $\boldsymbol{\Delta}_i^h$, $i = 1, \ldots, q$
4: Mark: Identify basis vectors to refine $I$
5: **for** $i \in I$ **do**
6: Refine: Split $\mathbf{v}_i$ into $\mathrm{card}\left(C\left(d_i\right)\right)$ vectors
7: **end for**
8: Compute QR factorization with column pivoting $\mathbf{V} = \mathbf{QR}$, $\mathbf{R}\bar{\mathbf{\Pi}} = \bar{\mathbf{Q}}\bar{\mathbf{R}}$
9: Ensure full-rank matrix $\mathbf{V} \leftarrow \mathbf{V}\left[\bar{\boldsymbol{\pi}}_1 \ \cdots \ \bar{\boldsymbol{\pi}}_r\right]$

# Previous example




- Generated by $\mathbf{V} \in \mathbb{R}^{250\times150}$ using $\tau_{\text{train}} \in [0, 2.5]$
- Now try *h*-adaptivity with $\mathbf{V}^{(0)} \in \mathbb{R}^{250\times10}$, $\tau_{\text{train}} \in [0, 2.5]$.

# Previous example with *h*-adaptivity (FOM tolerance $\epsilon = 0.05$)




- $\dim \mathbf{V}^{(0)} = 10$
- $\text{mean}(\dim \mathbf{V}) = 44.3$

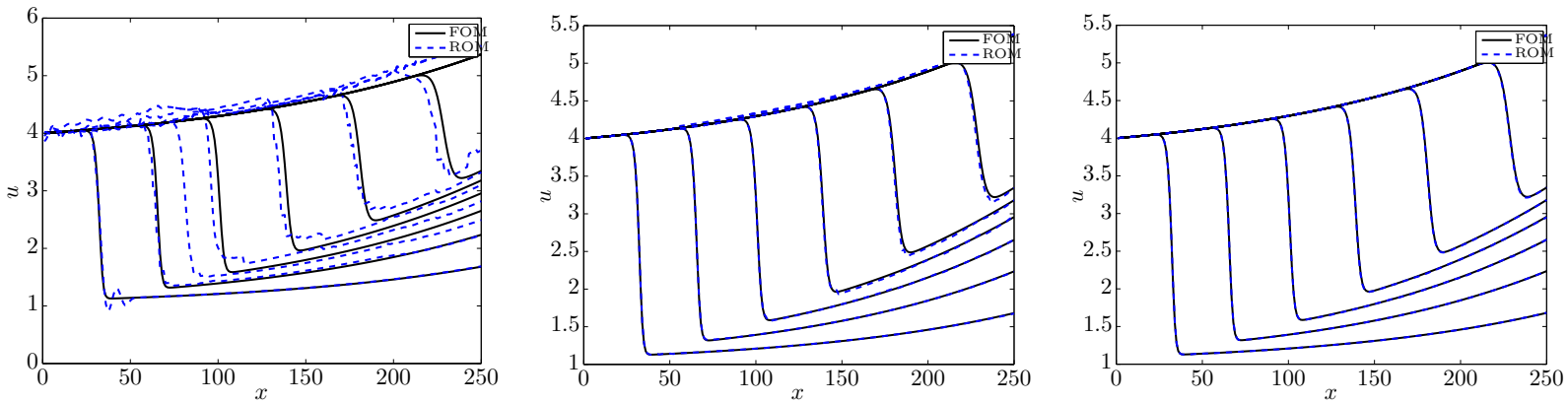
*h-adaptation allows the ROM to capture phenomena not present in the training data!*

# Inviscid Burgers equation: results

| | typical ROM | | | *h*-adaptive ROM | | | | |
|---|---|---|---|---|---|---|---|---|
| dim $\mathbf{V}^{(0)}$ | 10 | 45 | 150 | 5 | 10 | 20 | 10 | 10 |
| basis-reset frequency | | | | 50 | 50 | 50 | 100 | 25 |
| mean(dim $\mathbf{V}$) | 10 | 45 | 150 | 41.4 | 44.3 | 58 | 73 | 37 |
| Avg splits | | | | 0.20 | 0.19 | 0.14 | 0.13 | 0.28 |
| error (%) | 45.8 | 43.9 | 8.5 | 0.3 | 0.5 | 0.2 | 0.2 | 0.3 |
| online time (s) | 1.4 | 2.14 | 5.77 | 5.53 | 4.63 | 7.27 | 6.90 | 7.46 |

+ Low errors achievable only with *h*-adaptivity
- *Smaller initial basis*: smaller basis dimension, but more splits
- *More frequent basis resetting*: smaller basis dimension, but more splits

# $h$-adaptivity enables uncertainty/error control




(a) tolerance $\epsilon = 0.35$ (b) tolerance $\epsilon = 0.05$ (c) tolerance $\epsilon = 0.01$

| | $\epsilon = 0.35$ | $\epsilon = 0.05$ | $\epsilon = 0.01$ |
|---|---|---|---|
| average basis dimension per Newton iteration | 33.6 | 44.2507 | 53.9 |
| relative error (%) | 12.2 | 0.51 | 0.078 |
| online time (seconds) | 4.61 | 4.63 | 7.64 |

# Conclusions

- Adaptive *h*-refinement via splitting
  - \+ Incrementally improves ROM
  - \+ Does not require large-scale operations
  - \+ Enables uncertainty/error control
  - \+ Extends utility of ROMs to hyperbolic PDEs
- Future work
  - Production implementation
  - Adaptive *coarsening*
  - Adaptive *p*-refinement: add basis vectors from a library

# Error modeling

$$\bar{\mathbf{z}} = \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \boxed{\delta_{\mathbf{z}}(\boldsymbol{\mu}^\star)} + \varepsilon$$

*"An interesting future research direction is the inclusion of estimates of reduced model error as an additional source of uncertainty in the Bayesian formulation."*

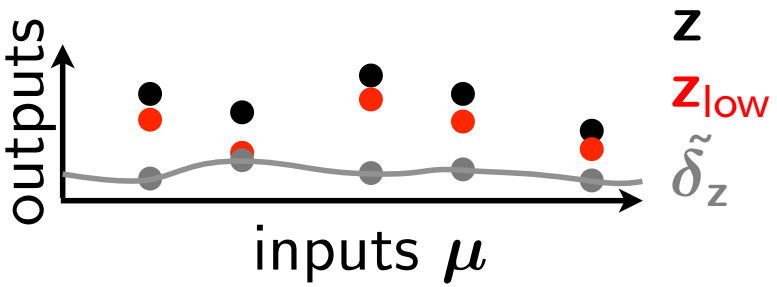
*[Galbally et al., 2009]*

**Our goals**:

1. construct a statistical model of this error
2. control this error

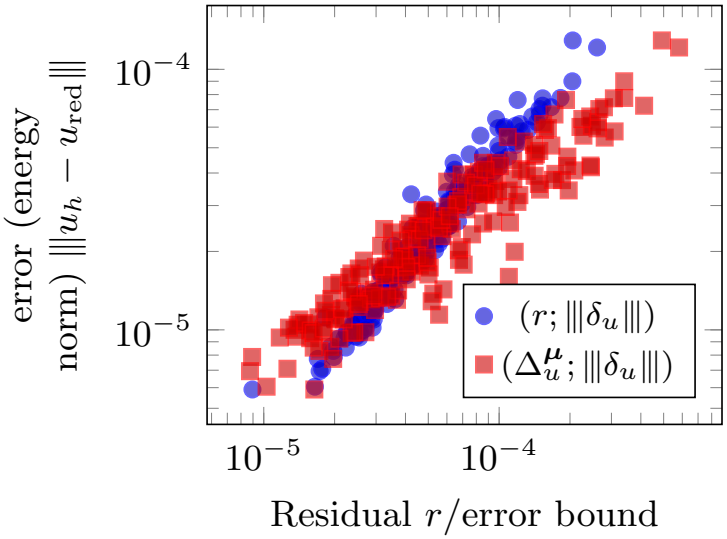
# Strategies for ROM error quantification

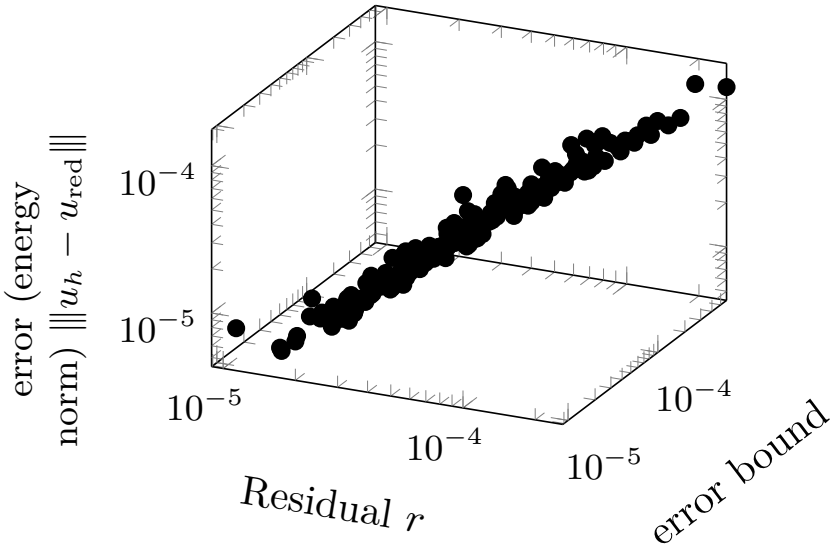
1. Rigorous error bounds
   - \+ independent of input-space dimension
   - \- not amenable to statistics
   - \- high effectivity (overestimation)
   - \- improving effectivity incurs high costs [Huynh et al., 2010, Wirtz et al., 2012] or intrusive reformulation of discretization [Yano et al., 2012]
2. Multifidelity correction [Eldred et al., 2004]




- model low-fidelity error as a function of inputs
- 'correct' low-fidelity outputs with model
- \+ amenable to statistics
- \- curse of dimensionality
- \- ROM errors highly oscillatory in the input space [Ng and Eldred, 2012]

# Our key observation

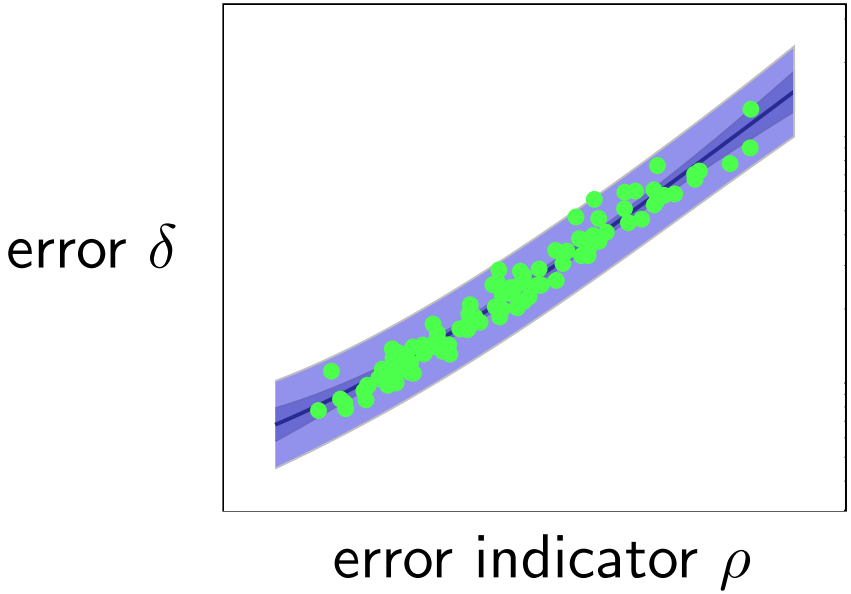



- ROMs generate **error indicators** that correlate with the error
- **Main idea**: construct a stochastic process that maps error indicators (not inputs $\boldsymbol{\mu}$!) to a distribution over the true error
  - \+ independent of input-space dimension
  - \+ quantifies ROM **epistemic uncertainty**

*Reduced-order model error surrogates*

# ROMES




- Construct a stochastic process of the ROM error $\widetilde{\delta}(\boldsymbol{\rho})$
- Select a *small number* of error indicators $\boldsymbol{\rho} = \boldsymbol{\rho}(\boldsymbol{\mu})$ that are
  1. cheaply computable online, and
  2. lead to low variance of the stochastic process.
- First attempt: Gaussian process (GP) such that random variables $(\widetilde{\delta}(\boldsymbol{\rho}_1), \widetilde{\delta}(\boldsymbol{\rho}_2), \ldots)$ have joint Gaussian distribution

# Gaussian process [Rasmussen and Williams, 2006]

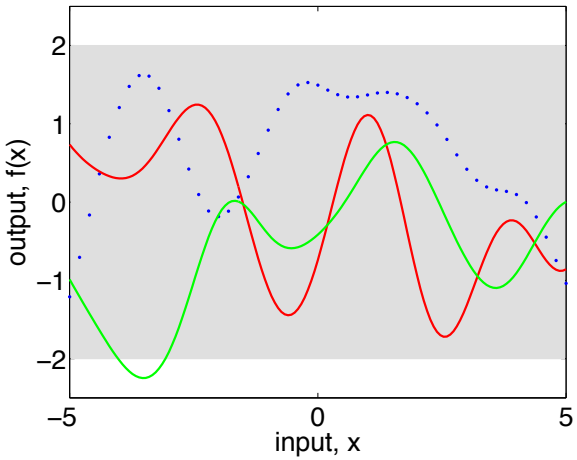
**Definition (Gaussian process)**

A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

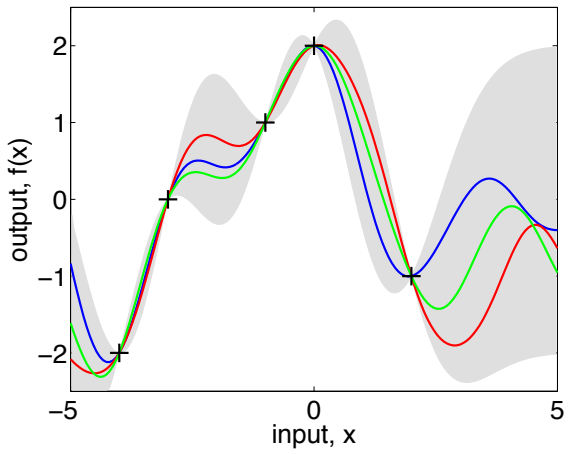
$$\widetilde{\delta}(\boldsymbol{\rho}) \sim \mathcal{GP}(m(\boldsymbol{\rho}), k(\boldsymbol{\rho}, \boldsymbol{\rho}'))$$

- mean function $m(\boldsymbol{\rho})$; covariance function $k(\boldsymbol{\rho}, \boldsymbol{\rho}')$
- given a training set $\{(\delta_i, \boldsymbol{\rho}_i)\}$, can infer $m(\boldsymbol{\rho})$ and $k(\boldsymbol{\rho}, \boldsymbol{\rho}')$
- consider two types of GPs
  1. kernel regression [Rasmussen and Williams, 2006]
  2. relevance vector machine (RVM) [Tipping, 2001]

# GP #1: Kernel regression [Rasmussen and Williams, 2006]




(d) prior




(e) posterior

- **prior**: $\widetilde{\delta}(\underline{\boldsymbol{\rho}}) \sim \mathcal{N}(0, K\left(\underline{\boldsymbol{\rho}}, \underline{\boldsymbol{\rho}}\right) + \sigma^2 \mathbf{I})$
  - $k(\boldsymbol{\rho}_i, \boldsymbol{\rho}_j) = \exp \frac{\|\boldsymbol{\rho}_i - \boldsymbol{\rho}_j\|^2}{r^2}$ is a positive definite kernel
  - $\underline{\boldsymbol{\rho}} := \left[\underline{\boldsymbol{\rho}}_{\text{train}} \ \underline{\boldsymbol{\rho}}_{\text{predict}}\right]^T$
- **posterior**: $\widetilde{\delta}(\boldsymbol{\rho}_{\text{predict}}) \sim \mathcal{N}(m(\boldsymbol{\rho}_{\text{predict}}), \mathrm{cov}(\boldsymbol{\rho}_{\text{predict}}))$
- infer hyperparameters $\sigma^2$ and $r^2$

# GP #2: Relevance vector machine [Tipping, 2001]

$$\widetilde{\delta}(\boldsymbol{\rho}) = \sum_{m=1}^{M} w_m \phi_m(\boldsymbol{\rho}) + \varepsilon$$

- fixed basis functions $\phi_m$ (e.g., polynomials)
- stochastic coefficients $w_m$
- noise $\varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$
- **prior**: $w \sim \mathcal{N}(0, \mathrm{diag}(\alpha_i))$
- **posterior**: $w \sim \mathcal{N}(\mathbf{m}, \boldsymbol{\Sigma})$ leads to posterior dist. of $\widetilde{\delta}(\boldsymbol{\rho})$
- infer hyperparameters $\sigma^2$ and $\alpha_i$

# ROMES Algorithm

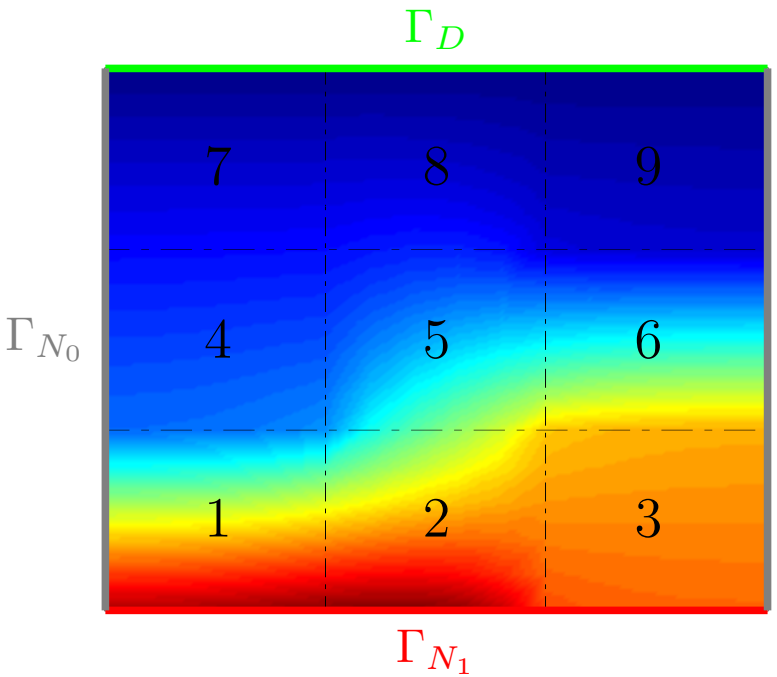
Offline

1. Populate ROMES database $\{(\delta(\boldsymbol{\mu}), \bar{\boldsymbol{\rho}}(\boldsymbol{\mu})) \mid \boldsymbol{\mu} \in \mathcal{D}_{\text{train}}\}$, where $\bar{\boldsymbol{\rho}}$ denotes candidate indicators.
2. Identify a few error indicators $\boldsymbol{\rho} \subset \bar{\boldsymbol{\rho}}$ that lead to a low-variance GP.
3. Construct the Gaussian process $\widetilde{\delta}(\boldsymbol{\rho}) \sim \mathcal{GP}(m(\boldsymbol{\rho}), k(\boldsymbol{\rho}, \boldsymbol{\rho}'))$ by Bayesian inference.

Online (for any $\boldsymbol{\mu}^\star \in \mathcal{D}$)

1. compute the ROM solution
2. compute error indicators $\boldsymbol{\rho}(\boldsymbol{\mu}^\star)$
3. obtain $\widetilde{\delta}(\boldsymbol{\rho}(\boldsymbol{\mu}^\star)) \sim \mathcal{N}(m(\boldsymbol{\rho}(\boldsymbol{\mu}^\star))), k(\boldsymbol{\rho}(\boldsymbol{\mu}^\star), \boldsymbol{\rho}(\boldsymbol{\mu}^\star))$
4. correct the ROM solution

# Thermal block (Parametrically coercive and compliant, affine, linear, elliptic)

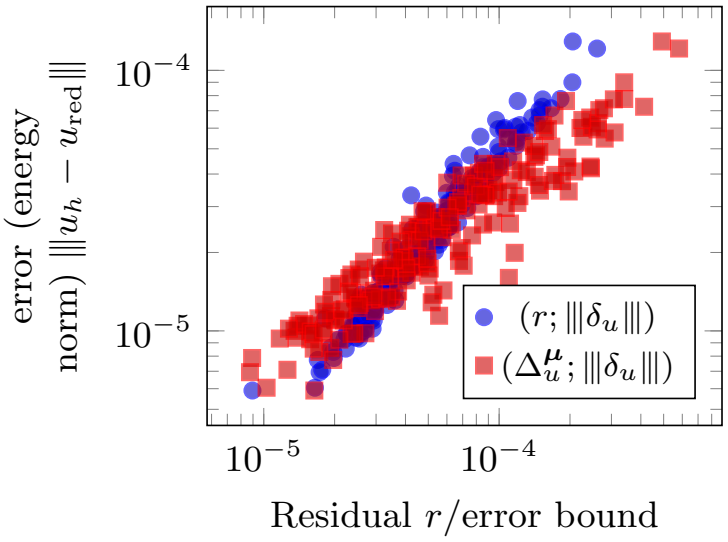


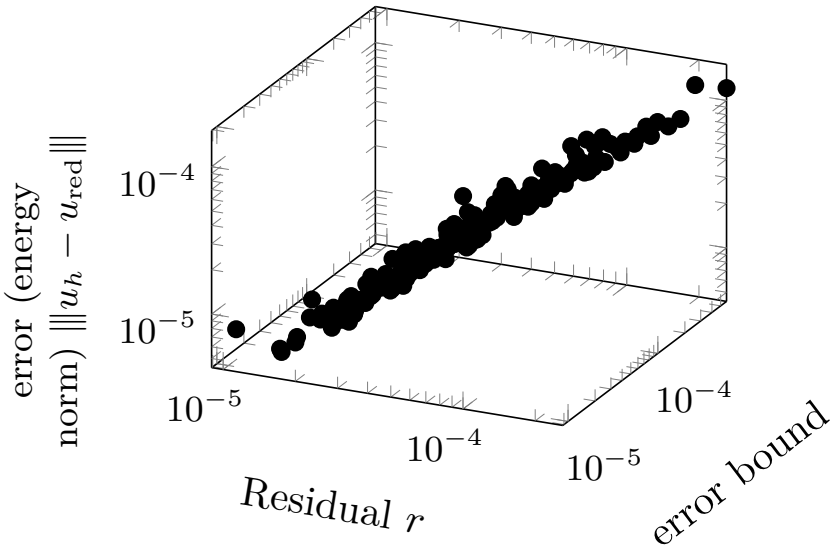

$$\triangle c(x;\boldsymbol{\mu})u(x;\boldsymbol{\mu}) = 0 \text{ in } \Omega \qquad \mathbf{x}(\boldsymbol{\mu}) = 0 \text{ on } \Gamma_D$$

$$\nabla c(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}) \cdot n = 0 \text{ on } \Gamma_{N_0} \qquad \nabla c(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}) \cdot n = 1 \text{ on } \Gamma_{N_1}$$

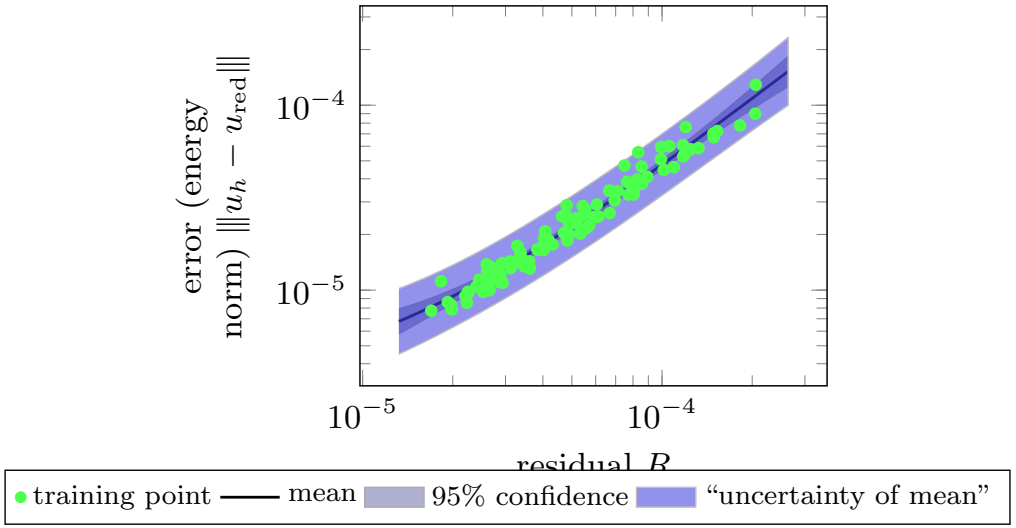
- Inputs $\boldsymbol{\mu} \in [0.1, 10]^9$ define diffusivity $c$ in subdomains
- Output $z(\boldsymbol{\mu}) = \int_{\Gamma_{N_1}} \mathbf{x}(\boldsymbol{\mu})\mathrm{d}x$ is compliant
- ROM constructed via RB–Greedy [Patera and Rozza, 2006]
- Consider two errors: 1) energy norm of state-space error $|||\mathbf{x}(\boldsymbol{\mu}) - \hat{\mathbf{x}}(\boldsymbol{\mu})|||$, 2) output bias $\mathbf{z}(\boldsymbol{\mu}) - \mathbf{z}_{\text{red}}(\boldsymbol{\mu})$

# Error #1: energy norm $|||\mathbf{x}(\boldsymbol{\mu}) - \hat{\mathbf{x}}(\boldsymbol{\mu})|||$



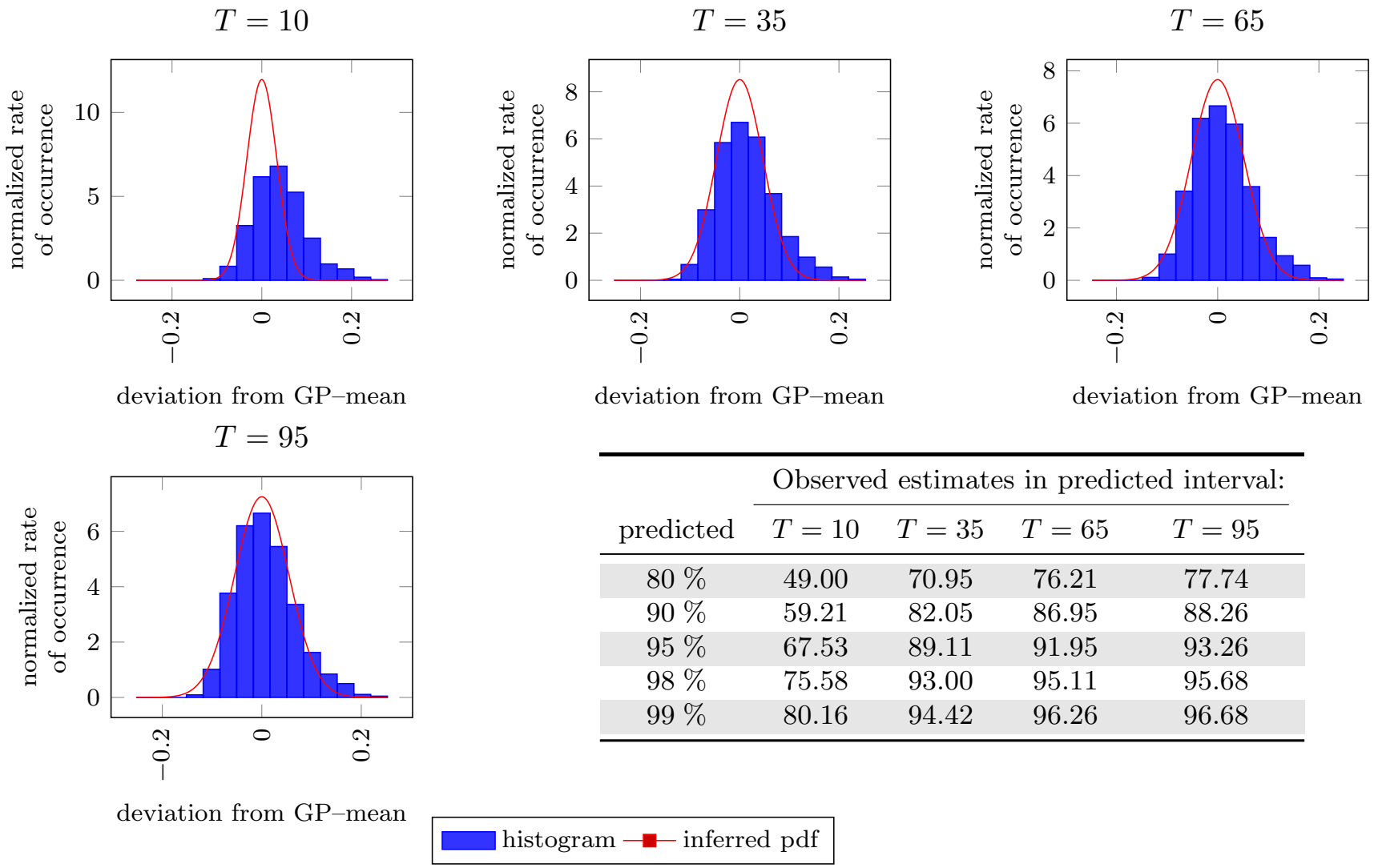




- Residual and error bound correlate with error



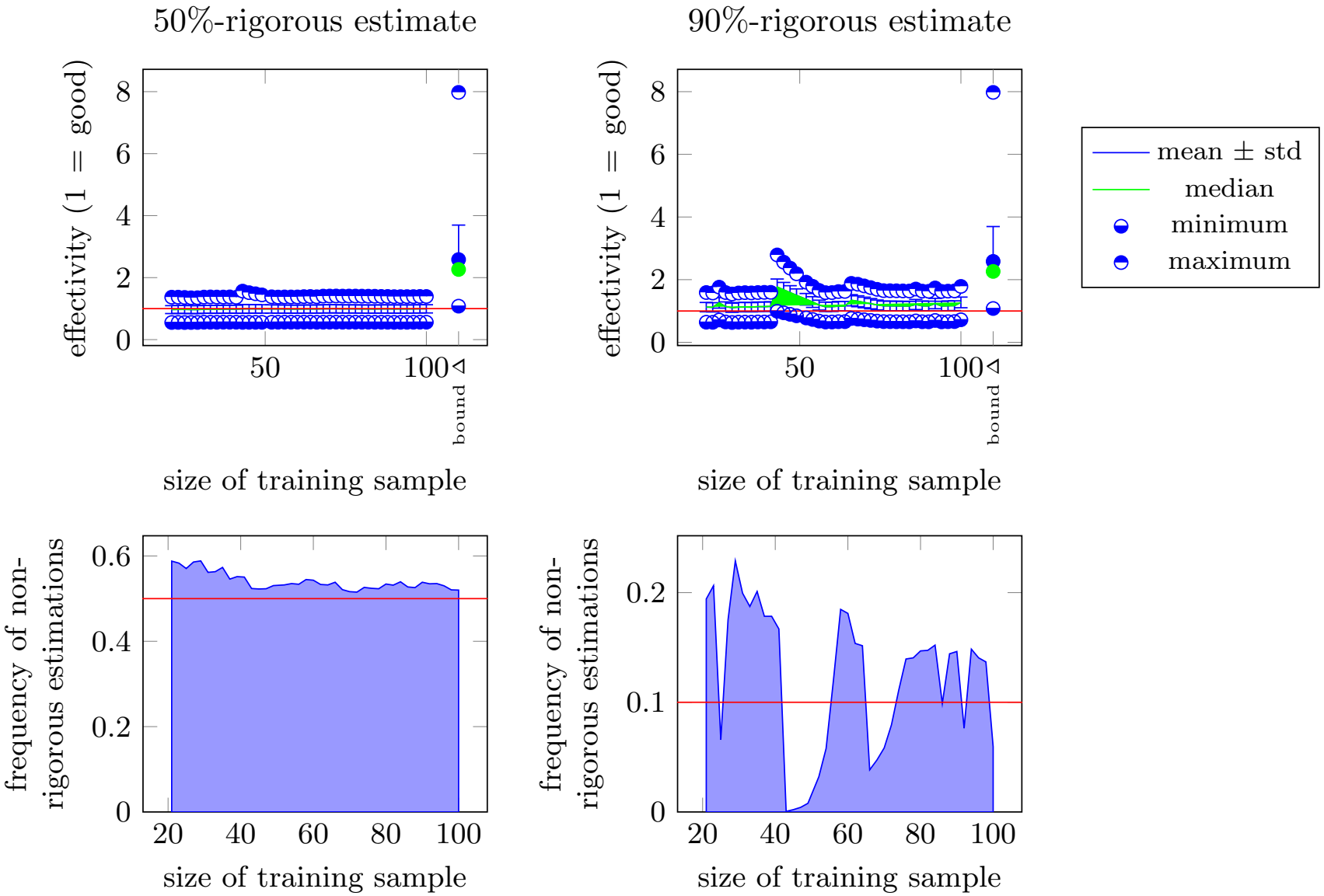

- ROMES (Kernel, residual indicator) in log-log space promising

# Gaussian-process assumptions verified (Kernel, residual indicator)

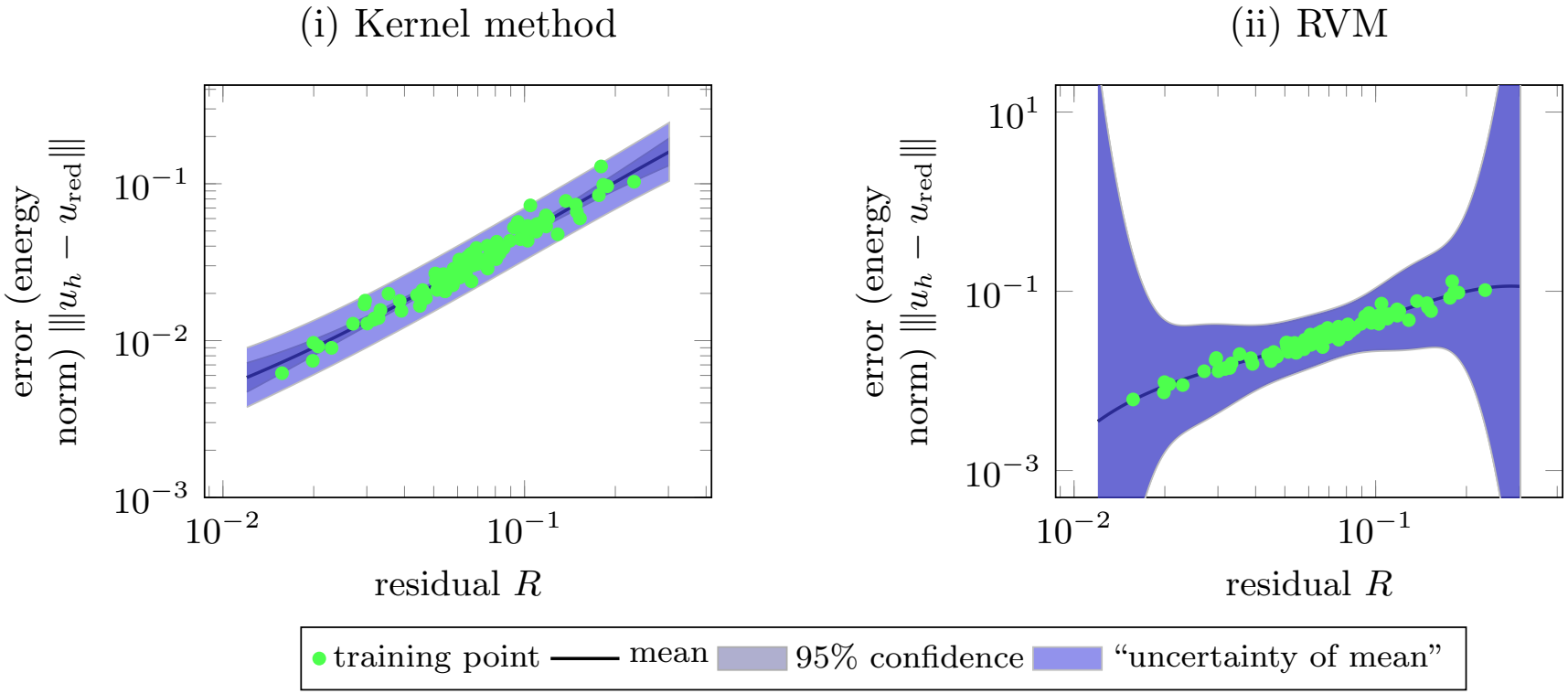



| predicted | Observed estimates in predicted interval: $T = 10$ | $T = 35$ | $T = 65$ | $T = 95$ |
|---|---|---|---|---|
| 80 % | 49.00 | 70.95 | 76.21 | 77.74 |
| 90 % | 59.21 | 82.05 | 86.95 | 88.26 |
| 95 % | 67.53 | 89.11 | 91.95 | 93.26 |
| 98 % | 75.58 | 93.00 | 95.11 | 95.68 |
| 99 % | 80.16 | 94.42 | 96.26 | 96.68 |

# Can achieve 'statistical rigor' (Kernel GP, residual indicator)

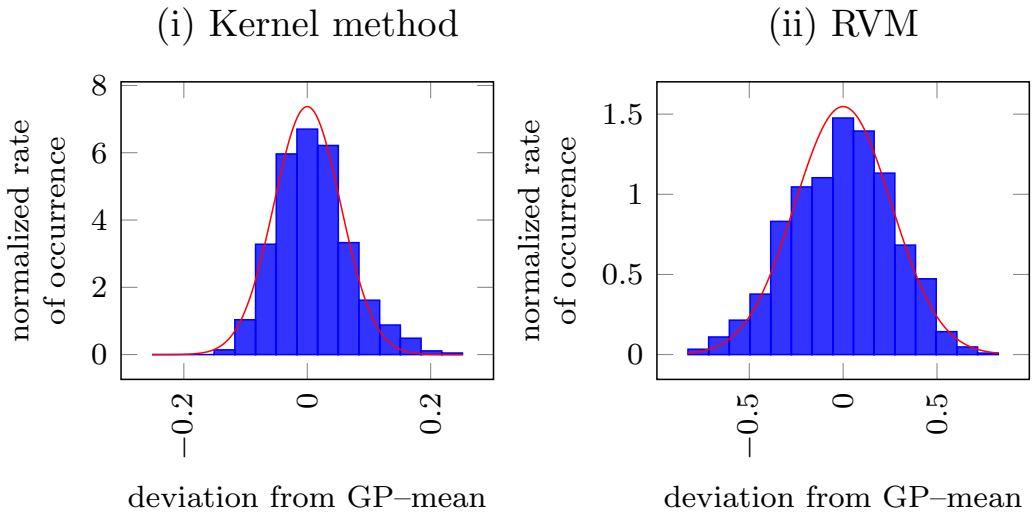


# ROMES: Kernel and RVM GP comparison



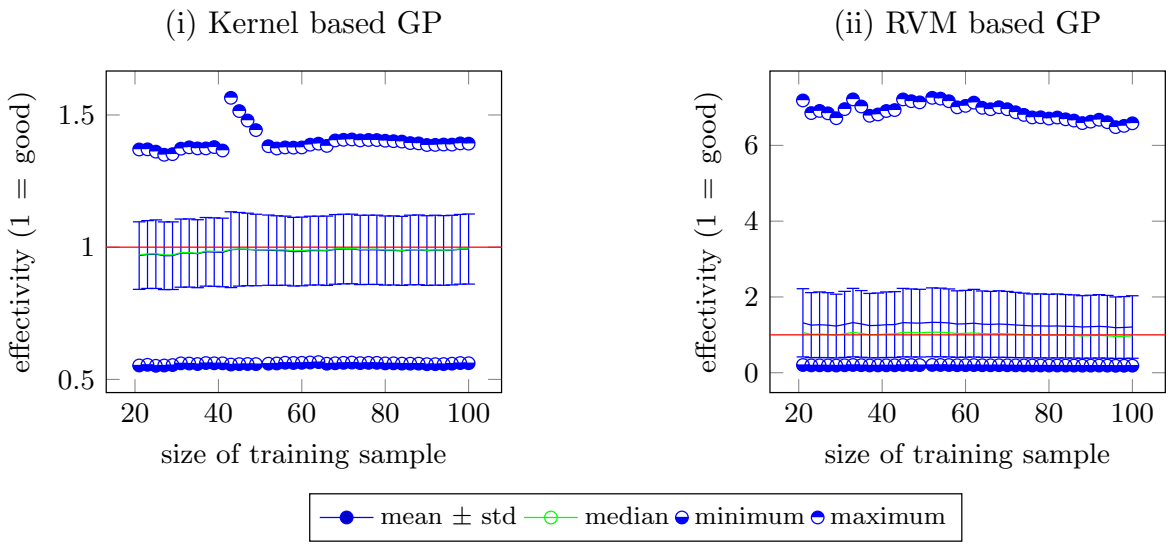

- RVM (Legendre-polynomial basis functions): significant uncertainty in mean's high-order polynomial coefficients

# ROMES: Kernel and RVM GP comparison




| $c$ | (i) | (ii) |
|---|---|---|
| 80 % | 77.7 | 77.9 |
| 90 % | 88.1 | 88.7 |
| 95 % | 92.9 | 94.7 |
| 98 % | 95.6 | 97.4 |
| 99 % | 96.6 | 99.2 |

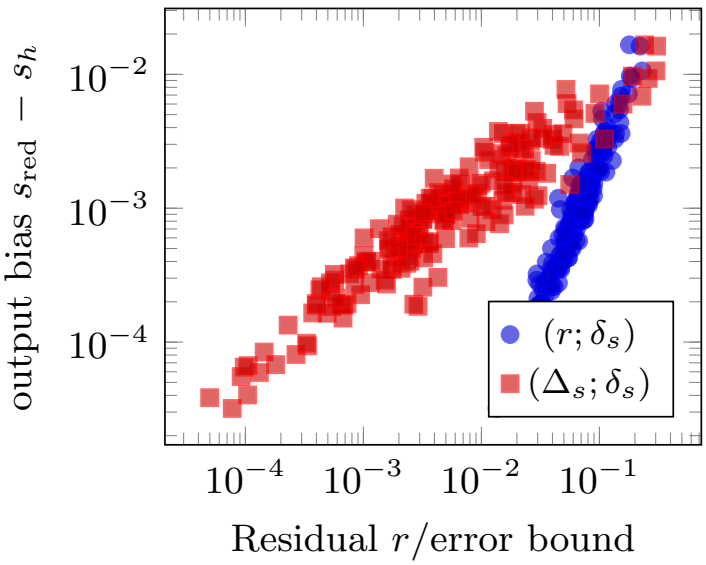
- GP structure and confidence intervals verified in both cases



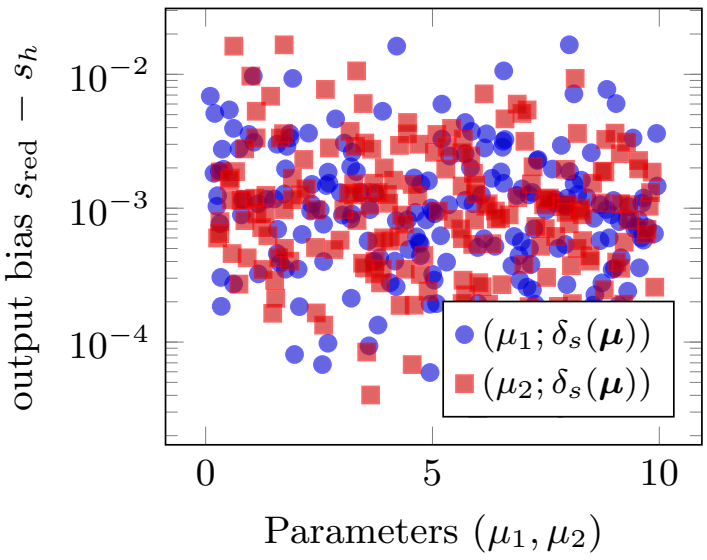

- Kernel GP produces better effectivity

# Error #2: output bias $\mathbf{z}(\boldsymbol{\mu}) - \mathbf{z}_{\text{red}}(\boldsymbol{\mu})$

(i) Indicators mapped to output bias



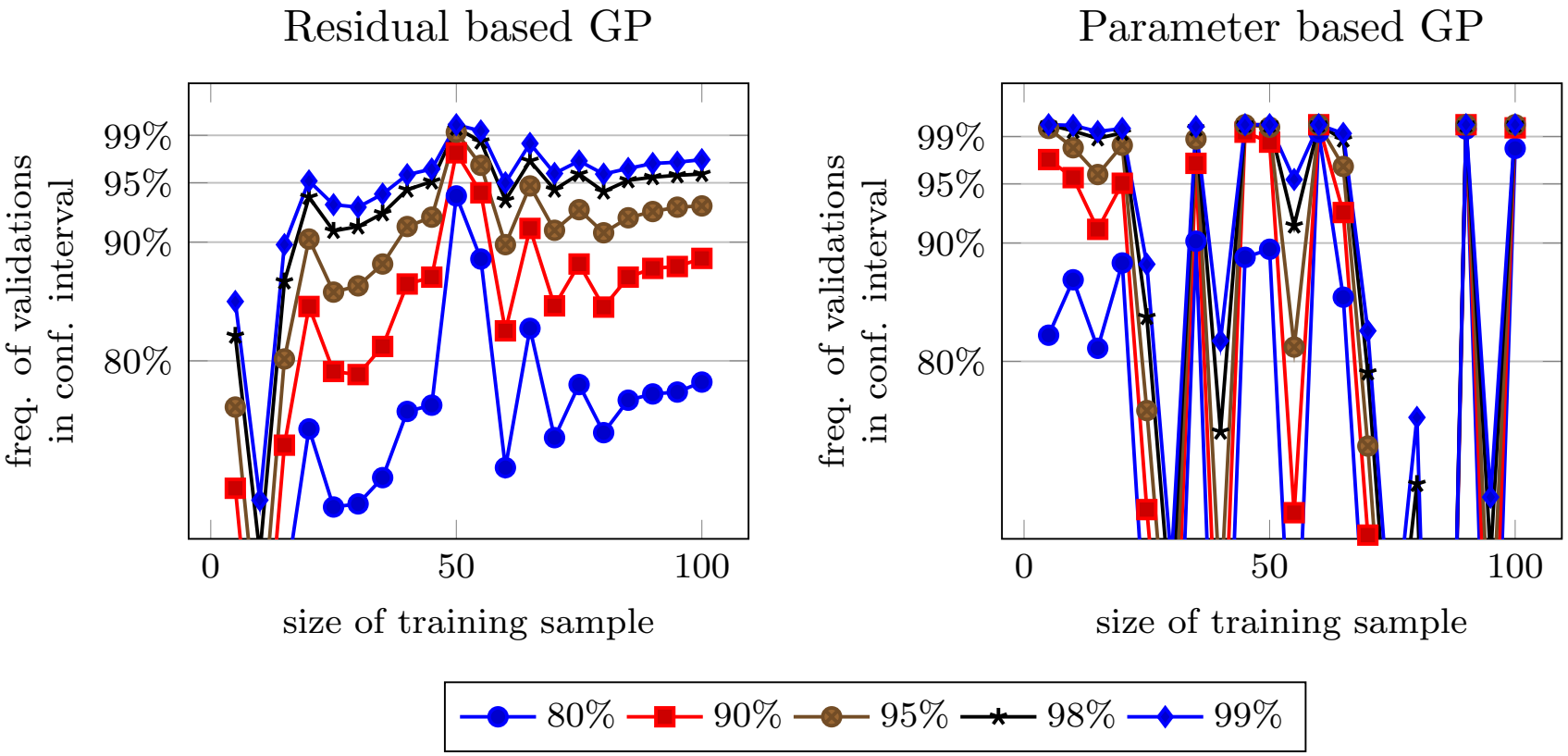

(ii) Parameters mapped to output bias




\+ Residual and error bound are good indicators (ROMES)

\- Inputs are poor indicators (Multifidelity correction)

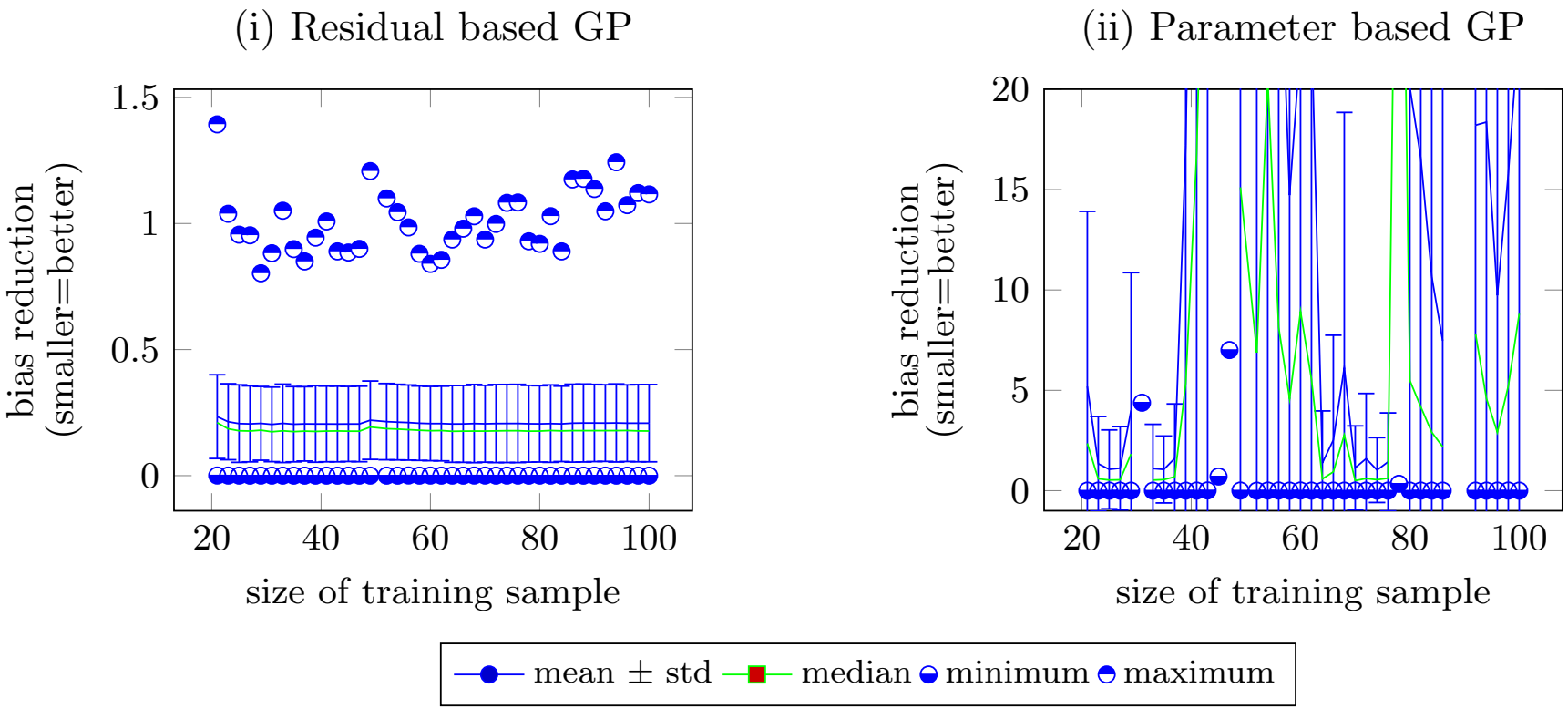
# Gaussian-process assumption verification




+ ROMES (Kernel GP, residual indicator) confidence intervals converge.
- Multifidelity correction (Kernel GP, input indicator) confidence intervals do not converge.

# Bias improvement

$$\text{bias reduction} = \frac{\mathsf{E}\left[\mathbf{z}_{\mathsf{red}}(\boldsymbol{\mu}) + \widetilde{\delta}_{\mathbf{z}}(\boldsymbol{\mu}) - \mathbf{z}(\boldsymbol{\mu})\right]}{\mathbf{z}_{\mathsf{red}}(\boldsymbol{\mu}) - \mathbf{z}(\boldsymbol{\mu})}$$




\+ ROMES reduces bias by roughly an order of magnitude

\- Multifidelity correction often *increases* the bias

# Conclusions

- ROMES
  - uses existing ROM error indicators to statistical quantify ROM error
  - 'statistical rigor' achievable
  - outperforms multifidelity correction (inputs = poor error indicators)
  - highlights strength of ROMs for data assimilation: other surrogates do not have such powerful error indicators
- Future work
  - apply to nonlinear, time-dependent problems
  - demonstrate on data-assimilation problem
  - automated selection of indicators and Gaussian process

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# Acknowledgments


- Matthew Zahr: providing the model-reduction testbed that was modified to generate the numerical results
- Seshadhri Comandur, Khachik Sargsyan: helpful discussions
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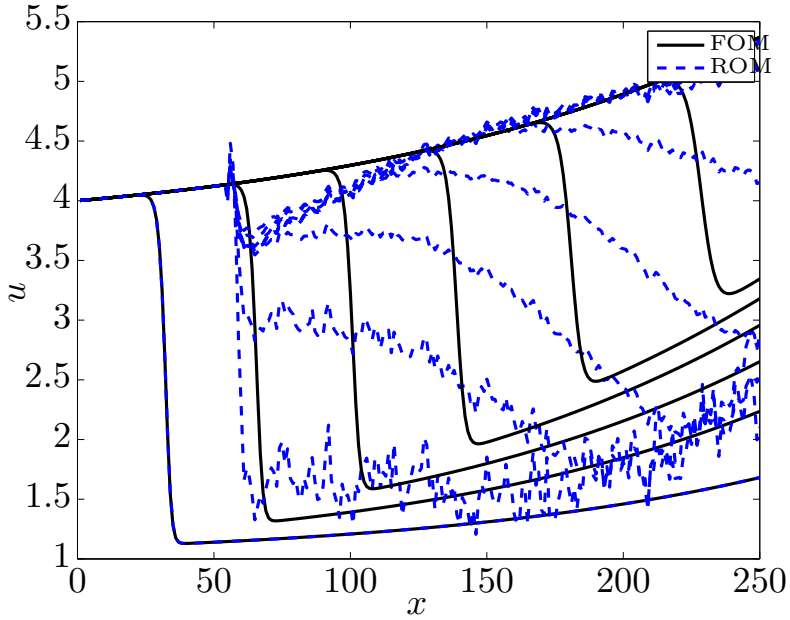
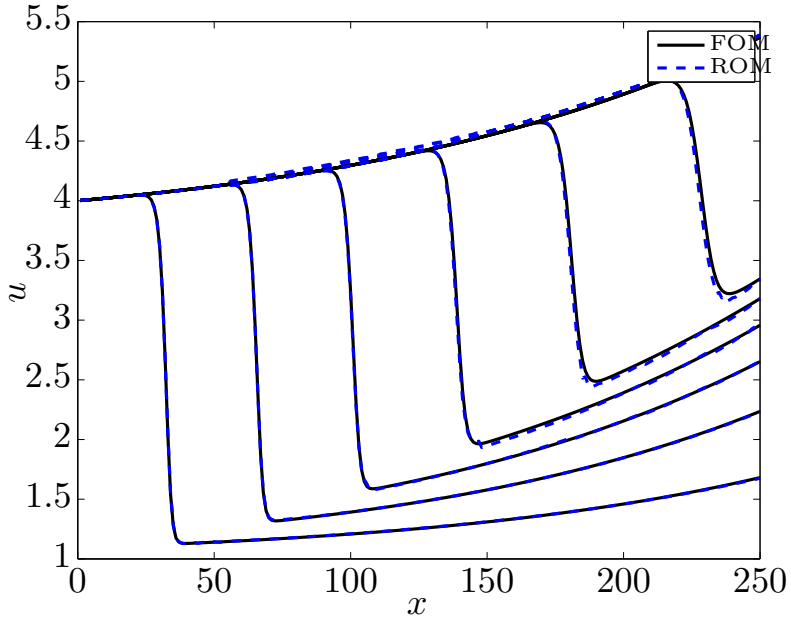
# Questions?

- **ROM error modeling**: M. Drohmann & K. Carlberg, "The ROMES method for statistical modeling of reduced-order-model error," arXiv e-print, (1404.0442), 2014.
- **ROM error control**: K. Carlberg. "Adaptive *h*-refinement for reduced-order models," International Journal for Numerical Methods in Engineering, in press (2014). doi:10.1002/nme.4800




(f) no adaptivity




(g) *h*-adaptivity

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