

Nonlinear model reduction:
discrete optimality, h -adaptivity, and error
surrogates

Kevin Carlberg

Sandia National Laboratories

Workshop on Data-Driven Model Order Reduction and
Machine Learning
April 1, 2016

Collaborators

2014–2015 M. Barone

Sandia National Laboratories

2014–2015 H. Antil

George Mason University

2015 L. Brencher, B. Haasdonk

University of Stuttgart

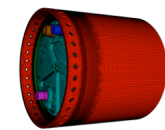
2010–2011 C. Farhat, C. Bou-Mosleh, J. Cortial, D. Amsallem

Stanford University

Computational barrier

High-fidelity simulation

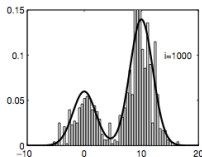
- + An indispensable tool
- Very high computational cost



Barrier

Time-critical applications

Many query



[Andrieu et al., 2003]

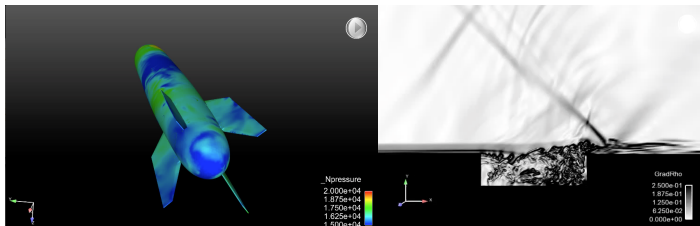
Real time



[Nat'l Power Grid Sim. Cap.]

Objective: break barrier

Computational barrier at Sandia



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

Barrier

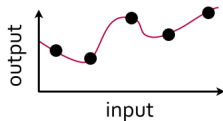
- Fast-turnaround design
- Uncertainty quantification (UQ)

Surrogate modeling

inputs $\mu \rightarrow$ **full-order model** \rightarrow outputs y

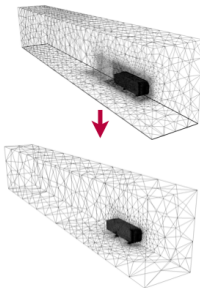
inputs $\mu \rightarrow$ **surrogate model** \rightarrow outputs y

1) Data fits



- Not physics based
- + High speedups

2) Coarsened physics



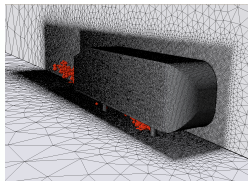
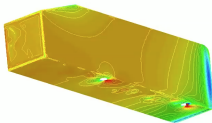
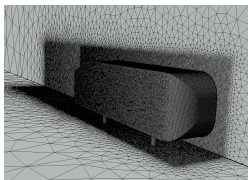
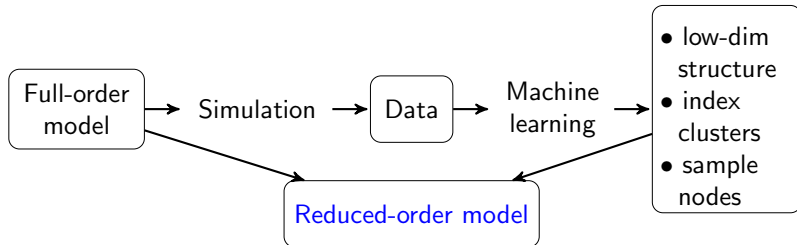
- + Physics based
- Low speedups

3) Reduced-order models (ROMs)

- + Physics based
- + High speedups
- + Preserve structure
- + Rigorous error analysis
- **Unproven for nonlinear dynamical systems**

ROM = data science + modeling and simulation

Goal: exploit **simulation data** to drastically **reduce simulation costs**



ROM: state of the art [Benner et al., 2015]

- Linear time-invariant systems: **mature** [Antoulas, 2005]
 - Balanced truncation [Moore, 1981]
 - Empirical balanced truncation [Willcox and Peraire, 2002, Rowley, 2005]
 - Moment matching
 - [Bai, 2002, Freund, 2003, Gallivan et al., 2004, Baur et al., 2011]
 - Loewner framework [Lefteriu and Antoulas, 2010, Ionita and Antoulas, 2014]
 - + *Reliable*: guaranteed stability, *a priori* error bounds
 - + *Certified*: sharp, computable *a posteriori* error bounds
- Elliptic/parabolic PDEs (FEM): **mature** [Rozza et al., 2008]
 - Reduced-basis method
 - [Prud'Homme et al., 2001, Veroy et al., 2003, Barrault et al., 2004]
 - Subsystem-based reduced-basis method
 - [Maday and Rønquist, 2002, Phuong Huynh et al., 2013, Eftang and Patera, 2013]
 - + *Reliable*: *a priori* error bounds
 - + *Certified*: sharp, computable *a posteriori* error bounds
- Nonlinear dynamical systems: **unproven**
 - Proper orthogonal decomposition (POD)–Galerkin
 - *Not reliable*: Stability and accuracy not guaranteed
 - *Not certified*: error bounds not sharp

My research goal

Nonlinear model-reduction methods that are
accurate, low cost, certified, and reliable.

+ Accuracy

- Improve projection technique [C. et al., 2011a, C. et al., 2015a]
- Preserve problem structure [C. et al., 2012, C. et al., 2015c]

+ Low cost

- Sample-mesh approach [C. et al., 2011b, C. et al., 2013]
- Leverage time-domain data [C. et al., 2015b]

+ Certification

- Error bounds [C. et al., 2015a]
- Statistical error modeling [Drohmman and C., 2015]

+ Reliability

- *A posteriori* h -refinement [C., 2015]

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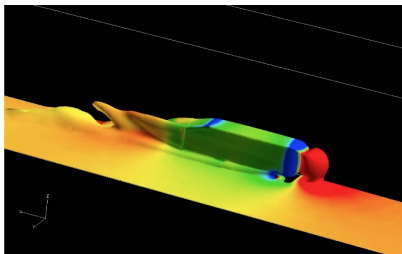
+ Reliability

- *A posteriori* h -refinement [C., 2015]

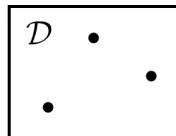
POD–Galerkin: offline data collection

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu}); \quad \mathbf{x}(0, \boldsymbol{\mu}) = \mathbf{x}^0(\boldsymbol{\mu}), \quad t \in [0, T], \quad \boldsymbol{\mu} \in \mathcal{D}$$

- 1 Collect ‘snapshots’ of the state



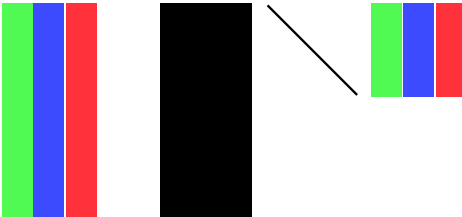
$\mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3$



POD–Galerkin: offline data collection

2 Data compression

■ Compute SVD: $[\mathbf{x}_1 \ \mathbf{x}_2 \ \mathbf{x}_3] = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^T$



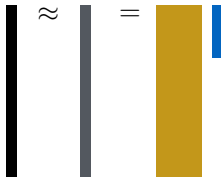
■ Truncate: $\Phi = [\mathbf{u}_1 \ \cdots \ \mathbf{u}_\rho]$

POD–Galerkin: online projection

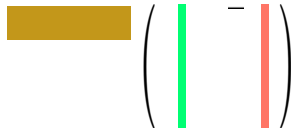
Full-order model:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \mu), \quad \mathbf{x}(0, \mu) = \mathbf{x}^0(\mu)$$

1 $\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \Phi \hat{\mathbf{x}}(t)$



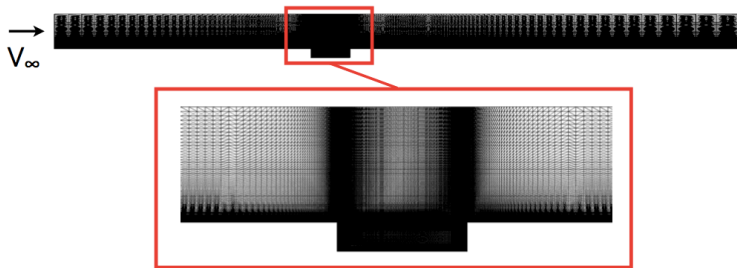
2 $\Phi^T \left(\mathbf{f}(\tilde{\mathbf{x}}; t, \mu) - \frac{d\tilde{\mathbf{x}}}{dt} \right) = 0$



Galerkin ROM:

$$\frac{d\hat{\mathbf{x}}}{dt} = \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}; t, \mu), \quad \hat{\mathbf{x}}(0, \mu) = \Phi^T \mathbf{x}^0(\mu)$$

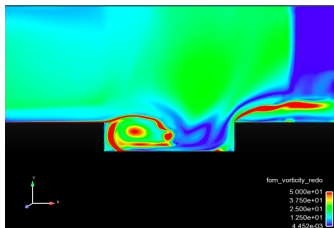
Cavity-flow problem. Collaborator: M. Barone (SNL)



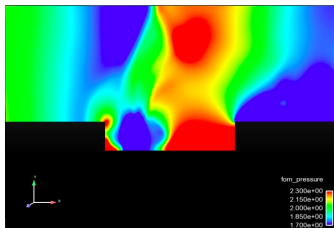
- Unsteady Navier–Stokes
- DES turbulence model
- 1.2 million degrees of freedom

- $\text{Re} = 6.3 \times 10^6$
 - $M_\infty = 0.6$
 - CFD code: AERO-F
- [Farhat et al., 2003]

Full-order model responses

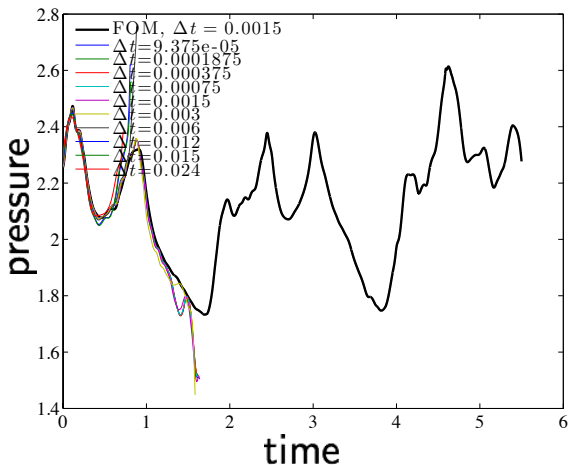


vorticity field



pressure field

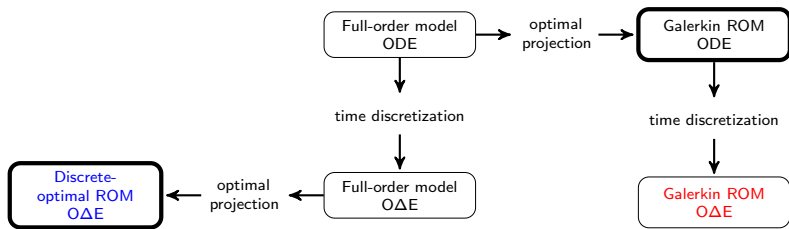
POD–Galerkin failure



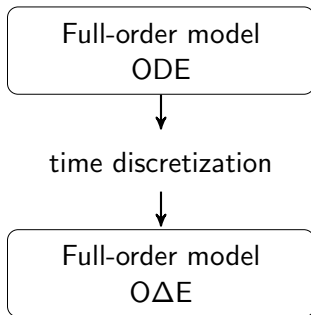
- Galerkin ROMs unstable

How to construct a ROM for nonlinear dynamical systems?

- Optimize then discretize? (Galerkin)
- Discretize then optimize? (discrete optimal)



- Outstanding questions:
 - 1 Which notion of optimality is better in practice?
 - 2 Are the two techniques ever equivalent?
 - 3 Discrete-time error bounds?



Full-order model (FOM)

- ODE: time continuous

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \quad \mathbf{x}(0) = \mathbf{x}^0, \quad t \in [0, T]$$

- OΔE, linear multistep schemes: $\boxed{\mathbf{r}^n(\mathbf{x}^n) = 0}$, $n = 1, \dots, N$

$$\mathbf{r}^n(\mathbf{x}) := \alpha_0 \mathbf{x} - \Delta t \beta_0 \mathbf{f}(\mathbf{x}, t^n) + \sum_{j=1}^k \alpha_j \mathbf{x}^{n-j} - \Delta t \sum_{j=1}^k \beta_j \mathbf{f}(\mathbf{x}^{n-j}, t^{n-j})$$

$$\mathbf{x}^n = \mathbf{x}^n \text{ (explicit state update)}$$

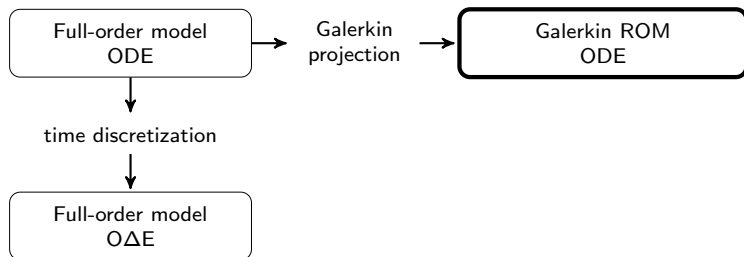
- OΔE, Runge–Kutta: $\boxed{\mathbf{r}_i^n(\mathbf{x}_1^n, \dots, \mathbf{x}_s^n) = 0}$, $i = 1, \dots, s$

$$\mathbf{r}_i^n(\mathbf{x}_1, \dots, \mathbf{x}_s) := \mathbf{x}_i - \mathbf{f}(\mathbf{x}^{n-1} + \Delta t \sum_{j=1}^s a_{ij} \mathbf{x}_j, t^{n-1} + c_i \Delta t)$$

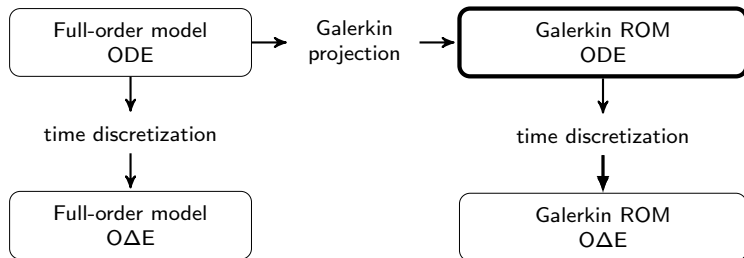
$$\mathbf{x}^n = \mathbf{x}^{n-1} + \Delta t \sum_{i=1}^s b_i \mathbf{x}_i^n \text{ (explicit state update)}$$

This talk focuses on linear multistep schemes.

Galerkin ROM: first optimize



Galerkin: first optimize, then discretize



Galerkin ROM

■ ODE

$$\frac{d\hat{\mathbf{x}}}{dt} = \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}, t), \quad \hat{\mathbf{x}}(0) = \Phi^T \mathbf{x}^0, \quad t \in [0, T]$$

+ Continuous velocity $\frac{d\hat{\mathbf{x}}}{dt}$ is **optimal**

Theorem (Galerkin ROM: continuous optimality)

The Galerkin ROM velocity minimizes the time-continuous FOM residual:

$$\frac{d\tilde{\mathbf{x}}}{dt}(\mathbf{x}, t) = \arg \min_{\mathbf{v} \in \text{range}(\Phi)} \|\mathbf{v} - \mathbf{f}(\mathbf{x}, t)\|_2^2$$

■ OΔE

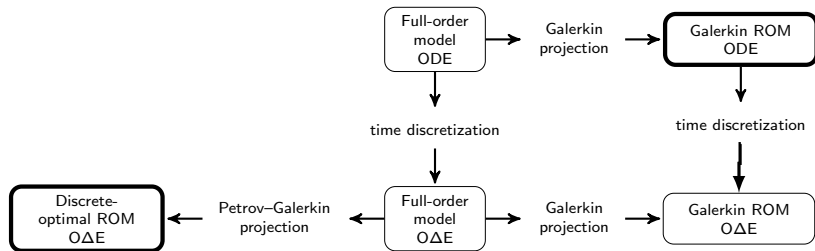
$$\hat{\mathbf{r}}^n(\hat{\mathbf{x}}^n) = 0, \quad n = 1, \dots, N$$

$$\hat{\mathbf{r}}^n(\hat{\mathbf{x}}) := \alpha_0 \hat{\mathbf{x}} - \Delta t \beta_0 \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}, t^n) + \sum_{j=1}^k \alpha_j \hat{\mathbf{x}}^{n-j} - \Delta t \sum_{j=1}^k \beta_j \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}^{n-j}, t^{n-j})$$

- Discrete state $\hat{\mathbf{x}}^n$ is **not generally optimal**

Can we fix this? Will doing so help?

Discrete-optimal ROM: first discretize, then optimize



Discrete-optimal ROM

- FOM $O(\Delta t)$

$$\mathbf{r}^n(\mathbf{x}^n) = 0, \quad n = 1, \dots, N$$

- Discrete-optimal ROM $O(\Delta t)$:

$$\hat{\mathbf{x}}^n = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \|\mathbf{A} \mathbf{r}^n(\Phi \hat{\mathbf{z}})\|_2^2.$$

$$\Updownarrow$$

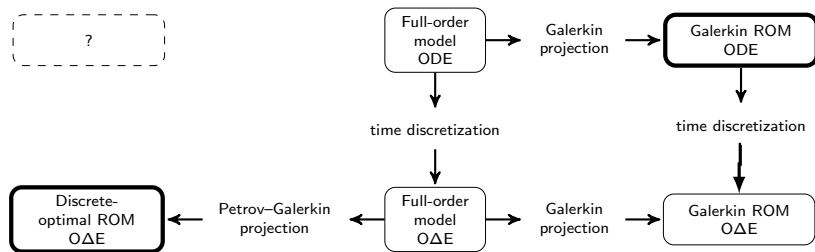
$$\boldsymbol{\Psi}^n(\hat{\mathbf{x}}^n)^T \mathbf{r}^n(\Phi \hat{\mathbf{x}}^n) = 0, \quad \boldsymbol{\Psi}^n(\hat{\mathbf{x}}) := \mathbf{A}^T \mathbf{A} \frac{\partial \mathbf{r}^n}{\partial \mathbf{x}}(\Phi \hat{\mathbf{x}})$$

- $\mathbf{A} = \mathbf{I}$: Least-squares Petrov–Galerkin

[LeGresley, 2006, Bui-Thanh et al., 2008, C. et al., 2011a]

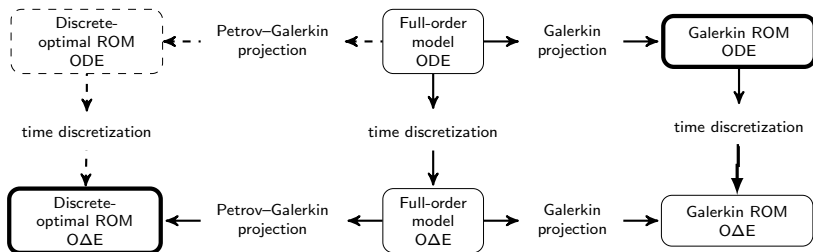
+ Discrete solution is optimal

Does the discrete-optimal ROM have a time-continuous representation?



Does the discrete-optimal ROM have a time-continuous representation?

Sometimes.



Discrete-optimal ROM: continuous representation

Theorem

The discrete-optimal ROM is equivalent to applying a Petrov–Galerkin projection to the FOM ODE with test basis

$$\Psi(\hat{\mathbf{x}}, t) = \mathbf{A}^T \mathbf{A} \left(\alpha_0 \mathbf{I} - \Delta t \beta_0 \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\mathbf{x}^0 + \Phi \hat{\mathbf{x}}, t) \right) \Phi$$

if

- 1** $\beta_j = 0, j \geq 1$ (e.g., a single-step method),
- 2** the velocity \mathbf{f} is linear in the state, or
- 3** $\beta_0 = 0$ (i.e., explicit schemes).

*Time-continuous test basis depends on
time-discretization parameters!*

Are the two approaches ever equivalent?

- Galerkin: $\Phi^T \mathbf{r}^n(\Phi \hat{\mathbf{x}}^n) = 0$
- Discrete-optimal: $\Psi^n(\hat{\mathbf{x}}^n)^T \mathbf{r}^n(\Phi \hat{\mathbf{x}}^n) = 0$

Does $\Psi^n(\hat{\mathbf{x}}^n) = \Phi$ ever?

Yes.

$$\Psi^n(\hat{\mathbf{x}}) := \mathbf{A}^T \mathbf{A} \frac{\partial \mathbf{r}^n}{\partial \mathbf{x}}(\Phi \hat{\mathbf{x}}) = \mathbf{A}^T \mathbf{A} \left(\alpha_0 \mathbf{I} - \Delta t \beta_0 \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\Phi \hat{\mathbf{x}}, t^n) \right) \Phi$$

Theorem

The two approaches are equivalent ($\Psi^n(\hat{\mathbf{x}}) = \Phi$)

- 1 *in the limit of $\Delta t \rightarrow 0$ with $\mathbf{A} = 1/\sqrt{\alpha_0} \mathbf{I}$,*
- 2 *if the scheme is explicit ($\beta_0 = 0$) with $\mathbf{A} = 1/\sqrt{\alpha_0} \mathbf{I}$, or*
- 3 *if $\frac{\partial \mathbf{r}^n}{\partial \mathbf{x}}$ is positive definite with $[\frac{\partial \mathbf{r}^n}{\partial \mathbf{x}}]^{-1} = \mathbf{A}^T \mathbf{A}$.*

Discrete-time error bound

Theorem

If the following conditions hold:

- 1 $\mathbf{f}(\cdot, t)$ is Lipschitz continuous with Lipschitz constant κ , and
- 2 Δt is such that $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$,

then

$$\|\delta \mathbf{x}_G^n\| \leq \frac{\Delta t}{h} \sum_{\ell=0}^k |\beta_\ell| \|(\mathbf{I} - \mathbb{V}) \mathbf{f}(\mathbf{x}_0 + \Phi \hat{\mathbf{x}}_G^{n-\ell})\| + \frac{1}{h} \sum_{\ell=1}^k (|\beta_\ell|\kappa\Delta t + |\alpha_\ell|) \|\delta \mathbf{x}_G^{n-\ell}\|$$
$$\|\delta \mathbf{x}_D^n\| \leq \frac{\Delta t}{h} \sum_{\ell=0}^k |\beta_\ell| \|(\mathbf{I} - \mathbb{P}^n) \mathbf{f}(\mathbf{x}_0 + \Phi \hat{\mathbf{x}}_D^{n-\ell})\| + \frac{1}{h} \sum_{\ell=1}^k (|\beta_\ell|\kappa\Delta t + |\alpha_\ell|) \|\delta \mathbf{x}_D^{n-\ell}\|,$$

with

- $\delta \mathbf{x}_G^n := \mathbf{x}_\star^n - \Phi \hat{\mathbf{x}}_G^n.$
- $\mathbb{V} := \Phi \Phi^T$
- $\delta \mathbf{x}_D^n := \mathbf{x}_\star^n - \Phi \hat{\mathbf{x}}_D^n$
- $\mathbb{P}^n := \Phi ((\Psi^n)^T \Phi)^{-1} (\Psi^n)^T$

Discrete-optimal ROM yields a smaller error bound

Theorem (Backward Euler)

If conditions (1) and (2) hold, then

$$\|\delta \mathbf{x}_G^n\| \leq \Delta t \sum_{j=0}^{n-1} \frac{1}{(h)^{j+1}} \underbrace{\|(\mathbf{I} - \mathbb{V}) \mathbf{f}(\mathbf{x}_0 + \Phi \hat{\mathbf{x}}_G^{n-j})\|}_{\varepsilon_G^{n-j}}$$

$$\|\delta \mathbf{x}_D^n\| \leq \Delta t \sum_{j=0}^{n-1} \frac{1}{(h)^{j+1}} \underbrace{\|(\mathbf{I} - \mathbb{P}^{n-j}) \mathbf{f}(\mathbf{x}_0 + \Phi \hat{\mathbf{x}}_D^{n-j})\|}_{\varepsilon_D^{n-j}}$$

$$\varepsilon_G^k = \|\Phi \hat{\mathbf{x}}_G^k - \Delta t \mathbf{f}(\mathbf{x}_0 + \Phi \hat{\mathbf{x}}_G^k) - \Phi \hat{\mathbf{x}}_G^{k-1}\|$$

$$\varepsilon_D^k = \|\Phi \hat{\mathbf{x}}_D^k - \Delta t \mathbf{f}(\mathbf{x}_0 + \Phi \hat{\mathbf{x}}_D^k) - \Phi \hat{\mathbf{x}}_D^{k-1}\| = \min_{\mathbf{y}} \|\Phi \mathbf{y} - \Delta t \mathbf{f}(\mathbf{x}_0 + \Phi \mathbf{y}) - \Phi \hat{\mathbf{x}}_D^{k-1}\|$$

Corollary (Discrete-optimal smaller error bound)

If $\hat{\mathbf{x}}_D^{k-1} = \hat{\mathbf{x}}_G^{k-1}$, then $\varepsilon_D^k \leq \varepsilon_G^k$.

Discrete-optimal ROM has an interesting time-step dependence

Corollary (Backward Euler)

Define

- $\Delta \hat{\mathbf{x}}_D^j := \hat{\mathbf{x}}_D^j - \hat{\mathbf{x}}_D^{j-1}$ and
- $\Delta \bar{\mathbf{x}}^j$: full-space solution increment from $\hat{\mathbf{x}}_D^{j-1}$.

Then, the discrete-optimal error can also be bounded as

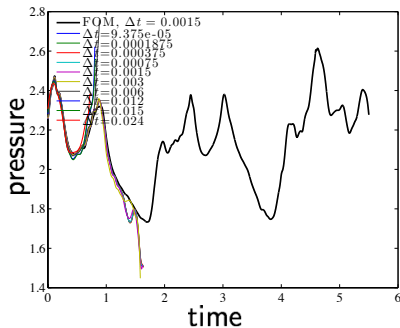
$$\|\delta \mathbf{x}_D^n\| \leq \Delta t(1 + \kappa \Delta t) \sum_{j=0}^{n-1} \frac{\mu^{n-j}}{(h)^{j+1}} \|\mathbf{f}(\hat{\mathbf{x}}_D^{j-1} + \Delta \bar{\mathbf{x}}^{n-j})\|$$

with $\mu^j := \|\Phi \Delta \hat{\mathbf{x}}_D^j - \Delta \bar{\mathbf{x}}^j\| / \|\Delta \bar{\mathbf{x}}^j\|$.

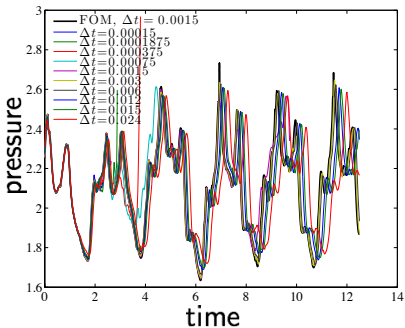
Effect of decreasing Δt :

- + The terms $\Delta t(1 + \kappa \Delta t)$ and $1/(h)^{j+1}$ decrease
- The number of total time instances n increases
- ? The term μ^{n-j} may **increase** or **decrease**, depending on the spectral content of the basis Φ

Galerkin and discrete-optimal responses for basis dimension $p = 204$



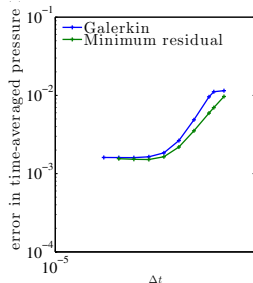
(a) Galerkin



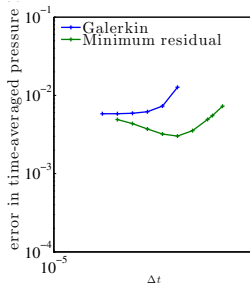
(b) Discrete optimal

- Galerkin ROMs unstable for long time intervals
(consistent with previous results [C. et al., 2013, C. et al., 2011a, C., 2011])
- + Discrete-optimal ROMs accurate and stable (most time steps)

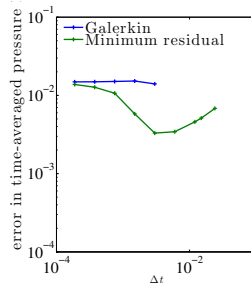
Discrete-optimal ROM: superior performance



(c) $0 \leq t \leq 0.55$



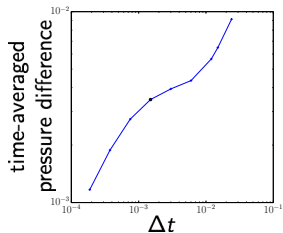
(d) $0 \leq t \leq 1.1$



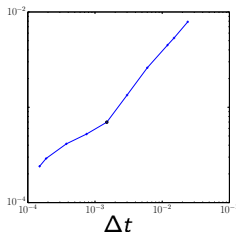
(e) $0 \leq t \leq 1.54$

- ✓ Discrete-optimal ROM yields a **smaller error** for all time intervals and time steps.

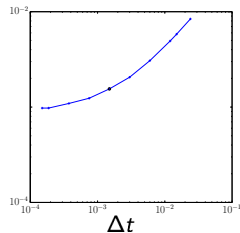
Limiting equivalence



(f) $p = 204$



(g) $p = 368$

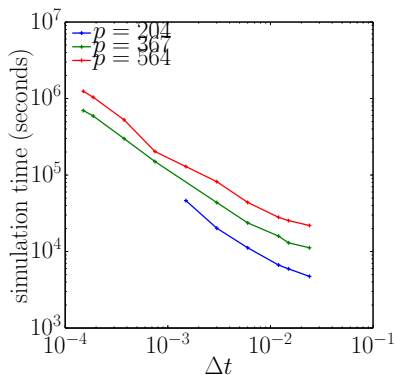
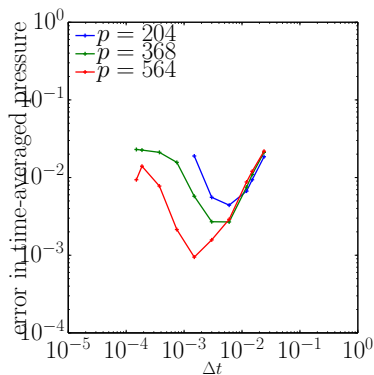


(h) $p = 564$

Galerkin/discrete-optimal difference in the stable Galerkin interval
 $0 \leq t \leq 1.1$.

- ✓ The discrete-optimal ROM converges to Galerkin as $\Delta t \rightarrow 0$.

Discrete-optimal performance ($t \leq 12.5$ sec)



✓ An intermediate Δt produces the **lowest error** and **better speedup**.

$p = 564$ case:

- $\Delta t = 1.875 \times 10^{-4}$ sec: relative error = **1.40%**, time = **289 hrs**
- $\Delta t = 1.5 \times 10^{-3}$ sec: relative error = **0.095%**, time = **35.8 hrs**

Summary: Improve projection technique

- Discrete optimality outperforms continuous optimality (Galerkin) in practice
- Equivalence conditions
 - 1 Limit of $\Delta t \rightarrow 0$
 - 2 Explicit schemes
 - 3 Positive definite residual Jacobians
- Discrete-time error bounds
 - Discrete-optimal ROM yields smaller error bound than Galerkin
 - Ambiguous role of time step Δt
- Numerical experiments
 - Discrete-optimal ROM yields a smaller error than Galerkin
 - Equivalent as $\Delta t \rightarrow 0$
 - Error minimized for intermediate Δt

My research goal

Nonlinear model-reduction methods that are
accurate, low cost, certified, and reliable.

+ Accuracy

- Improve projection technique [C. et al., 2011a, C. et al., 2015a]
- Preserve problem structure [C. et al., 2012, C. et al., 2015c]

+ Low cost

- Sample-mesh approach [C. et al., 2011b, C. et al., 2013]
- Leverage time-domain data [C. et al., 2015b]

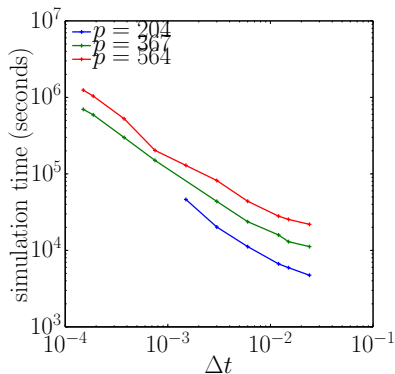
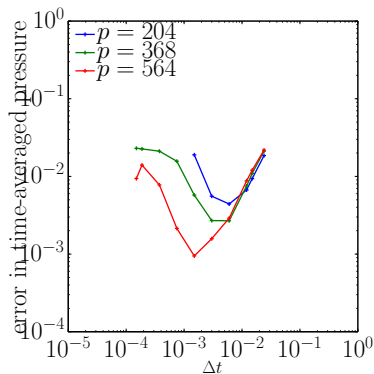
+ Certification

- Error bounds [C. et al., 2015a]
- Statistical error modeling [Drohmman and C., 2015]

+ Reliability

- *A posteriori* h -refinement [C., 2015]

Discrete-optimal performance ($t \leq 2.5$ sec)



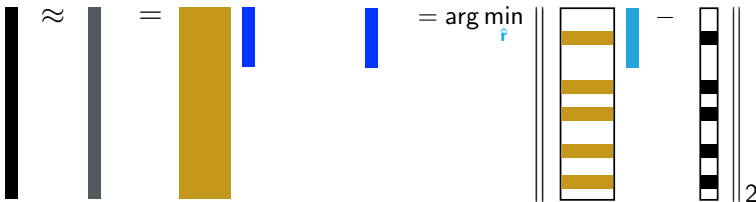
- + Always sub-3% errors
- More expensive than the FOM
 - FOM simulation: 1 hour, 48 CPU
 - Discrete-optimal ROM simulation (fastest): 1.3 hours, 48 CPU

Hyper-reduction via Gappy POD [Everson and Sirovich, 1995]

$$\hat{\mathbf{x}}^n = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \|\mathbf{A} \mathbf{r}^n(\Phi \hat{\mathbf{z}})\|_2^2.$$

Can we select \mathbf{A} to make this inexpensive?

$$1. \mathbf{r}^n(\mathbf{x}) \approx \tilde{\mathbf{r}}^n(\mathbf{x}) = \Phi_R \hat{\mathbf{r}}^n(\mathbf{x}) \quad 2. \hat{\mathbf{r}}^n(\mathbf{x}) = \arg \min_{\hat{\mathbf{r}}} \|\mathbf{P} \Phi_R \hat{\mathbf{r}} - \mathbf{P} \mathbf{r}^n(\mathbf{x})\|_2$$



$$\begin{aligned} \hat{\mathbf{x}}^n &= \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \|\tilde{\mathbf{r}}^n(\Phi \hat{\mathbf{z}})\|_2^2 = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \|\Phi_R \hat{\mathbf{r}}^n(\Phi \hat{\mathbf{z}})\|_2^2 = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \|\hat{\mathbf{r}}^n(\Phi \hat{\mathbf{z}})\|_2^2 \\ &= \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \underbrace{\|(\mathbf{P} \Phi_R)^+ \mathbf{P} \mathbf{r}^n(\Phi \hat{\mathbf{z}})\|_2^2}_{\mathbf{A}}. \end{aligned}$$

+ GNAT: $\mathbf{A} = (\mathbf{P} \Phi_R)^+ \mathbf{P}$ leads to low-cost

■ *Offline*: Construct Φ_R (POD) and \mathbf{P} (greedy method)

Sample mesh: HPC implementation

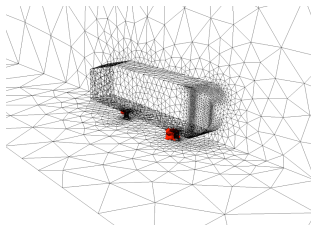
$$\hat{\mathbf{x}}^n = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \| (\mathbf{P}\Phi_R)^+ \mathbf{P}\mathbf{r}^n (\Phi\hat{\mathbf{z}}) \|_2^2$$

■ *Goals:*

- + Reuse existing computational-mechanics codes
- + Minimize number of required computing cores
- + Scalability

■ *Key:* GNAT samples only a few entries of the residual $\mathbf{P}\mathbf{r}^n$

■ *Idea:* Extract minimal subset of the mesh



Postprocessing mesh: HPC implementation

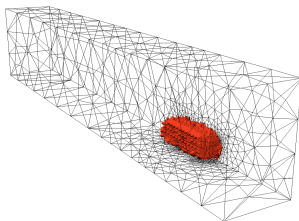
inputs $\mu \rightarrow$ reduced-order model \rightarrow outputs \mathbf{y}

- *Observations:*

- + Outputs \mathbf{y} are often defined **locally** in space (e.g., lift)
- Outputs **may not be computable** on sample mesh

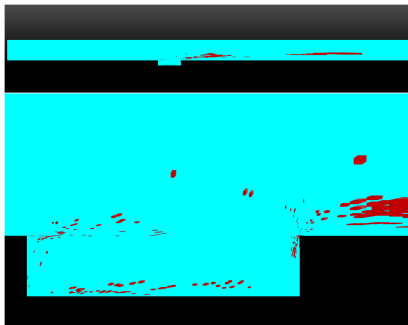
- *Output computation:*

- 1 Read reduced state $\hat{\mathbf{x}}^n$, $n = 1, \dots, M$ computed by GNAT
- 2 Assemble solution on minimal **output-computation mesh**
- 3 Compute outputs



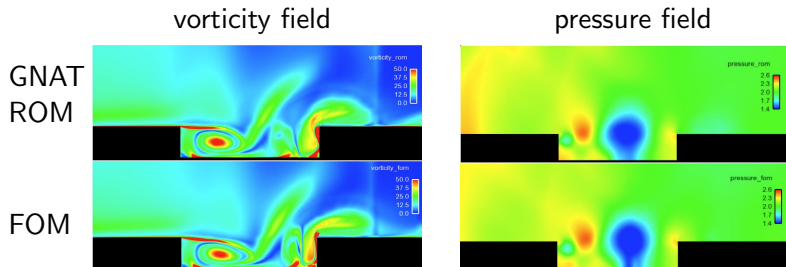
Cavity-flow problem: GNAT

$$\hat{\mathbf{x}}^n = \arg \min_{\hat{\mathbf{z}} \in \mathbb{R}^p} \| (\mathbf{P}\Phi_R)^+ \mathbf{P} \mathbf{r}^n (\Phi \hat{\mathbf{z}}) \|_2^2$$



- Sample mesh: 4.1% nodes, 3.0% cells
- + Small problem size: can run on many fewer cores

GNAT performance ($t \leq 12.5$ sec)



+ $< 1\%$ error in time-averaged drag

+ 229x CPU-hour savings

- FOM: 5 hour x 48 CPU
- GNAT ROM: 32 min x 2 CPU

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- Preserve problem structure [C. et al., 2012, C. et al., 2015c]

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- Leverage time-domain data [C. et al., 2015b]

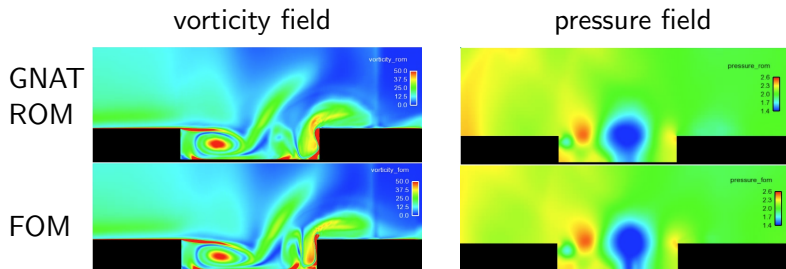
+ Certification

- Error bounds [C. et al., 2015a]
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- *A posteriori* h -refinement [C., 2015]

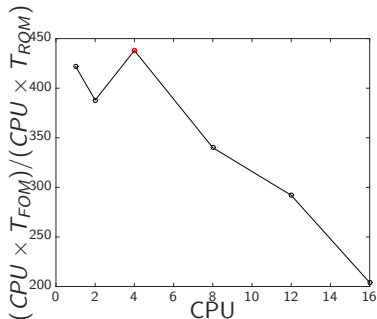
GNAT performance



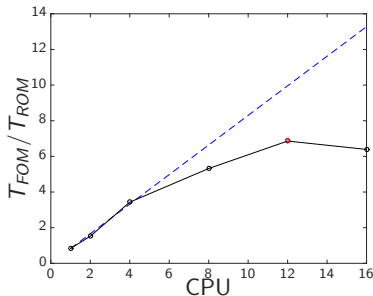
- FOM: 5 hour x 48 CPU
- GNAT ROM: 32 min x 2 CPU
- + 229x CPU-hour savings. Good for many query.
- 9.4x walltime savings. Bad for real time.

Why?

GNAT: strong scaling (Ahmed body) [C., 2011]



(e) CPU-hour savings



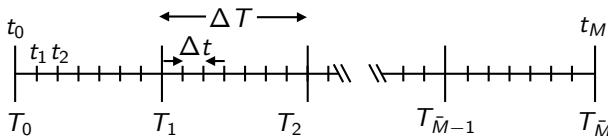
(f) Walltime savings

- + Significant CPU-hour savings (max: 438 for 4 CPU)
- Modest walltime savings (max: 7 for 12 CPU)

Spatial parallelism is quickly saturated!

Time-parallel algorithms [Lions et al., 2001a, Farhat and Chandesris, 2003]

Goal: expose more parallelism to reduce walltime



- Fine propagator: time step Δt

$$\mathcal{F}(\mathbf{x}; \tau_1, \tau_2)$$

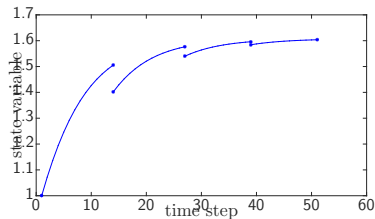
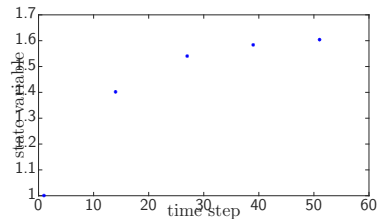
- Coarse propagator: time step ΔT

$$\mathcal{G}(\mathbf{x}; \tau_1, \tau_2)$$

- Parareal iteration k (sequential and parallel steps):

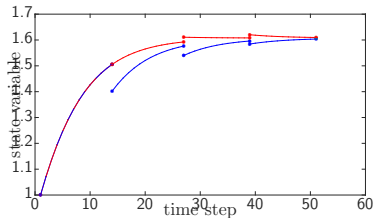
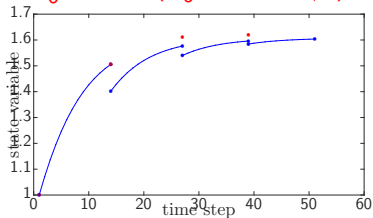
$$\mathbf{x}_{k+1}^{m+1} = \mathcal{G}(\mathbf{x}_{k+1}^m; T_m, T_{m+1}) + \mathcal{F}(\mathbf{x}_k^m; T_m, T_{m+1}) - \mathcal{G}(\mathbf{x}_k^m; T_m, T_{m+1})$$

Illustration: sequential and parallel steps



$$\mathbf{x}_0^{m+1} = \mathcal{G}(\mathbf{x}_0^m; T_m, T_{m+1})$$

$$\mathcal{F}(\mathbf{x}_0^m; T_m, T_{m+1})$$



$$\mathbf{x}_1^{m+1} = \mathcal{F}(\mathbf{x}_0^m; T_m, T_{m+1}) + \mathcal{G}(\mathbf{x}_1^m; T_m, T_{m+1}) - \mathcal{G}(\mathbf{x}_0^m; T_m, T_{m+1})$$

$$\mathcal{F}(\mathbf{x}_1^m; T_m, T_{m+1})$$

Coarse propagator

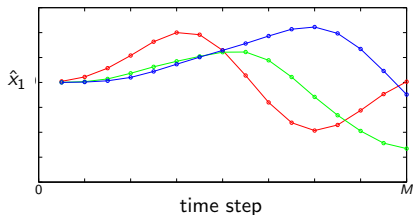
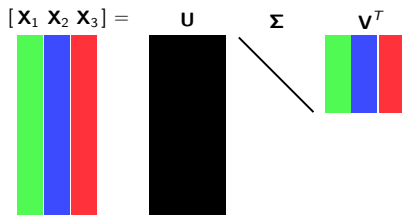
Critical: coarse propagator should be **fast**, **accurate**, **stable**

■ Existing coarse propagators

- Same integrator [Lions et al., 2001b, Bal and Maday, 2002]
- Coarse spatial discretization
[Fischer et al., 2005, Farhat et al., 2006, Cortial and Farhat, 2009]
- Simplified physics model [Baffico et al., 2002, Maday and Turinici, 2003, Blouza et al., 2011, Engblom, 2009, Maday, 2007]
- Relaxed solver tolerance [Guibert and Tromeur-Dervout, 2007]
- Reduced-order model (on the fly) [Farhat et al., 2006, Cortial and Farhat, 2009, Ruprecht and Krause, 2012, Chen et al., 2014]

Can we leverage offline data to improve the coarse propagator?

Revisit the SVD



First row of \mathbf{V}^T

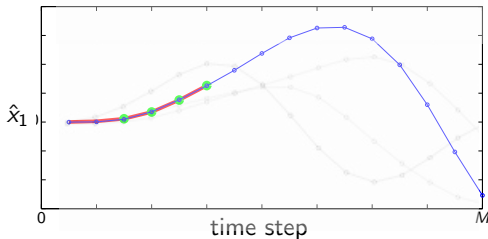
j th row of \mathbf{V}^T contains a basis for time evolution of \hat{x}_j

- Construct Ξ_j : basis for time evolution of \hat{x}_j

$$\Xi_j := \begin{bmatrix} \xi_j^1 & \cdots & \xi_j^{n_{\text{train}}} \end{bmatrix}, \quad \xi_j^i := [v_{M(i-1)+1,j} \ \cdots \ v_{Mi,j}]^T$$

Previous method [C. et al., 2015b]

- 1 compute forecast by gappy POD in time domain:

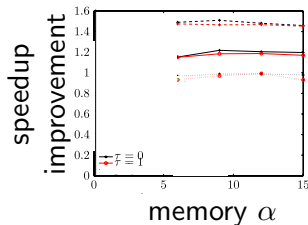
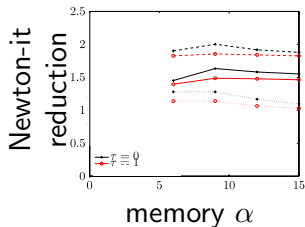


\hat{x}_1 so far; memory $\alpha = 4$; forecast; temporal basis

$$\mathbf{z}_j = \arg \min_{\mathbf{z} \in \mathbb{R}^{a_j}} \|\mathbf{Z}(m-1, \alpha) \Xi_j \mathbf{z} - \mathbf{Z}(m-1, \alpha) g(\hat{x}_j)\|_2$$

- Time sampling: $\mathbf{Z}(k, \beta) := [\mathbf{e}_{k-\beta} \cdots \mathbf{e}_k]^T$
 - Time unrolling: $g(\hat{x}_j) : \hat{x}_j \mapsto [\hat{x}_j(t_0) \cdots \hat{x}_j(t_M)]^T$
- 2 use $\mathbf{e}_m^T \Xi_j \mathbf{z}_j$ as *initial guess* for $\hat{x}_j(t_m)$ in Newton solver

Previous results: structural dynamics [C. et al., 2015b]

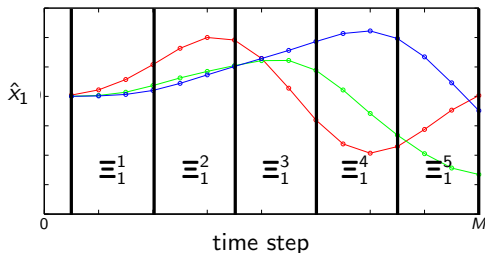


- + Newton iterations reduced by up to $\sim 2\times$
- + Speedup improved by up to $\sim 1.5\times$
- + No accuracy loss
- + Applicable to any nonlinear ROM
- Insufficient for real-time computation

Can we apply the same idea for the coarse propagator?

Coarse propagator for coordinate j and time interval m

- **Offline:** Construct time-evolution basis Ξ_j^m



- **Online:** Coarse propagator \mathcal{G}_j^m defined via forecasting:

- 1 Compute α time steps with fine propagator
- 2 Compute forecast via gappy POD
- 3 Select last timestep of forecast

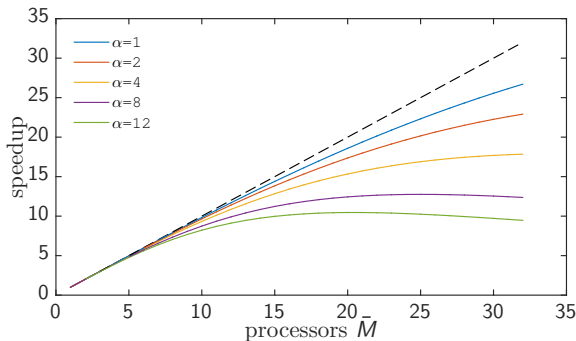
$$\mathcal{G}_j^m : (\hat{\mathbf{x}}_j; T_m, T_{m+1}) \mapsto \mathbf{e}_{\Delta T / \Delta t}^T \Xi_j^m [\mathbf{Z}(\alpha + 1, \alpha) \Xi_j^m]^+ \begin{bmatrix} \mathcal{F}(\hat{\mathbf{x}}_j; T_m, T_m + \Delta t) \\ \vdots \\ \mathcal{F}(\hat{\mathbf{x}}_j; T_m, T_m + \Delta t \alpha) \end{bmatrix}$$

Ideal-conditions speedup

Theorem

If $g(\hat{x}_j) \in \text{range}(\Xi_j)$, $j = 1, \dots, p$, then the proposed method converges in one parareal iteration and realizes a theoretical speedup of

$$\frac{\bar{M}}{\bar{M}(\bar{M} - 1)\alpha/M + 1}.$$



Ideal-conditions speedup for $M = 5000$

Ideal-conditions speedup with initial guesses

Corollary

If \mathbf{f} is nonlinear, $g(\hat{x}_j) \in \text{range}(\Xi_j)$, $j = 1, \dots, p$, and the forecasting method also provides Newton-solver initial guesses, then

- 1** *the method converges in **one parareal iteration**, and*
- 2** *only α nonlinear systems of algebraic equations are solved in each time interval.*

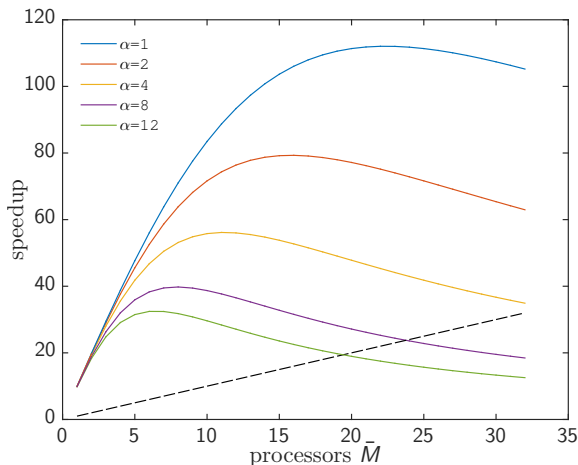
The method then realizes a theoretical speedup of

$$\frac{M}{(\bar{M}\alpha) + (M/\bar{M} - \alpha)\tau_r}$$

relative to the sequential algorithm without forecasting. Here,

$$\tau_r = \frac{\text{residual computation time}}{\text{nonlinear-system solution time}}.$$

Ideal-conditions speedup with initial-guesses



Ideal-condition speedup for $M = 5000$, $\tau_r = 1/10$

Significant speedups possible by leveraging time-domain data!

Theorem

If the fine propagator is stable, i.e.,

$$\|\mathcal{F}(\mathbf{x}; \tau_1, \tau_2)\| \leq (1 + C_{\mathcal{F}} \Delta T) \|\mathbf{x}\|,$$

then the proposed method is also stable, i.e.,

$$\|\hat{\mathbf{x}}_{k+1}^m\| \leq C_m \exp(C_F m \Delta T) \|\hat{\mathbf{x}}^0\|.$$

- $C_m := \sum_{k=1}^m \binom{k}{m} \beta_k \gamma^m \alpha^k (\Delta T / \Delta t)^{m-k}$
- $\beta_k := \exp(-C_{\mathcal{F}} k (\Delta T - \Delta t \alpha)) \leq 1$
- $\gamma := \max(\max_{m,j} 1 / \|\mathbf{Z}(\alpha+1, \alpha) \Xi_j^m\|, 1 / \sigma_{\min}(\mathbf{Z}(\alpha+1, \alpha) \Xi_j^m))$

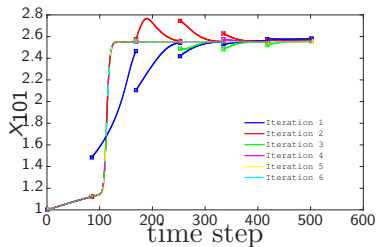
Example: inviscid Burgers equation [Rewiński, 2003]

$$\begin{aligned}\frac{\partial u(x, \tau)}{\partial \tau} + \frac{1}{2} \frac{\partial (u^2(x, \tau))}{\partial x} &= 0.02e^{\mu_2 x} \\ u(0, \tau) &= \mu_1, \quad \forall \tau \in [0, 25] \\ u(x, 0) &= 1, \quad \forall x \in [0, 100],\end{aligned}$$

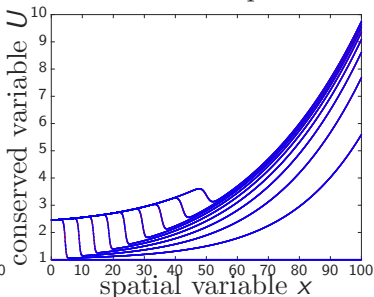
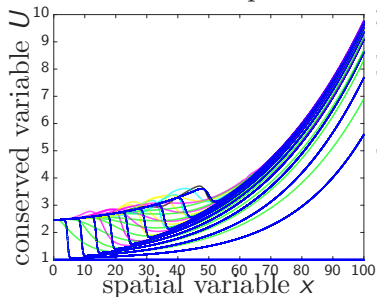
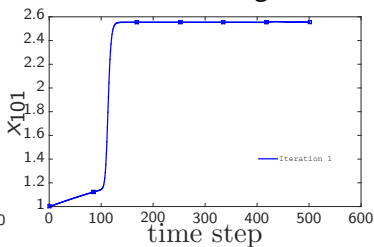
- Discretization: Godunov's scheme
- $(\mu_1, \mu_2) \in [2.5, 3.5] \times [0.02, 0.075]$
- $\Delta t = 0.1$, $M = 250$ fine time steps
- FOM: $N = 500$ degrees of freedom
- ROM: LSPG [C. et al., 2011a] with POD basis dimension $p = 100$
- $n_{\text{train}} = 4$ training points (LHS sampling); random online point
- Two coarse propagators: **Backward Euler** and **forecasting**

Forecasting outperforms backward Euler

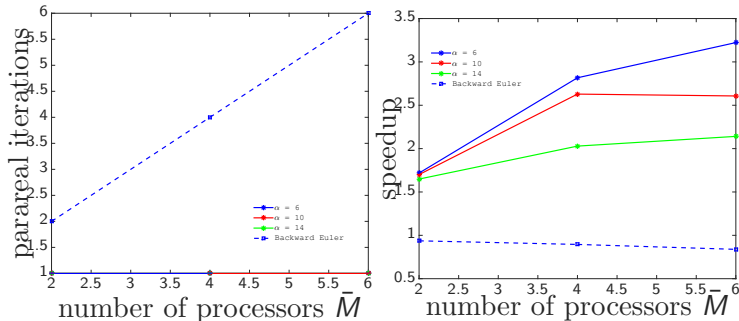
Backward Euler



Forecasting



Parareal performance



- + *Forecasting*: minimum possible iterations
- *Backward Euler*: maximum possible iterations

More parallelism successfully exposed!

Summary: Leverage time-domain data

Use temporal data to reduce ROM simulation time

- **offline:** time-evolution bases from right singular vectors
- **online:** use as coarse propagator
 - 1 compute α time steps with fine propagator
 - 2 use gappy POD to forecast
- + theory: excellent speedup and stability
- + ideal parareal performance observed
- + significant improvement over Backward Euler
- + no additional error introduced
- + generally applicable

Opportunities at Sandia National Laboratories, Livermore

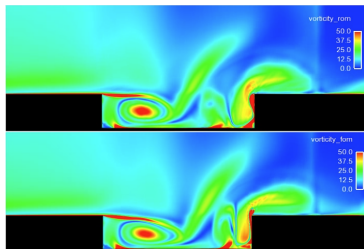
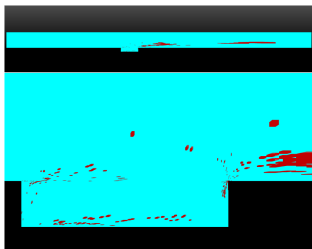
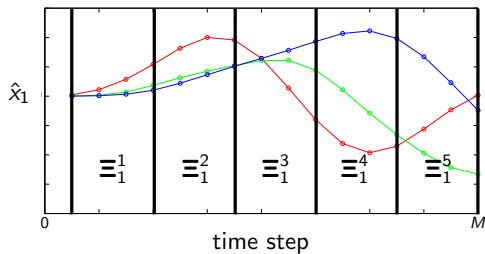


We are hiring summer interns, postdocs, and staff

- Model reduction
- Uncertainty quantification
- Machine learning
- High-performance computing
- Cybersecurity
- Data analytics

Email me if interested: ktcarlb@sandia.gov

Questions?



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- Improve projection technique [C. et al., 2011a, C. et al., 2015a]
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- Sample-mesh approach [C. et al., 2011b, C. et al., 2013]
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+ Certification

- Error bounds [C. et al., 2015a]
- Statistical error modeling [Drohmman and C., 2015]

+ Reliability

- *A posteriori* h -refinement [C., 2015]

Acknowledgments

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