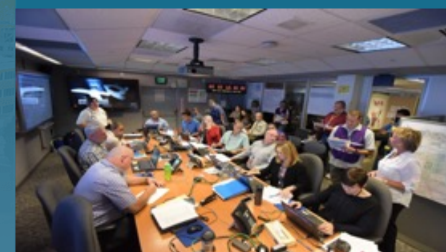
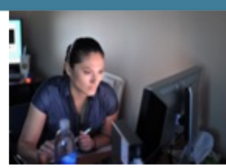
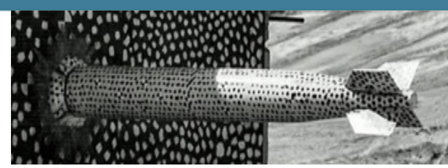
SAND2024-10112C

An optimization-based coupling of reduced order models with efficient reduced adjoint basis generation approach







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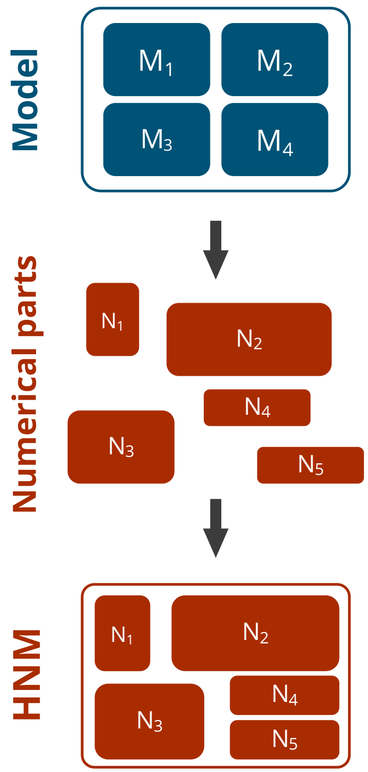
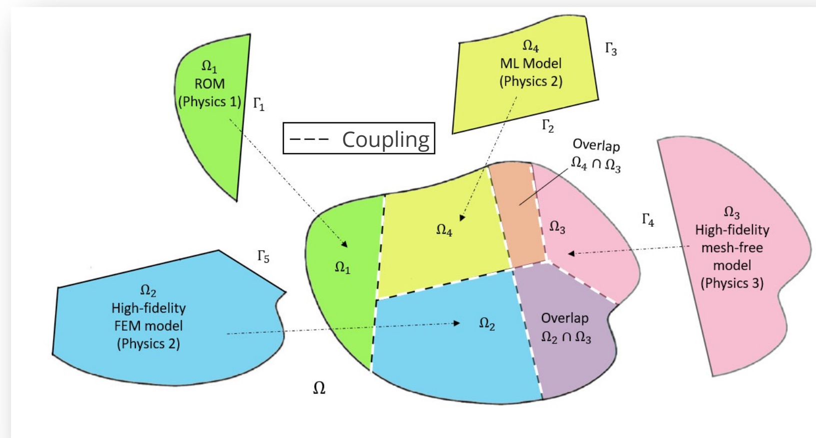
Heterogeneous Numerical Methods



DOE applications require **<u>diverse "mathematical parts"</u>**: PDEs, integral equations, classical DFT, potential-based atomistic…

Diverse math. models require **<u>diverse "numerical parts":</u>** mesh based (FE, FV, FD), meshless (SPH, MLS), implicit, explicit, Eulerian, Lagrangian…

HNM = Collection of **<u>diverse numerical parts</u>** from multiple disciplines functioning together as a **<u>unified simulation tool</u>**



Exemplar – Advection-Diffusion

Coupled problem with ”matching” interface conditions:

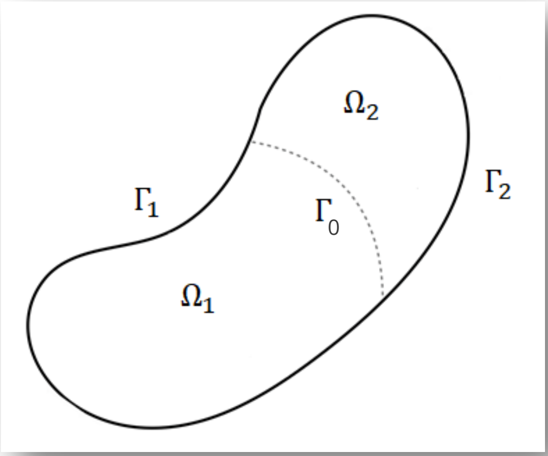
$$u_{i,t} - \nabla \cdot \sigma_i(_i) = f_i \text{ in } \Omega_i$$

$$u_i = 0 \text{ on } \Gamma_i$$

$$u_1 = u_2 \text{ on } \Gamma_0$$

$$\sigma_1(u_1) \cdot n_1 = -\sigma_2(u_2) \cdot n_2 \text{ on } \Gamma_0$$

where $\sigma_i(u) = \nu_i \nabla u - \mathbf{a}_i u$



Non-overlapping DD of $\Omega = \Omega_1 \cup \Omega_2$.

Review - Decomposition with Optimization-Based Coupling

$$J_\delta(u_1^n, u_2^n, g^n) := \frac{1}{2}\|u_1^n - u_2^n\|_{\Gamma_0}^2 + \frac{1}{2}\delta\|g^n\|_{\Gamma_0}^2$$

$$\min_{g^n} \quad J_\delta(u_1^n, u_2^n, g^n)$$

$$\text{s.t. finding } u_i^n \in X_i \text{ satisfying}$$

$$\frac{1}{\Delta t}(u_i^n - u_i^{n-1}, v) + (\sigma_i(u_i^n), \nabla v) = (f_i^n, v) + (-1)^i (g^n, v)_{\Gamma_0} \quad \forall v \in V_i$$

where $X_i = \{u \in H^1(\Omega_i) | u = 0 \text{ on } \Gamma_i\}, V_i = \{v \in H^1(\Omega_i) : v = 0 \text{ on } \Gamma_i\}$

Review - Relaxation with Lagrangian

We next introduce a Lagrangian in order to relax the constrained minimization problem,

$$\mathcal{L}(u_1^n, u_2^n, g,^n \mu_1, \mu_2) := J_\delta(u_1^n, u_2^n, g^n) + \sum_{i=1}^{2}[\frac{1}{\Delta t}(u_i^n - u_i^{n-1}, \mu_i) + (\sigma_i(u_i^n), \nabla \mu_i) - (f_i^n, \mu_i) + (-1)^{i+1}(g^n, \mu_i)_{\Gamma_0}]$$

and we solve for its stationary points.

$$\frac{\partial \mathcal{L}(u_1^n, u_2^n, g,^n \mu_1, \mu_2)}{\partial \mu_i} = 0 \quad \text{(State, primal problem)} \quad \frac{1}{\Delta t}(u_i^n - u_i^{n-1}, v) + (\sigma_i(u_i^n), \nabla v) = (f_i^n, v) + (-1)^i (g^n, v)_{\Gamma_0} \;\; \forall v \in V_i$$

$$\frac{\partial \mathcal{L}(u_1^n, u_2^n, g,^n \mu_1, \mu_2)}{\partial u_i^n} = 0 \quad \text{(Adjoint problem)} \quad \frac{1}{\Delta t}(\mu_i, \eta) + (\nu_i \nabla \mu_i + \mathbf{a}_i \mu_i, \nabla \eta) = (-1)^i (u_1^n - u_2^n, \eta)_{\Gamma_0} \;\; \forall \eta \in X_i^n$$

$$\frac{\partial \mathcal{L}(u_1^n, u_2^n, g,^n \mu_1, \mu_2)}{\partial g^n} = 0 \quad \text{(Informs update to control)} \quad \delta(\psi, g^n)_{\Gamma_0} = -(\psi, \mu_1 - \mu_2)_{\Gamma_0} \;\; \forall \psi \in L^2(\Gamma_0)$$

Gradient Descent $g^{n,(k)} = (1 - \alpha\delta) g^{n,(k-1)} - \alpha(\mu_1^{(k)} - \mu_2^{(k)})|_{\Gamma_0}$

Application of Finite Element Method to OBC

Find $\bar{u}_i^n \in \mathbb{R}^{N_i}$ satisfying

$$\frac{1}{\Delta t} M_i \bar{u}_i^n + (\nu_i K_i - A_i)\bar{u}_i^n = \bar{f}_i^n + (-1)^i M_{\Gamma_0,i} \bar{g}^n + \frac{1}{\Delta t} M_i \bar{u}_i^{n-1} \qquad \text{(FEM State)}$$

Find $\bar{\mu}_i \in \mathbb{R}^{N_i}$ satisfying

$$\frac{1}{\Delta t} M_i \bar{\mu}_i + (\nu_i K_i + A_i^T)\bar{\mu}_i = (-1)^i M_{\Gamma_0,i}(\bar{u}_1 - \bar{u}_2) \qquad \text{(FEM Adjoint)}$$

where $(M_i)_{k,j} := (\phi_{i,k}, \phi_{i,j})$, $(K_i)_{k,j} := (\nabla\phi_{i,k}, \nabla\phi_{i,j})$, $(A_i)_{k,j} := (\mathbf{a}\phi_{i,k}, \nabla\phi_{i,j})$, $(\bar{f}_i^n)_k := (f_i^n, \phi_{i,k})$, and $(M_{\Gamma_0,i})_{k,j} := (\xi_{\Gamma_0,j}, \xi_{i,k})$

FEM Gradient Descent

Given $\bar{g}^{n,(0)}$
for $k = 1, 2, \ldots$ **do**

Solve FEM state using $\bar{g}^{n,(k-1)}$ for $\bar{u}_1^n$ and $\bar{u}_2^n$

Solve FEM adjoint using $\bar{u}_1^n$ and $\bar{u}_2^n$ for $\bar{\mu}_1^{(k)}$ and $\bar{\mu}_2^{(k)}$

$\bar{g}^{n,(k)} = (1 - \alpha\delta)\bar{g}^{n,(k-1)} - \alpha(I_{1\to 0}\bar{\mu}_1^{(k)} - I_{2\to 0}\bar{\mu}_2^{(k)})|_{\Gamma_0}$

end for

Adaptation to ROM-ROM Coupling

Find $\hat{u}_i^n \in \mathbb{R}^{N_{u_i,r}}$ satisfying

$$\frac{1}{\Delta t}\hat{M}_i\hat{u}_i^n + (\nu_i\hat{K}_i - \hat{A}_i)\hat{u}_i^n = \hat{f}_i^n + (-1)^i M_{\Gamma_0,i}\bar{g} + \frac{1}{\Delta t}\hat{M}_i\hat{u}_i^{n-1}$$

(ROM State)

Find $\hat{\mu}_i \in \mathbb{R}^{N_{\mu_i,r}}$ satisfying

$$\frac{1}{\Delta t}\tilde{M}_i\hat{\mu}_i + (\nu_i\tilde{K}_i + \tilde{A}_i^T)\hat{\mu}_i = (-1)^i(\Psi_{\mu,i}^T M_{\Gamma_0,i}(\Psi_{u,1}\hat{u}_1^n - \Psi_{u,2}\hat{u}_2^n) + \Psi_{u,i}^T(\bar{\beta}_1^n - \bar{\beta}_2^n))$$

(ROM Adjoint)

where $\hat{M}_i := \Psi_{\mu,i}^T M_i \Psi_{\mu,i}$, $\hat{K}_i = \Psi_{\mu,i}^T K_i \Psi_{\mu,i}$, $\hat{A}_i := \Psi_{\mu,i}^T A_i \Psi_{u,i}$

with ROM change of basis:

$\Psi_{u,i}\hat{u}_i^n + \bar{\beta}_i^n = \bar{u}_i^n; \quad \hat{u}_i \in \mathbb{R}^{N_{u_i,r}}$

$\Psi_{\mu,i}\hat{\mu}_i = \bar{\mu}_i; \quad \hat{\mu}_i \in \mathbb{R}^{N_{\mu_i,r}}$

How is the adjoint reduced basis $\Psi_{\mu,i}$ generated?

ROM Gradient Descent

Given $\bar{g}^{n,(0)}$
for $k = 1, 2, \ldots$ **do**

Solve ROM state using $\bar{g}^{n,(k-1)}$ for $\hat{u}_1^n$ and $\hat{u}_2^n$

Solve ROM adjoint using $\hat{u}_1^n$, and $\hat{u}_2^n$ for $\hat{\mu}_1^{(k)}$ and $\hat{\mu}_2^{(k)}$

$\bar{g}^{n,(k)} = (1-\alpha\delta)\bar{g}^{n,(k-1)} - \alpha(I_{1\to 0}\Psi_{\mu,1}\hat{\mu}_1^{(k)} - I_{2\to 0}\Psi_{\mu,2}\hat{\mu}_2^{(k)})|_{\Gamma_0}$

end for

Adaptation to ROM-ROM Coupling

How do we most appropriately/efficiently generate snapshots for a suitable ROM basis for the adjoint system?

- Collecting snapshots of the state problem is well understood
- We make the assumption that the state snapshots are still available at the time of generating adjoint snapshots
- Below are several obvious ways to collect snapshots (**a,b**) and another way proposed
  by our group and investigated in this presentation (**c**):
  - **a)** Use state snapshots to form a reduced basis for the adjoint
  - **b)** Sequentially solve the FOM-FOM coupled problem with an OBC approach, storing all iterations at all timesteps
  - **c)** A modified version of b) that uses state snapshots to decouple timesteps and a fixed number of gradient descent iterations per timestep to reduce the adjoint snapshot size

Adaptation to ROM-ROM Coupling

Gradient Descent m for Reduced Adjoint

Given $\bar{g}^{n,(0)}$
for $k = 1, 2, \ldots$ **do**

Solve FEM state using $\bar{u}_1^{n-1}$, $\bar{u}_2^{n-1}$, and $\bar{g}^{n,(k-1)}$ for $\bar{u}_1^n$ and $\bar{u}_2^n$

Solve FEM adjoint using $\bar{u}_1^n$ and $\bar{u}_2^n$ for $\bar{\mu}_1^{(k)}$ and $\bar{\mu}_2^{(k)}$

$\bar{g}^{n,(k)} = (1 - \alpha\delta)\bar{g}^{n,(k-1)} - \alpha(I_{1\to 0}\bar{\mu}_1^{(k)} - I_{2\to 0}\bar{\mu}_2^{(k)})|_{\Gamma_0}$

end for

Modified Gradient Descent m for Reduced Adjoint

Given $\bar{g}^{n,(0)}$
for $k = 1, 2, \ldots$ **do**

Solve FEM state using $\bar{u}_{SNAP,1}^{n-1}$, $\bar{u}_{SNAP,2}^{n-1}$, and $\bar{g}^{n,(k-1)}$ for $\bar{u}_1^n$ and $\bar{u}_2^n$

Solve FEM adjoint using $\bar{u}_1^n$ and $\bar{u}_2^n$ for $\bar{\mu}_1^{(k)}$ and $\bar{\mu}_2^{(k)}$

$\bar{g}^{n,(k)} = (1 - \alpha\delta)\bar{g}^{n,(k-1)} - \alpha(I_{1\to 0}\bar{\mu}_1^{(k)} - I_{2\to 0}\bar{\mu}_2^{(k)})|_{\Gamma_0}$

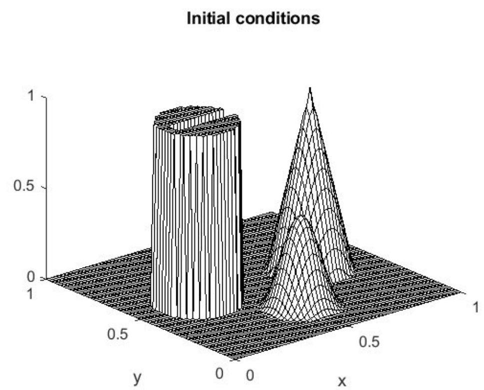
end for

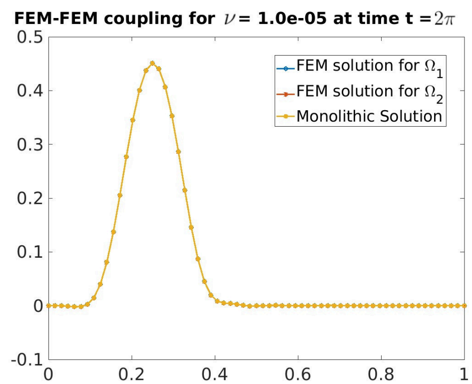
With traditional gradient descent, the solution at timestep (n-1) is needed and must be highly accurate (very tight tolerance for OBC)

Observation: Replace solution at previous timestep (n-1) with solution corresponding to that time in state snapshot matrix (breaks connection between timesteps [parallel] and allows GD tolerance to be loosened [cheaper])

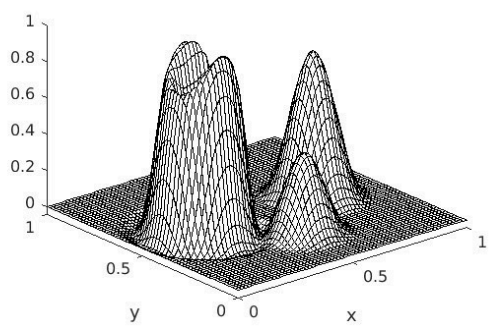
Leaves open the choice of what to choose for $\bar{g}^{n,(0)}$ at each timestep. We choose $\bar{g}^{n,(0)} = \vec{0}$.

Numerical Result – OBC FOM-FOM Coupled Problem

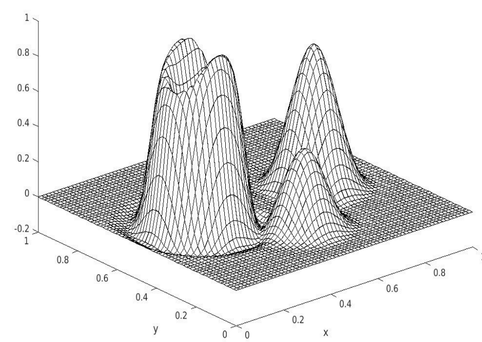




Monolithic FEM solution for $\nu = 1e - 5$ at time t=2π



FEM-FEM coupling for $\nu = 1e - 5$ at time t=2π



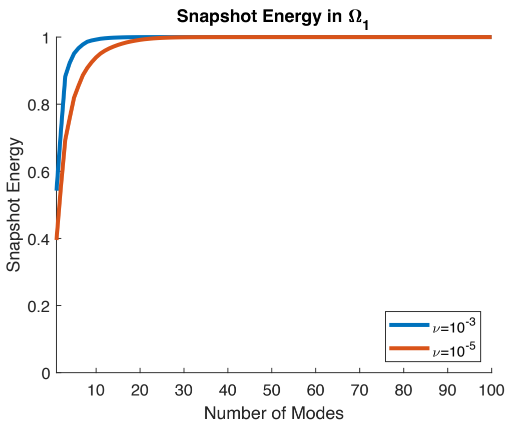
$\Delta t = 1.122398e - 3$ $\quad h = \frac{1}{64}$ $\quad \nu = 1e - 5$

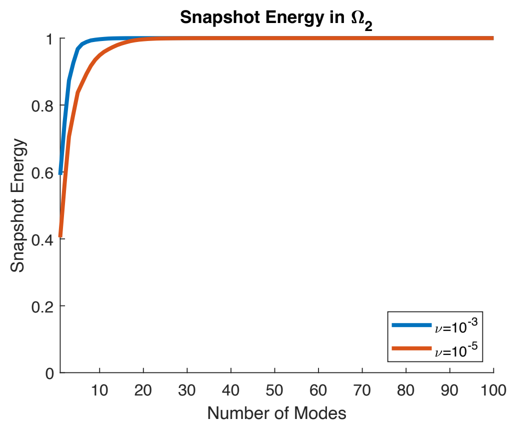
Coupled FEM-FEM results with $\delta = 1e - 16$ and tolerance of $1e - 14$ results in:

$$\frac{\|u_c - u_m\|_{L^2}}{\|u_m\|_{L^2}} = 7.8e - 8$$

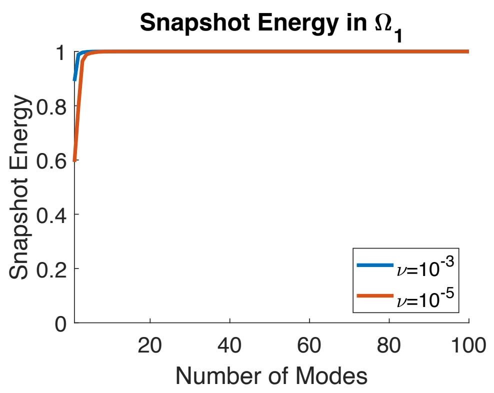
Balance of mismatched states and penalty term for the control indicates error should be roughly $\sqrt{tolerance}$

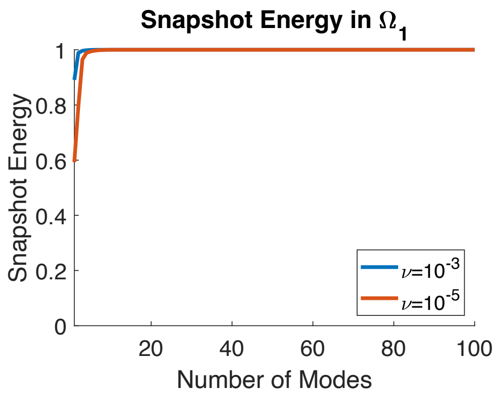
Numerical Result – Applicability of P-ROM





Snapshot energy in state solutions as a function of modes





Snapshot energy in adjoint solutions as a function of modes

Quick decay of snapshot energies w.r.t. # of modes

Numerical Result – Comparison Using Different Reduced Spaces for the Adjoint

RS - Reduced state
FS - FOM state

SRA - State solution-based reduced adjoint
MGD1RA - Modified gradient descent – *1 iteration*
FA - FOM adjoint

Takeaway #1: State solutions used to produce reduced basis for adjoint doesn't work until ~1500 modes retained. Replacing SRA with FA has significant impact. Can we do better?

	RS-FA	
Modes	Error	Iters.
50	10^{-4}	$*$
100	10^{-7}	50.1
250	10^{-7}	36.9
500	10^{-7}	21.4
1000	10^{-7}	9.8
1500	10^{-8}	4.4
1600	10^{-8}	4.4
1700	10^{-8}	4.4
1800	10^{-8}	4.4
2016	10^{-8}	3

	RS-SRA		FS-SRA	
Modes	Error	Iters.	Error	Iters.
50	10^{-3}	$*$	10^{-4}	$*$
100	10^{-3}	$*$	10^{-4}	$*$
250	10^{-5}	$*$	10^{-4}	$*$
500	10^{-6}	$*$	10^{-5}	$*$
1000	10^{-7}	$*$	10^{-6}	$*$
1500	10^{-7}	506.7	10^{-8}	139.8
1600	10^{-8}	68.6	10^{-8}	48.2
1700	10^{-8}	21.1	10^{-8}	11.9
1800	10^{-8}	14.8	10^{-8}	9
2016	10^{-8}	3	10^{-8}	3

	RS-MGD1RA		FS-MGD1RA	
Modes	Error	Iters.	Error	Iters.
50	10^{-4}	$*$	10^{-7}	$*$
100	10^{-5}	2342.8	10^{-8}	4.2
250	10^{-6}	401.5	10^{-8}	4
500	10^{-7}	102.8	10^{-8}	3.7
1000	10^{-7}	35.2	10^{-8}	3.7
1500	10^{-8}	7.8	10^{-8}	3.7
1600	10^{-8}	6.6	10^{-8}	3.7
1700	10^{-8}	6.5	10^{-8}	3.7
1800	10^{-8}	6.5	10^{-8}	3.7
2016	10^{-8}	3	10^{-8}	3

$\delta = 1e - 16$ and tolerance of $1e - 14$, $\nu = 1e - 5$

Numerical Result – Comparison Using Different Reduced Spaces for the Adjoint

RS - Reduced state
FS - FOM state

SRA - State solution-based reduced adjoint
MGD1RA - Modified gradient descent – *1 iteration*
FA - FOM adjoint

Takeaway #2: MGD1RA outperforms SRA and doesn't require many modes
(# of state modes kept is more important)

	RS-FA	
Modes	Error	Iters.
50	10^{-4}	$*$
100	10^{-7}	50.1
250	10^{-7}	36.9
500	10^{-7}	21.4
1000	10^{-7}	9.8
1500	10^{-8}	4.4
1600	10^{-8}	4.4
1700	10^{-8}	4.4
1800	10^{-8}	4.4
2016	10^{-8}	3

	RS-SRA		FS-SRA	
Modes	Error	Iters.	Error	Iters.
50	10^{-3}	$*$	10^{-4}	$*$
100	10^{-3}	$*$	10^{-4}	$*$
250	10^{-5}	$*$	10^{-4}	$*$
500	10^{-6}	$*$	10^{-5}	$*$
1000	10^{-7}	$*$	10^{-6}	$*$
1500	10^{-7}	506.7	10^{-8}	139.8
1600	10^{-8}	68.6	10^{-8}	48.2
1700	10^{-8}	21.1	10^{-8}	11.9
1800	10^{-8}	14.8	10^{-8}	9
2016	10^{-8}	3	10^{-8}	3

	RS-MGD1RA		FS-MGD1RA	
Modes	Error	Iters.	Error	Iters.
50	10^{-4}	$*$	10^{-7}	$*$
100	10^{-5}	2342.8	10^{-8}	4.2
250	10^{-6}	401.5	10^{-8}	4
500	10^{-7}	102.8	10^{-8}	3.7
1000	10^{-7}	35.2	10^{-8}	3.7
1500	10^{-8}	7.8	10^{-8}	3.7
1600	10^{-8}	6.6	10^{-8}	3.7
1700	10^{-8}	6.5	10^{-8}	3.7
1800	10^{-8}	6.5	10^{-8}	3.7
2016	10^{-8}	3	10^{-8}	3

$\delta = 1e - 16$ and tolerance of $1e - 14$, $\nu = 1e - 5$

Numerical Result – Projection Errors (State and Adjoint)

	RS	
Modes	$\mathcal{E}(u_1, \Psi_{u,1})$	$\mathcal{E}(u_2, \Psi_{u,2})$
50	10^{-3}	10^{-3}
100	10^{-8}	10^{-7}
250	10^{-9}	10^{-8}
500	10^{-9}	10^{-8}
1000	10^{-9}	10^{-8}
1500	10^{-9}	10^{-8}
2016	10^{-15}	10^{-15}

Projection of state solutions onto reduced basis generated from state solution snapshots

$\nu = 1e - 5$

	SRA	
Modes	$\mathcal{E}(\mu_1, \Psi_{u,1})$	$\mathcal{E}(\mu_2, \Psi_{u,2})$
50	10^{-1}	10^{-1}
2000	10^{-1}	10^{-1}
2001	10^{-2}	10^{-2}
2014	10^{-2}	10^{-2}
2015	10^{-3}	10^{-3}
2016	10^{-15}	10^{-15}

Projection of adjoint solutions onto reduced basis generated from state solution snapshots

Takeaway #3: State solutions should not be used to generate reduced basis for adjoint

	GDRA		MGD1RA	
Modes	$\mathcal{E}(\mu_1, \Psi_{\mu,1})$	$\mathcal{E}(\mu_2, \Psi_{\mu,2})$	$\mathcal{E}(\mu_1, \Psi_{\mu,1})$	$\mathcal{E}(\mu_2, \Psi_{\mu,2})$
50	$10^{-4} - 10^{-3}$	$10^{-6} - 10^{-5}$	$10^{-4} - 10^{-3}$	$10^{-6} - 10^{-5}$
100	$10^{-15} - 10^{-14}$	10^{-15}	$10^{-15} - 10^{-14}$	10^{-15}
500	$10^{-15} - 10^{-14}$	10^{-15}	$10^{-15} - 10^{-14}$	10^{-15}
1500	$10^{-15} - 10^{-14}$	10^{-15}	$10^{-15} - 10^{-14}$	10^{-15}
2016	10^{-15}	10^{-15}	10^{-15}	10^{-15}

Projection of adjoint solutions onto reduced basis generated from GDRA and MGD1RA

Numerical Result – Interplay of state and adjoint ROM modes

State/Adjoint Reduced Space Modal Size Comparison

RS Modes	50		100		250	
MGD1RA Modes	Avg. Iters.	Error	Avg. Iters.	Error	Avg. Iters.	Error
25	$*$	10^{-4}	4498.8	10^{-6}	$*$	10^{-4}
50	$*$	10^{-4}	761.5	10^{-6}	2119.8	10^{-6}
100	$*$	10^{-4}	2342.8	10^{-5}	536.9	10^{-6}

$\delta = 1e-16$ and tolerance of $1e-14$, $\nu = 1e-5$

RS Modes	50		100		250	
MGD1RA Modes	Avg. Iters.	Error	Avg. Iters.	Error	Avg. Iters.	Error
25	$*$	10^{-4}	349	10^{-5}	4246.4	10^{-6}
50	$*$	10^{-4}	170.7	10^{-5}	312.4	10^{-6}
100	$*$	10^{-4}	150.4	10^{-5}	129.5	10^{-5}

$\delta = 1e-14$ and tolerance of $1e-12$, $\nu = 1e-5$

RS Modes	50		100		250	
MGD1RA Modes	Avg. Iters.	Error	Avg. Iters.	Error	Avg. Iters.	Error
25	15.2	10^{-3}	9.3	10^{-4}	15.6	10^{-4}
50	18.9	10^{-3}	11.4	10^{-4}	8.8	10^{-4}
100	12.7	10^{-3}	8.4	10^{-4}	6.2	10^{-4}

$\delta = 1e-10$ and tolerance of $1e-8$, $\nu = 1e-5$

Takeaway #4:
Important to balance reduced space state and reduced space adjoint number of modes.
Also, loosening tolerance and increasing penalty increases rate of convergence.

Numerical Result – MGD*m*RA vs. GDRA
What is lost from limiting ourselves to m iterations?

Takeaway #5: Similar iterations and runtimes for GDRA and MGD1RA; both beating the FOM-FOM coupled problem

Average Iteration Comparison

RS Modes	100		250	
MGD1RA Modes	Avg. Iters.	Error	Avg. Iters.	Error
50	170.7	10^{-5}	312.4	10^{-6}
100	150.4	10^{-5}	129.5	10^{-5}
GDRA Modes				
50	170.7	10^{-5}	371.2	10^{-6}
100	242.1	10^{-5}	143.2	10^{-5}

$\nu = 1e - 5$

Runtime Comparison

$\nu = 10^{-5}$			$\nu = 10^{-3}$		
FOM	MGD1RA ROM	GDRA ROM	FOM	MGD1RA ROM	GDRA ROM
86 sec	33 sec	32 sec	131 sec	76 sec	76 sec

Conclusions

- Introduced a snapshot collection technique (MGDmRA) for producing a reduced basis for the adjoint of a ROM-ROM OBC problem

  - Broke the connection between timesteps by using state snapshot data
  - Fixed memory / computational footprint by selecting a fixed subset of gradient descent iterations per timestep

- Numerical experiments indicate:

  - State snapshots are not effective for producing a reduced basis for the adjoint
  - MGD*m*RA produces a basis that is competitive with the reduced basis generated by gradient descent (run sequentially with a tight tolerance) in iteration counts, projection errors, and computational time (with reduced offline cost).

Future Work

- Explore FOM-ROM combinations
- Improved optimization algorithms (far fewer iterations)

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