Discrete-optimal projection in nonlinear model reduction

SAND2015-9410C

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Workshop on Reduced Basis, POD and PGD Model Reduction Techniques
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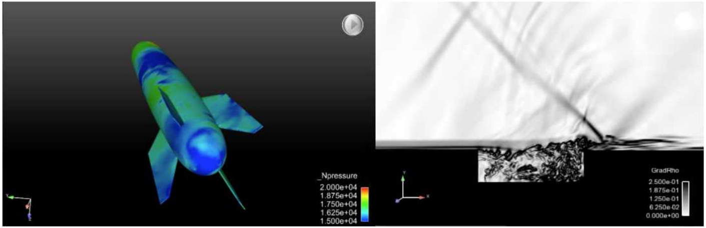


- CFD model
  - 100 million cells
  - 200,000 time steps
- High simulation costs
  - 6 weeks, 5000 cores
  - 6 runs maxes out Cielo

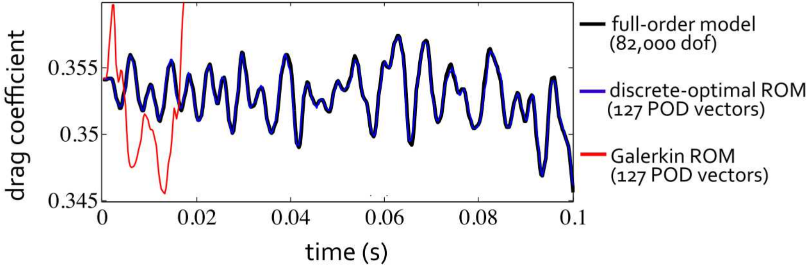
Barrier

- Design engineers require faster simulations
- Uncertainty quantification

Objective: break barrier

Discrete optimality outperforms Galerkin, but why?

- Discrete-optimal ROM outperforms Galerkin on large-scale compressible-flow problems [Carlberg, 2011, Carlberg et al., 2013]



- Strong performance attributed to discrete optimality
- Limited comparative analysis of the two approaches

Goal: Deeper understanding of Galerkin v. discrete-optimal projection for general time integrators

Outline

- Time-continuous and time-discrete representations
- Equivalence conditions
- Discrete-time error bounds

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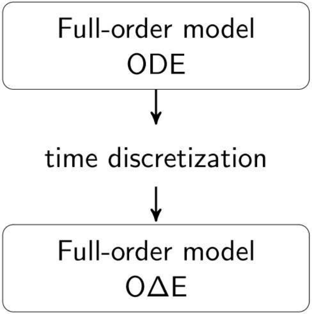
Continuous and discrete representations



Full-order model

- ODE (initial value problem)

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, t), \qquad \boldsymbol{x}(0) = \boldsymbol{x}_0,$$

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

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

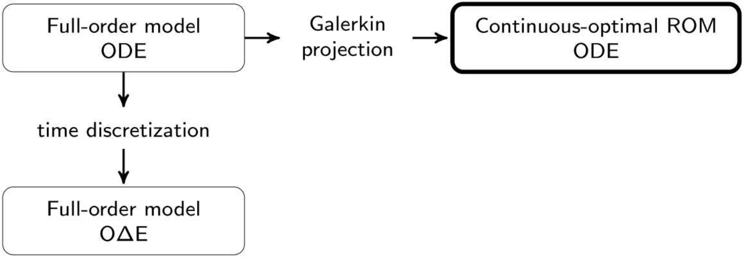
$\boldsymbol{x}^n = \boldsymbol{w}^n$ (explicit state update)

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

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

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

Continuous and discrete representations



Galerkin ROM: continuous representation

- ODE: Galerkin projection on FOM ODE

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

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

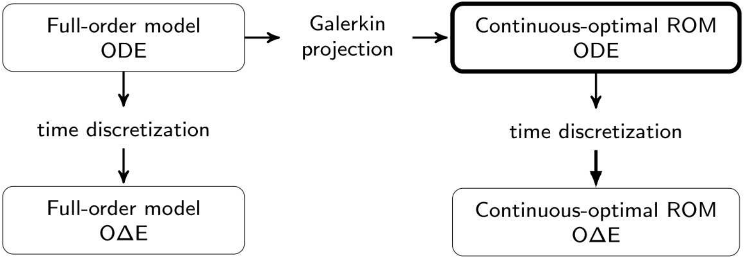
$$\frac{d\hat{\boldsymbol{x}}}{dt} = \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t), \qquad \hat{\boldsymbol{x}}(0) = \boldsymbol{\Phi}^T \boldsymbol{x}_0.$$

Theorem

The Galerkin ROM velocity minimizes the error in the FOM velocity $\boldsymbol{f}$ *over* range$(\boldsymbol{\Phi})$*:*

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

Continuous and discrete representations



Galerkin ROM: discrete representation

- OΔE, linear multistep schemes: $\boxed{\hat{\boldsymbol{r}}^n\left(\hat{\boldsymbol{w}}^n\right) = 0}$

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

$\hat{\boldsymbol{x}}^n = \hat{\boldsymbol{w}}^n$ (explicit state update)

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

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

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

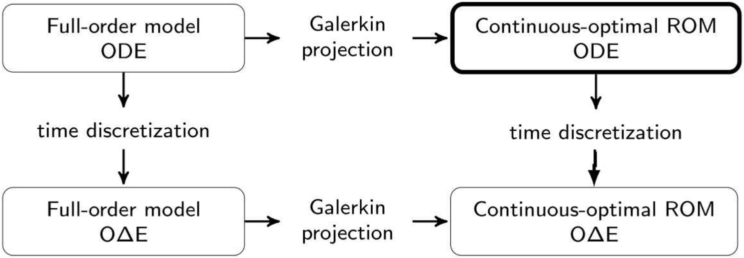
Galerkin ROM: Commutativity

Theorem

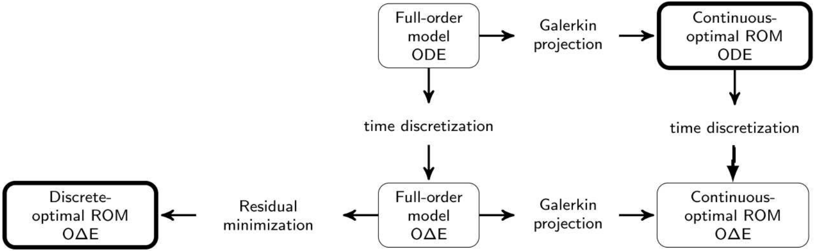
Projection and time discretization are commutative for Galerkin ROMs:

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

$$\hat{\boldsymbol{r}}_i^n(\hat{\boldsymbol{w}}_1, \ldots, \hat{\boldsymbol{w}}_s) = \boldsymbol{\Phi}^T \boldsymbol{r}_i^n(\boldsymbol{\Phi}\hat{\boldsymbol{w}}_1, \ldots, \boldsymbol{\Phi}\hat{\boldsymbol{w}}_s), \quad i = 1, \ldots, s,$$



Continuous and discrete representations



Discrete-optimal ROM: discrete representation

- OΔE, linear multistep schemes:

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

$$\Updownarrow$$

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

  - $\boldsymbol{A} = \boldsymbol{I}$: Least-squares Petrov–Galerkin [LeGresley, 2006, Carlberg et al., 2011]
  - $\boldsymbol{A} = (\boldsymbol{P}\boldsymbol{\Phi}_r)^+\boldsymbol{P}$: GNAT [Carlberg et al., 2013]
  - Alternative norm: ℓ^1 [Abgrall and Amsallem, 2015]

- OΔE, Runge–Kutta:

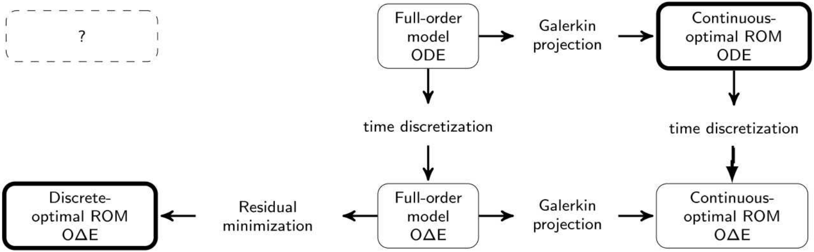
$$\left(\hat{\boldsymbol{w}}_1^n,\ldots,\hat{\boldsymbol{w}}_s^n\right) = \arg\min_{(\hat{\boldsymbol{z}}_1,\ldots,\hat{\boldsymbol{z}}_s)\in\mathbb{R}^{p\times s}} \sum_{i=1}^{s}\left\|\boldsymbol{A}_i\boldsymbol{r}_i^n\left(\boldsymbol{\Phi}\hat{\boldsymbol{z}}_1,\ldots,\boldsymbol{\Phi}\hat{\boldsymbol{z}}_s\right)\right\|_2^2$$

$$\Updownarrow$$

$$\sum_{j=1}^{s}\boldsymbol{\Psi}_{ij}^n(\hat{\boldsymbol{w}}_1^n,\ldots,\hat{\boldsymbol{w}}_s^n)^T\boldsymbol{r}_j^n\left(\boldsymbol{\Phi}\hat{\boldsymbol{w}}_1^n,\ldots,\boldsymbol{\Phi}\hat{\boldsymbol{w}}_s^n\right) = 0, \quad i = 1,\ldots,s$$

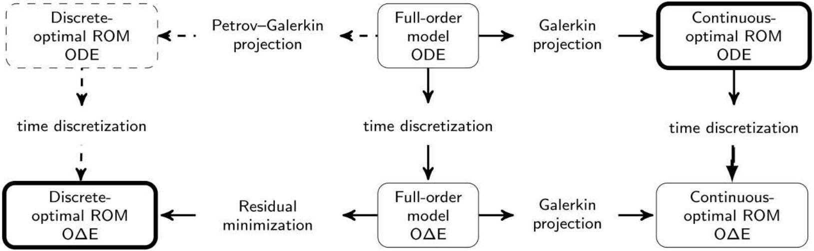
$$\boldsymbol{\Psi}_{ij}^n(\hat{\boldsymbol{w}}_1,\ldots,\hat{\boldsymbol{w}}_s) := \boldsymbol{A}_i^T\boldsymbol{A}_i\frac{\partial \boldsymbol{r}_i^n}{\partial \boldsymbol{w}_j}(\hat{\boldsymbol{w}}_1,\ldots,\hat{\boldsymbol{w}}_s)$$

Continuous and discrete representations



Continuous and discrete representations

The discrete-optimal ROM *sometimes* has a time-continuous representation.



Discrete-optimal ROM: continuous representation

Theorem (Linear multistep schemes)

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

$$\boldsymbol{\Psi}(\hat{\boldsymbol{x}}, t) = \boldsymbol{A}^T \boldsymbol{A} \left(\alpha_0 \boldsymbol{I} - \Delta t \beta_0 \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} (\boldsymbol{x}_0 + \boldsymbol{\Phi} \hat{\boldsymbol{x}}, t) \right) \boldsymbol{\Phi}$$

and subsequently applying time integration with time step Δt 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).*

Discrete-optimal ROM: continuous representation

Theorem (Runge–Kutta schemes)

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

$$\boldsymbol{\Psi}(\hat{\boldsymbol{x}}, t) = \boldsymbol{A}^T\boldsymbol{A}\left(\boldsymbol{I} - \Delta t a_{11}\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}(\boldsymbol{x}_0 + \boldsymbol{\Phi}\hat{\boldsymbol{x}}, t)\right)\boldsymbol{\Phi}$$

and subsequently applying time integration if either

1. $a_{ij} = 0\ \forall i \neq j$ *and* $a_{ii} = a_{jj}\ \forall i, j$, *or*
2. *the scheme is explicit, i.e.,* $a_{ij} = 0,\ \forall j \geq i$.

Outline

- Time-continuous and time-discrete representations
- Equivalence conditions
- Discrete-time error bounds

Equivalence

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

Theorem (Linear multistep schemes)

Galerkin projection is discrete-optimal ($\boldsymbol{\Psi}^n(\hat{\boldsymbol{w}}) = \boldsymbol{\Phi}$)

1. *in the limit of $\Delta t \to 0$ 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 $\frac{\partial \boldsymbol{r}^n}{\partial \boldsymbol{w}}$ is positive definite with $\boldsymbol{A}$ the Cholesky factor of $[\frac{\partial \boldsymbol{r}^n}{\partial \boldsymbol{w}}]^{-1}$*

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- Time-continuous and time-discrete representations
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Discrete-time error bound

Theorem (Linear multistep schemes)

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

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

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

with

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

Discrete-time error bound

Theorem (Backward Euler)

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

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

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

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

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

Corollary (Discrete-optimal smaller error bound)

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

Discrete-optimal time-step dependence

Corollary

Define $\bar{\mathbf{x}}^j$ *as the full-space solution centered at the discrete-optimal solution:*

$$\bar{\mathbf{x}}^j = \Delta t \boldsymbol{f}\left(\mathbf{x}_0 + \bar{\mathbf{x}}^j\right) + \boldsymbol{\Phi}\hat{\mathbf{x}}_D^{j-1}, \quad j = 1, \ldots, n.$$

Then, the discrete-optimal error can be bounded as

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

with

- $\Delta \bar{\mathbf{x}}^j := \bar{\mathbf{x}}^j - \boldsymbol{\Phi}\hat{\mathbf{x}}_D^{j-1}$
- $\Delta \hat{\mathbf{x}}_D^j := \hat{\mathbf{x}}_D^j - \hat{\mathbf{x}}_D^{j-1}$
- $\mu^j := \left\|\boldsymbol{\Phi}\Delta\hat{\mathbf{x}}_D^j - \Delta\bar{\mathbf{x}}^j\right\| / \Delta\bar{\mathbf{x}}^j$

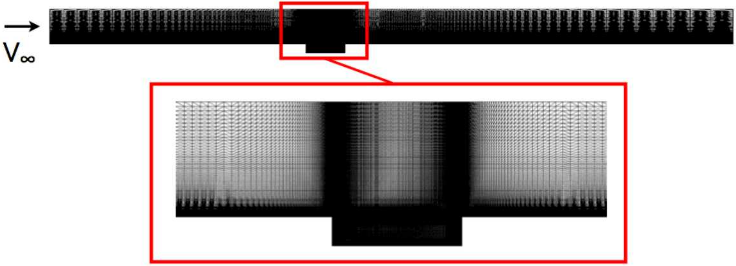
Effect of decreasing Δt:

\+ 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 $\boldsymbol{\Phi}$

Example: Cavity-flow problem



- Unsteady Navier–Stokes
- DES turbulence model
- 1.2 million degrees of freedom
- Linear multistep: BDF2
- $\Delta t_\star = 1.5 \times 10^{-3}$ sec by time-step verification study
- $\text{Re} = 6.3 \times 10^6$
- $M_\infty = 0.6$

FOM responses

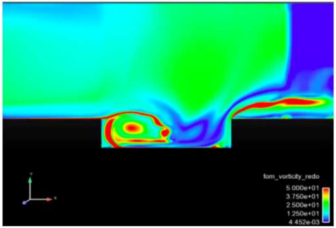


Figure: vorticity field

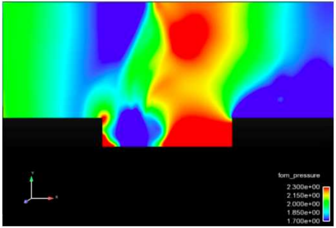
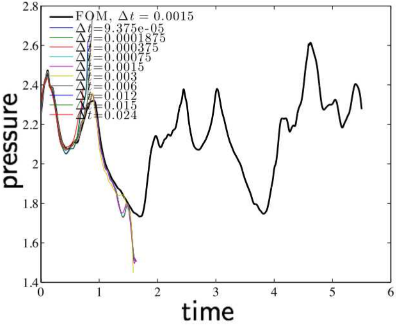
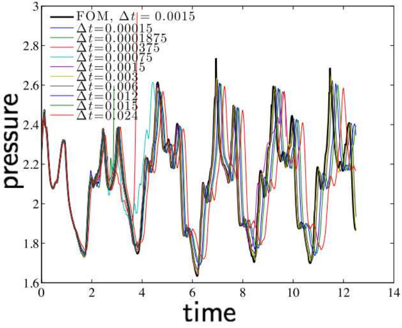


Figure: pressure field

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



(a) Galerkin

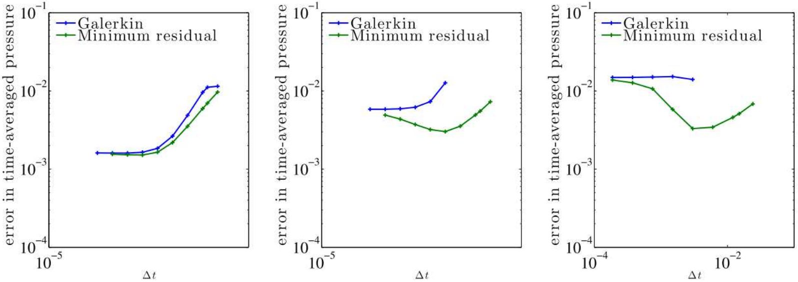


(b) Discrete optimal

- Galerkin ROMs unstable for all time steps. Consistent with previous results [Carlberg et al., 2013, Carlberg et al., 2011, Carlberg, 2011]

+ Discrete-optimal ROMs accurate and stable, with a clear dependence on the time step Δt.

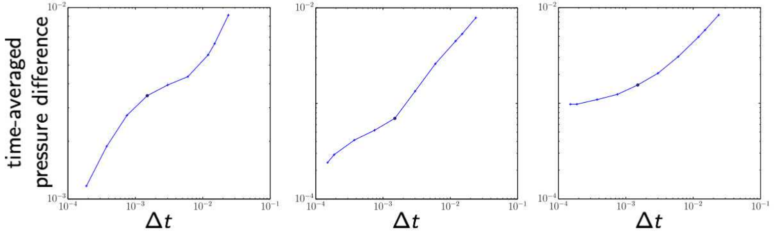
Superior performance ($p = 204$)



(c) $0 \leq t \leq 0.55$ (d) $0 \leq t \leq 1.1$ (e) $0 \leq t \leq 1.54$

✓ When Galerkin is stable, the discrete-optimal ROM yields a smaller error for all time intervals and time steps.

Limiting equivalence



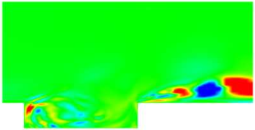
(f) $p = 204$ (g) $p = 368$ (h) $p = 564$

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

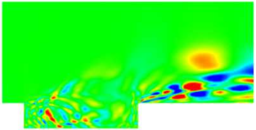
✓ The discrete-optimal ROM converges to Galerkin as $\Delta t \to 0$.

POD basis spectral analysis

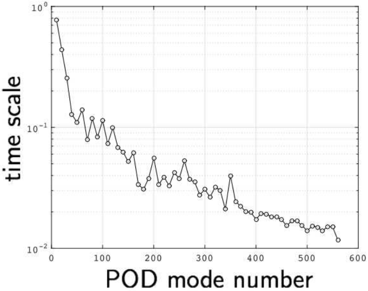
(a) mode 1



(b) mode 21



(c) mode 101

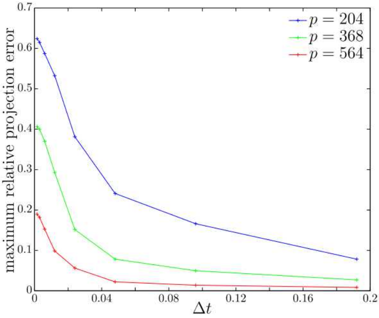


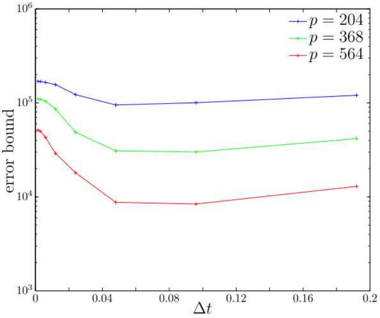
- Higher modes numbers associate with smaller spatial and temporal scales.

Backward Euler error bound

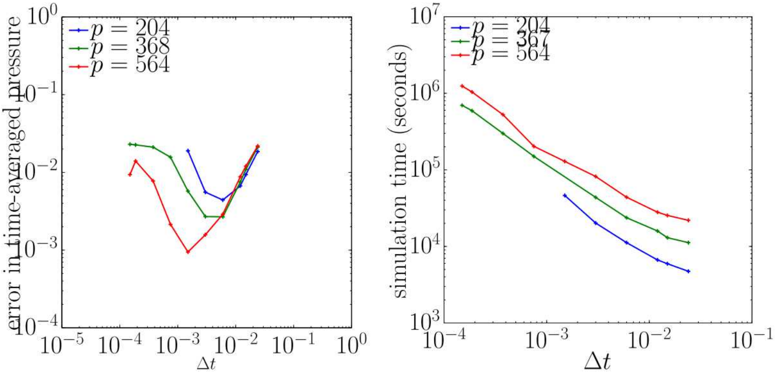
$$\left\|\delta \boldsymbol{x}_D^n\right\| \le \Delta t(1+\kappa\Delta t)\sum_{j=0}^{n-1}\frac{\boxed{\mu^{n-j}}}{(h)^{j+1}}\left\|\boldsymbol{f}(\bar{\boldsymbol{x}}^{n-j})\right\|$$

Approximate $\mu^k := \left\|\boldsymbol{\Phi}\Delta\hat{\boldsymbol{x}}_D^k - \Delta\bar{\boldsymbol{x}}^k\right\| / \Delta\bar{\boldsymbol{x}}^k$ with relative projection error.





1. Adding basis vectors for larger time steps yields little improvement
2. Approximated error bound: intermediate time step → lowest bound



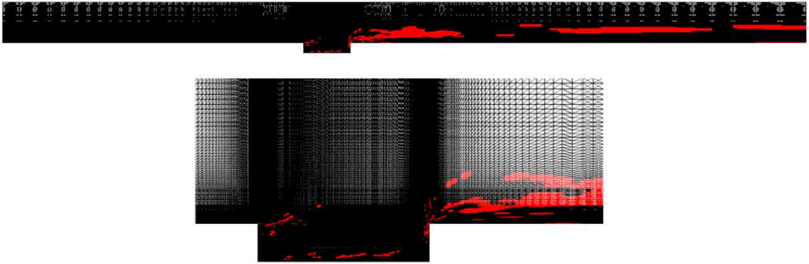
1. Adding basis vectors for larger time steps yields little improvement
2. Intermediate time step → lowest error

$p = 564$ 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

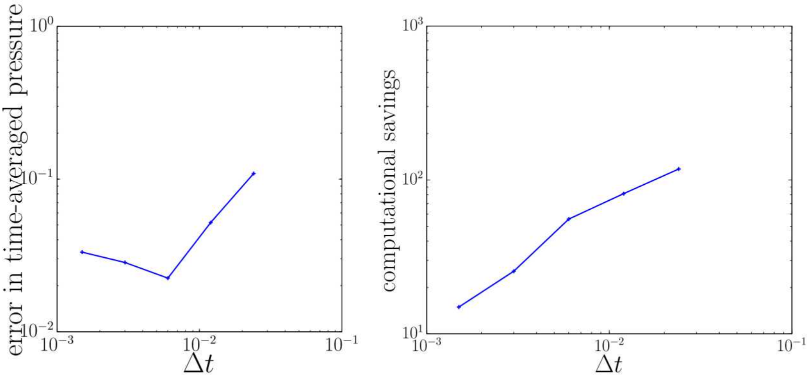
GNAT model

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



- Sample mesh [Carlberg et al., 2013]: 4.1% nodes, 3.0% original cells
- \+ Allows GNAT to run on 2 cores instead of 48 cores

GNAT performance



- 1.5×10^{-3} sec: relative error $= 3.32\%$, cpu savings $= 14.9$
- 6.0×10^{-3} sec: relative error $= 2.25\%$, cpu savings $= 55.7$

Conclusions

- Time-continuous and time-discrete representations
  - Galerkin: projection and time-discretization are commutative
  - Discrete-optimal: a continuous representation sometimes exists
- Equivalence conditions
  1. Limit of $\Delta t \to 0$
  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
- Numerical experiments
  - Discrete-optimal ROM always yields a smaller error than Galerkin
  - Equivalent as $\Delta t \to 0$
  - Approximated error bound and actual error minimized for intermediate Δt

Acknowledgments

- Charbel Farhat: permitting the open use of AERO-F
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Questions?

- K. Carlberg, M. Barone, H. Antil. "Galerkin v. discrete-optimal projection in nonlinear model reduction," arXiv e-Print 1504.03749 (2015).

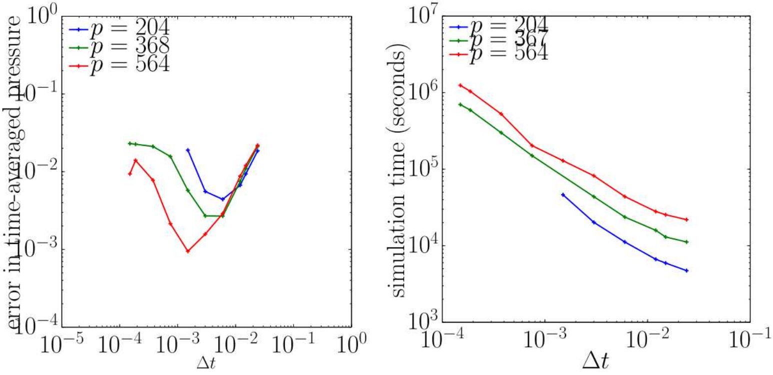

Figure: Discrete-optimal ROM performance.

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