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Nonlinear model reduction: discrete optimality and time parallelism

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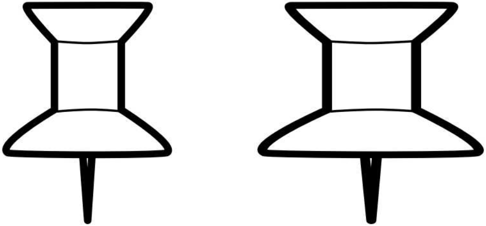
Computational barrier at Sandia



- 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

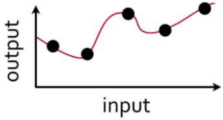
Objective: break barrier via nonlinear model reduction

Surrogate modeling

inputs $\boldsymbol{\mu}$ → full-order model → outputs $\mathbf{y}$

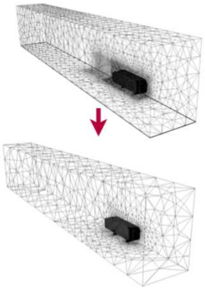
inputs $\boldsymbol{\mu}$ → surrogate model → outputs $\mathbf{y}_s$

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: 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, Or and Speyer, 2010, Ma et al., 2011]
  - 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 [Drohmann and C., 2015]
- Reliability
  - *A posteriori h*-refinement [C., 2015]

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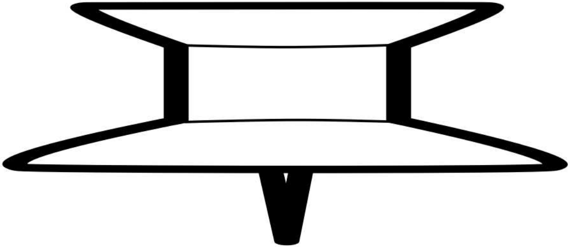
Collaborators: M. Barone (Sandia), H. Antil (GMU)

POD–Galerkin: offline data collection

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

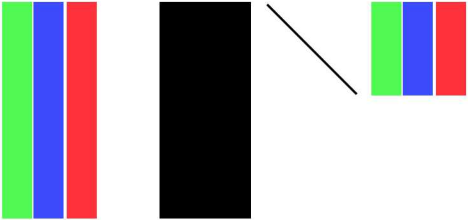
1 Collect 'snapshots' of the state



POD–Galerkin: offline data collection

2 Data compression

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

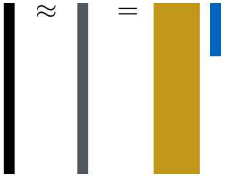


- Truncate: $\boldsymbol{\Phi} = [\boldsymbol{u}_1\ \cdots\ \boldsymbol{u}_p]$

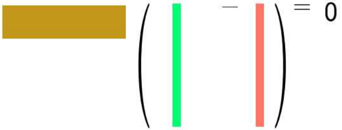
POD–Galerkin: online projection

Full-order model: $$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}; t, \boldsymbol{\mu}), \quad \boldsymbol{x}(0, \boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu})$$

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

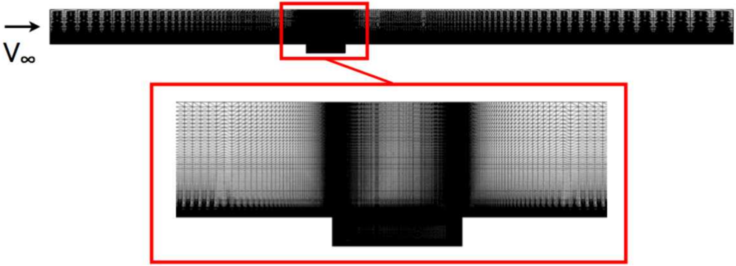


2 $\boldsymbol{\Phi}^T\left(\boldsymbol{f}(\tilde{\boldsymbol{x}}; t, \boldsymbol{\mu}) - \frac{d\tilde{\boldsymbol{x}}}{dt}\right) = 0$



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

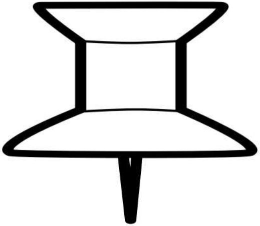
Cavity-flow problem. Collaborator: M. Barone (SNL)



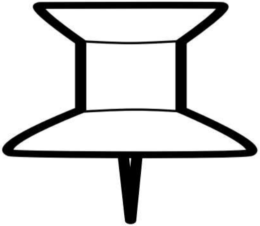
- Unsteady Navier–Stokes
- DES turbulence model
- 1.2 million degrees of freedom

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

Full-order model responses

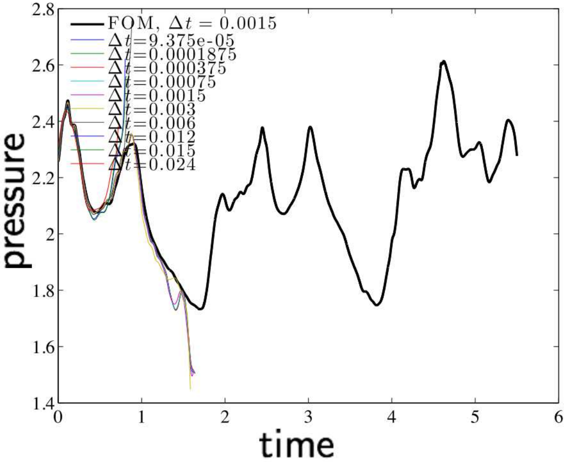


vorticity field



pressure field

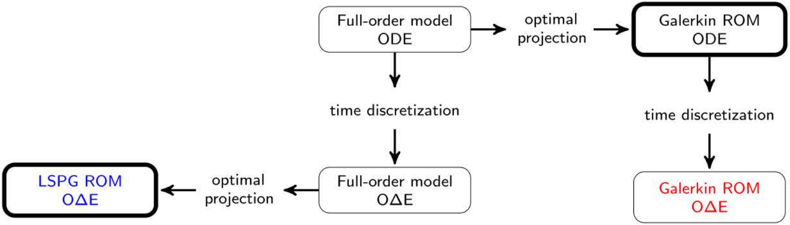
POD–Galerkin failure



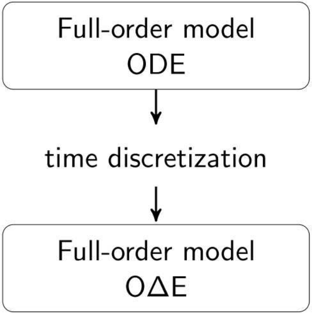
- Galerkin ROMs unstable

How to construct a ROM for nonlinear dynamical systems?

- Optimize then discretize? (Galerkin)
- Discretize then optimize? (Least-squares Petrov–Galerkin)



- Outstanding questions:
  1. Which notion of optimality is better in practice?
  2. Discrete-time error bounds?
  3. Time step selection?


Full-order model
ODE
time discretization
Full-order model
OΔE

Full-order model (FOM)

- ODE: time continuous

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

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

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

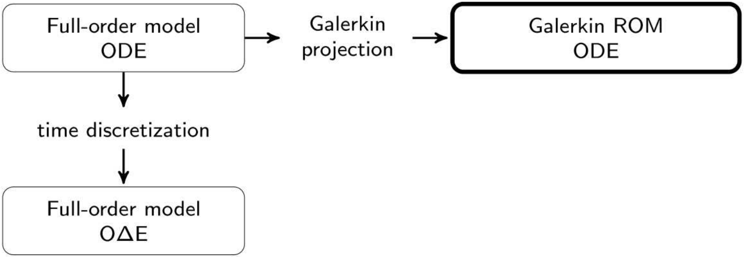
- OΔE, Runge–Kutta: $\boxed{\boldsymbol{r}_i^n(\boldsymbol{x}_1^n, \ldots, \boldsymbol{x}_s^n) = 0}$, $i = 1, \ldots, s$

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

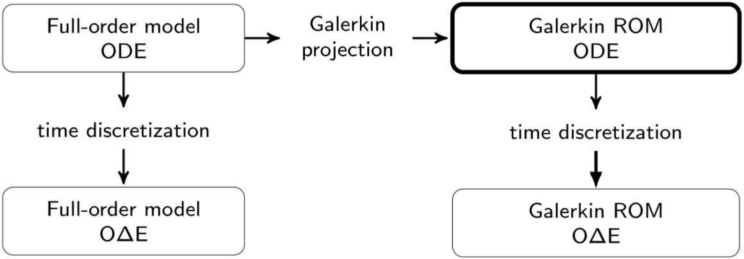
$$\boldsymbol{x}^n = \boldsymbol{x}^{n-1} + \Delta t \sum_{i=1}^{s} b_i \boldsymbol{x}_i^n \text{ (explicit state update)}$$

This talk focuses on linear multistep schemes.

Galerkin ROM: first optimize



Galerkin: first optimize, then discretize



Galerkin ROM

- ODE

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

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

Theorem (Galerkin ROM: continuous optimality)

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

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

- OΔE

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

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

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

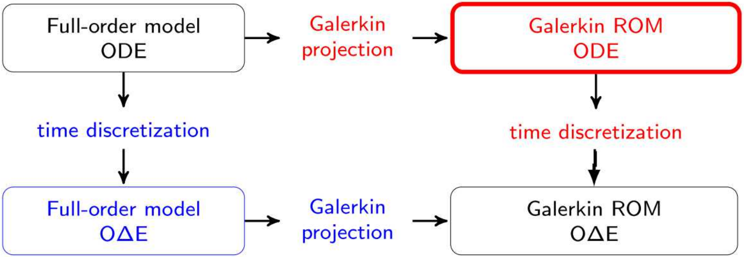
Can we fix this? Will doing so help?

Galerkin ROM: Commutativity

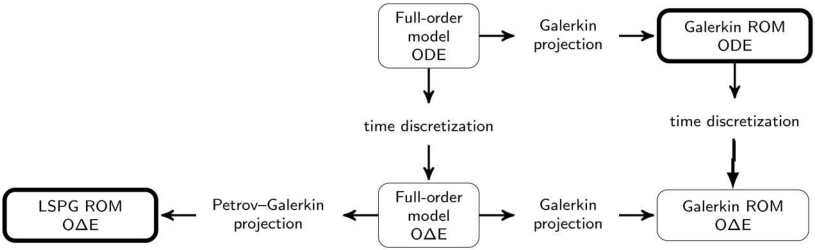
Theorem

Projection and time discretization are commutative for Galerkin ROMs:

$$\hat{\boldsymbol{r}}^n(\hat{\boldsymbol{x}}) = \boldsymbol{\Phi}^T \boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{x}})$$



LSPG ROM: first discretize, then optimize



LSPG ROM

- FOM OΔE

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

- LSPG ROM OΔE:

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

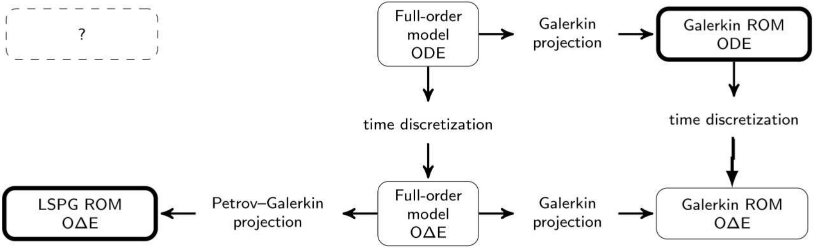
$$\Updownarrow$$

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

  - $\boldsymbol{A} = \boldsymbol{I}$: LSPG [LeGresley, 2006, Bui-Thanh et al., 2008, C. et al., 2011a]

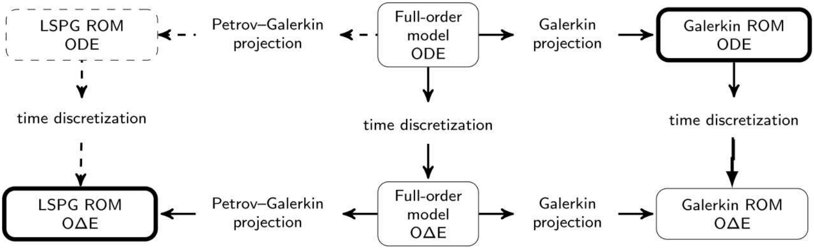
\+ Discrete solution is optimal

Does the LSPG ROM have a time-continuous representation?



Does the LSPG ROM have a time-continuous representation?

Sometimes.



LSPG ROM: continuous representation

Theorem

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

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

if

1. $\beta_j = 0$, $j \geq 1$ *(e.g., a single-step method),*
2. *the velocity* $\boldsymbol{f}$ *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: $$\boldsymbol{\Phi}^T \boldsymbol{r}^n (\boldsymbol{\Phi}\hat{\boldsymbol{x}}^n) = 0$$
- LSPG: $$\boldsymbol{\Psi}^n(\hat{\boldsymbol{x}}^n)^T \boldsymbol{r}^n (\boldsymbol{\Phi}\hat{\boldsymbol{x}}^n) = 0$$

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

Yes.

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

Theorem

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

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

Discrete-time error bound

Theorem

If the following conditions hold:

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

then

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

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

with

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

LSPG ROM yields a smaller error bound

Theorem (Backward Euler)

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

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

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

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

$$\varepsilon_L^k = \|\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^k - \Delta t \boldsymbol{f}\left(\boldsymbol{x}_0 + \boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^k\right) - \boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^{k-1}\| = \min_{\boldsymbol{y}} \|\boldsymbol{\Phi}\boldsymbol{y} - \Delta t \boldsymbol{f}\left(\boldsymbol{x}_0 + \boldsymbol{\Phi}\boldsymbol{y}\right) - \boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^{k-1}\|$$

Corollary (LSPG smaller error bound)

If $\hat{\boldsymbol{x}}_L^{k-1} = \hat{\boldsymbol{x}}_G^{k-1}$, *then* $\varepsilon_L^k \leq \varepsilon_G^k$.

LSPG ROM has an interesting time-step dependence

Corollary (Backward Euler)

Define

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

Then, the LSPG error can also be bounded as

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

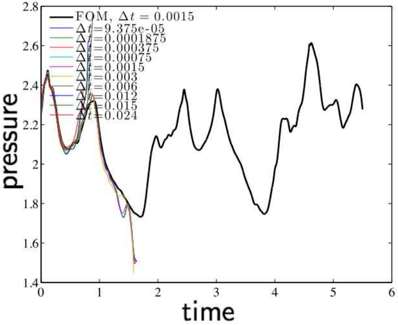
with $\mu^j := \|\boldsymbol{\Phi}\Delta\hat{\mathbf{x}}_L^j - \Delta\bar{\mathbf{x}}^j\|/\|\Delta\bar{\mathbf{x}}^j\|$.

Effect of decreasing Δt:

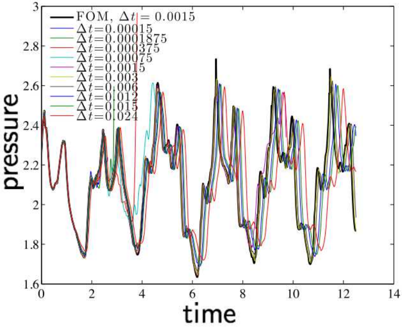
+ The terms $\Delta t(1+\kappa\Delta t)$ and $1/(h)^{j+1}$ decrease
- The number of total time instances n increases

? The term μ^{n-j} may increase or decrease, depending on the spectral content of the basis $\boldsymbol{\Phi}$

Galerkin and LSPG responses for basis dimension $p = 204$



(a) Galerkin

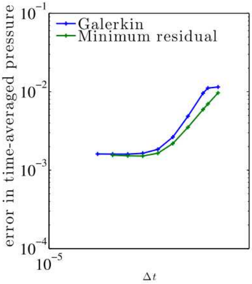


(b) LSPG

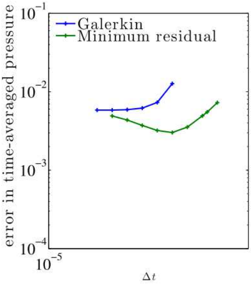
- Galerkin ROMs unstable for long time intervals

+ LSPG ROMs accurate and stable (most time steps)

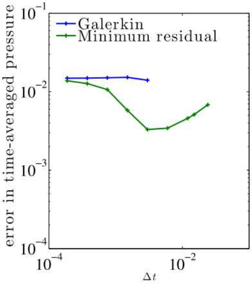
LSPG ROM: superior performance



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



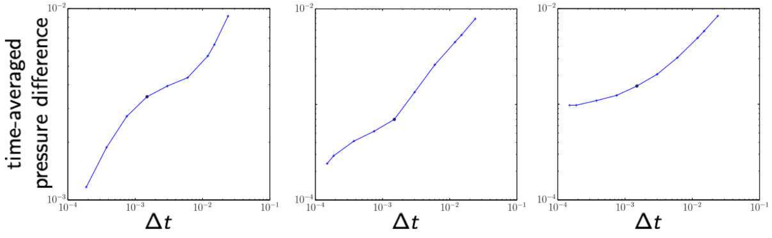
(d) $0 \leq t \leq 1.1$



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

✓ LSPG ROM yields a smaller error for all time intervals and time steps.

Limiting equivalence

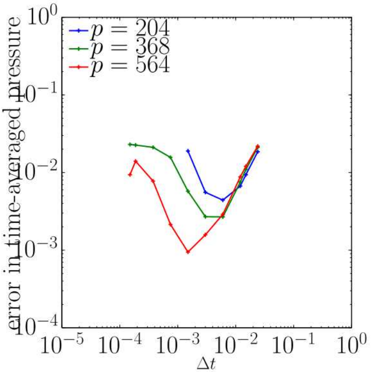


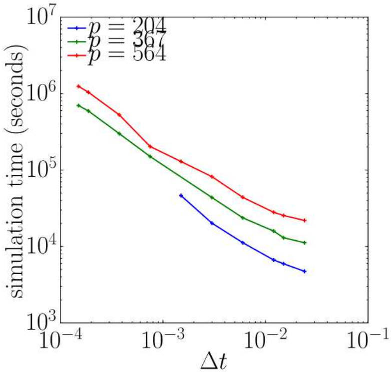
(f) $p = 204$ (g) $p = 368$ (h) $p = 564$

Galerkin/LSPG difference in the stable Galerkin interval $0 \leq t \leq 1.1$.

✓ The LSPG ROM converges to Galerkin as $\Delta t \to 0$.

LSPG 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

- *Galerkin*: projection and time-discretization are commutative
- *LSPG*: a continuous representation sometimes exists
- Equivalence conditions
  1. Limit of $\Delta t \rightarrow 0$
  2. Explicit schemes
  3. Positive definite residual Jacobians
- Discrete-time error bounds
  - LSPG ROM yields smaller error bound than Galerkin
  - Ambiguous role of time step Δt
- Numerical experiments
  - LSPG ROM yields a smaller error than Galerkin
  - Equivalent as $\Delta t \rightarrow 0$
  - Error minimized for intermediate Δt
- **Reference**: C., Barone, and Antil. Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction. *arXiv e-print*, (1504.03749), 2015.

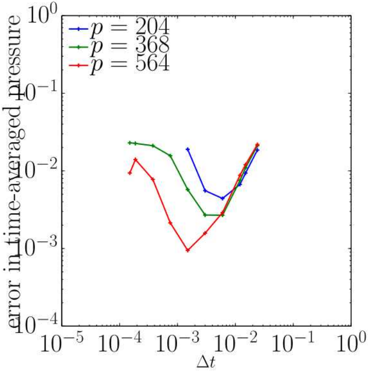
My research goal

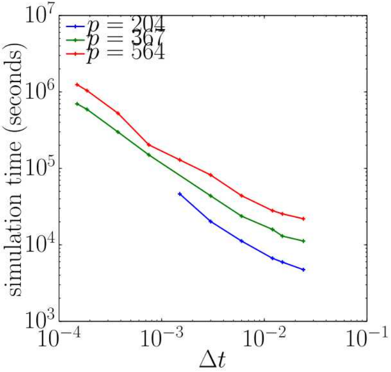
Nonlinear model-reduction methods that are
accurate, low cost, certified, and reliable.

+ 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 [Drohmann and C., 2015]
+ Reliability
  - *A posteriori h*-refinement [C., 2015]

Collaborators: C. Farhat, J. Cortial (Stanford)

LSPG performance ($t \leq 2.5$ sec)





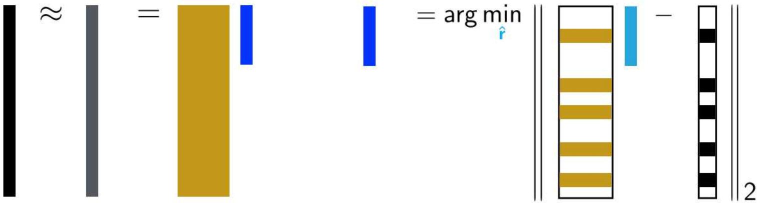
+ Always sub-3% errors
- More expensive than the FOM
  - FOM simulation: 1 hour, 48 CPU
  - LSPG ROM simulation (fastest): 1.3 hours, 48 CPU

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

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

Can we select $\boldsymbol{A}$ *to make this inexpensive?*

1. $\boldsymbol{r}^n(\boldsymbol{x}) \approx \tilde{\boldsymbol{r}}^n(\boldsymbol{x}) = \boldsymbol{\Phi}_R\hat{\boldsymbol{r}}^n(\boldsymbol{x})$
2. $\hat{\boldsymbol{r}}^n(\boldsymbol{x}) = \arg\min_{\hat{\boldsymbol{r}}} \|\boldsymbol{P}\boldsymbol{\Phi}_R\hat{\boldsymbol{r}} - \boldsymbol{P}\boldsymbol{r}^n(\boldsymbol{x})\|_2$



$$\hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\tilde{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2 = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\boldsymbol{\Phi}_R\hat{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2 = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\hat{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2$$

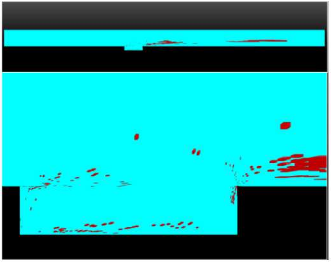
$$= \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\underbrace{(\boldsymbol{P}\boldsymbol{\Phi}_R)^+\boldsymbol{P}}_{\boldsymbol{A}}\boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2.$$

- \+ GNAT: $\boldsymbol{A} = (\boldsymbol{P}\boldsymbol{\Phi}_R)^+\boldsymbol{P}$ leads to low-cost
- *Offline*: Construct $\boldsymbol{\Phi}_R$ (POD) and $\boldsymbol{P}$ (greedy method)

Sample mesh: HPC implementation

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

- *Key*: GNAT samples only a few entries of the residual $\boldsymbol{P}\boldsymbol{r}^n$
- *Idea*: Extract minimal subset of the mesh



- Sample mesh: 4.1% nodes, 3.0% cells

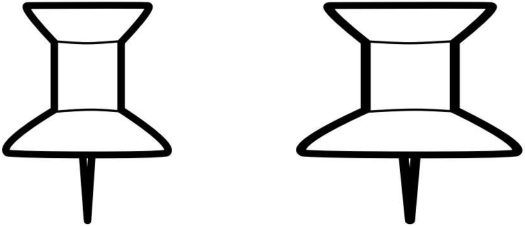
+ Small problem size: can run on many fewer cores

GNAT performance ($t \leq 12.5$ sec)

vorticity field pressure field

GNAT ROM

FOM



- $+$ $< 1\%$ 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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  - Improve projection technique [C. et al., 2011a, C. et al., 2015a]
  - Preserve problem structure [C. et al., 2012, C. et al., 2015c]
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  - Error bounds [C. et al., 2015a]
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+ Reliability
  - *A posteriori* *h*-refinement [C., 2015]

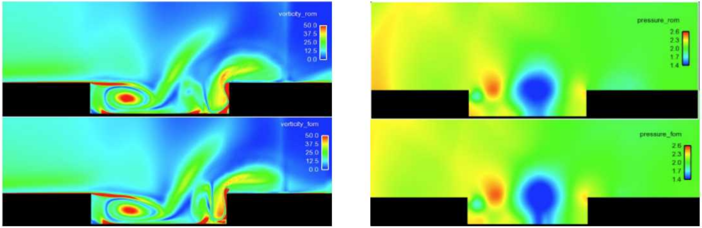
Collaborators: L. Brencher, B. Haasdonk, A. Barth (U Stuttgart)

GNAT performance

vorticity field | pressure field

GNAT ROM

FOM



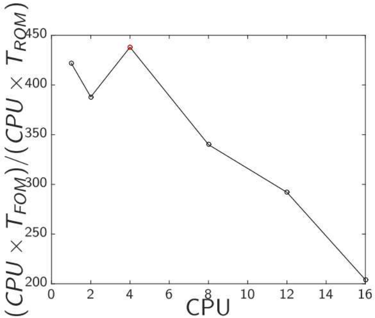
- FOM: 5 hour x 48 CPU
- GNAT ROM: 32 min x 2 CPU.

\+ 229x CPU-hour savings. Good for many query.

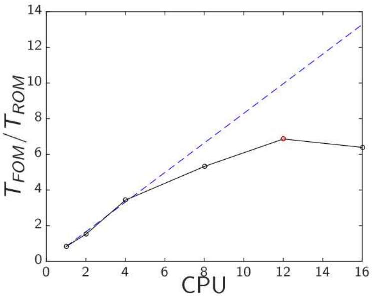
\- 9.4x walltime savings. Bad for real time.

Why?

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



(e) CPU-hour savings



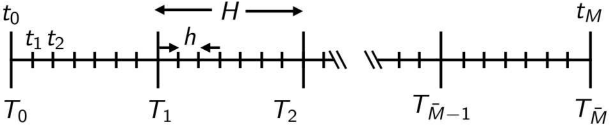
(f) Walltime savings

+ 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

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

- Coarse propagator: time step ΔT

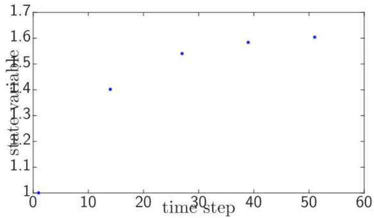
$$\mathcal{G}(\boldsymbol{x}; \tau_1, \tau_2)$$

- Parareal iteration k (sequential and parallel steps):

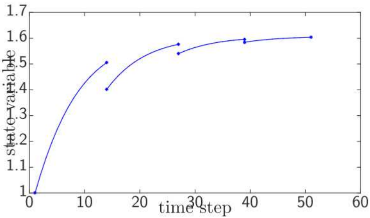
$$\boldsymbol{x}_{k+1}^{m+1} = \mathcal{G}(\boldsymbol{x}_{k+1}^{m}; T_m, T_{m+1}) + \mathcal{F}(\boldsymbol{x}_{k}^{m}; T_m, T_{m+1}) - \mathcal{G}(\boldsymbol{x}_{k}^{m}; T_m, T_{m+1})$$

- Interpretations [Gander and Vandewalle, 2007, Falgout et al., 2014]:
  - Deferred/residual-correction scheme $\mathcal{B}(\boldsymbol{x}_{k+1}) = \mathcal{B}(\boldsymbol{x}_k) - \mathcal{A}(\boldsymbol{x}_k)$
  - Multiple shooting method with FD Jacobian approximation
  - Two-level multigrid

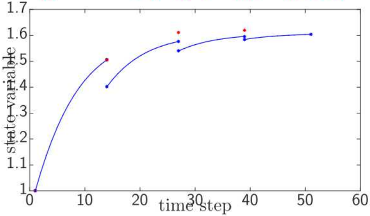
Parareal: sequential and parallel steps [Lions et al., 2001a]



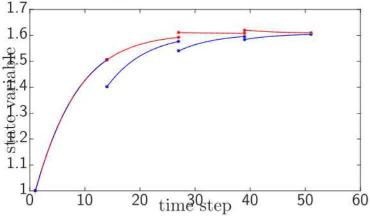
$$\mathbf{x}_0^{m+1} = \mathcal{G}(\mathbf{x}_0^m; T_m, T_{m+1})$$



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



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



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

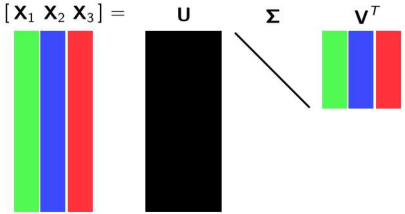
Coarse propagator

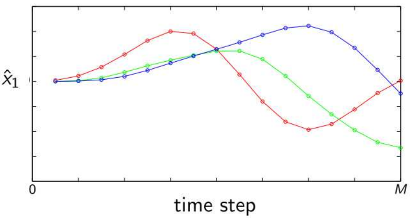
Critical: coarse propagator should be fast, accurate, stable

- 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]

ROM context: can we leverage offline data to improve the coarse propagator?

Revisit the SVD





First row of $\boldsymbol{V}^T$

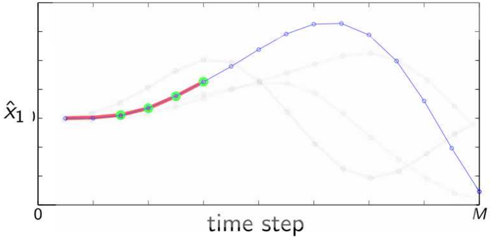
jth row of $\boldsymbol{V}^T$ contains a basis for time evolution of $\hat{x}_j$

- Construct $\boldsymbol{\Xi}_j$: **global time-evolution basis** for $\hat{x}_j$

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

First attempt [C. et al., 2015b]

1. compute **global forecast** by gappy POD in time domain:



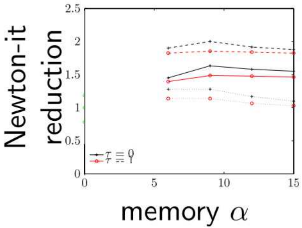
$\hat{\mathbf{x}}_1$ so far; memory $\alpha = 4$; forecast; temporal basis

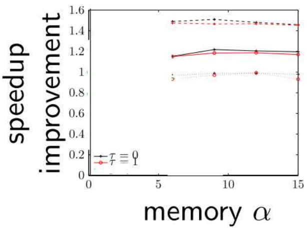
$$\boldsymbol{z}_j = \arg\min_{\boldsymbol{z} \in \boldsymbol{R}^{a_j}} \| \boldsymbol{Z}(m-1,\alpha)\boldsymbol{\Xi}_j \boldsymbol{z} - \boldsymbol{Z}(m-1,\alpha) g(\hat{x}_j) \|_2$$

- Time sampling: $\boldsymbol{Z}(k,\beta) := \left[\boldsymbol{e}_{k-\beta} \; \cdots \; \boldsymbol{e}_k\right]^T$
- Time unrolling: $g(\hat{x}_j) : \hat{x}_j \mapsto [\hat{x}_j(t_0) \; \cdots \; \hat{x}_j(t_M)]^T$

2. use $\boldsymbol{e}_m^T \boldsymbol{\Xi}_j \boldsymbol{z}_j$ as <u>initial guess</u> for $\hat{x}_j(t_m)$ in Newton solver

First attempt: structural dynamics [C. et al., 2015b]



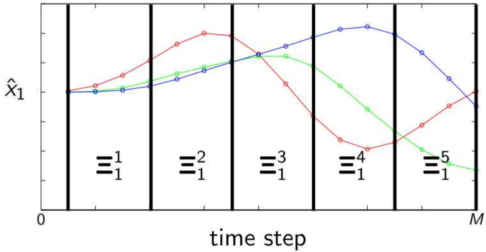


+ Newton iterations reduced by up to ∼2x
+ Speedup improved by up to ∼1.5x
+ No accuracy loss
+ Applicable to any nonlinear ROM
- Insufficient for real-time computation

Can we apply the same idea for the coarse propagator?

Coarse propagator via local forecasting

- **Offline**: Construct **local time-evolution basis** $\boldsymbol{\Xi}_j^m$



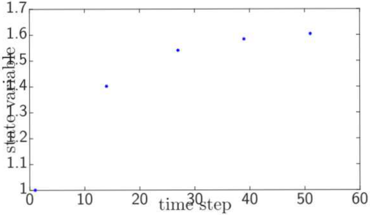
- **Online**: Coarse propagator $\mathcal{G}_j^m$ defined via forecasting:
  1. Compute α time steps with fine propagator
  2. Compute **local forecast** via gappy POD
  3. Select last timestep of **local forecast**

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

Initial seed

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

How to compute initial seed $\mathbf{x}_0^m$, $m = 0, \ldots, \bar{M}$*?*



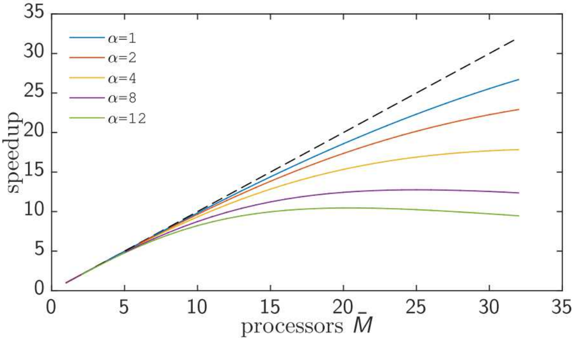
1. Typical time integrator
2. Local forecast
3. Global forecast

Ideal-conditions speedup

Theorem

If $g(\hat{x}_j) \in \mathrm{range}(\boldsymbol{\Xi}_j)$, $j = 1, \ldots, p$, then the proposed method converges in one parareal iteration and realizes a 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, $g(\hat{x}_j) \in \mathrm{range}(\boldsymbol{\Xi}_j)$, $\quad j = 1, \ldots, p$, 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.*

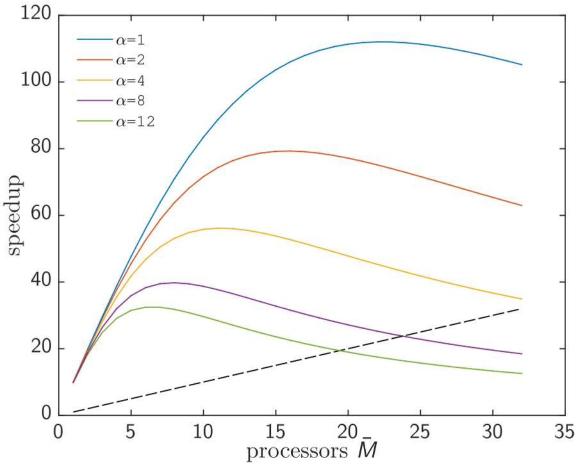
The method then realizes a theoretical speedup of

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

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!

Stability

Theorem

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

$$\|\mathcal{F}(\boldsymbol{x};\tau,\tau+\Delta T)\| \leq (1+C_{\mathcal{F}}\Delta T)\|\boldsymbol{x}\|, \quad \forall 0 \leq \tau \leq \tau+\Delta T$$

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

$$\|\hat{\boldsymbol{x}}_{k+1}^{m}\| \leq C_m \exp(C_{\mathcal{F}} m \Delta T)\|\hat{\boldsymbol{x}}^0\|.$$

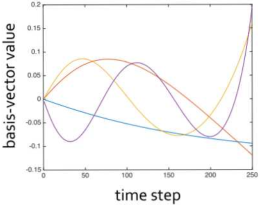
- $C_m := \sum_{k=1}^{m} \binom{k}{m} \beta_k \gamma^m \alpha^k (\Delta T/\Delta t)^{m-k}$
- $\beta_k := \exp(-C_{\mathcal{F}} k(\Delta T - \Delta t \alpha)) \leq 1$
- $\gamma := \max(\max_{m,j} 1/\|\boldsymbol{Z}(\alpha+1,\alpha)\boldsymbol{\Xi}_j^m\|, 1/\sigma_{\min}(\boldsymbol{Z}(\alpha+1,\alpha)\boldsymbol{\Xi}_j^m))$

Example: inviscid Burgers equation [Rewienski, 2003]

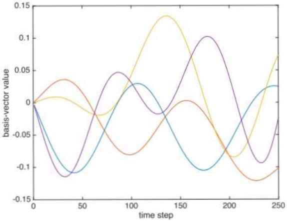
$$\frac{\partial u(x,\tau)}{\partial \tau} + \frac{1}{2}\frac{\partial\left(u^2(x,\tau)\right)}{\partial x} = 0.02e^{\mu_2 x}$$
$$u(0,\tau) = \mu_1,\ \forall \tau \in [0,25]$$
$$u(x,0) = 1,\ \forall x \in [0,100],$$

- Discretization: Godunov's scheme
- $(\mu_1, \mu_2) \in [2.5, 3.5] \times [0.02, 0.03]$
- $\Delta t = 0.1$, $M = 250$ fine time steps
- FOM: $N = 500$ degrees of freedom
- ROM: LSPG [C. et al., 2011a], POD basis dimension $p = 100$
- $n_{\text{train}} = 4$ training points (LHS sampling); random online point
- **2 coarse propagators**: Backward Euler and local forecast
- **3 initial seeds**: Backward Euler, local forecast, global forecast

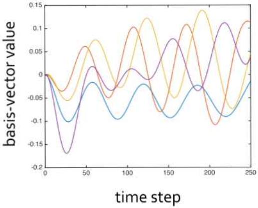
Global temporal bases



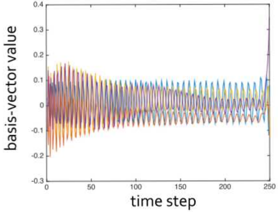
(a) coordinate 1



(b) coordinate 5



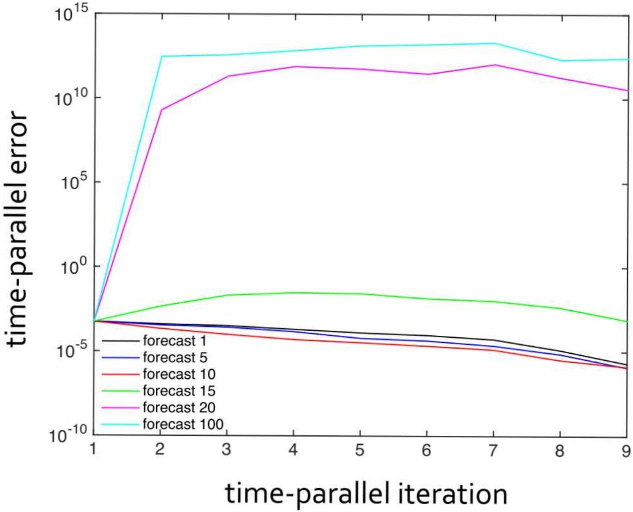
(c) coordinate 10



(d) coordinate 100

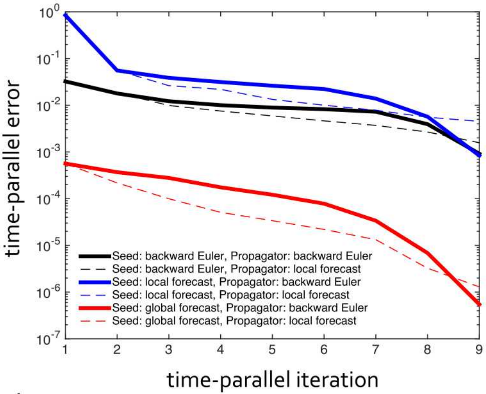
Higher-index generalized coordinates not ‘forecastable’

Forecasting 'high-frequency' coordinates is dangerous



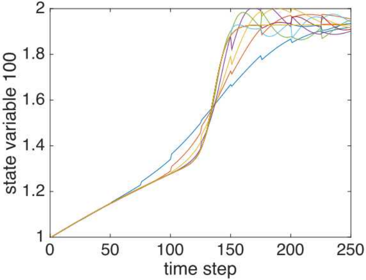
Proceed by forecasting the first 10 coordinates

Comparison: Initial seed and coarse propagator

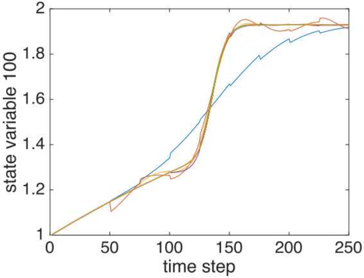


- Initial seed:
  - \+ best performance: global forecast
  - \- worst performance: local forecast (error accumulation)
- Coarse propagator:
  - \+ local forecast outperforms backward Euler

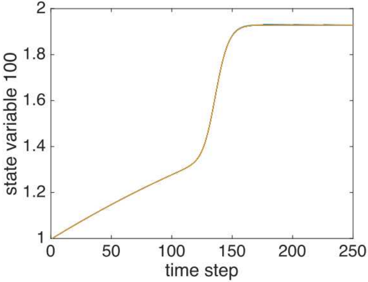
Forecasting improves improves initial seed and coarse propagator!



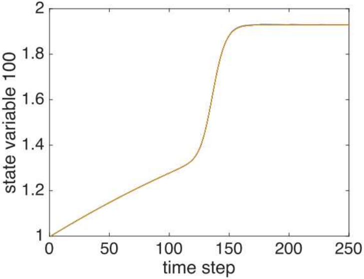
(e) Seed: Euler, Prop: Euler



(f) Seed: Euler, Prop: local forecast

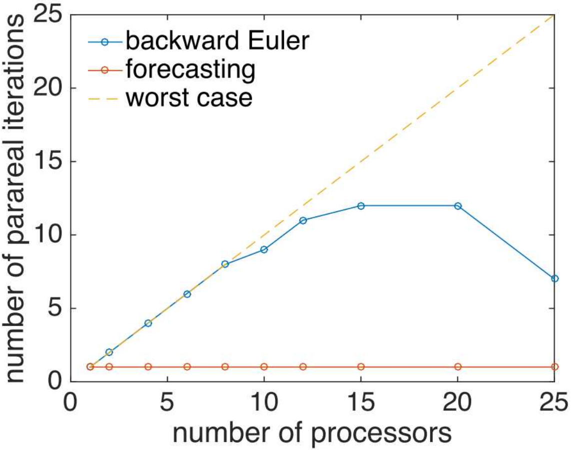


(g) Seed: glob forecast, Prop: Euler



(h) Seed: glob forecast, Prop: loc fore-

Parareal performance



+ *Forecasting*: minimum possible iterations
- *Backward Euler*: often close to worst-case performance

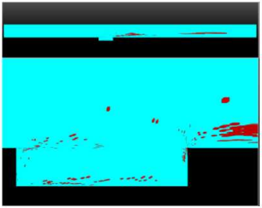
Conclusions

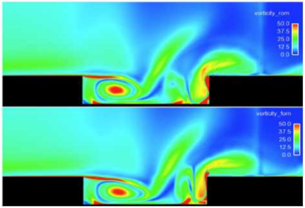
Use temporal data to reduce ROM simulation time

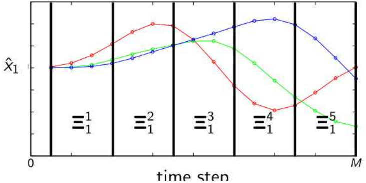
- **offline**: time-evolution bases from right singular vectors
- **online**:
  1. global forecast as initial seed
  2. local forecast as coarse propagator
- \+ theory: excellent speedup and stability
- \+ ideal parareal performance observed
- \+ significant improvement over Backward Euler
- \+ no additional error introduced
- **References**:

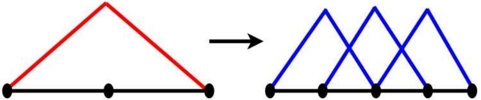
  - K. Carlberg, L. Brencher, B. Haasdonk, and A. Barth. "Data-driven time parallelism with application to reduced-order models," *in preparation*.
  - K. Carlberg, J. Ray, and B. van Bloemen Waanders. "Decreasing the temporal complexity for nonlinear, implicit reduced-order models by forecasting," CMAME, Vol. 289, p. 79–103 (2015).

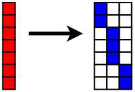
Questions?











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