Reduced basis modeling of complex flow systems

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Center for Biomedical Computing

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Reduced basis modeling of complex flow systems

Outline

- The reduced basis method
- The reduced basis element method
- Offline/online decoupling: Empirical interpolation

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- Multi-block flow systems
- Summary





Main idea

Assume a parameter dependent problem

 $F(u; \mu) = 0.$





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$$F(u;\mu)=0.$$

For small changes in the parameter $\mu,$ the corresponding solution u often varies in a smooth fashion.





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Parameter dependent problems: $F(u; \mu) = 0$ Given $\mu \in \mathcal{D} \subset \mathbb{R}^p$, find $u \in X_N$ such that $a(u, v; \mu) = \ell(v) \quad \forall v \in X_N, \quad \mathcal{N} \gg 1$

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Reduced basis procedure

Offline:

Basis functions defined on X_N span the reduced basis approximation space $X_N = span\{u_i\}_{i=1}^N, N \ll N$

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Reduced basis procedure

Offline:

Basis functions defined on X_N span the reduced basis approximation space $X_N = span\{u_i\}_{i=1}^N, N \ll N$

Online:

Find the reduced basis approximation:

$$u_N(\mu) = \sum_{i=1}^N \alpha_i(\mu) u_i,$$

such that

$$a(u_N, v; \mu) = \ell(v) \quad \forall \ v \in X_N$$

Offline/online decoupling

- ► GOAL: Avoid online computations on the underlying FEM basis.
- ▶ All basis functions in X_N are stored in the FEM basis, so both $a(u_N, v; \mu)$ and $\ell(v)$ involve computations on the FEM basis.
- $\ell(v)$ is independent of the parameter, so this can be done offline.

Offline/online decoupling

If the problem has affine parameter dependence, we may decouple the bilinear form such that

$$\mathsf{a}(u,v;\mu) = \sum_{q=1}^{Q} \sigma^{q}(\mu) \mathsf{a}^{q}(u,v).$$

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Offline we compute $A_{ij}^q = a^q(u_j, u_i)$, i, j = 1, ..., N, q = 1, ..., Q, and $\ell_i = \ell(u_i)$, i = 1, ..., N using $\mathcal{O}(QN^2\mathcal{N})$ operations.

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Online we then solve the algebraic equations

$$(\sum_{q=1}^{Q} \sigma^{q}(\mu) A^{q}) \underline{\alpha} = \underline{\ell},$$

using $\mathcal{O}(QN^2)$ operations on assembly, and $\mathcal{O}(N^3)$ operations to find $\underline{\alpha}$.

Output of interest

The reduced basis approximation $u_N(\mu) = \sum_{i=1}^N \alpha_i(\mu) u_i$ needs $\mathcal{O}(N\mathcal{N})$ operations for assembly.

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Output of interest

The reduced basis approximation $u_N(\mu) = \sum_{i=1}^N \alpha_i(\mu) u_i$ needs $\mathcal{O}(N\mathcal{N})$ operations for assembly.

A derived quantity (or output of interest) $s(u) = f(u(\mu))$ (e.g., drag force, volume flow rate,) may be computed as

$$s(u_N) = f(u_N(\mu)) = f(\sum_{i=1}^N \alpha_i(\mu)u_i) = \sum_{i=1}^N \alpha_i(\mu)f_i$$

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where $f_i = f(u_i)$ may be computed offline. We thus only need N operations to find $s(u_N)$ once $\underline{\alpha}$ is found. Recall $N \ll \mathcal{N}$.

A posteriori error estimation

For a given output of interest s(u), Prud'homme et al. (2002) present upper and lower bounds, such that

$$s^-(u_N) \leq s(u) \leq s^+(u_N)$$

For affine parameter dependence they also show that through offline/online decoupling of the computations, the online work needed to find the output bounds only depends on N.

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Adaptive reduced basis method

Based on the bound gap

$$\Delta s(u_N) = s^+(u_N) - s^-(u_N),$$

Veroy et al. (2003) present an adaptive method to control the number of basis functions N used in the reduced basis approximation.

A greedy approach

Recall that $\mu \in \mathcal{D} \subset \mathbb{R}^{p}$, and let $\Xi_{n} \equiv \{\mu_{1}^{*}, ..., \mu_{n}^{*}\}$ be a finite dimensional substitute for \mathcal{D} . For an initial subset $S_{N_{0}} = \{\mu_{1}, ..., \mu_{N_{0}}\} \subset \Xi_{n}$, and $X_{N_{0}} = \text{span } \{u(\mu_{1}), ..., u(\mu_{N_{0}})\}$

for
$$N = N_0 + 1$$
: N_{\max}
 $\mu_N = \arg \max_{\mu \in \Xi_n} \Delta s(u_{N-1}(\mu))$
if $\Delta s(u_{N-1}(\mu_N)) \leq \text{tol}$
exit
end
 $S_N = S_{N-1} \cup \mu_N$
 $X_N = X_{N-1} + \text{span } \{u(\mu_N)\}$
end



Main idea

Combine the reduced basis method with domain decomposition to solve PDEs in complex geometries

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Applications

- ▶ Repetitive geometry: Thermal fin and Hierarchical systems
- Repetitive solves: Optimization and Control



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Building blocks

$$\overline{\Omega} = \bigcup_{k=1}^{K} \overline{\Omega}^{k} = \bigcup_{k=1}^{K} \overline{\Phi^{k}(\hat{\Lambda})}$$

Pipes $\{\Omega^k = \Phi^k(\hat{\Omega})\}_{k=1}^{K_P}$, Bifurcations $\{\Omega^k = \Phi^k(\hat{\mathcal{B}})\}_{k=K_P+1}^{K_P+K_B}$.

Building blocks: pipes



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The geometry as a parameter

$$a(\mathbf{v},\mathbf{w};\Phi) =
u \int_{\Omega}
abla \mathbf{v} \cdot
abla \mathbf{w} d\Omega, \quad \Omega = \Phi(\hat{\Lambda})$$

The geometry as a parameter

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abla &= \mathcal{J}^{- au}(\Phi) \hat{
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abla} \end{aligned}$$

$$a(\mathbf{v},\mathbf{w};\Phi) = \nu \int_{\hat{\Lambda}} \mathcal{J}^{-T}(\Phi) \hat{\nabla}(\mathbf{v} \circ \Phi) \cdot \mathcal{J}^{-T}(\Phi) \hat{\nabla}(\mathbf{w} \circ \Phi) |J(\Phi)| \ d\hat{\Lambda}.$$

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The steady Stokes equations: weak form Let $\Omega = \Phi(\hat{\Lambda})$. Find $\mathbf{u} \in X(\Omega)$ and $p \in M(\Omega)$, such that $a(\mathbf{u}, \mathbf{v}; \Phi) + b(\mathbf{v}, p; \Phi) = \ell(\mathbf{v}; \Phi) \quad \forall \mathbf{v} \in X(\Omega)$

$$b(\mathbf{u}, q; \Phi) = 0 \quad \forall q \in M(\Omega)$$

$$X(\Omega) = \{\mathbf{v} \in (H^1(\Omega))^2, \mathbf{v}^w = 0, v_t^{in} = v_t^{out} = 0\}$$

$$M(\Omega) = L^2(\Omega)$$

$$a(\mathbf{v}, \mathbf{w}) = \nu \int_{\Omega} \nabla \mathbf{v} \cdot \nabla \mathbf{w} d\Omega$$

$$b(\mathbf{v}, q) = -\int_{\Omega} q \nabla \cdot \mathbf{v} d\Omega$$

Neumann type boundary conditions by specifying $\sigma_n = \frac{\partial u_n}{\partial n} - p$ to be $\sigma_n^{in} = -1$ along Γ_{in} , and $\sigma_n^{out} = 0$ along Γ_{out} .

Preselected geometries



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The reduced basis spaces The parameter space $S_N = {\{\Phi_i\}}_{i=1}^N$.

Preselected geometries



The reduced basis spaces

The parameter space $S_N = \{\Phi_i\}_{i=1}^N$. The velocity space $\hat{X}_N^0 = span\{\hat{\mathbf{u}}_i = \Psi_i(\mathbf{u}_i) = \mathcal{J}_i^{-1}(\mathbf{u}_i \circ \Phi_i)|J_i|\}_{i=1}^N$.

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Preselected geometries



The reduced basis spaces

The parameter space $S_N = \{\Phi_i\}_{i=1}^N$. The velocity space $\hat{X}_N^0 = span\{\hat{\mathbf{u}}_i = \Psi_i(\mathbf{u}_i) = \mathcal{J}_i^{-1}(\mathbf{u}_i \circ \Phi_i)|J_i|\}_{i=1}^N$. The pressure space $\hat{M}_N = span\{\hat{p}_i = p_i \circ \Phi_i\}_{i=1}^N$.

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Reduced basis steady Stokes approximation Find $\mathbf{u}_N \in X_N(\Omega)$ and $p_N \in M_N(\Omega)$, such that $a(\mathbf{u}_N, \mathbf{v}; \Phi) + b(\mathbf{v}, p_N; \Phi) = \ell(\mathbf{v}; \Phi) \quad \forall \mathbf{v} \in X_N(\Omega)$ $b(\mathbf{u}_N, q; \Phi) = 0 \quad \forall q \in M_N(\Omega)$

Reduced basis steady Stokes approximation Find $\mathbf{u}_N \in X_N^0(\Omega)$, such that $a(\mathbf{u}_N, \mathbf{v}; \Phi) = \ell(\mathbf{v}; \Phi) \quad \forall \mathbf{v} \in X_N^0(\Omega)$

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Reduced basis steady Stokes approximation Find $\mathbf{u}_N \in X_N(\Omega)$ and $p_N \in M_N(\Omega)$, such that $a(\mathbf{u}_N, \mathbf{v}; \Phi) + b(\mathbf{v}, p_N; \Phi) = \ell(\mathbf{v}; \Phi) \quad \forall \mathbf{v} \in X_N(\Omega)$ $b(\mathbf{u}_N, q; \Phi) = 0 \quad \forall q \in M_N(\Omega)$

Reduced basis steady Stokes approximation Find $\mathbf{u}_N \in X_N(\Omega)$ and $p_N \in M_N(\Omega)$, such that $a(\mathbf{u}_N, \mathbf{v}; \Phi) + b(\mathbf{v}, p_N; \Phi) = \ell(\mathbf{v}; \Phi) \quad \forall \mathbf{v} \in X_N(\Omega)$ $b(\mathbf{u}_N, q; \Phi) = 0 \quad \forall q \in M_N(\Omega)$

Enriched reduced basis velocity space For each $\hat{p}_i \in \hat{M}_N$ we find $\hat{\mathbf{v}}_i \in \hat{X}_N = X_N(\hat{\Lambda})$ such that $\hat{\mathbf{v}}_i = \arg \max_{\hat{\mathbf{u}} \in \hat{X}_N} \frac{\int_{\hat{\Lambda}} \hat{p}_i \hat{\nabla} \cdot \hat{\mathbf{u}} d\hat{\Lambda}}{|\hat{\mathbf{u}}|_{H^1}}.$

The enriched reduced basis velocity space on Ω is then

 $X_N(\Omega) = \{ \mathbf{v} \in X^0_N(\Omega) \oplus X^e_N(\Omega) \},$ where $X^0_N(\Omega) = \{ \Psi^{-1}(\hat{\mathbf{u}}_i) \}_{i=1}^N$, and $X^e_N(\Omega) = \{ \Psi^{-1}(\hat{\mathbf{v}}_i) \}_{i=1}^N$.

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Compliant output of interest Volume flow rate: $s(\mathbf{u}) = \ell(\mathbf{u}; \Phi)$

Compute output bounds: $s^-(\mathbf{u}_N) \leq s(\mathbf{u}) \leq s^+(\mathbf{u}_N)$

The output bounds for steady Stokes flow

$$egin{aligned} s^-(\mathbf{u}_N) &= \ell(\mathbf{u}_N; \Phi) \ s^+(\mathbf{u}_N) &= \ell(\mathbf{u}_N; \Phi) + \hat{a}(\mathbf{e}, \mathbf{e}; \Phi) \ \hat{a}(\mathbf{v}, \mathbf{w}; \Phi) &= \int_{\hat{\Lambda}} q(\Phi) \hat{
abla}(\mathbf{v} \circ \Phi) \cdot \hat{
abla}(\mathbf{w} \circ \Phi) d\hat{A} \end{aligned}$$

The reconstructed error \mathbf{e} satisfies the residual equation

$$\hat{a}(\mathbf{e},\mathbf{v};\Phi) = \ell(\mathbf{v};\Phi) - a(\mathbf{u}_N,\mathbf{v};\Phi) - b(\mathbf{v},p_N;\Phi) \quad \forall \ \mathbf{v} \in \widetilde{X}_{\mathcal{N}}(\Omega)$$



The reduced basis steady Stokes error on a pipe

Ν	$ \mathbf{u}_N - \mathbf{u}_N _{H^1}$	$ p_N - p_N _{L^2}$	$s(\mathbf{u}_{\mathcal{N}}) - s^{-}(\mathbf{u}_{N})$	$s^+({f u}_N)-s({f u}_{\mathcal N})$
3	$1.2 \cdot 10^{-2}$	$1.6 \cdot 10^{-1}$	$1.4 \cdot 10^{-4}$	$9.7 \cdot 10^{-2}$
6	$8.6 \cdot 10^{-3}$	$5.2 \cdot 10^{-2}$	$7.4 \cdot 10^{-5}$	$6.9 \cdot 10^{-3}$
9	$2.6 \cdot 10^{-3}$	$1.4 \cdot 10^{-2}$	$7.0 \cdot 10^{-6}$	$1.6 \cdot 10^{-3}$
12	$1.8 \cdot 10^{-3}$	$9.5 \cdot 10^{-3}$	$3.2 \cdot 10^{-6}$	$6.2 \cdot 10^{-4}$
15	$1.4\cdot10^{-3}$	$8.6\cdot10^{-3}$	$1.9\cdot 10^{-6}$	$3.8\cdot10^{-4}$



The reduced basis steady Stokes error on a bifurcation

Ν	$ \mathbf{u}_N - \mathbf{u}_N _{H^1}$	$ p_N - p_N _{L^2}$	$s(\mathbf{u}_{\mathcal{N}}) - s^{-}(\mathbf{u}_{N})$	$s^+(u_N)-s(u_\mathcal{N})$
1	$1.4 \cdot 10^{-2}$	$8.8 \cdot 10^{-2}$	$2.1 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$
5	$5.0 \cdot 10^{-4}$	$4.8 \cdot 10^{-3}$	$2.5 \cdot 10^{-7}$	$1.1 \cdot 10^{-5}$
10	$9.9 \cdot 10^{-6}$	$7.2 \cdot 10^{-5}$	$9.8\cdot10^{-11}$	$7.3 \cdot 10^{-9}$
15	$4.0 \cdot 10^{-6}$	$7.3 \cdot 10^{-6}$	$1.6\cdot10^{-11}$	$1.5\cdot10^{-11}$

Affine parameter dependence

$$m{a}(\mathbf{v},\mathbf{w};\mu) = \sum_{q=1}^Q \sigma^q(\mu) m{a}^q(\mathbf{v},\mathbf{w})$$

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Offline: Compute $A_{ij}^q = a^q(\mathbf{u}_i, \mathbf{u}_j)$ for q = 1, ..., Q and i, j = 1, ..., N. Online: Assemble A in $\mathcal{O}(QN^2)$ operations, and solve the reduced problem in $\mathcal{O}(N^3)$ operations.

Non-affine parameter dependence

$$a(\mathbf{v},\mathbf{w};\Phi) = \nu \int_{\hat{\Lambda}} \mathcal{J}^{-T}(\Phi) \hat{\nabla}(\mathbf{v} \circ \Phi) \cdot \mathcal{J}^{-T}(\Phi) \hat{\nabla}(\mathbf{w} \circ \Phi) |J(\Phi)| \ d\hat{\Lambda}.$$

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Non-affine parameter dependence

$$\begin{split} a(\mathbf{v},\mathbf{w};\Phi) &= \nu \int_{\hat{\Lambda}} \mathcal{J}^{-T}(\Phi) \hat{\nabla} (\mathbf{v} \circ \Phi) \cdot \mathcal{J}^{-T}(\Phi) \hat{\nabla} (\mathbf{w} \circ \Phi) |J(\Phi)| \ d\hat{\Lambda}. \\ a(\mathbf{v},\mathbf{w};\Phi) &= \nu \sum_{q=1}^{Q} \int_{\hat{\Lambda}} g^{q}(\Phi) a^{q}(\hat{\mathbf{v}},\hat{\mathbf{w}}) \ d\hat{\Lambda} \end{split}$$

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Non-affine parameter dependence

$$a(\mathbf{v},\mathbf{w};\Phi) =
u \int_{\hat{\Lambda}} \mathcal{J}^{-T}(\Phi) \hat{
abla} (\mathbf{v}\circ\Phi) \cdot \mathcal{J}^{-T}(\Phi) \hat{
abla} (\mathbf{w}\circ\Phi) |J(\Phi)| \ d\hat{\Lambda}.$$

$$a(\mathbf{v},\mathbf{w};\Phi) =
u \sum_{q=1}^{Q} \int_{\hat{\Lambda}} g^{q}(\Phi) a^{q}(\hat{\mathbf{v}},\hat{\mathbf{w}}) \ d\hat{\Lambda}$$

$$a(\mathbf{v},\mathbf{w};\Phi) pprox
u \sum_{q=1}^{Q} \sum_{m=1}^{M} eta_{m}^{q}(\Phi) \int_{\hat{\Lambda}} \tilde{g}^{q}(\Phi_{m}) a^{q}(\hat{\mathbf{v}},\hat{\mathbf{w}}) \ d\hat{\Lambda}$$

Offline: compute $A_{ij}^{qm} = \tilde{g}^q(\Phi_m)a^q(\mathbf{u}_i, \mathbf{u}_j)$ for q = 1, ..., Q, m = 1, ..., M, and i, j = 1, ..., N. Online: Find $\beta_m^q(\Phi)$, assemble A in $\mathcal{O}(QMN^2)$ operations, and solve the reduced problem in $\mathcal{O}(N^3)$ operations

Empirical interpolation

Find the constants $\beta_m^q(\Phi)$, m = 1, ..., M such that.

$$\sum_{m=1}^M eta_m^q(\Phi) g^q(\Phi_m) pprox g^q(\Phi).$$

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Projection gives

$$\begin{bmatrix} b_{mn} \end{bmatrix} [\beta_n] = [g_m] \,,$$

where $b_{mn} = \int_{\hat{\Lambda}} g^q(\Phi_m) g^q(\Phi_n) d\hat{\Lambda}$
and $g_m = \int_{\hat{\Lambda}} g^q(\Phi) g^q(\Phi_m) d\hat{\Lambda}.$

Empirical interpolation

Barrault et al. (2004) introduced magic points $\{t_m^q \in \hat{\Lambda}\}_{m=1}^M$ and corresponding operators $\{\tilde{g}^q(\Phi_m(x))\}_{m=1}^M$ such that

$$\tilde{g}^{q}(\Phi_{m}(t_{m}^{q})) = 1, \quad m = 1, ..., M$$
 $\tilde{g}^{q}(\Phi_{m}(t_{n}^{q})) = 0, \quad m < n.$

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The matrices B^q defined by $B^q_{mn} = \tilde{g}^q(\Phi_m(t^q_n))$ are lower triangular.

Empirical interpolation

Online we only need to find the coefficients $\beta_m^q(\Phi)$ to compute

$$a(\mathbf{u},\mathbf{v};\Phi) \approx \nu \sum_{q_1}^{Q} \sum_{m=1}^{M} \beta_m^q(\Phi) \int_{\hat{\Omega}} \tilde{g}^q(\Phi_m) a^q(\hat{\mathbf{u}},\hat{\mathbf{v}}) \ d\hat{\Omega}$$

The coefficients are found by solving

$$\sum_{n=1}^M B^q_{mn}eta^q_n(\Phi) = g(\Phi(t^q_m)), \quad 1\leq m\leq M$$

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New features

- Boundary conditions
- Continuity across block interfaces
- Nonconforming reduced basis element solution



Boundary conditions

- Construct one set of basis functions, and use the reflection across the vertical axis on the reference domain to deal with symmetric boundary conditions.
- Construct several sets of basis functions, each set corresponding to different boundary conditions.

Constraints ("gluing")
Let
$$\overline{\Gamma}_{kl} = \overline{\mathcal{B}}^k \bigcap \overline{\mathcal{B}}^l$$

$$\int_{\Gamma_{kl}} (\mathbf{v}^k - \mathbf{v}^l) \cdot \mathbf{n} \psi \, ds = 0, \quad \forall \, \psi \in W_{k,l}^n, \quad \forall k, l, \qquad (1)$$

$$\int_{\Gamma_{kl}} (\mathbf{v}^k - \mathbf{v}^l) \cdot \mathbf{t} \psi \, ds = 0, \quad \forall \, \psi \in W_{k,l}^t, \quad \forall k, l, \qquad (2)$$

Constraints ("gluing")
Let
$$\overline{\Gamma}_{kl} = \overline{\mathcal{B}}^k \bigcap \overline{\mathcal{B}}^l$$

$$\int_{\Gamma_{kl}} (\mathbf{v}^k - \mathbf{v}^l) \cdot \mathbf{n} \psi \, ds = 0, \quad \forall \, \psi \in W_{k,l}^n, \quad \forall k, l, \qquad (1)$$

$$\int_{\Gamma_{kl}} (\mathbf{v}^k - \mathbf{v}^l) \cdot \mathbf{t} \psi \, ds = 0, \quad \forall \, \psi \in W_{k,l}^t, \quad \forall k, l, \qquad (2)$$

Reduced basis approximation (nonconforming) Find $\mathbf{u}_N \in X_N(\Omega)$ and $p_N \in M_N(\Omega)$, such that

$$\begin{array}{ll} a(\mathbf{u}_N,\mathbf{v};\Phi) + b(\mathbf{v},p_N;\Phi) &= \ell(\mathbf{v};\Phi) & \forall \mathbf{v} \in X_N(\Omega) \\ b(\mathbf{u}_N,q;\Phi) &= 0 & \forall q \in M_N(\Omega) \end{array}$$

where $X_N(\Omega) = \{ \mathbf{v} \in X^0_N(\Omega) \oplus X^e_N(\Omega), \text{ s.t.}(1) \text{ and } (2) \text{ hold } \}.$

Example I: Three pipe segments



The reduced basis error

Ν	N_1	$ \mathbf{u}_N - \mathbf{u}_N _{H^1}$	$ p_N - p_N _{L^2}$
27	9	$2.3 \cdot 10^{-3}$	$3.6 \cdot 10^{-1}$
33	11	$1.2 \cdot 10^{-3}$	$5.8 \cdot 10^{-2}$
39	13	$9.7 \cdot 10^{-4}$	$4.4 \cdot 10^{-3}$
45	15	$8.4\cdot10^{-4}$	$3.6 \cdot 10^{-3}$

Example II: Hierarchical flow system



Reduced basis error

Ν	N_1	N_2	$ \mathbf{u}_N - \mathbf{u}_N _{H^1}$	$ p_N - p_N _{L^2}$
36	9	9	$2.6 \cdot 10^{-3}$	$4.0 \cdot 10^{-1}$
44	11	11	$1.7 \cdot 10^{-3}$	$6.6 \cdot 10^{-2}$
52	13	13	$1.2 \cdot 10^{-3}$	$4.9 \cdot 10^{-2}$
65	15	15	$1.1 \cdot 10^{-3}$	$3.7 \cdot 10^{-2}$
105	15	30	$4.2 \cdot 10^{-4}$	$6.3\cdot10^{-3}$

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Example III: A "bypass"



Reduced basis error

Ν	N_1	<i>N</i> ₂	$ \mathbf{u}_N - \mathbf{u}_N _{H^1}$	$ p_N - p_N _{L^2}$
45	9	9	$9.3 \cdot 10^{-3}$	3.3 · 10
55	11	11	$3.1 \cdot 10^{-3}$	$5.3\cdot10^{-1}$
65	13	13	$2.3 \cdot 10^{-3}$	$9.0 \cdot 10^{-2}$
75	15	15	$1.4 \cdot 10^{-3}$	$5.3 \cdot 10^{-2}$
105	15	30	$5.4\cdot10^{-4}$	$3.0\cdot10^{-2}$

Reduced basis modeling of complex flow systems

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Key features

- Geometry as a parameter
- Output bounds
- Offline/online decoupling
- Building blocks
- Lagrange multipliers

Reduced basis modeling of complex flow systems

Key features

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Future work/ongoing work

A posteriori bounds on multi-block geometries

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- Three dimensional domains
- Time dependent problems
- Fluid-structure interaction

Thank you!

