

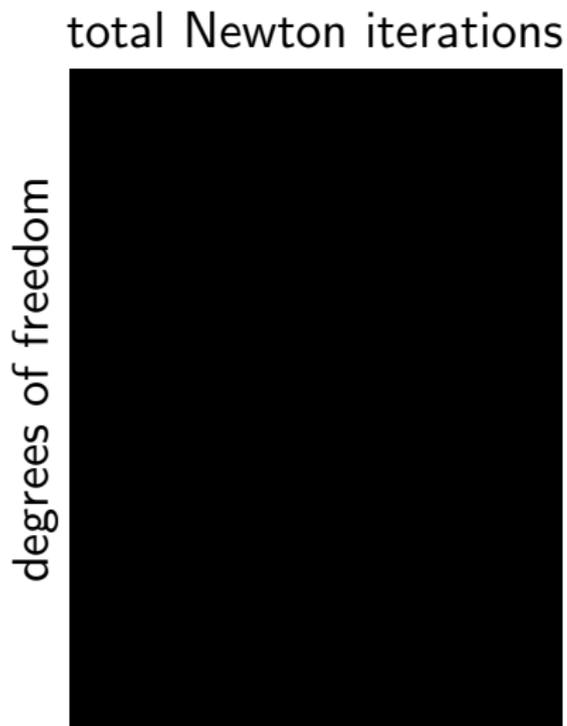
# A forecasting method for decreasing the temporal complexity in implicit, nonlinear model reduction

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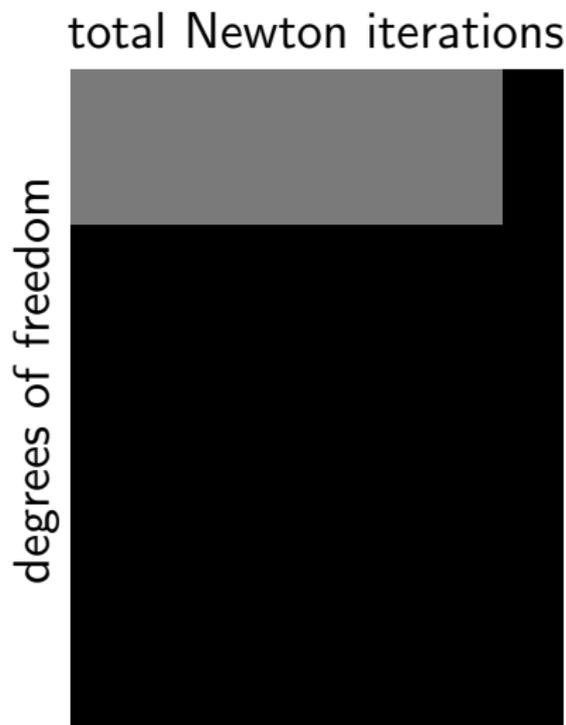
Sandia National Laboratories

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# Nonlinear ODE, implicit time integration

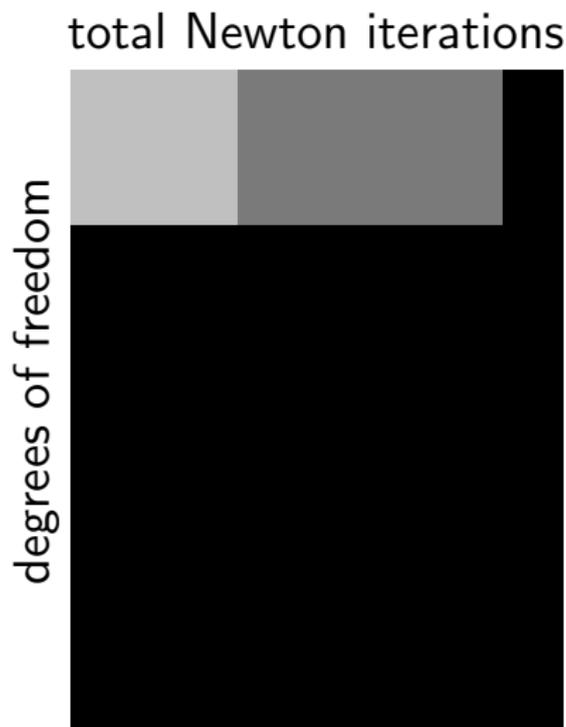


# Reduced-order model (ROM): computed unknowns



Exploit *spatial-behavior* data to decrease # unknowns.

**Can we do more?**



Exploit *temporal-behavior* data to decrease total Newton iterations.

# Main idea

- full-order model
  - 1st- or 2nd-order nonlinear ODE
  - implicit time integrator
- computational complexity
  - each time step, solve a large-scale system of nonlinear equations with a Newton-like method
  - **spatial complexity**: cost of each Newton iteration (i.e., linear-system solve)
  - **temporal complexity**: number of Newton iterations
- ROM: use *spatial-behavior* data to decrease *spatial complexity*
- goals
  - 1 exploit *temporal-behavior* data to decrease *temporal complexity*
  - 2 introduce *no additional error* to ROM solution

- 1 Motivation
- 2 Problem formulation
  - full-order model
  - reduced-order model
- 3 Temporal-complexity reduction
  - overview
  - offline/online decomposition
  - algorithm sketch
- 4 Numerical experiments

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# Parameterized, nonlinear ODE

- for simplicity, consider first-order ODEs

$$\begin{aligned}\dot{x} &= f(x; t, \mu) \\ x(0; \mu) &= x^0(\mu)\end{aligned}$$

- state:  $x \equiv x(t; \mu) \in \mathbb{R}^N$
- $f$  nonlinear in  $x$
- inputs:  $\mu \in \mathcal{D}$
- initial condition:  $x^0(\mu) \in \mathbb{R}^N$

# Implicit time integration

- for simplicity, consider only single-stage methods
- system of nonlinear equations solved at each time step:

$$R^n(w^n; \mu) = 0, \quad n = 1, \dots, M$$

- unknowns  $w^n$ : state or velocity at  $t \in [t^{n-1}, t^n]$
- after computing  $w^n$ , explicitly update the state:

$$x^n = \gamma x^{n-1} + \beta w^n$$

# Full-order model: computational burden

Solve

$$R^n(w^n; \mu) = 0, \quad n = 1, \dots, M$$

with a Newton-like method

- solve one  $N$ -dimensional linear system per Newton iteration
- **spatial complexity**: cost of each linear-system solve
  - direct solver:  $\mathcal{O}(\omega^2 N)$  flops<sup>1</sup>
  - iterative solver:  $\mathcal{O}(L\omega N)$  flops<sup>2</sup>
  - $N$  large  $\rightarrow$  spatial complexity large
- **temporal complexity**: total number of Newton iterations
  - $N$  large  $\rightarrow M$  large  $\rightarrow$  temporal complexity large

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<sup>1</sup> $\omega$ : average number of nonzeros per row of  $\frac{\partial R^n}{\partial w}$

<sup>2</sup> $L$ : average number of linear-solver iterations per Newton iteration

# Projection-based model reduction

- **Offline:** exploit knowledge of *spatial behavior* to compute basis  $\Phi \in \mathbb{R}^{N \times \hat{N}}$  with  $\hat{N} \ll N$  (e.g., POD)
- **Online:** approximate state by  $\tilde{x}$  in low-dim trial subspace:

$$\tilde{x}(t; \mu) = x^0(\mu) + \Phi \hat{x}(t; \mu) \quad (1)$$

$$\dot{\tilde{x}}(t; \mu) = \Phi \dot{\hat{x}}(t; \mu) \quad (2)$$

- substituting (1)–(2) into ODE (with  $x = \tilde{x}$ ) yields

$$\Phi \dot{\hat{x}} = f(x^0(\mu) + \Phi \hat{x}; t, \mu). \quad (3)$$

- ODE (3) may not be solvable, because  $\text{image}(f) \not\subset \text{range}(\Phi)$

# Project, then discretize in time

**Goal:** compute solution to overdetermined ODE

- enforce orthogonality of ODE residual to range of  $\Psi \in \mathbb{R}^{N \times \hat{N}}$

$$\Psi^T \Phi \dot{\hat{x}} = \Psi^T f(x^0(\mu) + \Phi \hat{x}; t, \mu)$$

$$\dot{\hat{x}} = \left(\Psi^T \Phi\right)^{-1} \Psi^T f(x^0(\mu) + \Phi \hat{x}; t, \mu) \quad (4)$$

- solve (4) with the same implicit numerical integrator

$$\left(\Psi^T \Phi\right)^{-1} \Psi^T R^n(w^0(\mu) + \Phi \hat{w}^n; \mu) = 0, \quad n = 1, \dots, M$$

- $\hat{w}^n \in \mathbb{R}^{\hat{N}}$ : generalized unknowns at time step  $n$

# Discretize in time, then project

**Goal:** compute solution to overdetermined ODE

- 1 apply time integrator to overdetermined ODE
- 2 minimize discrete residual over the trial subspace

[LeGresley, 2006, Carlberg et al., 2011]

$$\hat{w}^n = \arg \min_{y \in \mathbb{R}^{\hat{N}}} \|R^n(w^0(\mu) + \Phi y; \mu)\|^2$$

- solve with nonlinear least-squares method, e.g., Gauss–Newton

**Problem:** spatial complexity still scales with  $N$

# Hyperreduction

**Goal:** reduce spatial complexity by approximating nonlinear terms

- collocation [Astrid et al., 2008, Ryckelynck, 2005, LeGresley, 2006]

$$\tilde{R}^n = Z^T Z R^n$$

$Z$  (sampling matrix): selected rows of  $I_{N \times N}$

- empirical interpolation/gappy POD

[Astrid et al., 2008, Bos et al., 2004, Chaturantabut and Sorensen, 2010, Galbally et al., 2009, Drohmann et al., 2012, Carlberg et al., 2011]

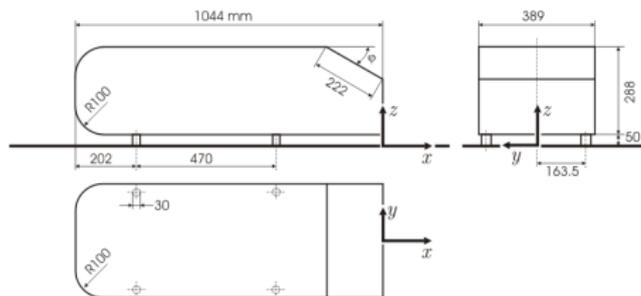
$$\tilde{f} = \Phi_f (Z \Phi_f)^+ Z f$$

or

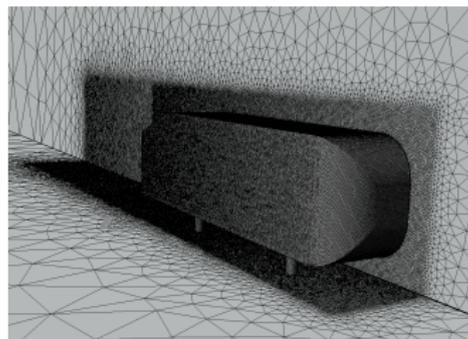
$$\tilde{R}^n = \Phi_R (Z \Phi_R)^+ Z R^n$$

$\Phi_R, \Phi_f$ : bases that exploit observed spatial behavior

# Example: Ahmed body



(a) Ahmed body [Hinterberger et al., 2004]



(b) mesh

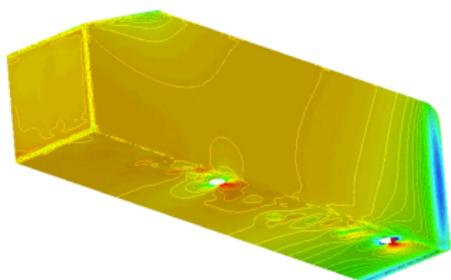
compressible Navier–Stokes (finite volume, AERO-F)

- DES turbulence model
- $Re = 4.48 \times 10^6$
- $M_\infty = 0.175$
- 3-point BDF integrator (implicit)
- FOM:  $N = 1.73 \times 10^7$

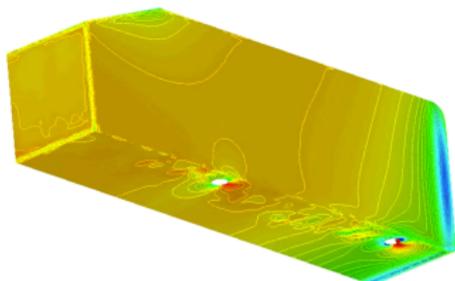
GNAT nonlinear ROM [Carlberg et al., 2011]

- discretize in time, then project (minimize discrete residual)
- hyperreduction: gappy POD applied to residual

# Example: GNAT nonlinear model reduction [Carlberg et al., 2012]



(c) full-order ( $1.73 \times 10^7$  dofs)



(d) GNAT (283 dofs)

surface pressure at  $t = 0.1$  seconds

<i>model</i>	<i>error in drag</i>	<i>cost, core-hours</i>	<i>Newton iterations per time step</i>
full-order model		6810	4.0
reduced-order model	0.68%	16	2.75

# Complexity reduction

- **spatial complexity**: decreased by factor of **637**
- **temporal complexity**: decreased by factor of **1.5**

**Can we do more?**

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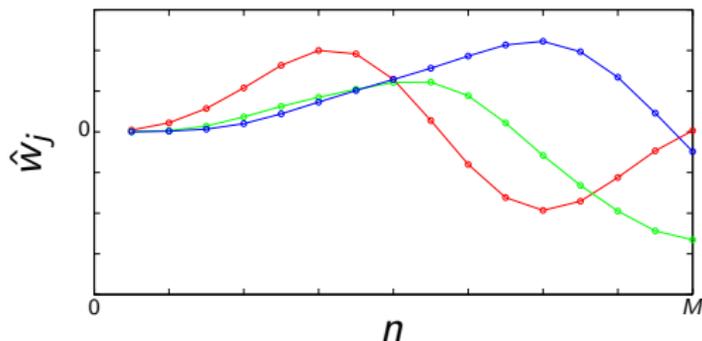
**Goal:** exploit temporal-behavior data to reduce temporal complexity

- 1 during ROM simulation, apply gappy POD *in the time domain* to generate a forecast for the generalized unknowns
  - 2 use the forecast as an *accurate initial guess* for the Newton-like solver
- + good guess  $\rightarrow$  few Newton its  $\rightarrow$  low temporal complexity
  - + introduces *no additional error*

# Offline: compute time-evolution POD bases $\Psi_j$

- 1 collect snapshots of the *temporal behavior* of the  $j$ th generalized unknown:

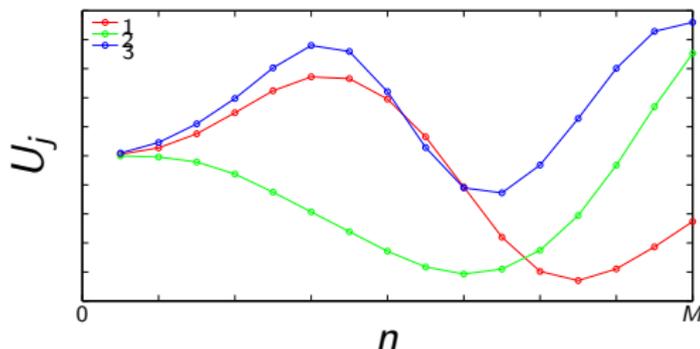
$$\hat{w}_j^n(\mu), \quad n = 1, \dots, M, \quad \mu \in \{\bar{\mu}_i\}_{i=1}^{n_{\text{train}}}$$



example with 3 training configurations ( $n_{\text{train}} = 3$ )

# Offline: compute time-evolution POD bases $\Psi_j$

- 2 compute SVD of temporal-behavior snapshots



$$\begin{bmatrix} \hat{w}_j^1(\bar{\mu}_1) & \cdots & \hat{w}_j^1(\bar{\mu}_{n_{\text{train}}}) \\ \vdots & \ddots & \vdots \\ \hat{w}_j^M(\bar{\mu}_1) & \cdots & \hat{w}_j^M(\bar{\mu}_{n_{\text{train}}}) \end{bmatrix} = U_j \Sigma_j V_j^T$$

- 3 truncate: keep only  $a_j \leq n_{\text{train}}$  vectors:  $\Psi_j = U_j(:, 1 : a_j)$

## Time-evolution bases: example

- implicit linear multi-step scheme:  $w^n = x^n$
- one training configuration ( $n_{\text{train}} = 1$ )
- POD model reduction

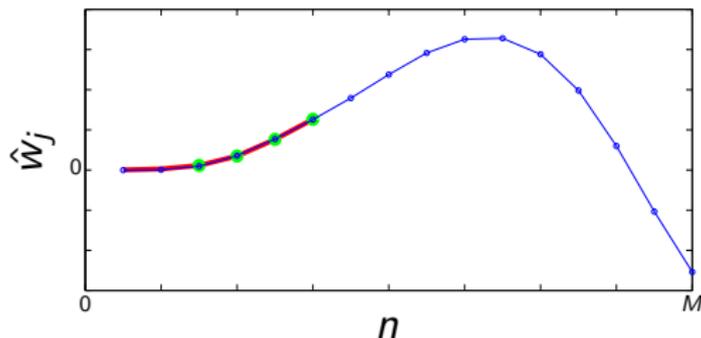
Here, the time-evolution bases  $\Psi_j$  are the *right singular vectors* generated when computing  $\Phi$ :

$$\left[ x^1(\bar{\mu}_1) \cdots x^M(\bar{\mu}_1) \right] = U \Sigma V^T$$

- $\Phi = U$
- $\Psi_j = V(:, j)$  for  $j = 1, \dots, M$

# Online: compute forecast, use as initial guess

- 1 compute forecast by gappy POD in time domain:  
match generalized unknowns at previous  $\alpha$  time steps



$\hat{w}_j$  so far; memory  $\alpha = 4$ ; forecast

$$z_j = \arg \min_{z \in \mathbb{R}^{a_j}} \left\| \begin{bmatrix} \Psi_j(n - \alpha, 1) & \cdots & \Psi_j(n - \alpha, a_j) \\ \vdots & \ddots & \vdots \\ \Psi_j(n - 1, 1) & \cdots & \Psi_j(n - 1, a_j) \end{bmatrix} z - \begin{bmatrix} \hat{w}_j^{n-\alpha} \\ \vdots \\ \hat{w}_j^{n-1} \end{bmatrix} \right\|_2$$

- 2 use forecast  $\Psi_j z_j$  as an *accurate initial guess* for Newton solver

# Online algorithm sketch

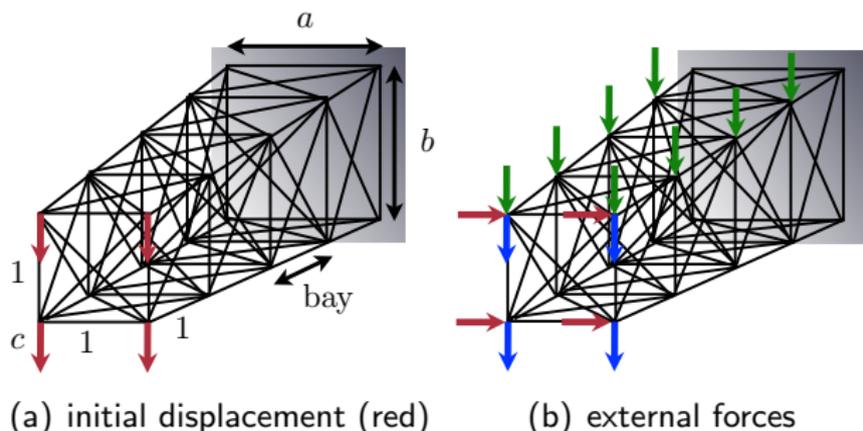
- 1: **for**  $n = 1, \dots, M$  **do**
- 2:   **if** forecast is available **then**
- 3:     use forecast as initial guess for generalized unknowns
- 4:   **end if**
- 5:   solve reduced-order equations with a Newton-like method
- 6:   **if**  $\#$  Newton iterations  $> \tau$  **then** {recompute forecast}
- 7:     compute forecast using generalized unknowns at previous  
       $\alpha$  time steps
- 8:   **end if**
- 9: **end for**

- many Newton iterations: heuristic for poor forecast

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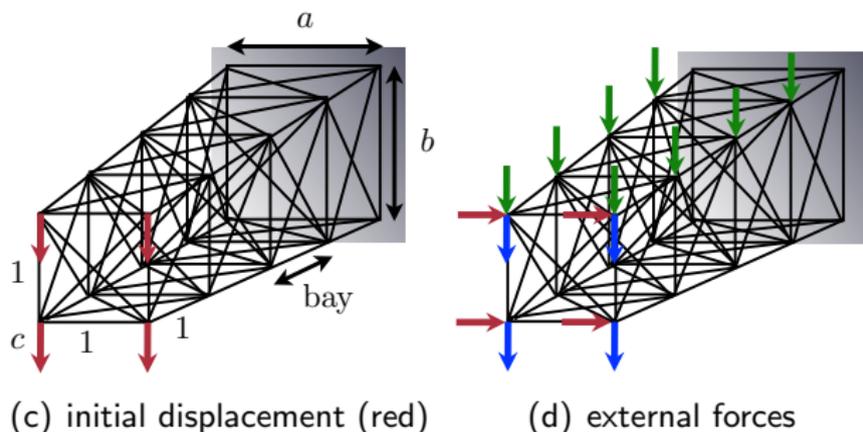
# Clamped-free truss structure, geometric nonlinearity



$$M(\mu)\ddot{x} + C(\mu)\dot{x} + f^{\text{int}}(x; \mu) = f^{\text{ext}}(t; \mu)$$

- $M$ : mass matrix
- $C = \alpha M + \beta \nabla_x f^{\text{int}}(x^0)$ : Rayleigh damping matrix
- $f^{\text{int}}$ : internal force, *nonlinear in  $x$*
- $f^{\text{ext}}$ : sum of three sinusoidal forces, activated at  $n = M/2$
- $N = 9000$  degrees of freedom in full-order model
- implicit midpoint rule:  $w^n = \ddot{x}(t^{n-1} + 1/2\Delta t)$

# Clamped-free truss structure, geometric nonlinearity



9 inputs:

- 3 material properties: density, bar cross-sectional area, modulus of elasticity
- 2 geometrical parameters: base width  $a$ , base height  $b$
- 1 initial-displacement magnitude
- 3 external-force magnitudes

# Three reduced-order models compared

## 1 Galerkin projection

$$\Phi^T M(\mu) \ddot{\hat{x}} + \Phi C(\mu) \Phi \dot{\hat{x}} + \Phi^T f^{\text{int}}(x^0(\mu) + \Phi \hat{x}; \mu) = \Phi^T f^{\text{ext}}(t; \mu)$$

## 2 Galerkin projection + collocation

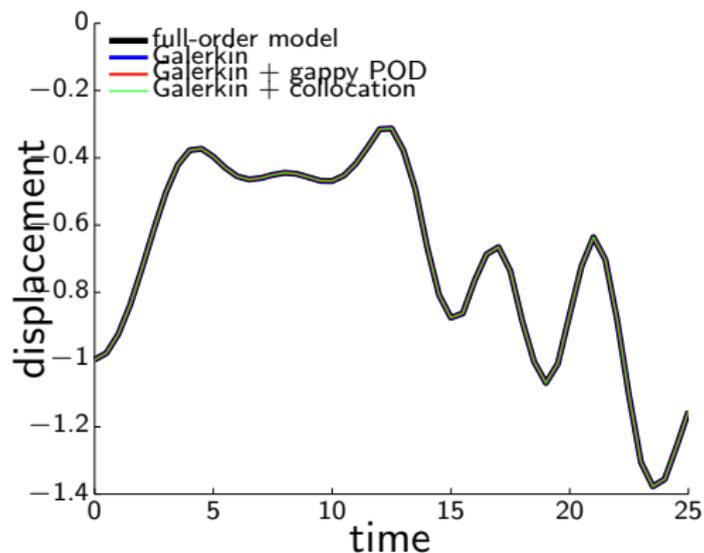
$$\Phi^T Z^T Z \left( M(\mu) \ddot{\hat{x}} + C(\mu) \Phi \dot{\hat{x}} + f^{\text{int}}(x^0(\mu) + \Phi \hat{x}; \mu) - f^{\text{ext}}(t; \mu) \right) = 0$$

## 3 Galerkin projection + gappy POD approximation of residual

$$\Phi^T \Phi_R (Z \Phi_R)^+ Z \left( M(\mu) \ddot{\hat{x}} + C(\mu) \Phi \dot{\hat{x}} + f^{\text{int}}(x^0(\mu) + \Phi \hat{x}; \mu) \right) = \Phi^T \Phi_R (Z \Phi_R)^+ Z f^{\text{ext}}(t; \mu)$$

- forecasting: memory  $\alpha = 12$ , Newton threshold  $\tau = 0$

## Case 1 (ideal): fixed inputs, no truncation of bases



- all responses nearly exact (as expected)

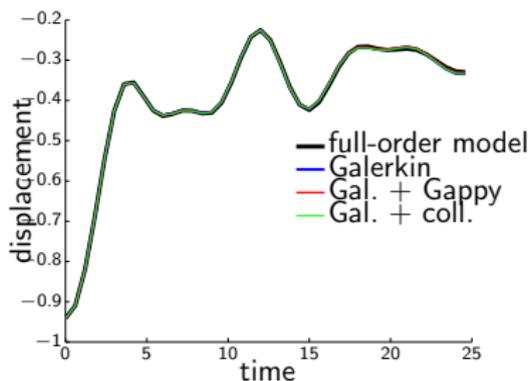
## Case 1: forecasting drastically improves performance

ROM method	relative error	total Newton its		wall-time speedup	
		no forecast	forecast	no forecast	forecast
Galerkin	$8.64 \times 10^{-12}$	99	2	1.01	1.84
Gal + Gappy	$8.64 \times 10^{-12}$	99	2	36.4	69.3
Gal + coll	$2.12 \times 10^{-5}$	100	16	36.5	61.9

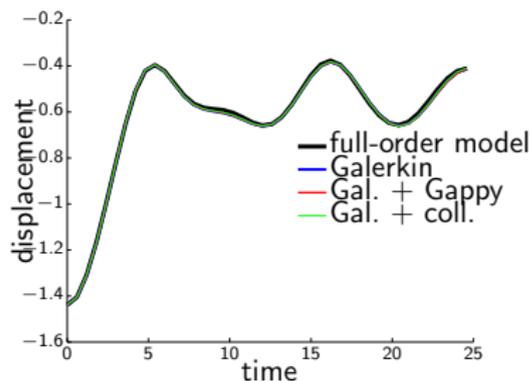
- + forecast 'perfect': computation *only at first time step* for ROMs 1 and 2

## Case 2: unforced dynamics, varying structure

- six varied inputs: material properties, geometry, initial cond
- six randomly chosen training configurations
- two randomly chosen online configurations
- 99.99% energy criterion for POD



(e) online configuration 1



(f) online configuration 2

+ all relative errors less than 1%

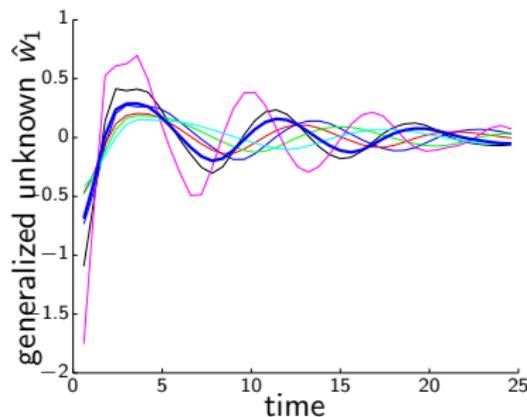
## Case 2: forecasting improves performance by $\sim 60\%$

online config	ROM method	Newton its		wall-time speedup	
		no forecast	forecast	no forecast	forecast
1	Galerkin	82	49	0.998	1.71
	Gal + Gappy	82	48	58.2	82.4
	Gal + coll	82	48	59.4	80.8
2	Galerkin	82	48	1.03	1.55
	Gal + Gappy	82	48	54.0	86.1
	Gal + coll	82	48	55.5	88.7

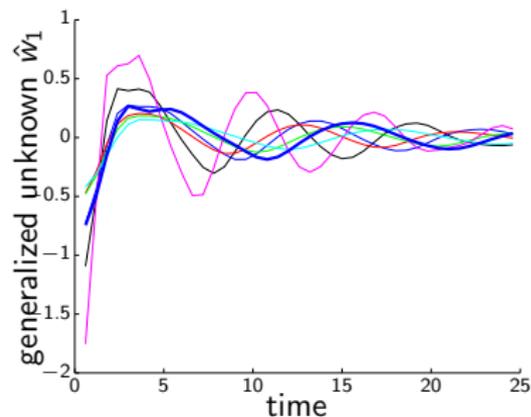
- + forecasting cuts Newton steps nearly in half
- + wall-time speedup increases by roughly 60%
- performance less impressive than ideal case

## Case 2: temporal behavior similar across input variation

- temporal behavior of first generalized unknown  $\hat{w}_1$  (bold=online; thin=training):



(g) online configuration 1

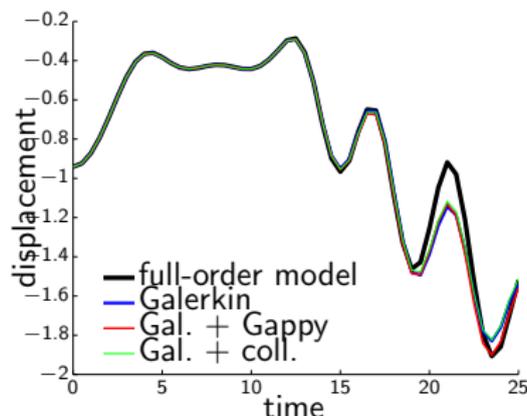


(h) online configuration 2

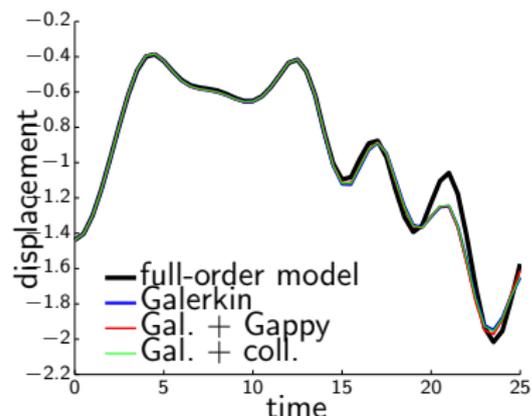
- temporal behavior similar across input variation: this explains the method's effectiveness
- + method seems to handle frequency shifts

## Case 3: forced dynamics, fixed structure

- four varied inputs: external-force magnitudes, initial condition



(i) online configuration 1



(j) online configuration 2

+ relative errors roughly 1.5%

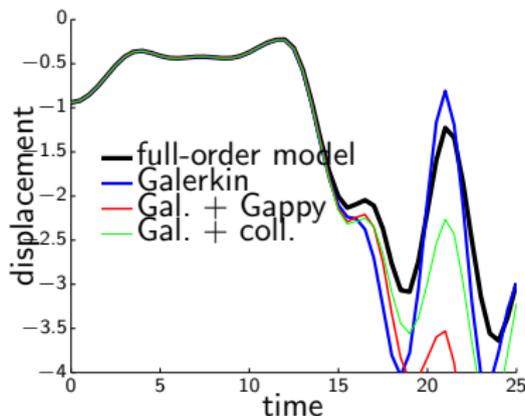
## Case 3: forecasting improves performance by $\sim 50\%$

online config	ROM method	Newton its		wall-time speedup	
		no forecast	forecast	no forecast	forecast
1	Galerkin	100	60	1.02	1.47
	Gal + Gappy	100	61	52.7	75.2
	Gal + coll	100	71	49.5	70.9
2	Galerkin	100	60	1.02	1.52
	Gal + Gappy	100	61	52.1	73.2
	Gal + coll	100	68	54.3	71.8

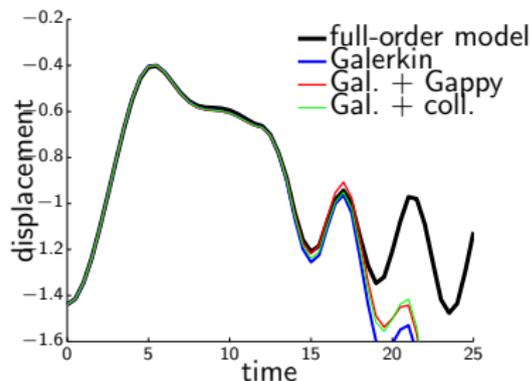
- + forecasting cuts Newton steps by 40%
- + wall-time speedup increases by roughly 50%
- performance again slightly worse (richer dynamics)

## Case 4: forced dynamics, varying structure

- nine varied inputs: external-force magnitudes, initial condition



(k) online configuration 1



(l) online configuration 2

- ROMs increasingly inaccurate after forces activated ( $t = 12.5$ )
- relative errors between 5% and 17%

## Case 4: forecasting improves performance by $\sim 35\%$

online config	ROM method	Newton its		wall-time speedup	
		no forecast	forecast	no forecast	forecast
1	Galerkin	104	109	1.21	1.38
	Gal + Gappy	124	94	8.0	9.48
	Gal + coll	120	90	8.12	11
2	Galerkin	95	62	1.04	1.47
	Gal + Gappy	95	64	7.47	10.4
	Gal + coll	100	73	7.36	9.98

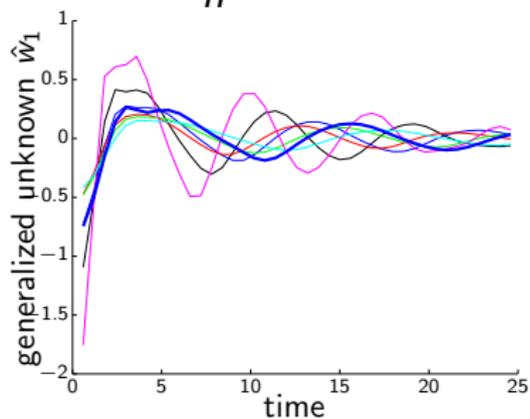
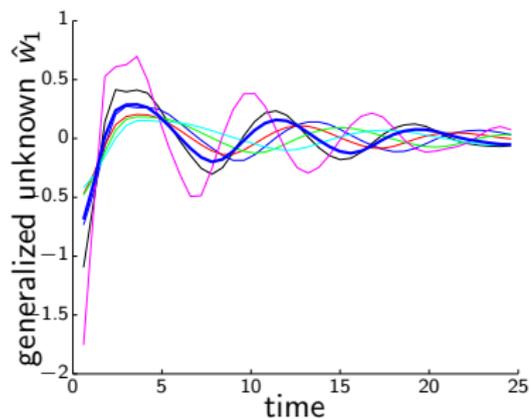
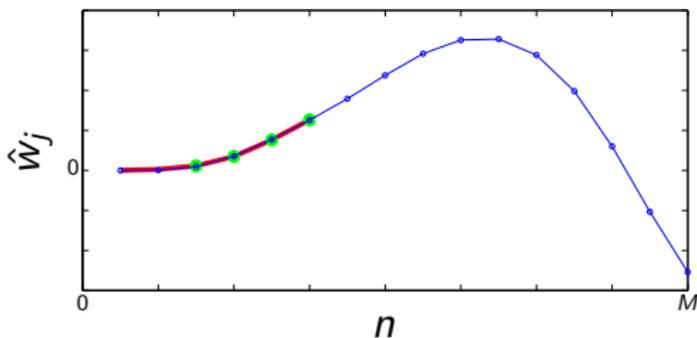
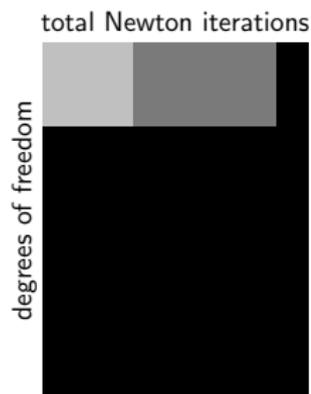
- forecasting method does not always help: number of Newton steps **increases** in one case
- + forecasting cuts Newton steps by 25% in most cases
- + wall-time speedup increases by roughly 35%

# Conclusions

## use temporal-behavior data to reduce ROM simulation time

- offline: compute time-evolution bases
- online:
  - 1 use gappy POD to forecast generalized unknowns
  - 2 use forecast as initial guess in ROM Newton solver
- + observed decrease in temporal complexity
- + observed decrease in ROM simulation wall time
- + no additional error introduced
- best performance occurs in the case of:
  - 1 smooth dynamics (low frequency)
  - 2 temporal behavior similar across input variation
  - 3 accurate ROM
- **Reference:** K. Carlberg, J. Ray, and B. van Bloemen Waanders. 'Decreasing the temporal complexity for nonlinear, implicit reduced-order models by forecasting,' arXiv e-Print 1209.5455 (2012). (submitted to CMAME)

# Questions?



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