Adaptive *h*-refinement in nonlinear model reduction: capturing moving discontinuities

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Parameterized PDEs at Sandia

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

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Barrier

- Design engineers require faster simulations
- Uncertainty quantification

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Objective: break barrier

Reduced-order modeling: accuracy limitation

- Full-order model (FOM)

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

  - residual: $\boldsymbol{r}^k \in \mathbb{R}^n$
  - state: $\boldsymbol{x}^k \in \mathbb{R}^n$

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  2. *Online*: approximate $\boldsymbol{x}^k \approx \boldsymbol{V}\hat{\boldsymbol{x}}^k$

$$\text{solve } \boldsymbol{V}^T\boldsymbol{r}^k(\boldsymbol{V}\hat{\boldsymbol{x}}^k;\boldsymbol{\mu}) = 0, \quad k = 1,\ldots,t \tag{2}$$

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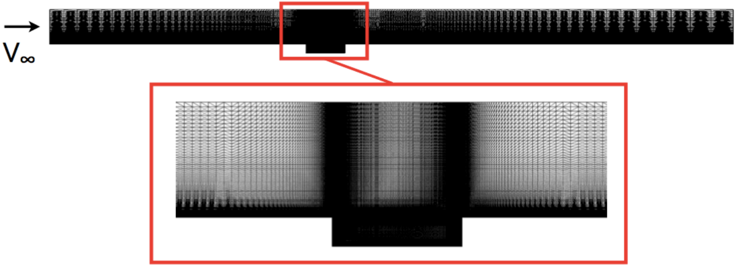
\+ ROMs are almost always *fast* ($p \ll n$).

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



- FOM: Compressible Navier–Stokes
  - Nonlinear dynamical system
  - 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 [?]
  - 179 degrees of freedom

When a ROM works

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- FOM: 48 cpu x 5 hours
- ROM: 2 cpu x 31 min = 229X cpu savings

When a ROM works

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

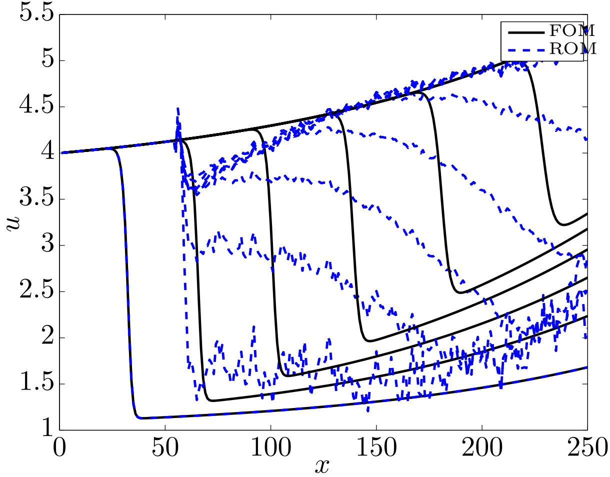
ROM accuracy is limited by the information in $\boldsymbol{V}$.

Example: inviscid Burgers equation [?]

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

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

ROM accuracy limited by relevance of training data



- ROM inaccurate when outside predictive domain of $\boldsymbol{V}$

Existing *a posteriori* ROM adaptation methods

- Revert to the FOM, solve it, and add solution to the basis [?, ?, ?]

\+ Improves the ROM *a posteriori*

\- Incurs large-scale operations

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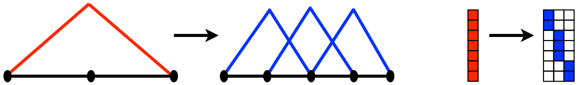
Goal: *Cheap, a posteriori improvement of the ROM*

Main idea

ROM analog to mesh-adaptive h-refinement

- 'Split' basis vectors



finite element h-refinement *ROM h-refinement*

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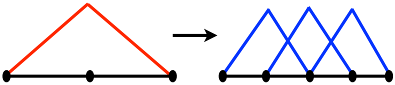

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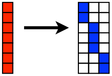
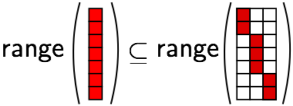


ROM h-refinement

- Generate hierarchical subspaces



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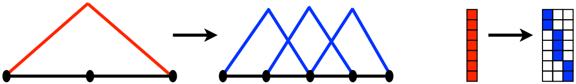

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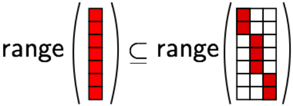
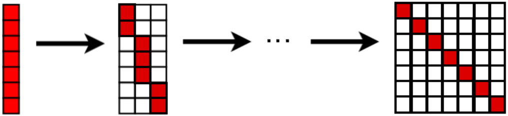
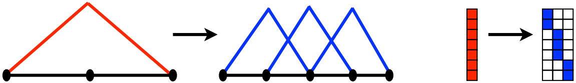


- ROM converges to the FOM



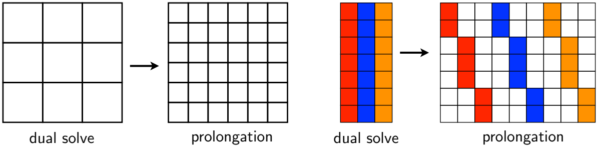
h-refinement ingredients

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)



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

Ingredient 1: Refinement

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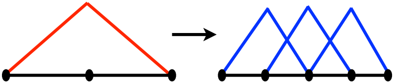

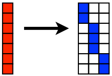

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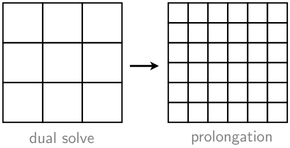

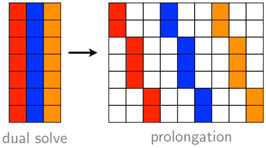

finite element h-refinement *ROM h-refinement*

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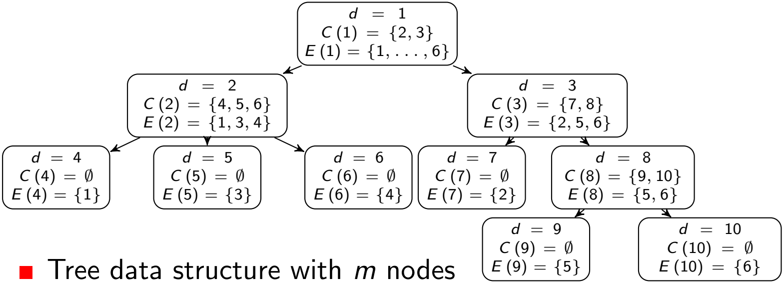
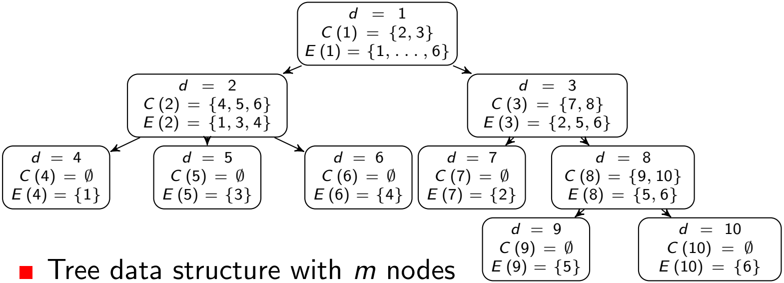
Tree structure



- Tree data structure with m nodes
  - *child* function $C : \mathbb{N}(m) \rightarrow \mathcal{P}(\mathbb{N}(m))$
  - *element* function $E : \mathbb{N}(m) \rightarrow \mathcal{P}(\mathbb{N}(n))$
  - each vector $\mathbf{v_i}$ assigned a node d_i, support $E(d_i)$, splits $C(d_i)$

Tree structure



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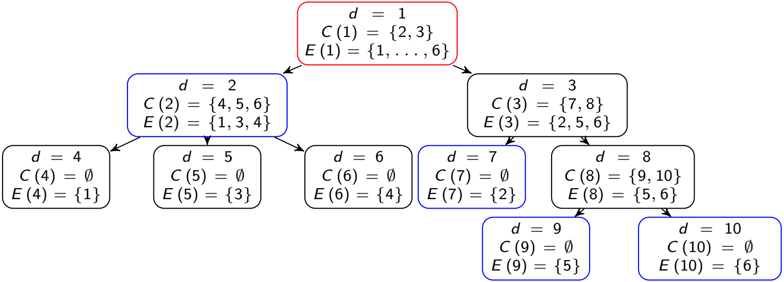
- Requirements
  1. Root node includes all elements $E(1)$
  2. Each element has a single leaf node
  3. Disjoint support of children $E(j) \cap E(k) = \emptyset, \ \forall j \neq k \in C(i)$
  4. $\cup_{j \in C(i)} E(j) = E(i)$
  - + **??–??** ensure the ROM converges to the FOM
  - + **??** ensures hierarchical refined subspaces

Tree example: $n = 6$



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

Tree construction

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

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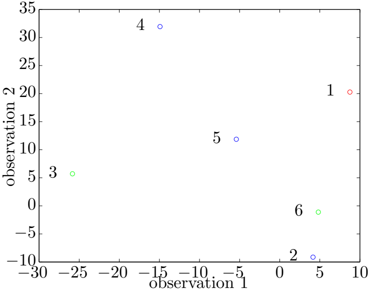
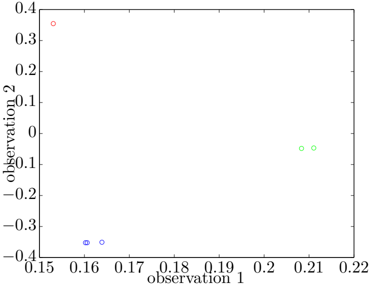
State variables that are strongly **correlated** *or* **anticorrelated** *should reside in the same tree node.*

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



(a) before modification

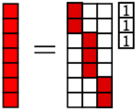


(b) after modification

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

Refinement machinery

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



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

- **Main idea**: ROM analog to mesh-adaptive *h*-refinement
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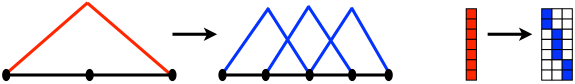
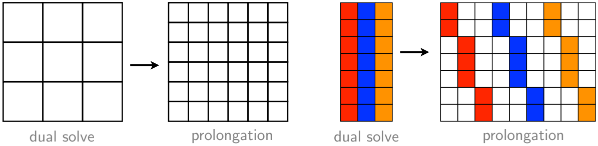


finite element h-refinement *ROM h-refinement*

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



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

Dual-weighted residual error indicators

- **Goal-oriented**: reduce the error in output $z(\boldsymbol{x})$
- Analogous to duality-based error control for
  - differential equations [?, ?]
  - finite elements [?, ?, ?, ?, ?, ?],
  - finite volumes [?, ?, ?, ?]
  - discontinuous Galerkin methods [?, ?]

Dual-weighted residual error indicators

- Approximate fine output:

$$z(\boldsymbol{V}^h\hat{\boldsymbol{x}}^h) \approx z(\boldsymbol{V}^H\hat{\boldsymbol{x}}^H) + \frac{\partial z}{\partial \boldsymbol{x}}(\boldsymbol{V}^H\hat{\boldsymbol{x}}^H)\boldsymbol{V}^h(\hat{\boldsymbol{x}}^h - \boldsymbol{I}_H^h\hat{\boldsymbol{x}}^H) \quad (3)$$

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- Approximate the fine residual:

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

- Solve for the error:

$$(\hat{\boldsymbol{x}}^h - \boldsymbol{I}_H^h \hat{\boldsymbol{x}}^H) \approx -[(\boldsymbol{V}^h)^T \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{x}}(\boldsymbol{V}^H \hat{\boldsymbol{x}}^H)\boldsymbol{V}^h]^{-1}(\boldsymbol{V}^h)^T \boldsymbol{r}(\boldsymbol{V}^H \hat{\boldsymbol{x}}^H) \quad (4)$$

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- Substitute (**??**) in (**??**):

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

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

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

Dual-weighted residual error indicators

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

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

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

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- Substituting $\hat{\boldsymbol{y}}^h_H$ for $\hat{\boldsymbol{y}}^h$ in (**??**) yields cheaply computable

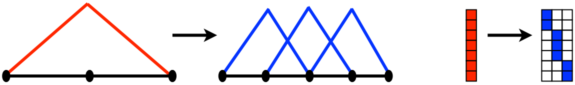
$$z(\boldsymbol{V}^h\hat{\boldsymbol{x}}^h) - z(\boldsymbol{V}^H\hat{\boldsymbol{x}}^H) \approx -(\hat{\boldsymbol{y}}^h_H)^T(\boldsymbol{V}^h)^T\boldsymbol{r}(\boldsymbol{V}^H\hat{\boldsymbol{x}}^H).$$

- The RHS can be bounded by cheaply computable error indicators

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

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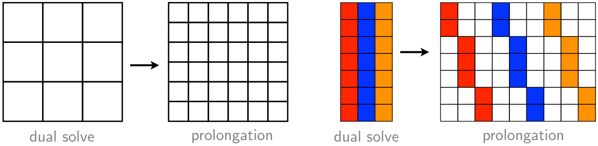
  2. *Error indicators*: a) dual solve (coarse), b) prolongation (fine)



finite element h-refinement *ROM h-refinement*

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

Adaptive algorithm

Algorithm 1 Outer loop

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

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

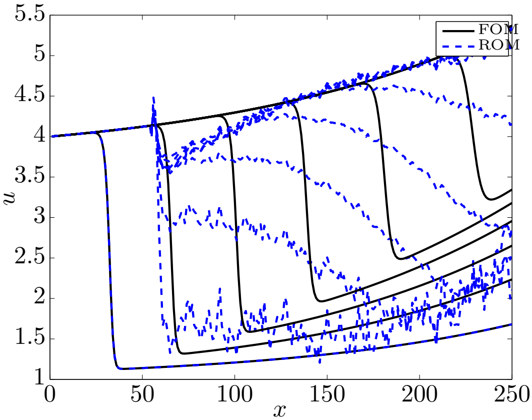
Adaptive algorithm

Algorithm 2 Refine

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

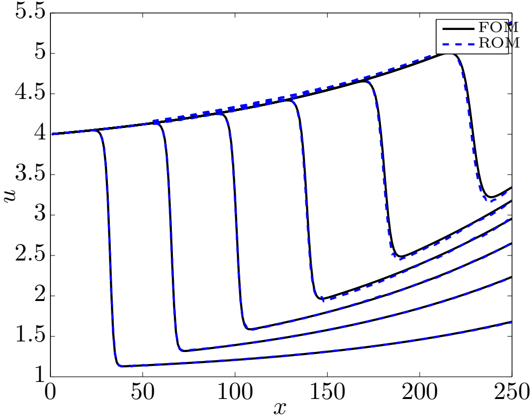
Compute prolongation operator $\boldsymbol{I}_H^h$ and fine basis $\boldsymbol{V}^h$
Solve: Compute coarse adjoint solution $\hat{\boldsymbol{y}}^H$ and prolongation $\hat{\boldsymbol{y}}_H^h$
Estimate: Compute fine error indicators $\boldsymbol{\Delta}_i^h$, $i = 1, \ldots, q$
Mark: Identify basis vectors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

Previous example



- Generated by $\boldsymbol{V} \in \mathbb{R}^{250\times 150}$ using $\tau_{\text{train}} \in [0, 2.5]$
- Now try *h*-adaptivity with $\boldsymbol{V}^{(0)} \in \mathbb{R}^{250\times 10}$, $\tau_{\text{train}} \in [0, 2.5]$.

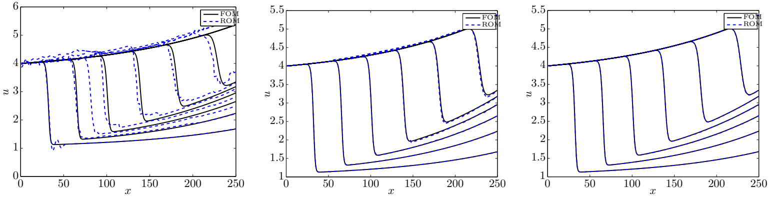
Previous example with h-adaptivity (FOM tolerance $\epsilon = 0.05$)



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

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

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 (%) online time (seconds)	12.2 4.61	0.51 4.63	0.078 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

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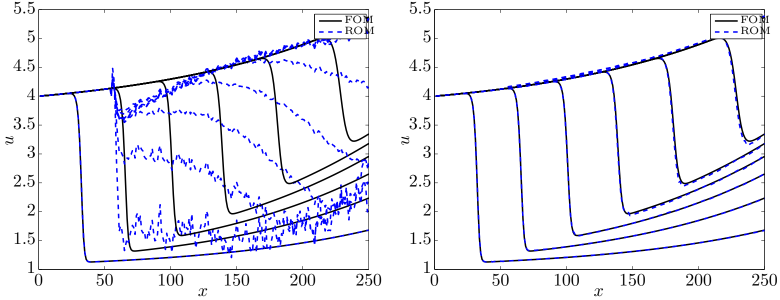
Questions?

- K. Carlberg. "Adaptive *h*-refinement for reduced-order models," International Journal for Numerical Methods in Engineering, in press (2014). doi:10.1002/nme.4800



(d) no adaptivity (e) *h*-adaptivity

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Inviscid Burgers equation: results

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