Adaptive *h*-refinement for reduced-order models with application to uncertainty control

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Motivation: Bayesian inference

- Structural health monitoring

source: Holger Speckmann, Airbus

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

- Bayesian inference problem

Bayesian inference

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

- Bayes' theorem

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

  - measured outputs $\bar{\mathbf{z}} = \mathbf{z}(\boldsymbol{\mu}^\star) + \varepsilon$ with noise $\varepsilon \sim \mathcal{N}(0, \sigma^2\mathbf{I})$
  - posterior $P(\boldsymbol{\mu}|\bar{\mathbf{z}})$ is sought
  - prior $P(\boldsymbol{\mu})$ is given
  - normalizing factor $P(\bar{\mathbf{z}})$ is handled indirectly
  - likelihood $P(\bar{\mathbf{z}}|\boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{z}(\boldsymbol{\mu}), \sigma^2\mathbf{I})$ sampling requires **full-order model evaluations**
- Objective: numerically sample the posterior distribution
  - \+ achievable in principle, e.g., by MCMC or importance sampling.
  - \- barrier: sampling requires full-order forward solves

Reduced-order modeling and Bayesian inference

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

- Replace the full-order model (FOM) with reduced-order model (ROM)
  - measured outputs $\bar{\mathbf{z}} = \mathbf{z}(\boldsymbol{\mu}^\star) + \varepsilon \approx \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \varepsilon$
  - likelihood $P(\bar{\mathbf{z}}|\boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{z}_{\text{red}}(\boldsymbol{\mu}), \sigma^2\mathbf{I})$ sampling requires **reduced-order model evaluations**
- **Problem**: neglects ROM errors

$$\bar{\mathbf{z}} = \mathbf{z}(\boldsymbol{\mu}^\star) + \varepsilon \tag{1}$$

$$= \mathbf{z}_{\text{red}}(\boldsymbol{\mu}^\star) + \boxed{\delta_{\mathbf{z}}(\boldsymbol{\mu}^\star)} + \varepsilon \tag{2}$$

- "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 (next talk)
  2. **control this error (this talk)**

Reduced-order modeling: accuracy limitation

- FOM: parameterized sequence of systems of equations

$$\mathbf{r}^k(\mathbf{x}^k; \boldsymbol{\mu}) = 0, \quad k = 1, \ldots, t \tag{3}$$

  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

$$\mathbf{V}^T \mathbf{r}^k(\mathbf{V}\hat{\mathbf{x}}^k; \boldsymbol{\mu}) = 0, \quad k = 1, \ldots, t \tag{4}$$

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

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

\- ROMs are not guaranteed to be *accurate*.

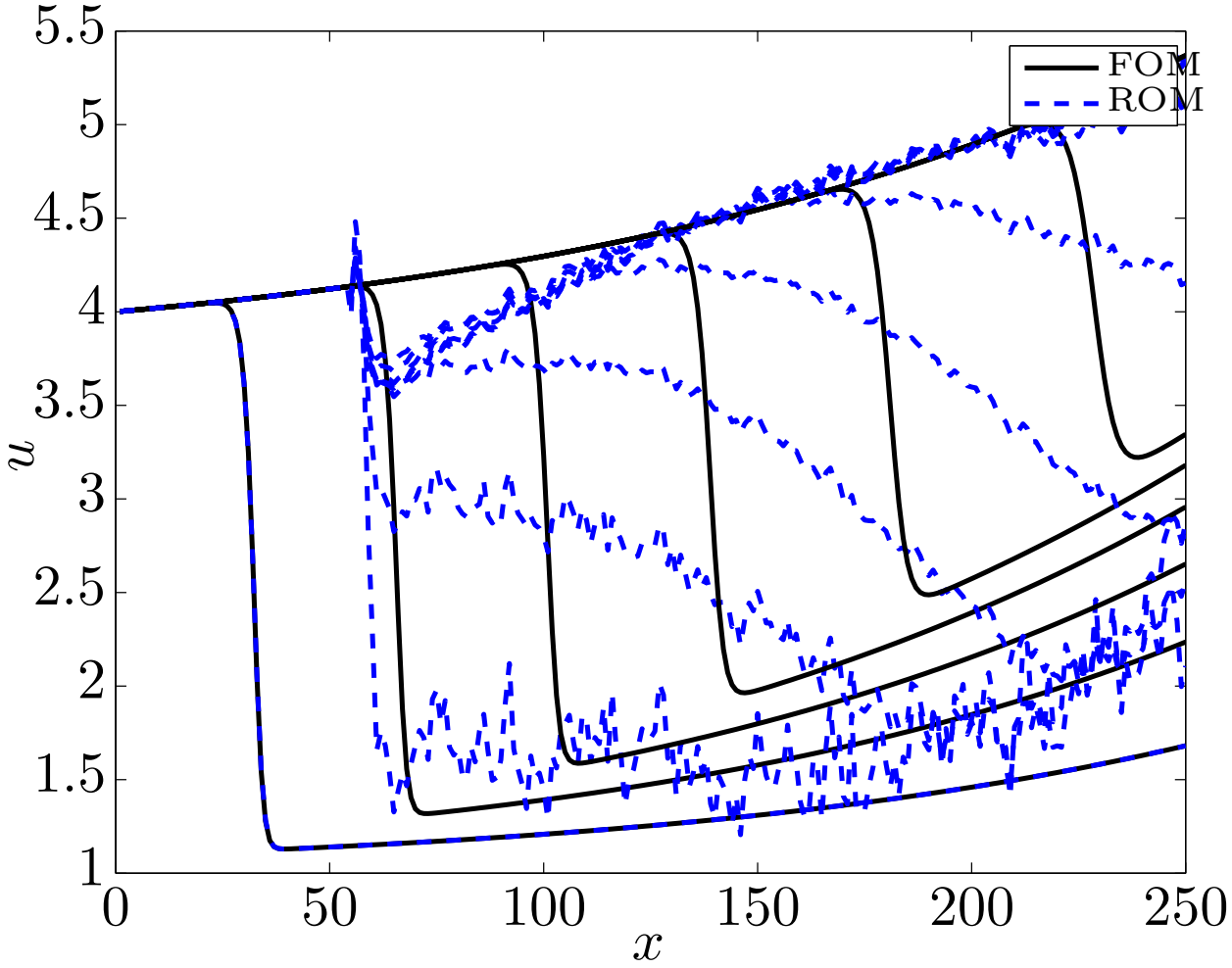
ROM accuracy is limited by the information in $\mathbf{V}$.

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
- $x_i = i \times (100/250)$, $i = 0, \ldots, 250$. Thus, $n = 250$.
- $\tau \in [0, 50]$ with time-step size $\Delta t = 0.05$
- POD–Galerkin ROM: $\mathbf{V} \in \mathbb{R}^{250\times 150}$ from 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**

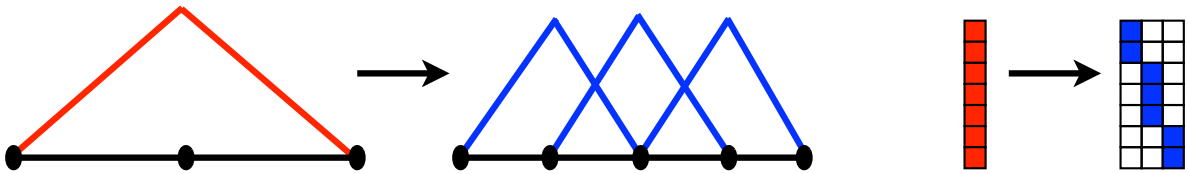
Existing ROM adaptation methods

- *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., 2013]
  - time domain [Drohmann et al., 2011, Dihlmann et al.,]
  - state space [Amsallem et al., 2012, Washabaugh et al., 2012, Peherstorfer et al., 2013].
  - \+ 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

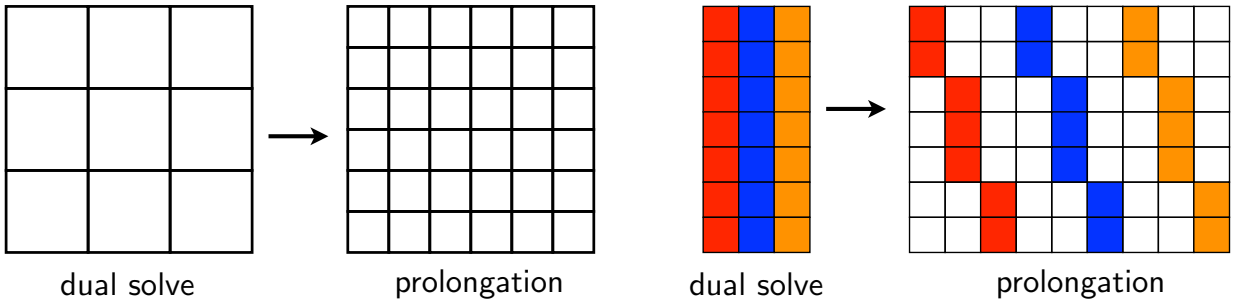
Adaptive *h*-refinement

- **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)

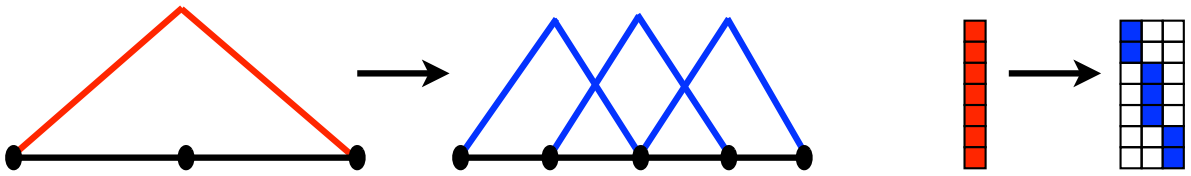


finite element h-refinement *ROM h-refinement*

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

Ingredient 1: Refinement

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



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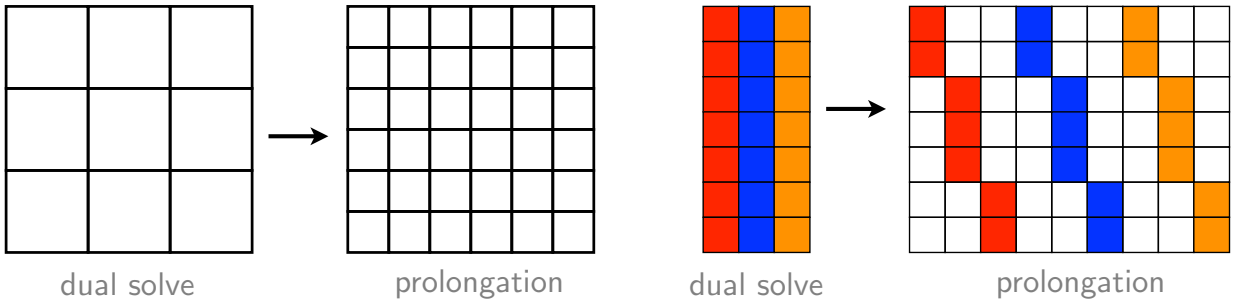
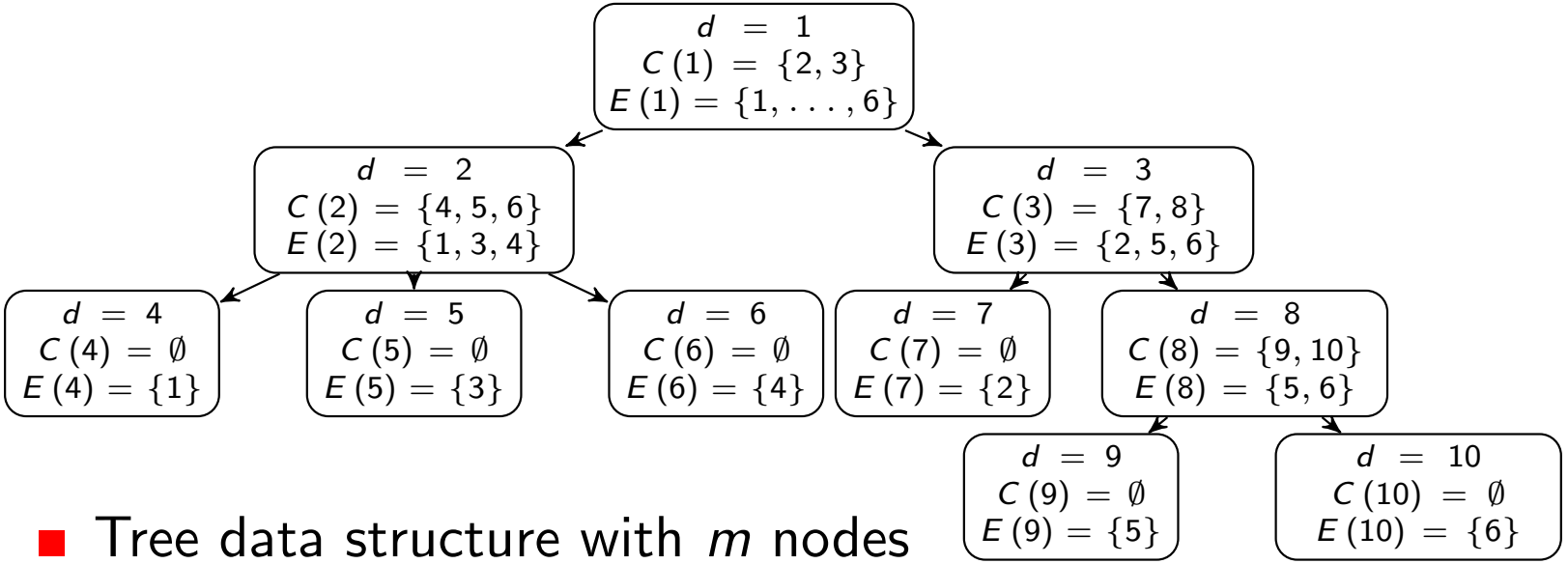


finite element h-refinement *ROM h-refinement*

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

Refinement via splitting: Tree data structure

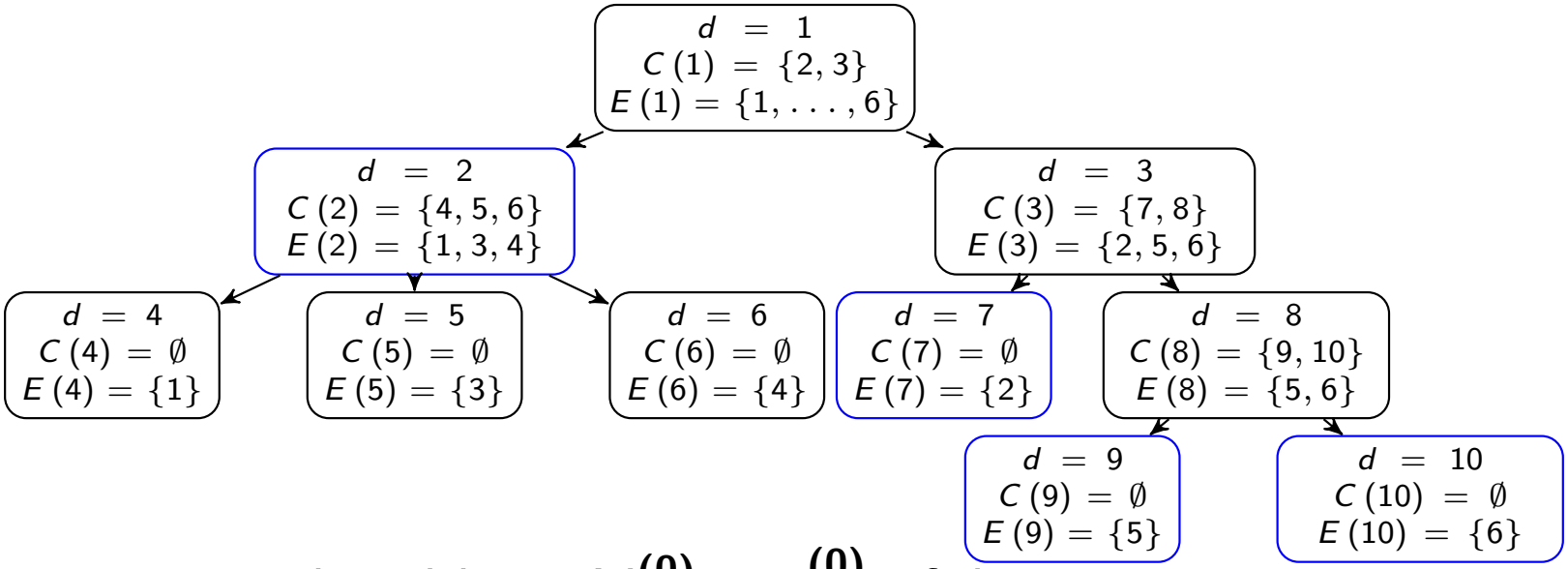


- Tree data structure with m nodes
  - *child* function $C : \mathbb{N}(m) \to \mathcal{P}(\mathbb{N}(m))$
  - *element* function $E : \mathbb{N}(m) \to \mathcal{P}(\mathbb{N}(n))$
  - each basis vector i characterized by a node d_i
- Requirements
  1. Root node includes all elements $E(1)$
  2. Each 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. $\cup_{j \in C(i)} E(j) = E(i)$

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

  \+ Requirement 4 ensures hierarchical refined subspaces

Tree example: $n = 6$



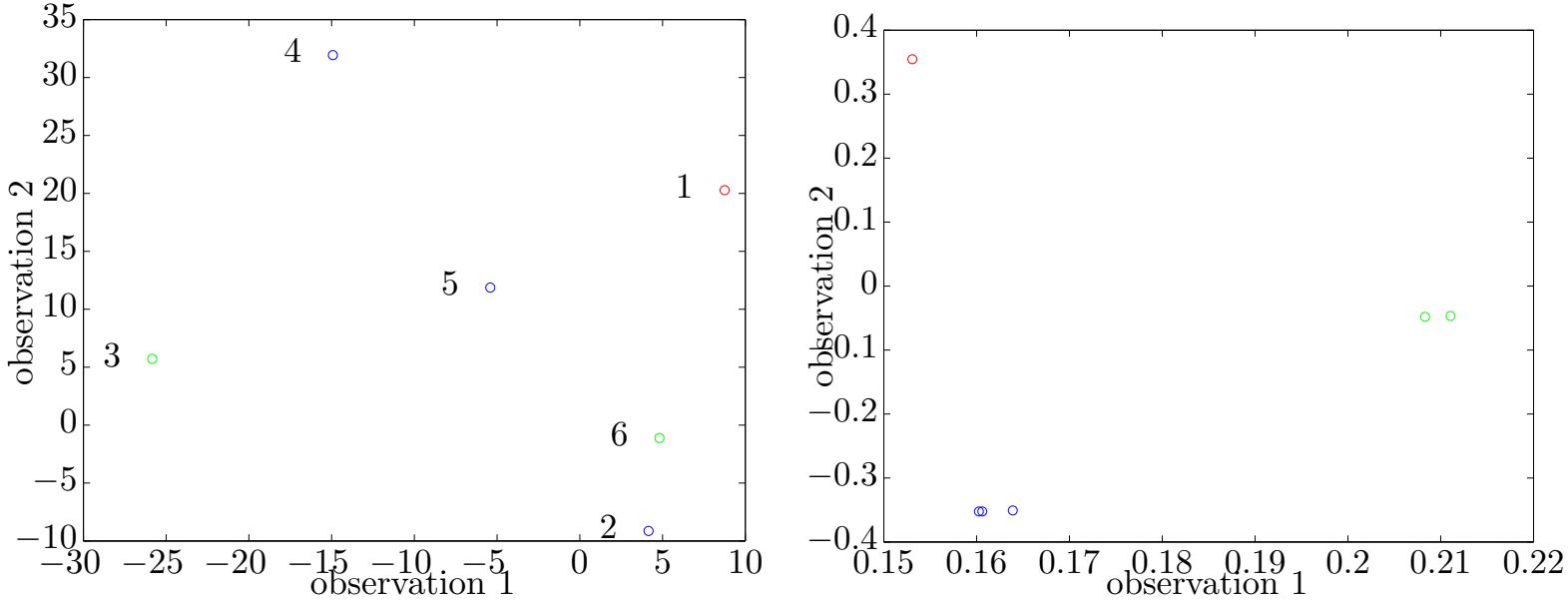
- Initial reduced basis $\mathbf{V}^{(0)} = \mathbf{v}_1^{(0)}$ of dimension 1
- Basis has been split into $p = 4$ vectors
- $d_1 = 2$, $d_2 = 7$, $d_3 = 9$, and $d_4 = 10$
- Refined reduced basis with $\text{range}(\mathbf{V}^{(0)}) \subset \text{range}(\mathbf{V})$ is

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_{11}^{(0)} & 0 & 0 & 0 \\ 0 & \mathbf{v}_{21}^{(0)} & 0 & 0 \\ \mathbf{v}_{31}^{(0)} & 0 & 0 & 0 \\ \mathbf{v}_{41}^{(0)} & 0 & 0 & 0 \\ 0 & 0 & \mathbf{v}_{51}^{(0)} & 0 \\ 0 & 0 & 0 & \mathbf{v}_{61}^{(0)} \end{bmatrix}.$$

Tree construction: k-means clustering of state variables

State variables x_i that tend to be strongly positively or negatively correlated can be accurately represented by the same generalized coordinate, and should therefore reside in the same tree node.

- Recursively apply k-means clustering to snapshots after
  1. Normalizing snapshot history of each state variable
  2. Flipping over the origin if the first snapshot is negative



(a) before processing (variables labeled) (b) after processing

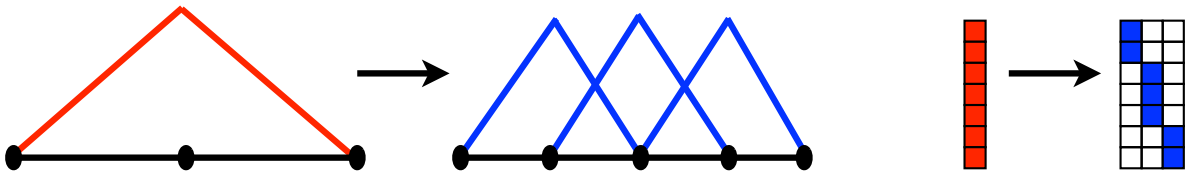
Refinement machinery

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

- coarse basis $\mathbf{V}^H \in \mathbb{R}^{n \times p}$ (initially equal to the $\mathbf{V}^{(0)}$)
- fine basis $\mathbf{V}^h \in \mathbb{R}^{n \times q}$ with $q = \sum_{i=1}^{p} \operatorname{card}\left(C\left(d_i\right)\right)$
- prolongation operator $\mathbf{I}_H^h \in \{0,1\}^{q \times p}$ constructed from tree
- restriction operator (not unique) $\mathbf{I}_h^H = \left(\mathbf{I}_H^h\right)^+$
- prolongated generalized coordinates $\hat{\mathbf{x}}_H^h = \mathbf{I}_H^h \hat{\mathbf{x}}^H$

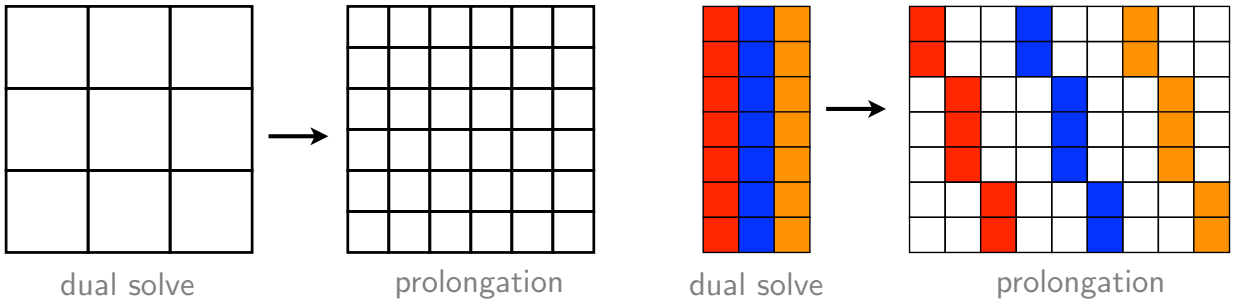
Ingredient 2: Error indicators

- **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: aims to reduce the error in output $z(\mathbf{x})$ via targeted refinement
- Analogy to duality-based error-control methods 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 the output due to the (unknown) fine solution:

$$z(\mathbf{V}^h\hat{\mathbf{x}}^h) \approx z(\mathbf{V}^H\hat{\mathbf{x}}^H) + \frac{\partial z}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)\mathbf{V}^h(\hat{\mathbf{x}}^h - \mathbf{I}_H^h\hat{\mathbf{x}}^H) \quad (5)$$

- Approximate the fine residual:

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

  and solve for the error

$$(\hat{\mathbf{x}}^h - \mathbf{I}_H^h\hat{\mathbf{x}}^H) \approx -[(\mathbf{V}^h)^T\frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)\mathbf{V}^h]^{-1}(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H). \quad (6)$$

- Substituting (6) in (5) yields

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

  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

$$\boxed{z(\mathbf{V}^h\hat{\mathbf{x}}^h) - z(\mathbf{V}^H\hat{\mathbf{x}}^H) \approx -(\hat{\mathbf{y}}^h)^T(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H)} \tag{7}$$

$$\boxed{(\mathbf{V}^h)^T\frac{\partial \mathbf{r}^k}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T\mathbf{V}^h\hat{\mathbf{y}}^h = (\mathbf{V}^h)^T\frac{\partial z}{\partial \mathbf{x}}(\mathbf{V}^H\hat{\mathbf{x}}^H)^T} \tag{8}$$

- We want to avoid fine solves like (8), 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 (7) yields a cheaply computable

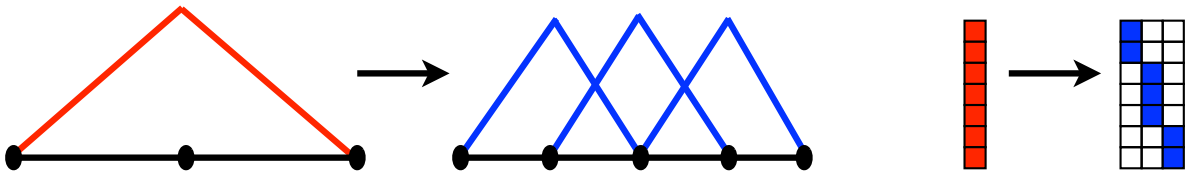
$$z(\mathbf{V}^h\hat{\mathbf{x}}^h) - z(\mathbf{V}^H\hat{\mathbf{x}}^H) \approx -(\hat{\mathbf{y}}^h_H)^T(\mathbf{V}^h)^T\mathbf{r}(\mathbf{V}^H\hat{\mathbf{x}}^H).$$

- The RHS can be bounded by cheaply computable fine error indicators

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

Ingredient 3: Adaptive algorithm

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



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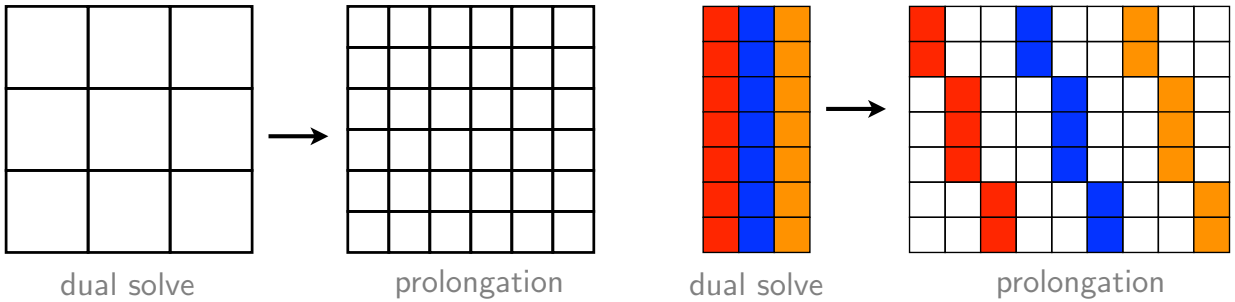

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  3. *Adaptive algorithm*: refine basis vecs with large error indicators

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** Output error estimate $\delta_{\mathbf{z}}$ '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**

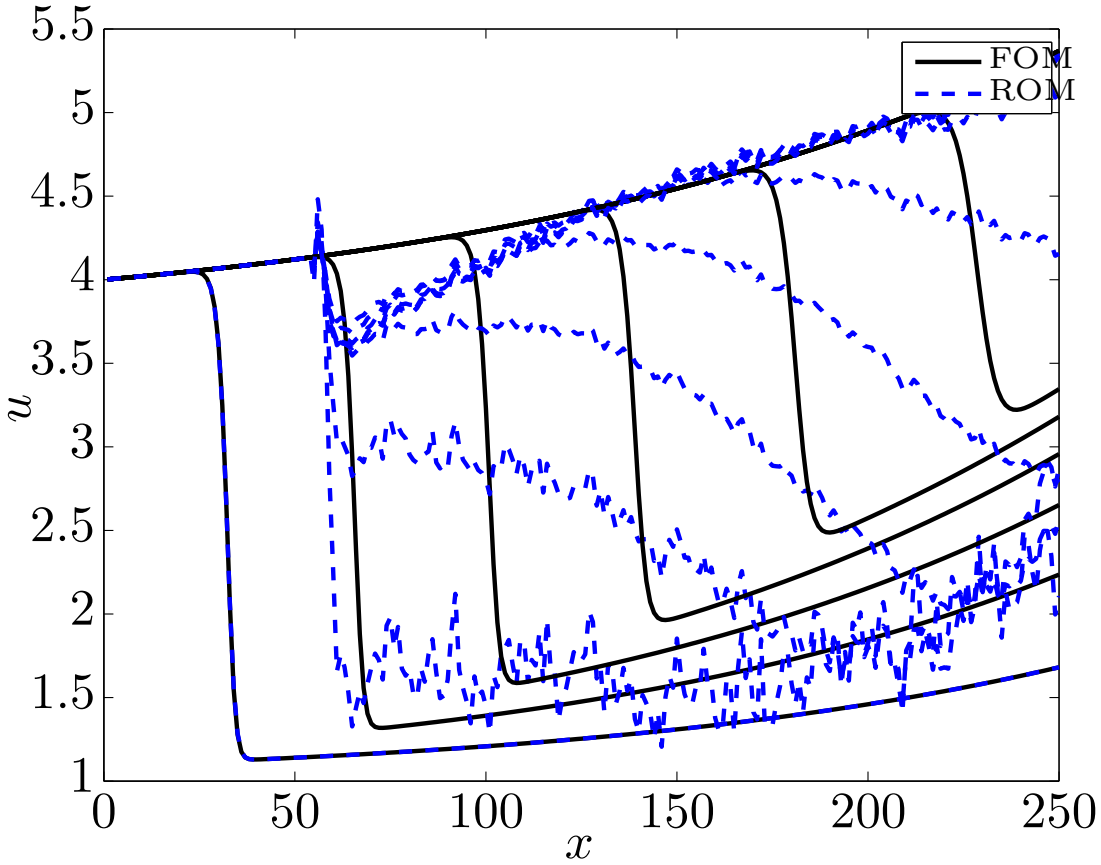
Adaptive algorithm

Algorithm 2 Refine

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

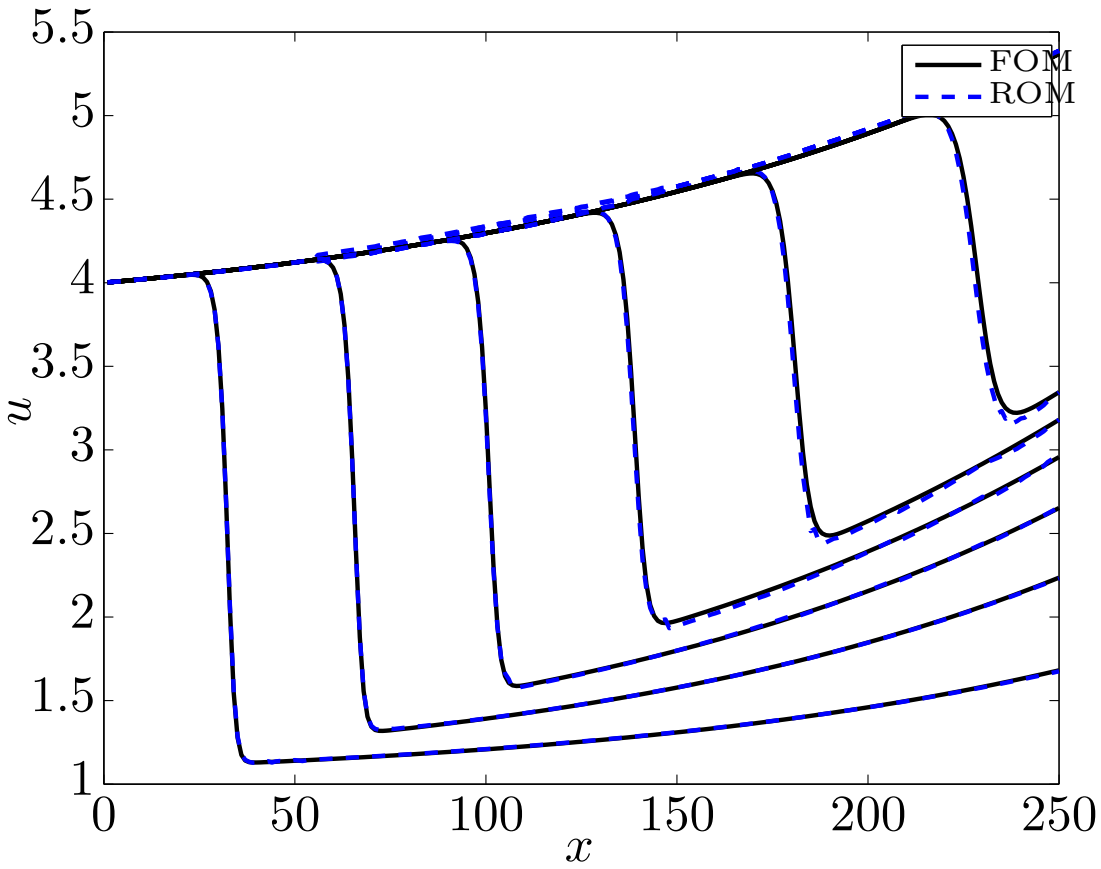
1: Compute prolongation operator $\mathbf{I}_H^h$ and fine reduced basis $\mathbf{V}^h$
2: Compute coarse adjoint solution $\hat{\mathbf{y}}^H$ and prolongation $\hat{\mathbf{y}}_H^h$
3: Compute fine error indicators δ_i^h, $i = 1, \ldots, q$
4: Identify basis vectors to refine I: those whose children contribute have above-average contributions to the total estimated error
5: **for** $i \in I$ **do**
6: Split $\mathbf{v}_i$ into card $(C(d_i))$ vectors
7: **end for**
8: Compute QR factorization with column pivoting $\mathbf{V} = \mathbf{Q}\mathbf{R}$, $\mathbf{R}\bar{\mathbf{\Pi}} = \bar{\mathbf{Q}}\bar{\mathbf{R}}$.
9: Ensure full-rank matrix $\mathbf{V} \leftarrow \mathbf{V}\left[\bar{\boldsymbol{\pi}}_1 \ \cdots \ \bar{\boldsymbol{\pi}}_r\right]$, with r the rank of $\mathbf{R}$.

Previous example



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

Previous example with *h*-adaptivity



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

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

Conclusions

- Adaptive *h*-refinement via splitting
  - Incrementally improves ROM without requiring large-scale operations or solves
  - Enables uncertainty control
  - Extends utility of ROMs to highly nonlinear problems
- Future work
  - Nonlinear model reduction: incorporating complexity reduction (e.g., empirical interpolation, gappy POD) into refinement
  - Adaptive *coarsening* instead of (simple) basis resetting
  - Adaptive *p*-refinement: add other basis vectors (e.g., truncated POD vectors, discrete wavelets) from a library

Acknowledgments

- Matthew Zahr: providing the model-reduction testbed that was modified to generate the numerical results
- Seshadhri Comandur: helpful discussions related to tree construction and clustering.
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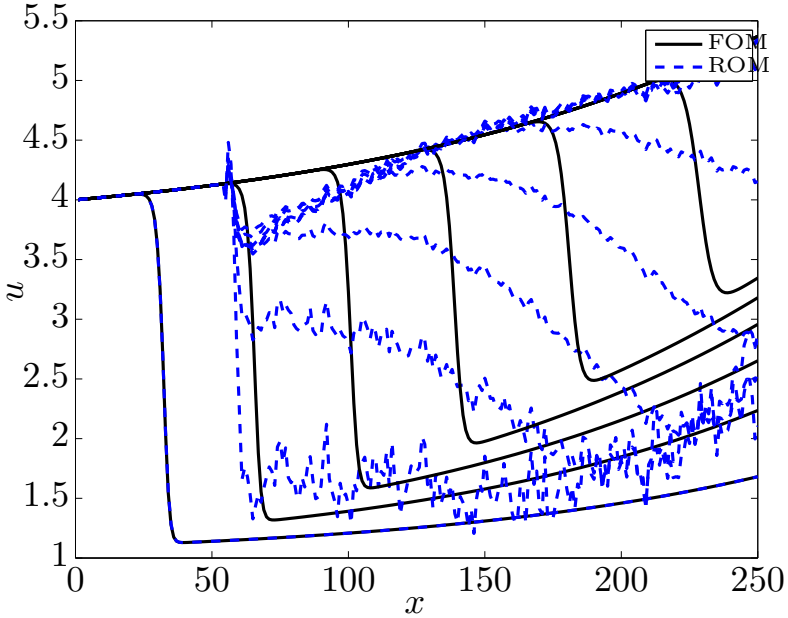
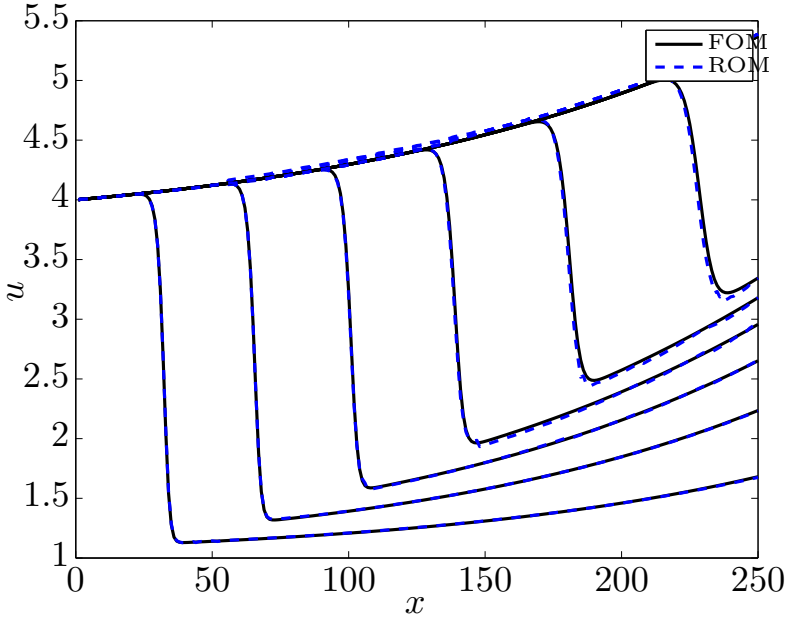
Questions?

- K. Carlberg, "Adaptive *h*-refinement for reduced-order models," *on arXiv later this week.*



(a) no adaptivity



(b) *h*-adaptivity

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