Time-parallel reduced-order models via forecasting

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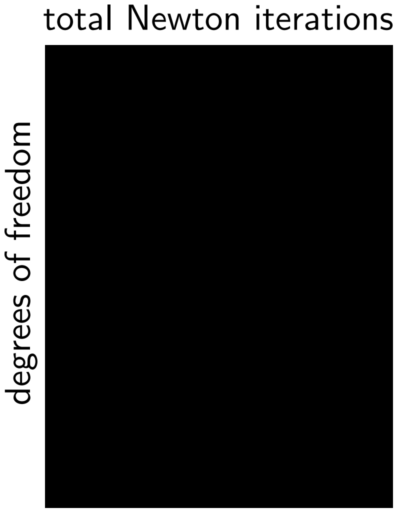
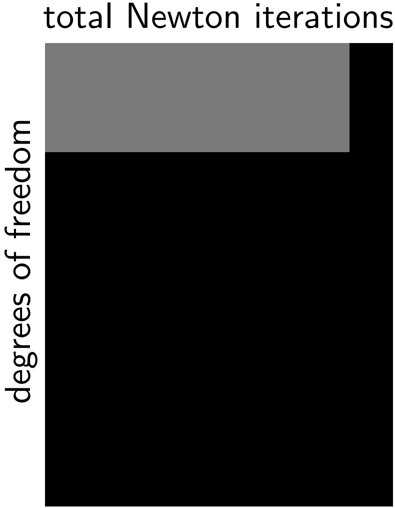
Nonlinear ODE, implicit time integration



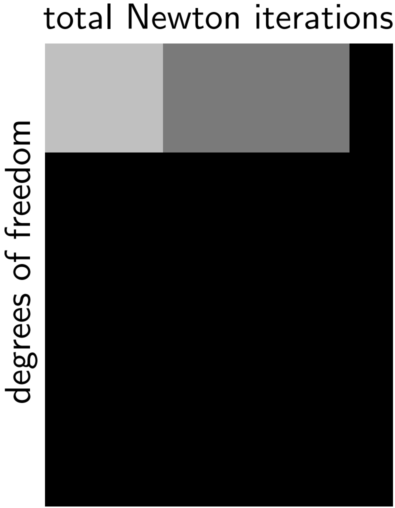
Reduced-order model (ROM): computed unknowns



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

Can we do more?

Goal



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 additonal error* to ROM solution

Outline

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Parameterized, nonlinear ODE

- for simplicity, consider first-order ODEs

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

- 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:

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

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

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

Full-order model: computational burden

Solve

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

with a Newton-like method

- solve one N-dimensional linear system per Newton iteration
- **spatial complexity**: cost of each linear-system solve
  - direct solver: $\mathcal{O}\left(\omega^2 N\right)$ flops[1]
  - iterative solver: $\mathcal{O}\left(L\omega N\right)$ flops[2]
  - 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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[1] ω: average number of nonzeros per row of $\frac{\partial R^n}{\partial w}$

[2] 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

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

- 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 $\Psi \in \mathbb{R}^{N\times\hat{N}}$

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

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

- solve (4) with the same implicit numerical integrator

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

- $\hat{w}^n \in \mathbb{R}^{\hat{N}}$: 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]

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

- 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]

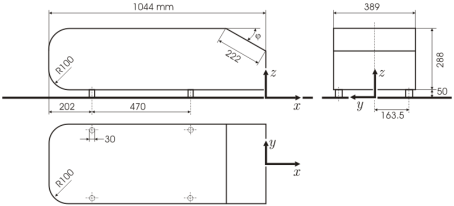
$$\tilde{f} = \Phi_f \left(Z \Phi_f \right)^+ Z f$$

or

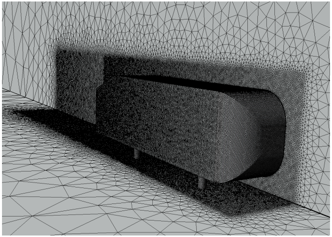
$$\tilde{R}^n = \Phi_R \left(Z \Phi_R \right)^+ Z R^n$$

Φ_R, Φ_f: bases that exploit observed spatial behavior

Example: Ahmed body



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



(b) mesh

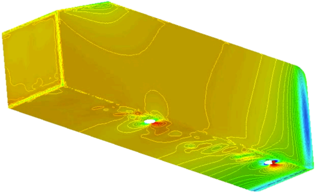
compressible Navier–Stokes (finite volume, AERO-F)

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

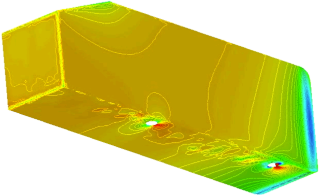
GNAT nonlinear ROM [Carlberg et al., 2011]

- 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 (1.73×10^7 dofs)



(d) GNAT (283 dofs)

surface pressure at $t = 0.1$ seconds

model	*error in drag*	*cost, core-hours*	*Newton iterations per time step*
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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Overview

Goal: exploit temporal-behavior data to reduce temporal complexity

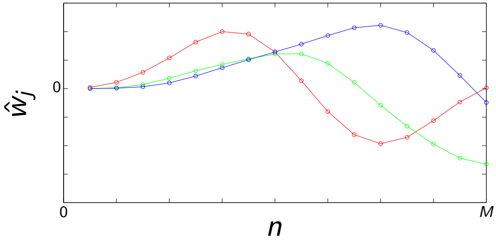
1. during ROM simulation, apply gappy POD *in the time domain* to generate a forecast for the generalized unknowns
2. use the forecast as an *accurate initial guess* for the Newton-like solver

+ good guess $\rightarrow$ few Newton its $\rightarrow$ low temporal complexity
+ introduces *no additional error*

Offline: compute time-evolution POD bases Ψ_j

1. collect snapshots of the *temporal behavior* of the jth generalized unknown:

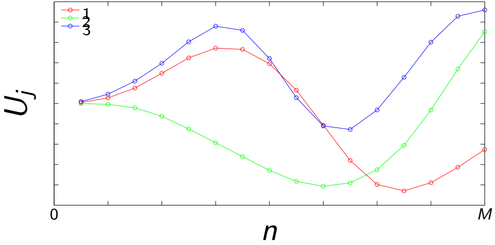
$$\hat{w}_j^n(\mu), \quad n = 1, \ldots, M, \ \mu \in \{\bar{\mu}_i\}_{i=1}^{n_{\text{train}}}$$



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

Offline: compute time-evolution POD bases Ψ_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

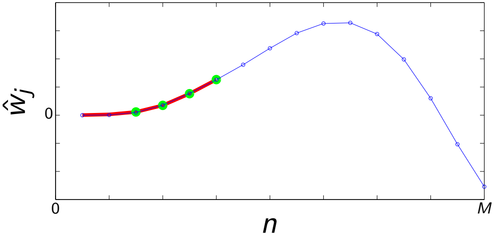
Here, the time-evolution bases Ψ_j are the *right singular vectors* generated when computing Φ:

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

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

Online: compute forecast, use as initial guess

1. compute forecast by gappy POD in time domain: match generalized unknowns at previous α time steps



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

$$z_j = \arg\min_{z \in \mathbb{R}^{a_j}} \left\| \begin{bmatrix} \Psi_j(n-\alpha, 1) & \cdots & \Psi_j(n-\alpha, a_j) \\ \vdots & \ddots & \vdots \\ \Psi_j(n-1, 1) & \cdots & \Psi_j(n-1, a_j) \end{bmatrix} z - \begin{bmatrix} \hat{w}_j^{n-\alpha} \\ \vdots \\ \hat{w}_j^{n-1} \end{bmatrix} \right\|_2^2$$

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

Online algorithm sketch

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

- many Newton iterations: heuristic for poor forecast

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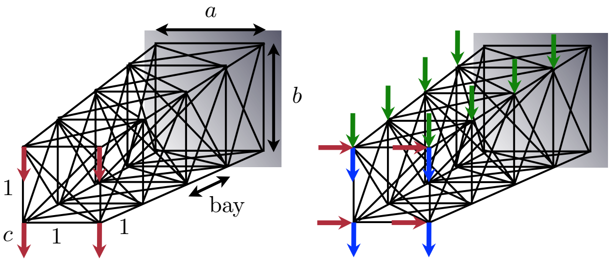
Clamped-free truss structure, geometric nonlinearity

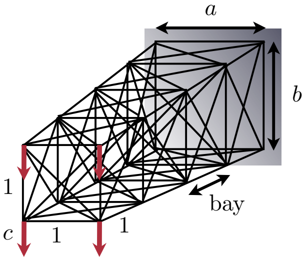


(a) initial displacement (red) (b) external forces

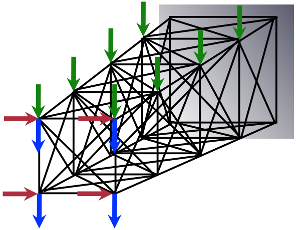
$$M(\mu)\ddot{x} + C(\mu)\dot{x} + f^{\text{int}}(x;\mu) = f^{\text{ext}}(t;\mu)$$

- M: mass matrix
- $C = \alpha M + \beta \nabla_x f^{\text{int}}(x^0)$: Rayleigh damping matrix
- f^{int}: internal force, *nonlinear in x*
- f^{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



(c) initial displacement (red)



(d) external forces

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

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

2. Galerkin projection + collocation

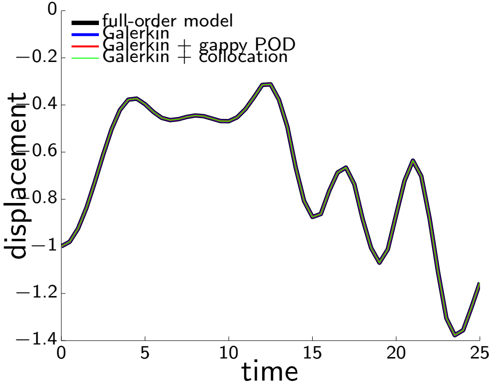
$$\Phi^T Z^T Z\left(M(\mu)\ddot{\hat{x}} + C(\mu)\Phi\dot{\hat{x}} + f^{\text{int}}\left(x^0(\mu) + \Phi\hat{x};\mu\right) - f^{\text{ext}}(t;\mu)\right) = 0$$

3. Galerkin projection + gappy POD approximation of residual

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

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

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



- all responses nearly exact (as expected)

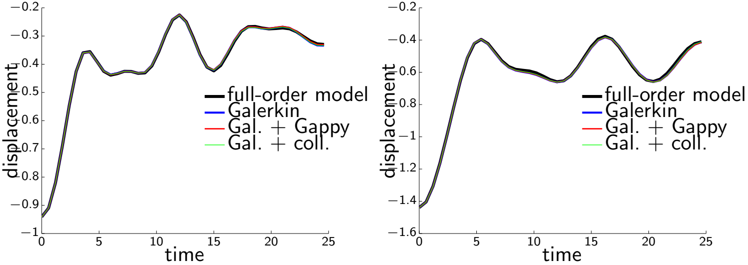
Case 1: forecasting drastically improves performance

ROM method	relative error	total Newton its		wall-time speedup	
		no forecast	forecast	no forecast	forecast
Galerkin	8.64×10^{-12}	99	2	1.01	1.84
Gal + Gappy	8.64×10^{-12}	99	2	36.4	69.3
Gal + coll	2.12×10^{-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%

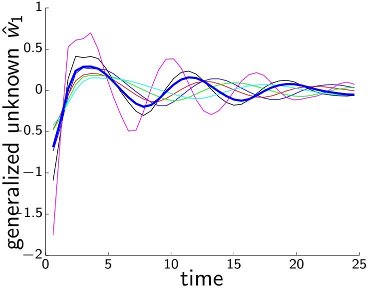
Case 2: forecasting improves performance by $\sim$ 60%

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

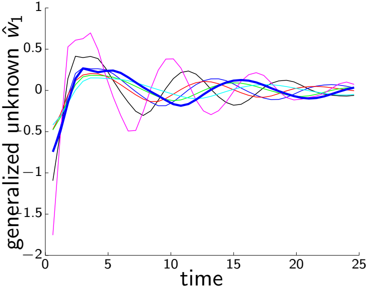
+ forecasting cuts Newton steps nearly in half
+ wall-time speedup increases by roughly 60%
- performance less impressive than ideal case

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



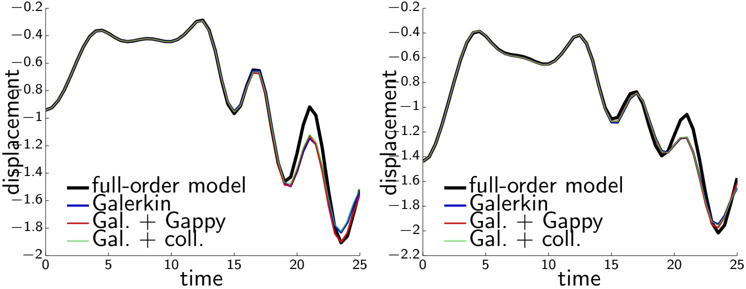
(h) online configuration 2

- 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%

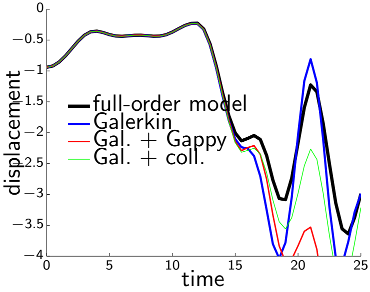
Case 3: forecasting improves performance by $\sim$ 50%

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

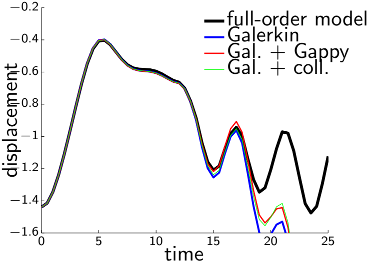
+ forecasting cuts Newton steps by 40%
+ wall-time speedup increases by roughly 50%
- performance again slightly worse (richer dynamics)

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

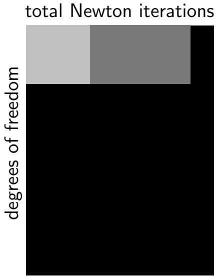
use temporal-behavior data to reduce ROM simulation time

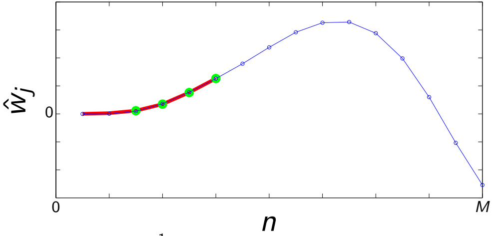
- offline: compute time-evolution bases
- online:
  1. use gappy POD to forecast generalized unknowns
  2. use forecast as initial guess in ROM Newton solver

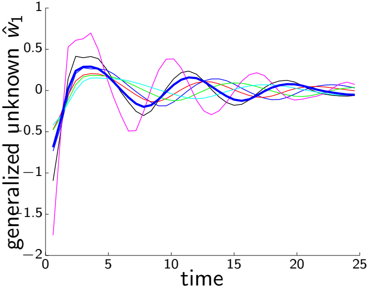
+ observed decrease in temporal complexity
+ observed decrease in ROM simulation wall time
+ no additional error introduced

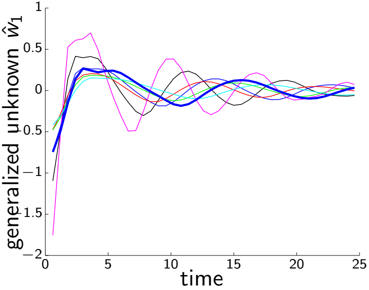
- best performance occurs in the case of:
  1. smooth dynamics (low frequency)
  2. temporal behavior similar across input variation
  3. accurate ROM
- **Reference**: K. Carlberg, J. Ray, and B. van Bloemen Waanders. 'Decreasing the temporal complexity for nonlinear, implicit reduced-order models by forecasting,' arXiv e-Print 1209.5455 (2012). (submitted to CMAME)

Questions?


total Newton iterations
degrees of freedom


$\hat{w}_j$
0
0
M
n


generalized unknown $\hat{w}_1$
time
1
0.5
0
−0.5
−1
−1.5
−2
0
5
10
15
20
25


generalized unknown $\hat{w}_1$
time
1
0.5
0
−0.5
−1
−1.5
−2
0
5
10
15
20
25

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