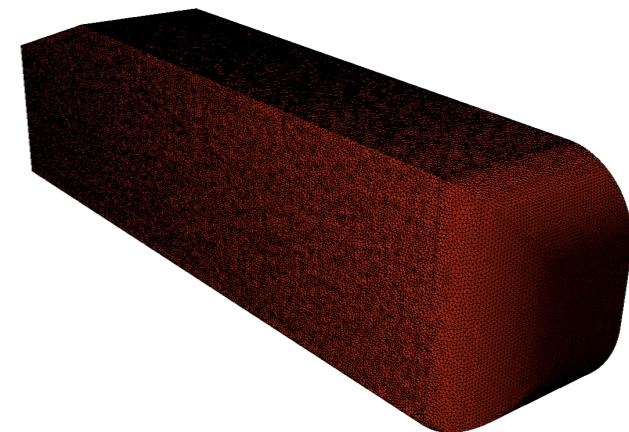
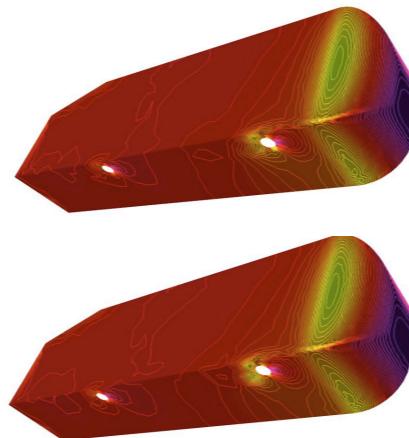
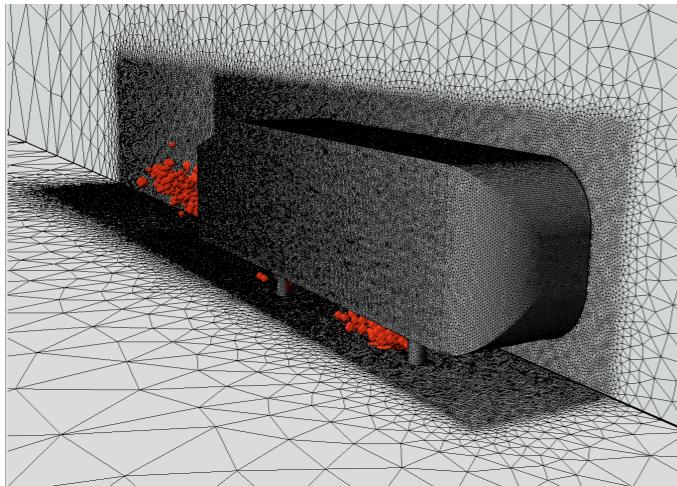


The GNAT Nonlinear Model-Reduction Method with Application to Large-Scale Turbulent Flows



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4th IWMRRF
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The punchline

- **Goal:** practical model reduction for large-scale nonlinear ODEs
- **Problem:** POD–Galerkin often fails
 - lacks *discrete optimality*
- **New method:** GNAT model reduction
 - *discrete-optimal* approximations
 - effective ‘sample mesh’ implementation
 - works on large-scale problems

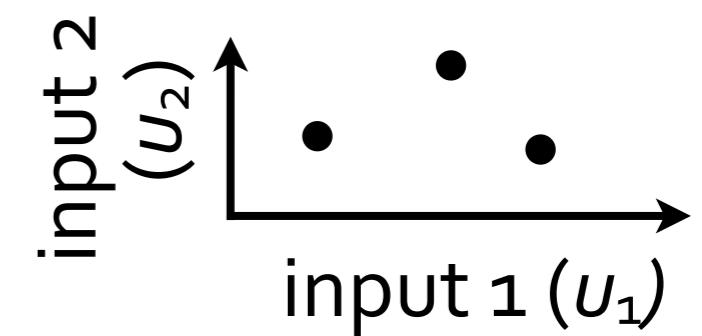
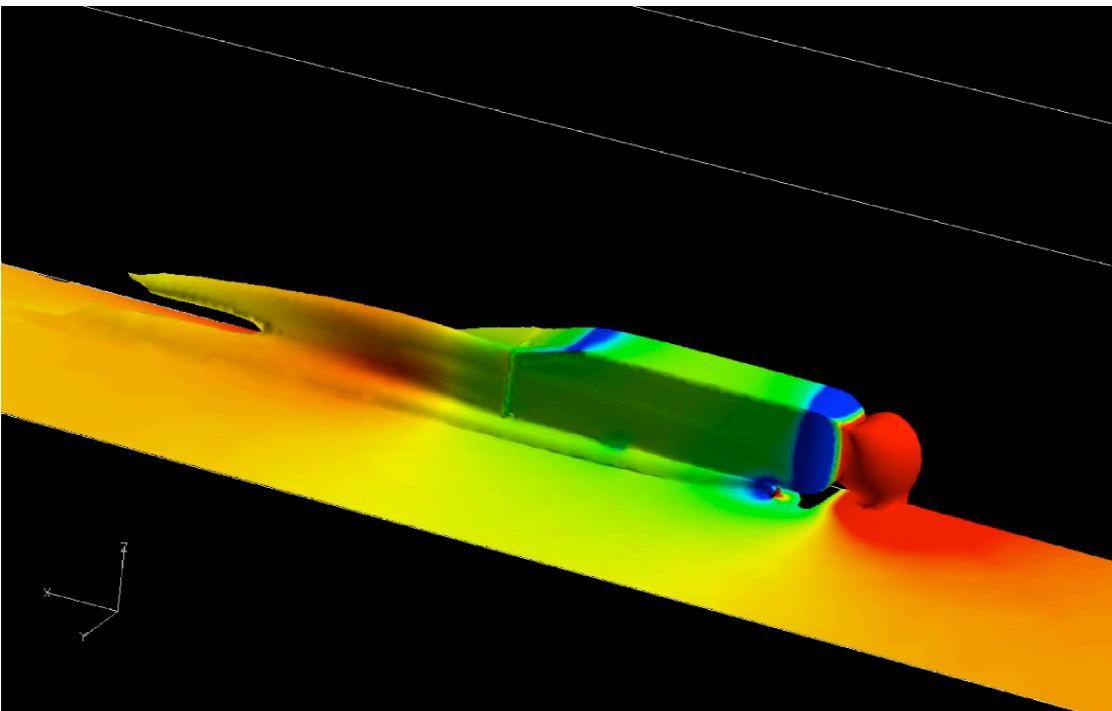


POD–Galerkin

step 1: training (expensive)

$$\dot{y} = f(y; t, u)$$

1. Collect snapshots of the state vector



2. Compression
 - a. compute singular value decomposition

$$Y = U \Sigma V^T$$

b. truncate

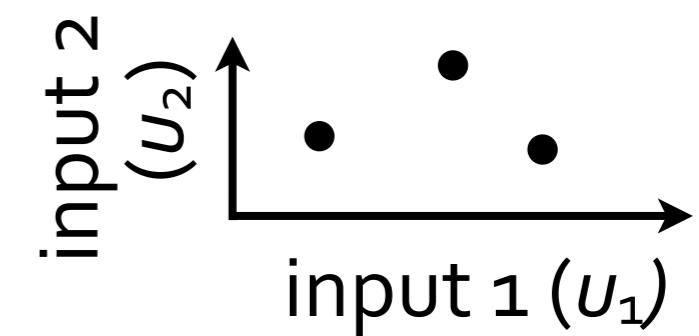
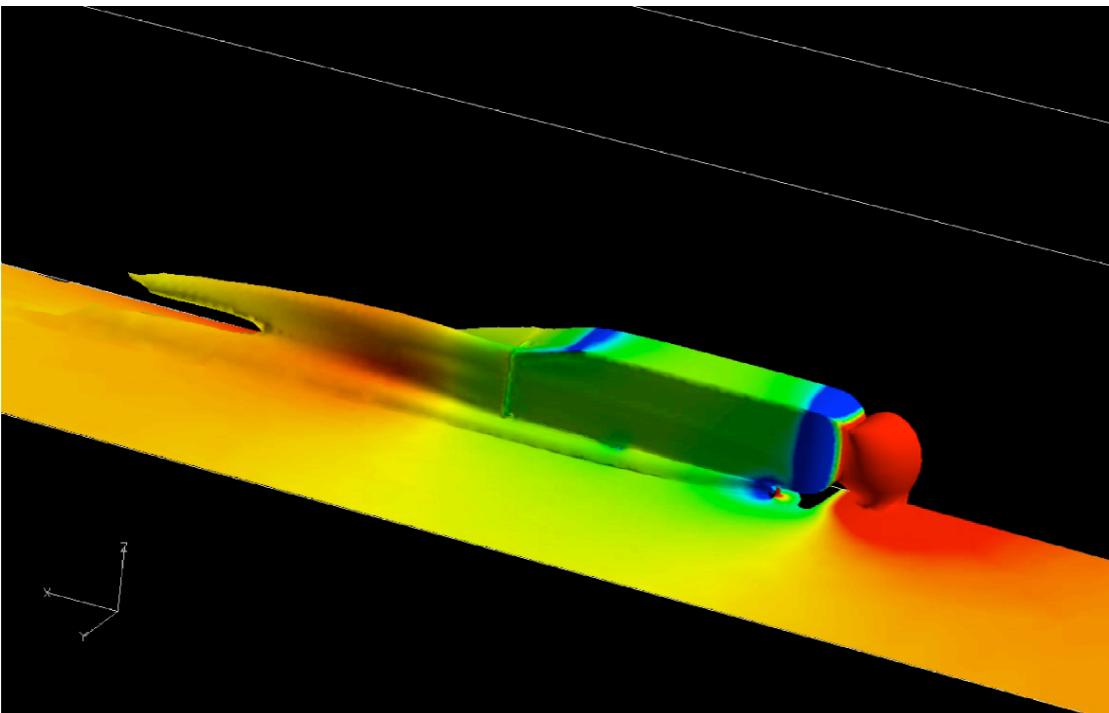
$$U$$

POD–Galerkin

step 1: training (expensive)

$$\dot{y} = f(y; t, u)$$

1. Collect snapshots of the state vector



2. Compression
 - a. compute singular value decomposition

$$Y = U \Sigma V^T$$

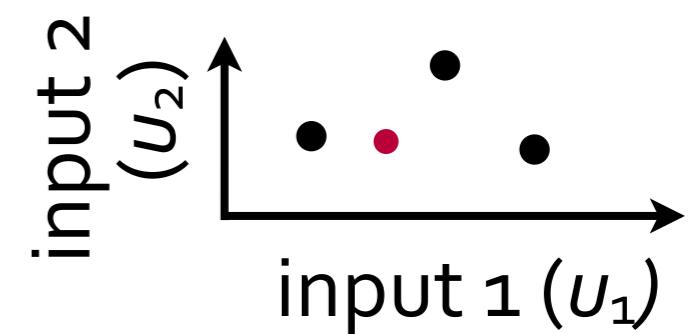
b. truncate Φ



POD–Galerkin

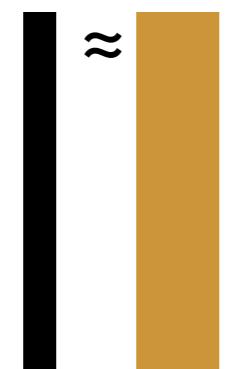
step 2: Galerkin projection (cheap)

$$\dot{y} = f(y; t, u)$$



reduce # unknowns

$$y \approx \Phi y_r$$



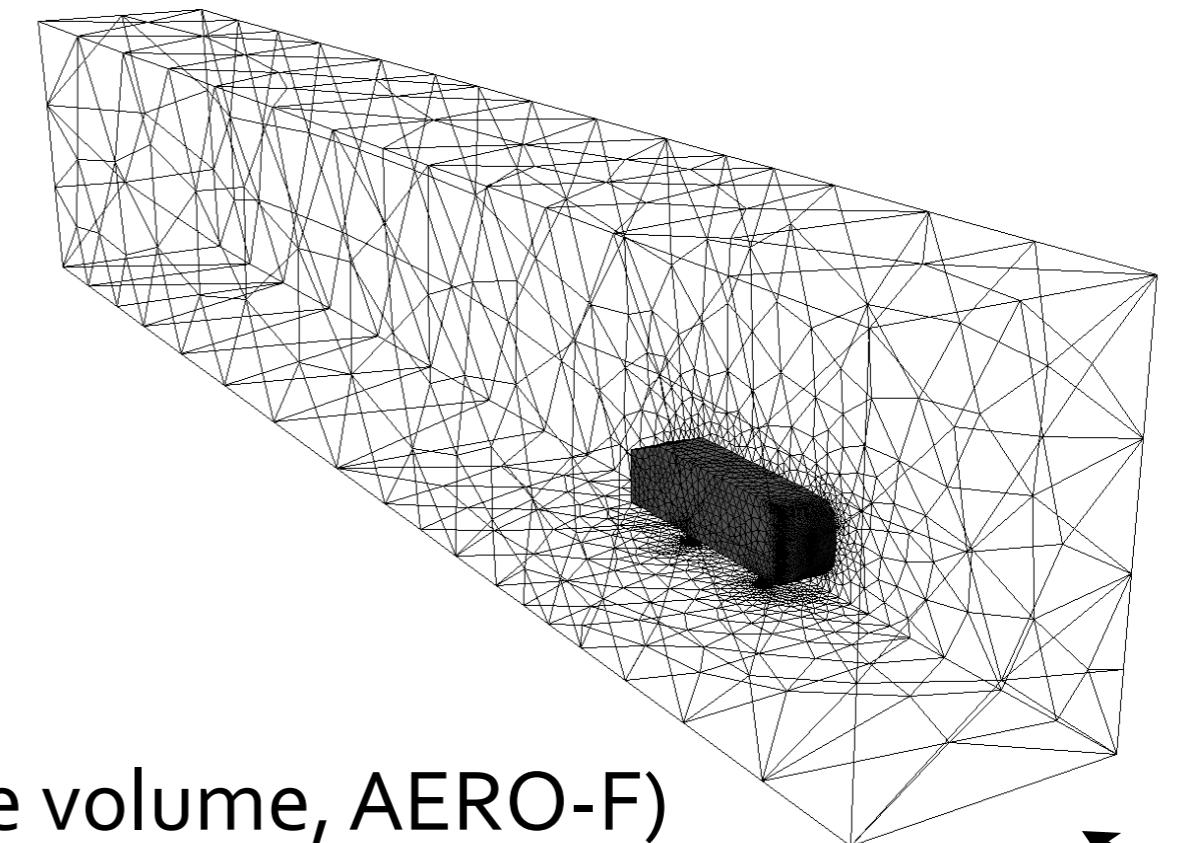
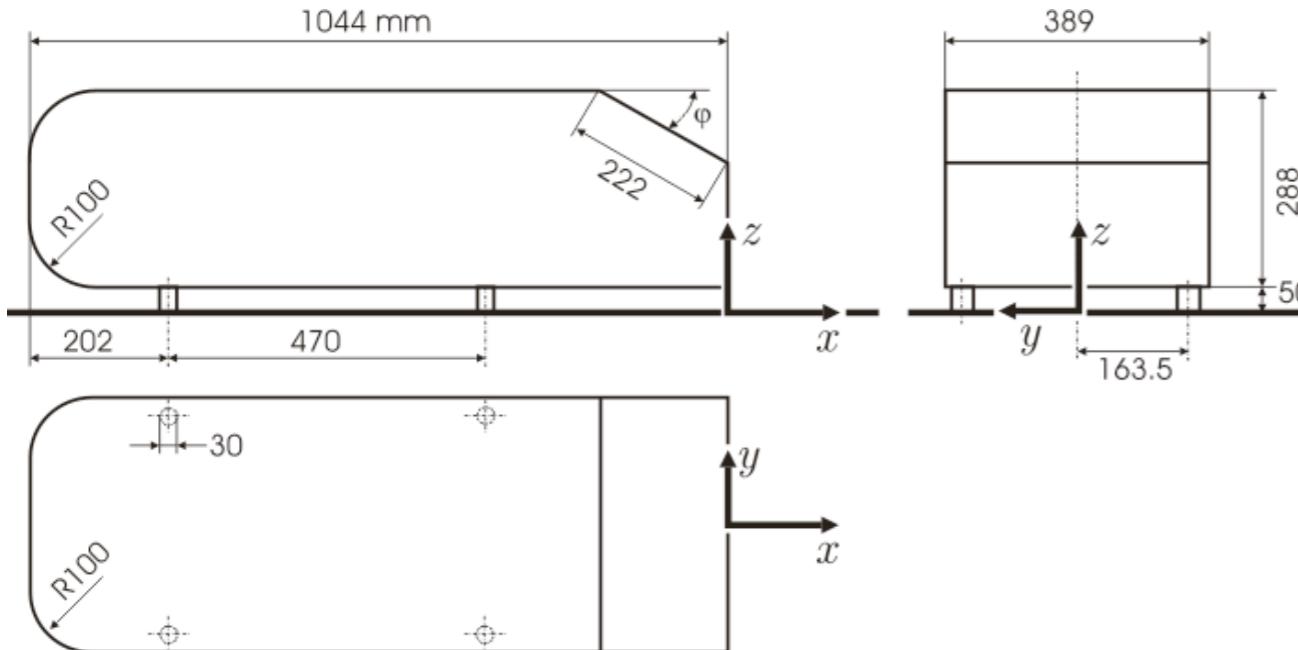
reduce # equations

$$\Phi^T [\dot{y} - f(y; t, u)] = 0$$



$$\dot{y}_r = \Phi^T f(\Phi y_r; t, u)$$

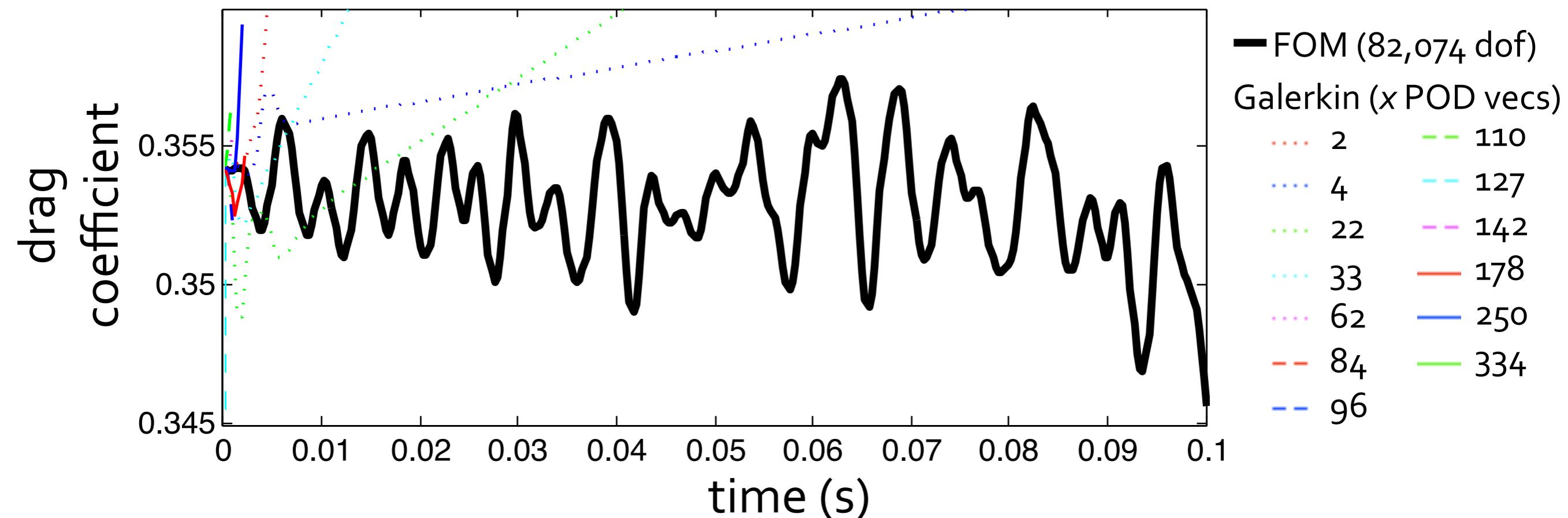
Benchmark: Ahmed body



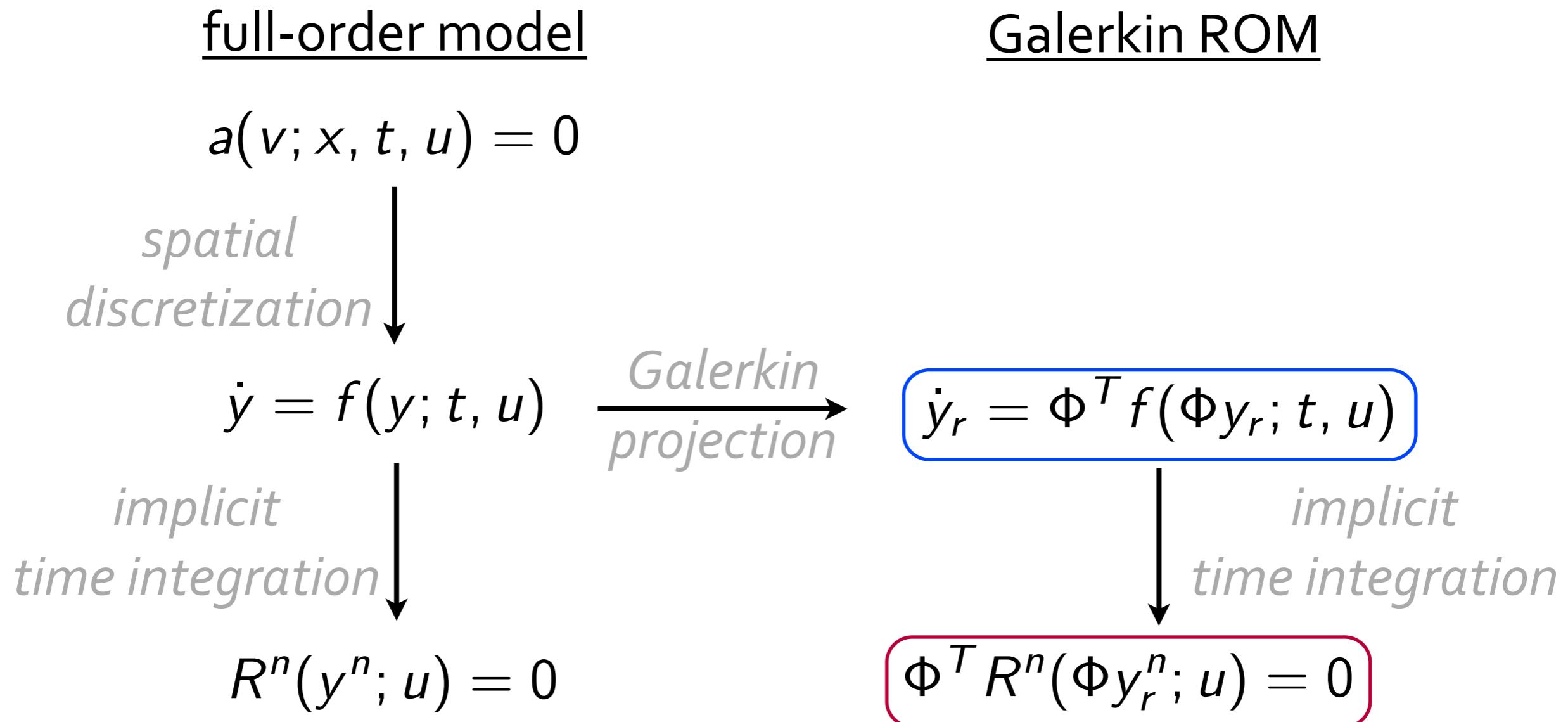
- Compressible Navier-Stokes (finite volume, AERO-F)

- Re = 4.48×10^6
- $M_\infty = 0.175$ (134 mph)
- steady-state initial condition
- 2nd order flux reconstruction
- DES turbulence model
- Spalart–Allmaras RANS
- $\Delta t = 3 \times 10^{-4}$
- 82,074** degrees of freedom (dof)

POD–Galerkin is unstable



Galerkin projection: not 'discrete optimal'

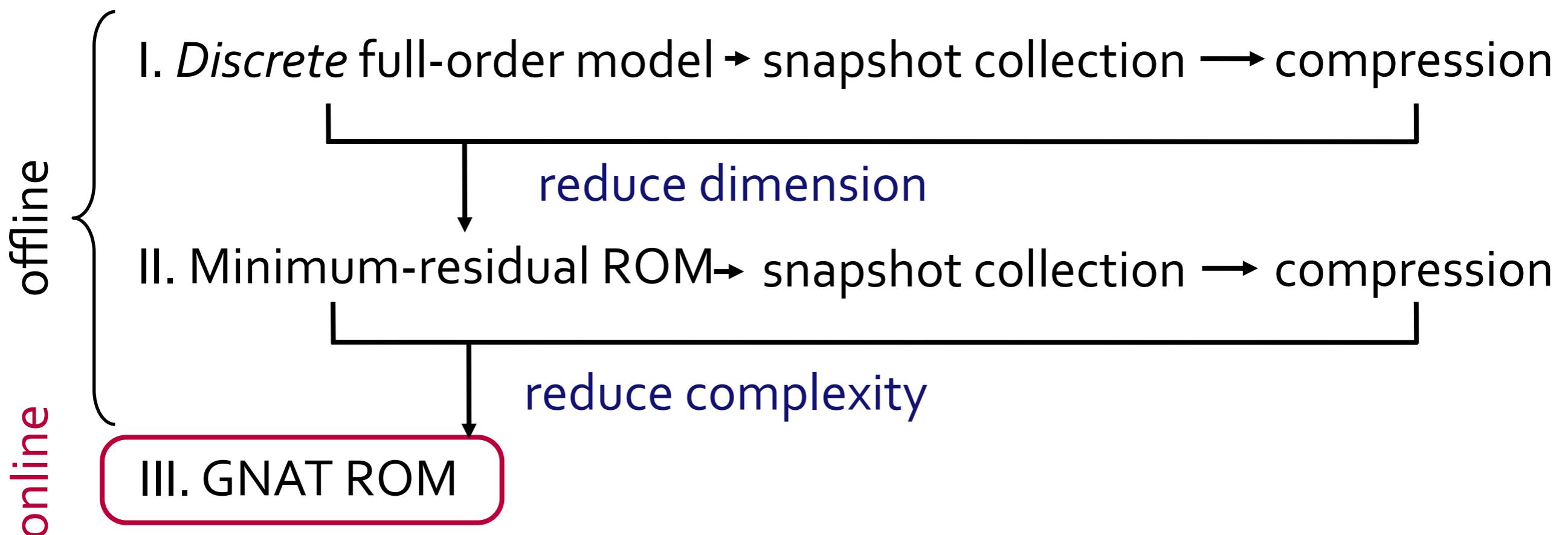


+ Semi-discrete optimal: $\Phi \dot{y}_r = \arg \min_{x \in \text{range}(\Phi)} \|\dot{y} - x\|_2$

- Not discrete optimal: $\begin{cases} \Phi \dot{y}_r \neq \arg \min_{x \in \text{range}(\Phi)} \|y^n - x\| \\ \Phi y_r^n \neq \arg \min_{x \in \text{range}(\Phi)} \|R^n(x)\| \end{cases}$

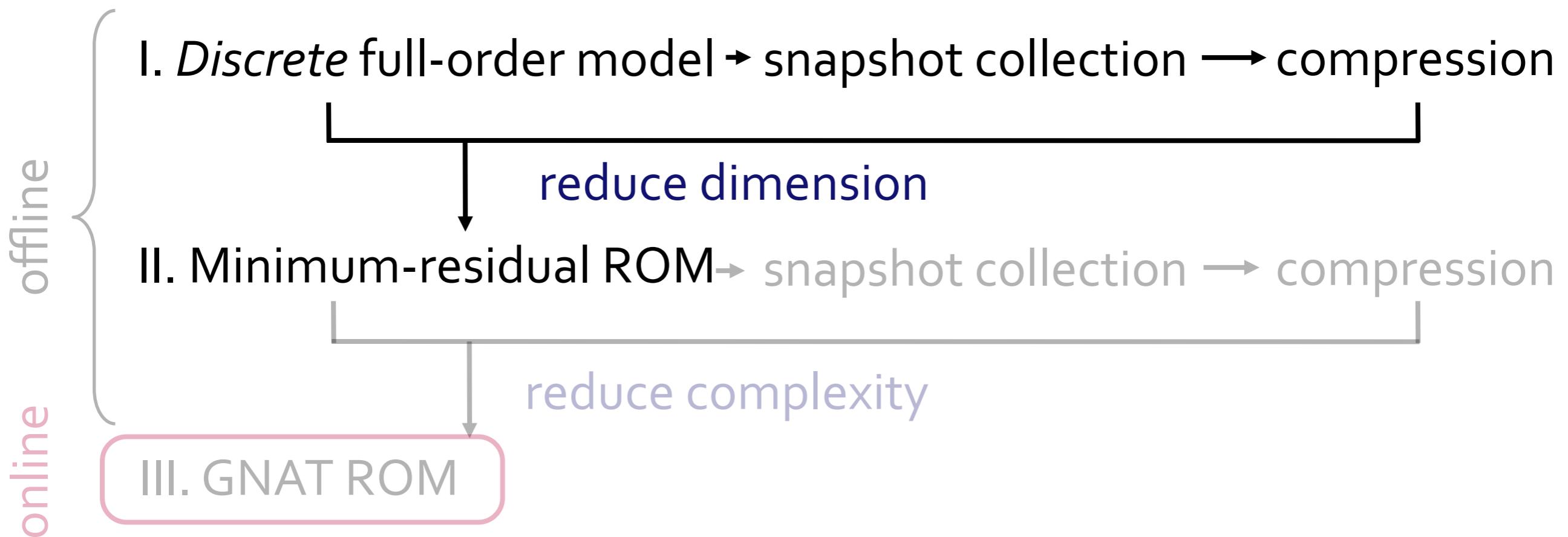
GNAT strategy

- Discrete-optimal approximations



GNAT strategy

- Discrete-optimal approximations



Minimum-residual ROM is discrete optimal

Minimum-residual ROM

not defined

full-order model

$$a(v; x, t, u) = 0$$

*spatial
discretization*



$$\dot{y} = f(y; t, u) \rightarrow$$

$$\dot{y}_r = \Phi^T f(\Phi y_r; t, u)$$

*implicit
time integration*

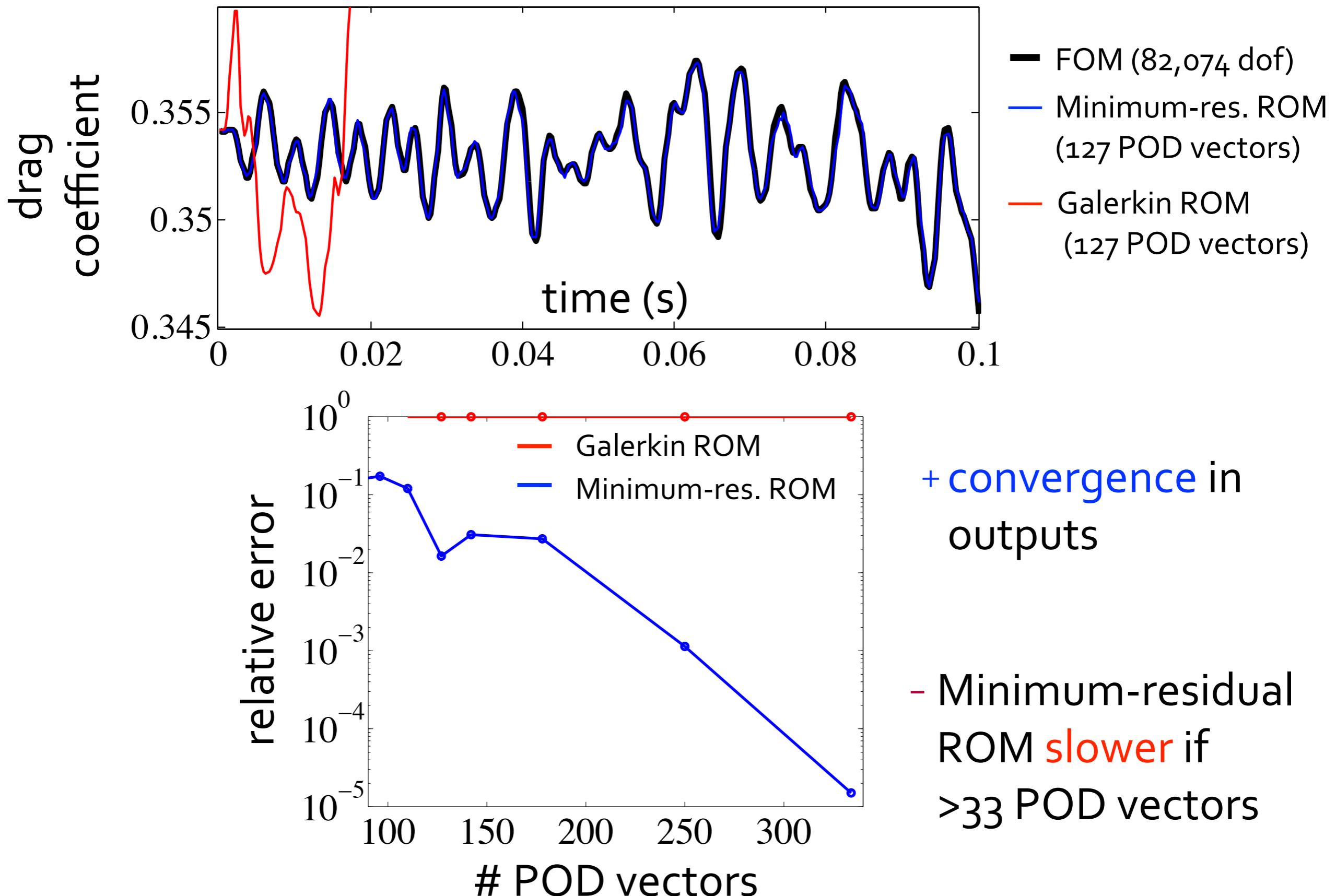


$$y_r^n = \arg \min_x \|R^n(\Phi x; u)\|_2 \leftarrow R^n(y^n; u) = 0$$

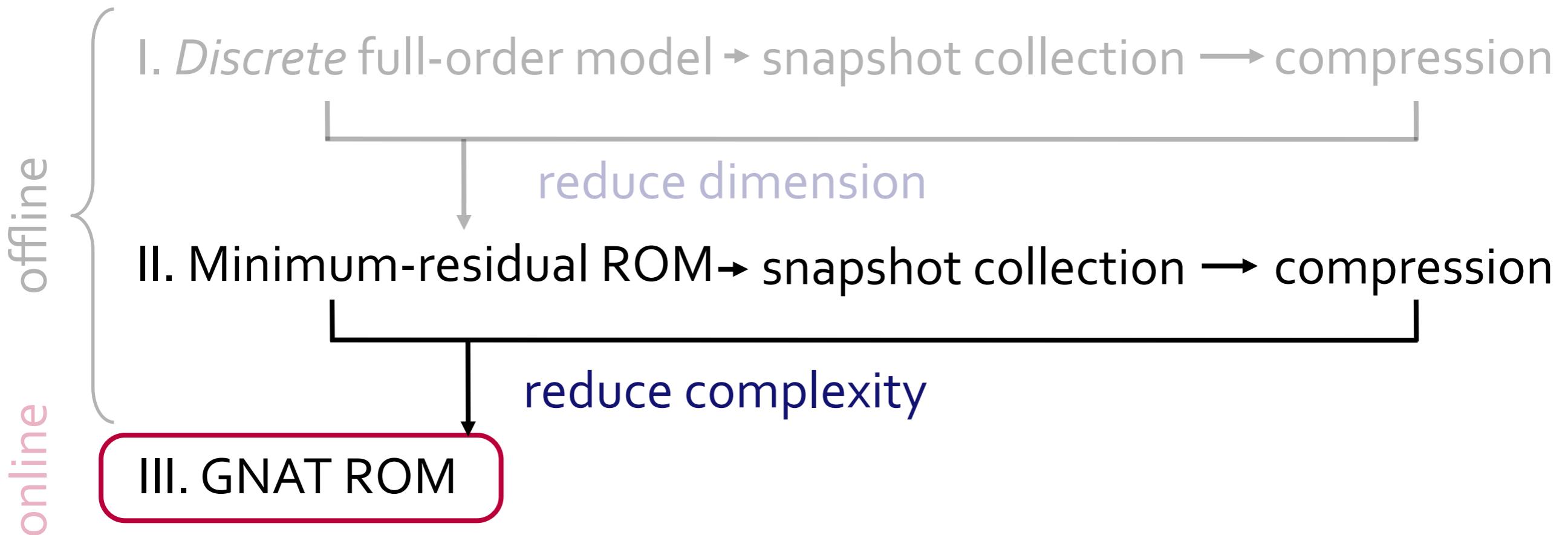
$$\Phi^T R^n(\Phi y_r^n; u) = 0$$

- + Discrete optimal
- Not defined at the semi-discrete level
- Other least-squares ROM methods: Legresley & Alonso, 2001;
Bui-Thanh, *et al.* 2008; Constantine & Wang, 2012

Minimum-residual ROM is accurate



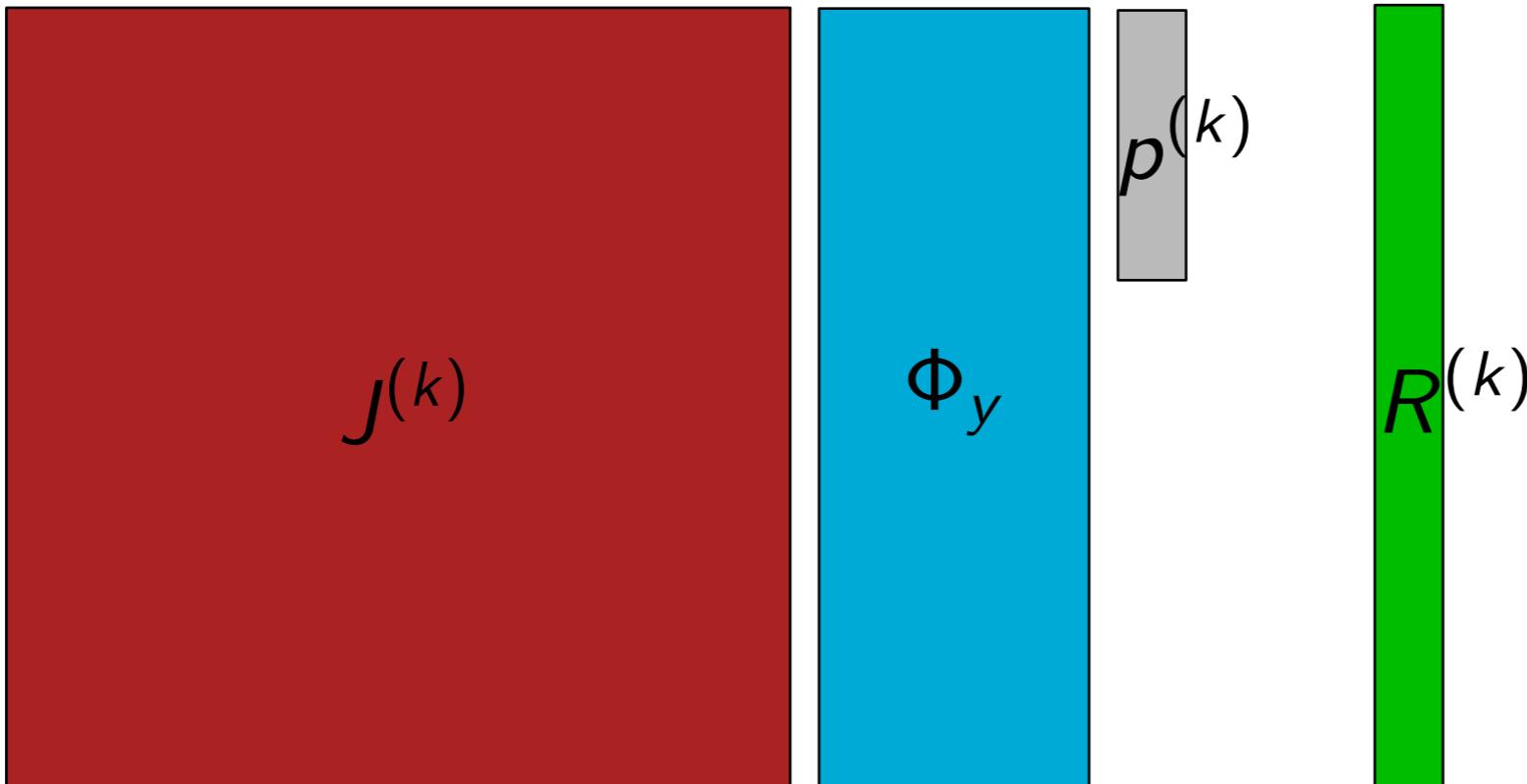
GNAT strategy



Low dimension \neq low cost

- Minimum-residual ROM iterations are

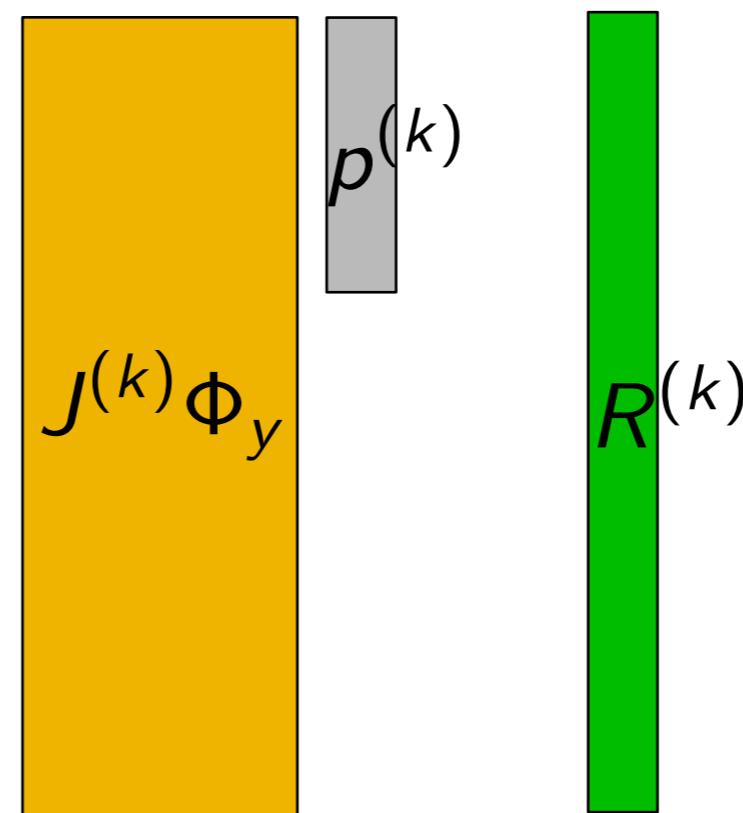
$$\underset{p^{(k)}}{\text{minimize}} \| J^{(k)} \Phi_y p^{(k)} + R^{(k)} \|_2$$



Low dimension \neq low cost

- Minimum-residual ROM iterations are

$$\underset{p^{(k)}}{\text{minimize}} \| J^{(k)} \Phi_y p^{(k)} + R^{(k)} \|_2$$



- Large operation count **even though** $p^{(k)}$ is low-dimensional!

- Goal: approximate $R^{(k)}$
- Given: i) basis Φ_R
ii) a few sampled entries of $R^{(k)}$

$$R^{(k)} = \begin{array}{c} \text{[Color-coded matrix]} \\ \vdots \\ \text{[Color-coded matrix]} \end{array}$$

$$\Phi_R = \begin{array}{c} \text{[Color-coded matrix]} \\ \vdots \\ \text{[Color-coded matrix]} \end{array}$$

1. Least squares minimization
on sampled entries

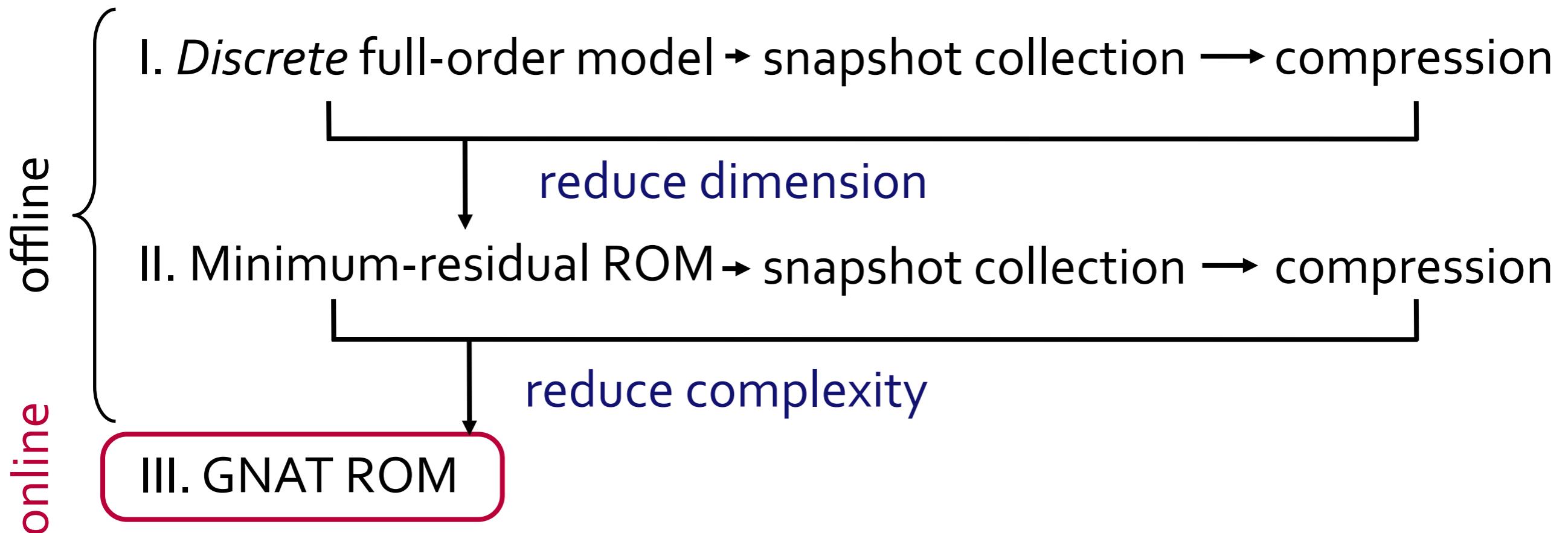
$$x^* = \arg \min_{x \in \mathbb{R}^p}$$

$$\left\| \begin{array}{c} \text{[Color-coded matrix]} \\ \vdots \\ \text{[Color-coded matrix]} \end{array} - \begin{array}{c} x \\ \vdots \\ x \end{array} \right\|_2^2$$

2. Reconstruct all entries:

$$R^{(k)} \approx \begin{array}{c} \text{[Color-coded matrix]} \\ \vdots \\ \text{[Color-coded matrix]} \end{array} \Phi_R \begin{array}{c} x^* \\ \vdots \\ x^* \end{array}$$

- + Discrete optimality
- + Complexity reduction



GNAT = discrete-residual minimization + Gappy POD approximation

Error bound

- Assumptions:

1. backward Euler: $R^n(y^n; u) = y^n - y^{n-1} - \Delta t f(y^n; t^n, u)$
2. inverse Lipschitz continuity for $G : (y; t, u) \mapsto y - \Delta t f(y; t, u)$
3. full-order simulation convergence criterion: $\|R^n(y^n; u)\| \leq \epsilon$

Proposition [Carlberg et al., 2012]

The global error at time step n for **any sequence** $(y^0, \tilde{y}^1, \dots, \tilde{y}^{n_t})$ is

$$\|y^n - \tilde{y}^n\| \leq \sum_{k=0}^{n-1} a^k b_{n-k} \leq \sum_{k=0}^{n-1} a^k c_{n-k}$$

Proposition [Carlberg et al., 2012]

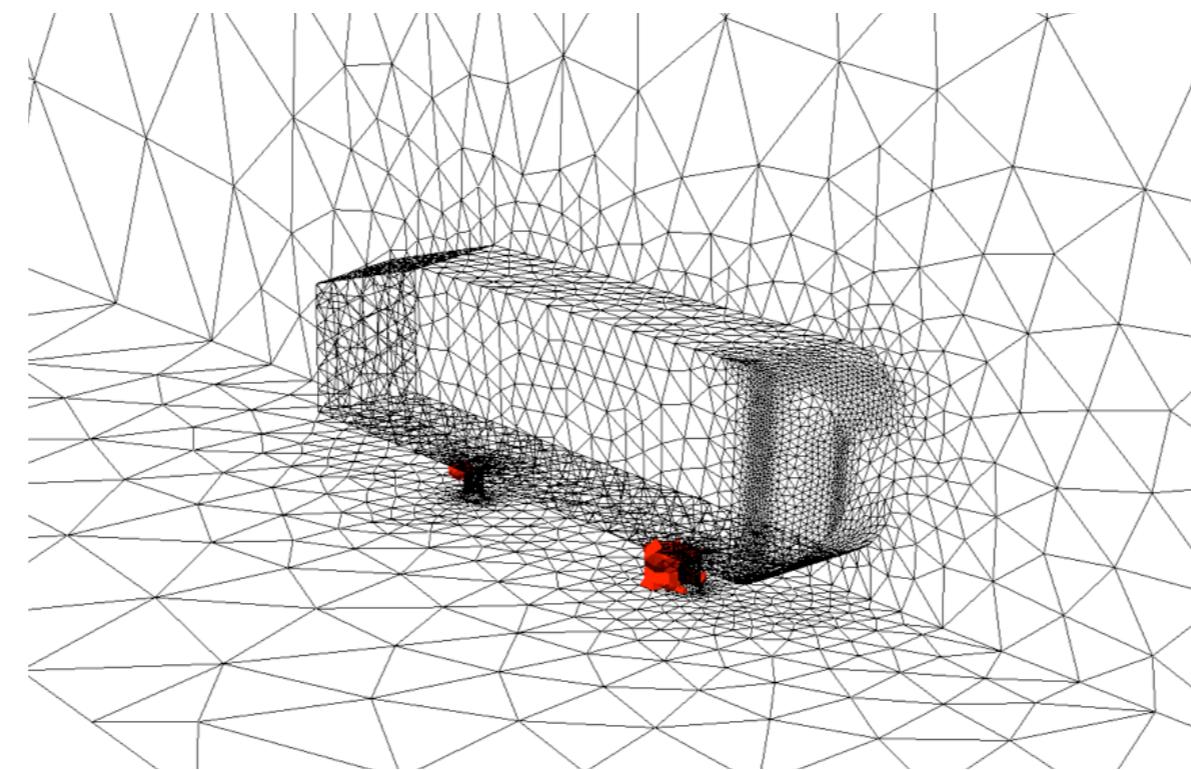
The global error at time step n for **any sequence** $(y^0, \tilde{y}^1, \dots, \tilde{y}^{n_t})$ is

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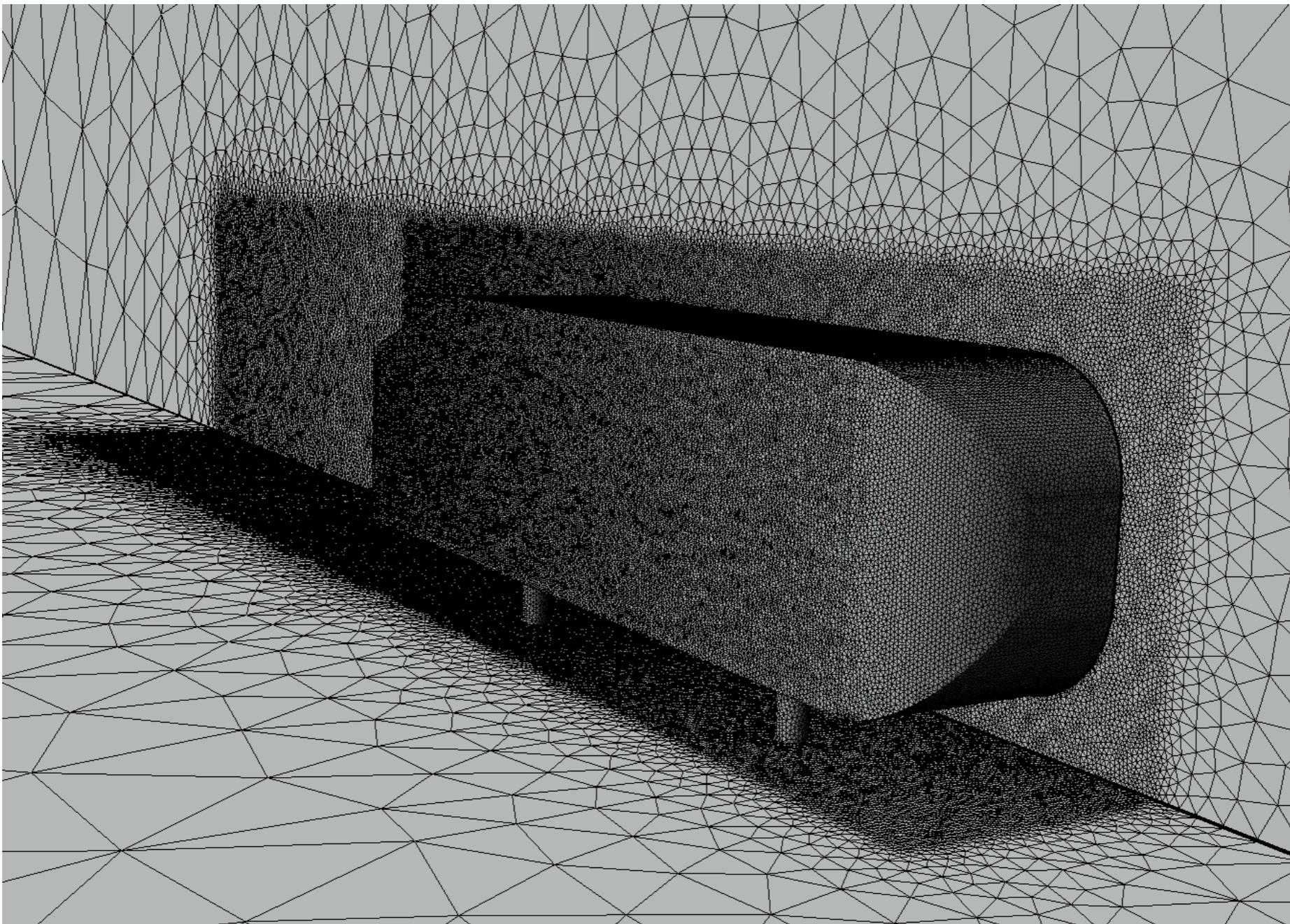
- a : inverse Lipschitz constant ‣ \tilde{R} : residual for sequence $\{\tilde{y}^n\}$
 - $b_n = \epsilon + \|\tilde{R}^n(\tilde{y}^n; u)\|$ ‣ P : Gappy POD operator
 - $c_n = \epsilon + \|P\tilde{R}^n(\tilde{y}^n; u)\| + \|(I - P)\tilde{R}^n(\tilde{y}^n; u)\|$
-
- + Minimum-residual ROM solutions minimize b_n
 - + GNAT solutions minimize $\|P\tilde{R}^n(\tilde{y}^n; u)\|$
 - + sampling algorithm: heuristic for minimizing $\|(I - P)\tilde{R}^n(\tilde{y}^n; u)\|$
 - discrete optimality enables this!

Sample mesh implementation

- *Goals:*
 - reuse existing simulation codes
 - minimize computing cores
 - scalability
- *Key:* GNAT samples only **a few** entries of the residual
- *Idea:* extract minimal subset of mesh

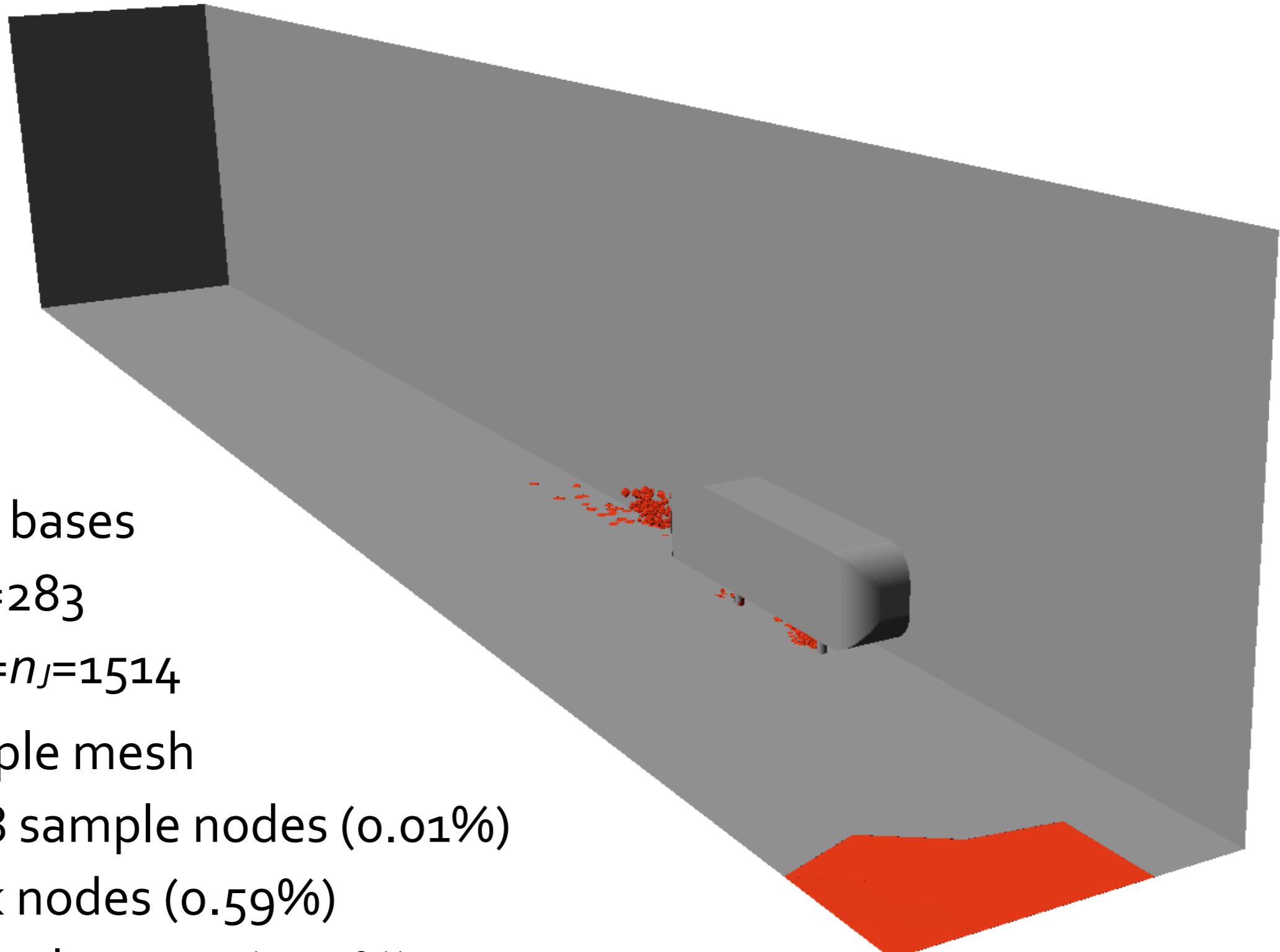


Example: Ahmed body (fine mesh)



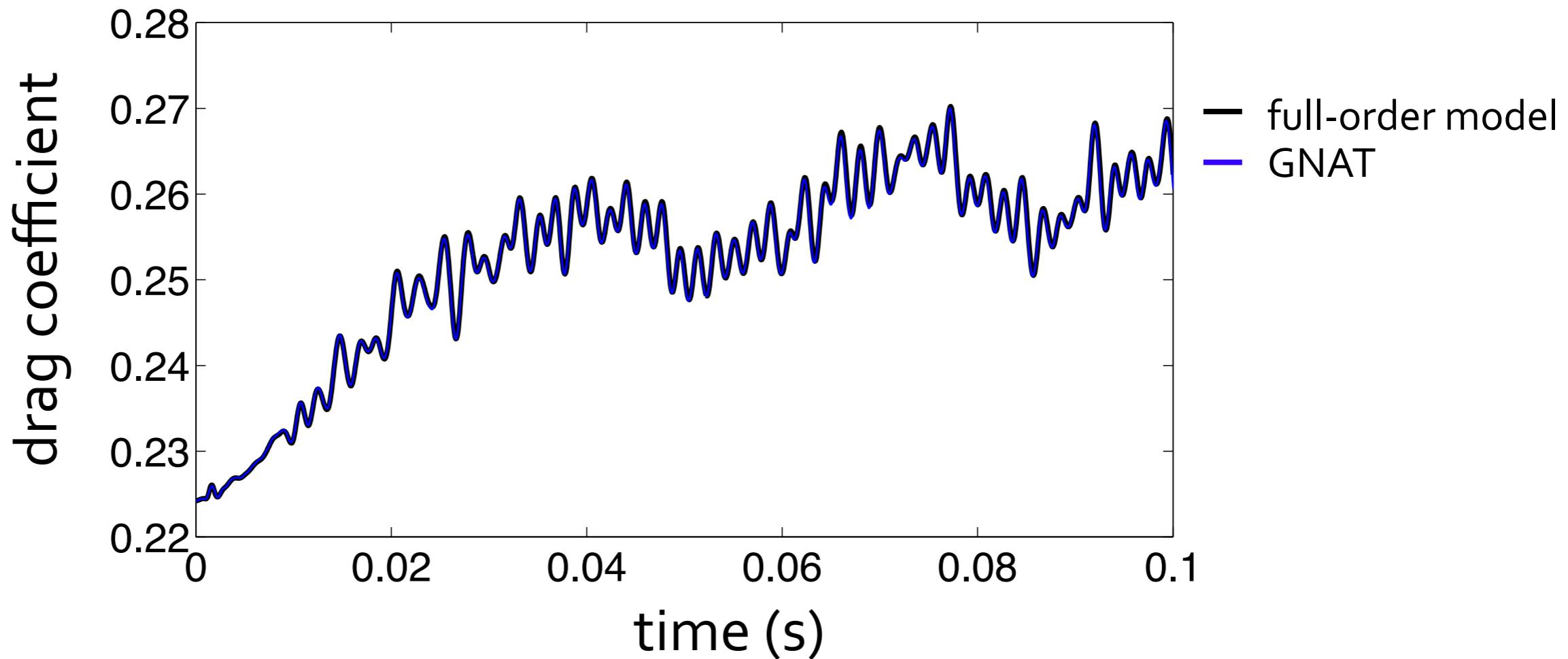
- 2.89×10^6 nodes, 1.70×10^7 tetrahedral volumes
- 1.73×10^7 degrees of freedom

GNAT model



- POD bases
 - $n_y=283$
 - $n_R=n_J=1514$
- Sample mesh
 - 378 sample nodes (0.01%)
 - 17k nodes (0.59%)
 - 56k elements (0.33%)

GNAT results: accurate and fast

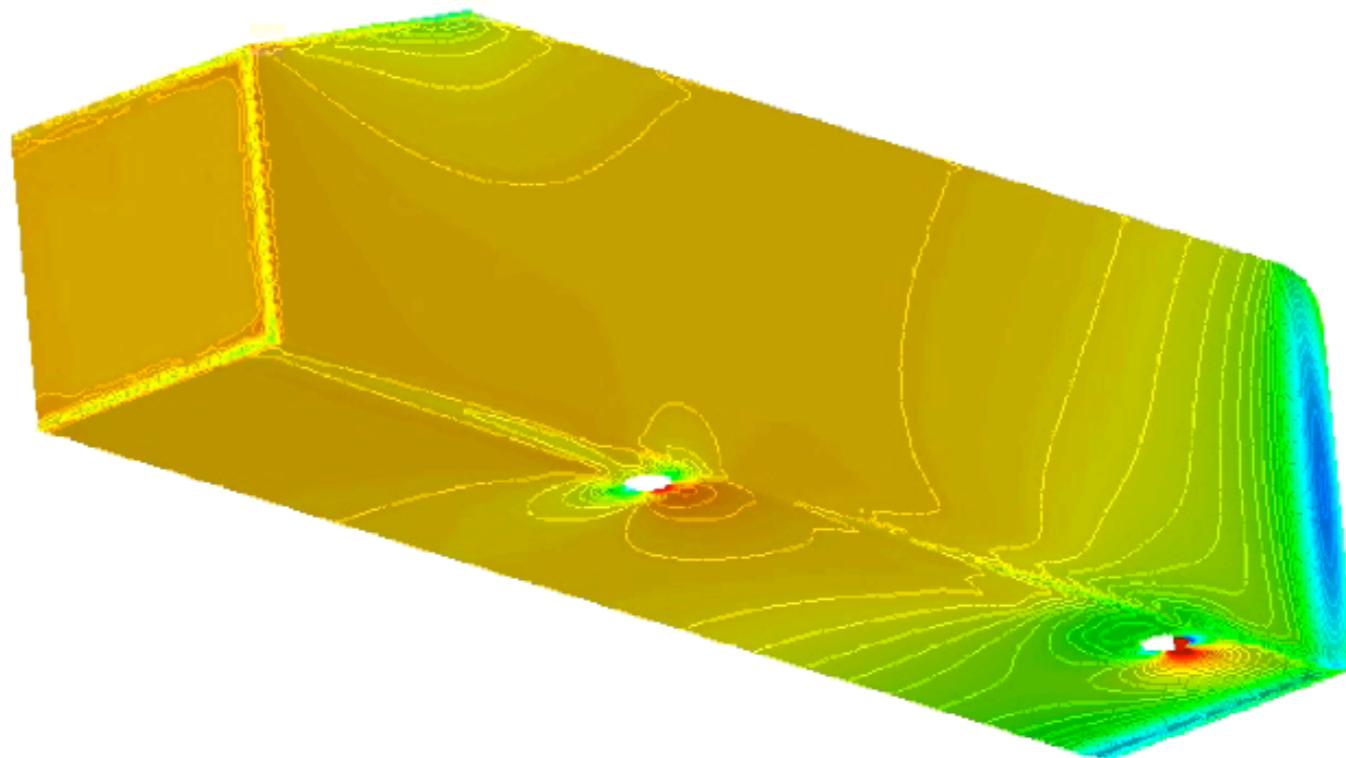


model	relative error	# cores	time, hours	speedup in cpu resources
FOM	-	512	13.3	-
GNAT	0.68%	4	3.88	438

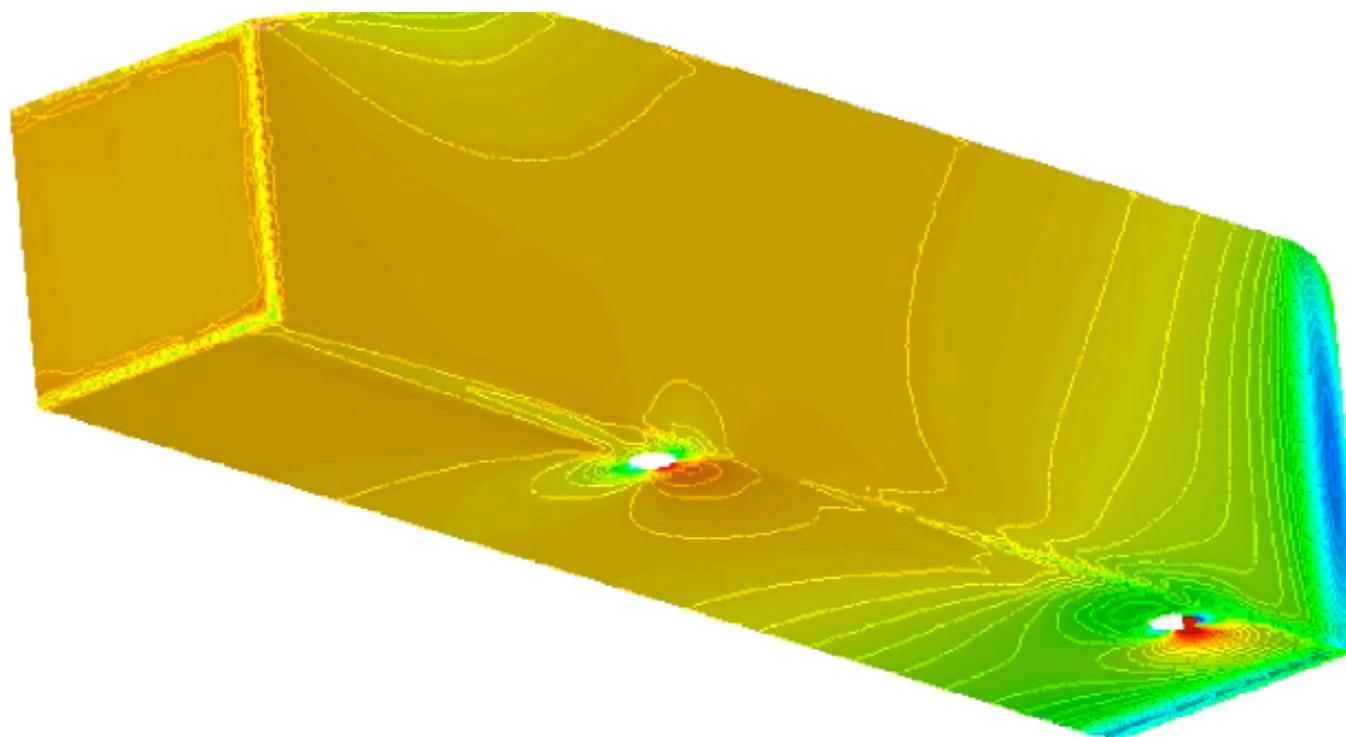
+ negligible error + wall-time decrease + supercomputer → desktop

GNAT results: accurate pressure contours

full-order
model

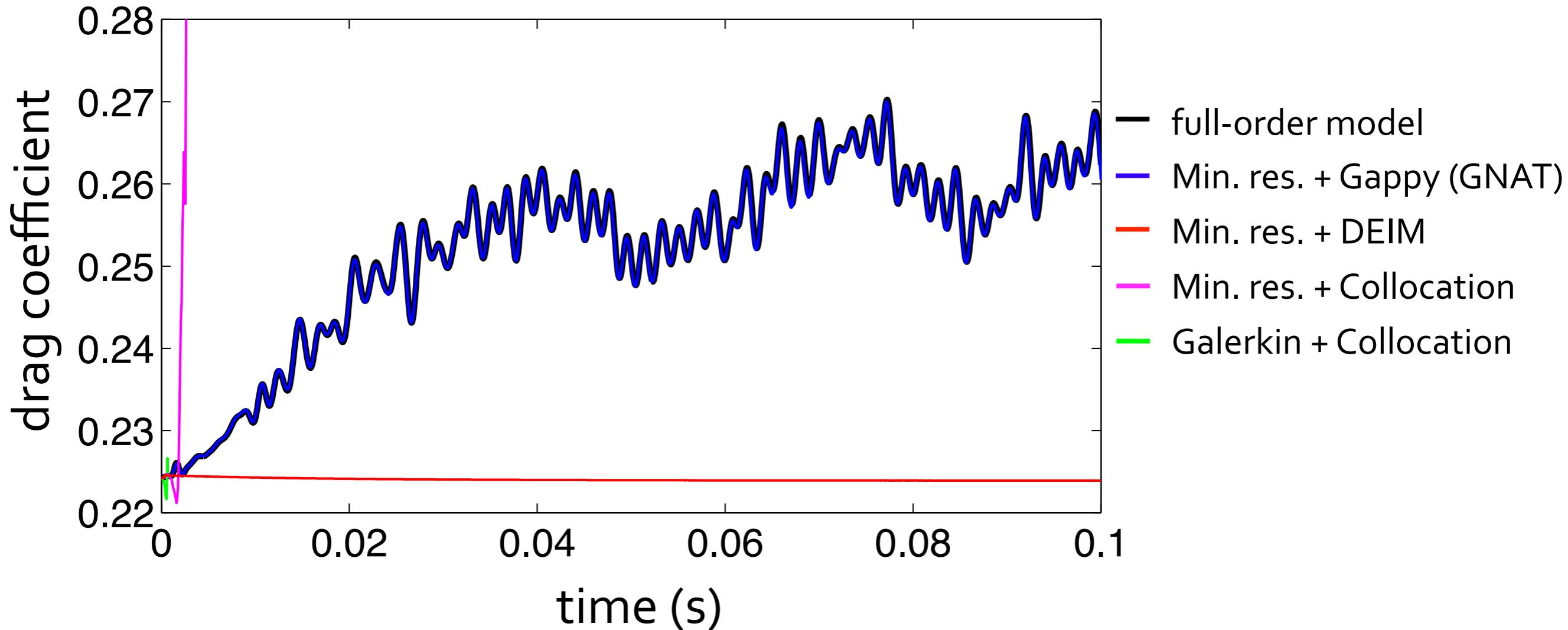


GNAT



GNAT performs better than other ROM methods

- Fixed POD basis and sample mesh (378 sample nodes)



- Galerkin ROM fails
 - discrete optimality important
- Gappy POD: only complexity-reduction method that works!

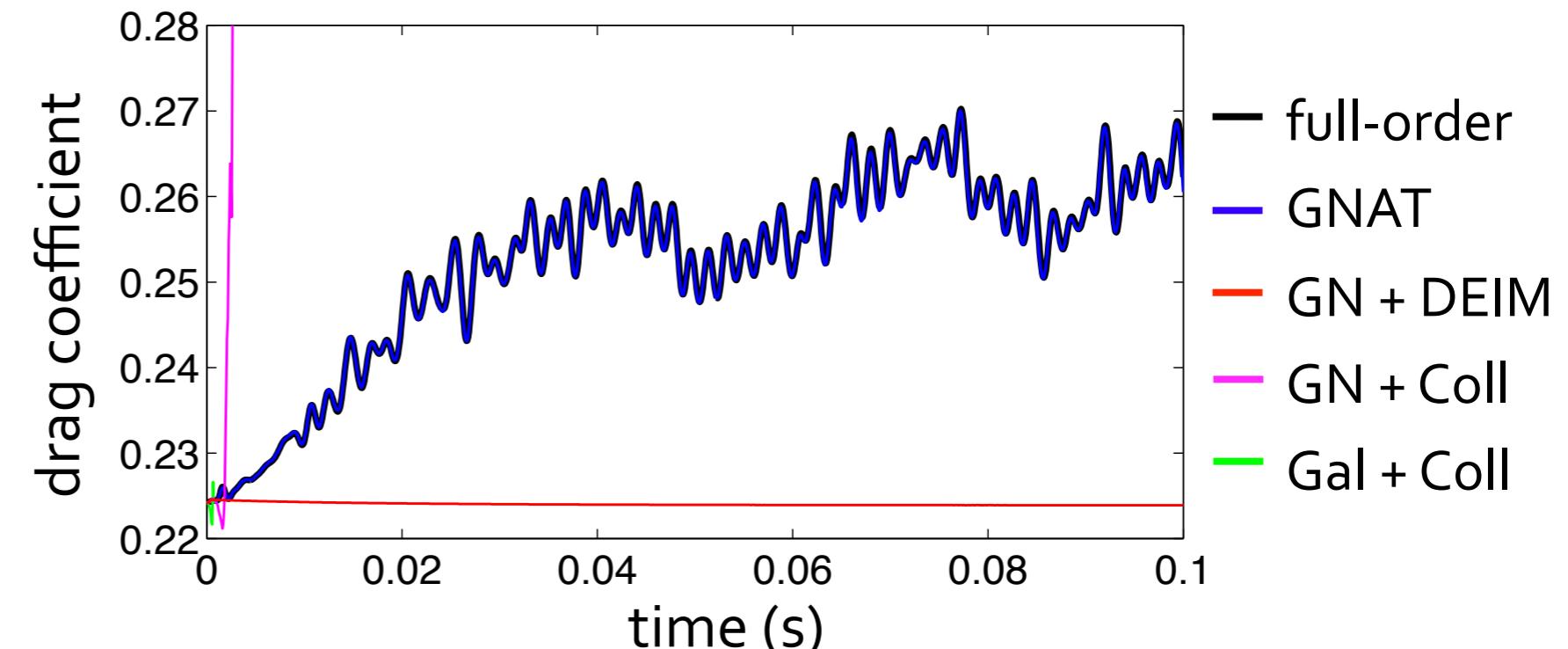
Summary

- GNAT method
 - ▶ discrete-optimal approximations
 - ▶ error bound justifies its design
- Sample mesh concept enables many fewer cores
 - ▶ supercomputer → desktop
- Ahmed body example
 - ▶ speedups over 400, error less than 1%
 - ▶ other model-reduction methods failed
- Key papers: sandia.gov/~ktcarlb
 - ▶ K. Carlberg, C. Bou-Mosleh, and C. Farhat. "Efficient non-linear model reduction via a least-squares Petrov–Galerkin projection and compressive tensor approximations," International Journal for Numerical Methods in Engineering, Vol. 86, No. 2, p. 155–181 (2011).
 - ▶ K. Carlberg, C. Farhat, J. Cortial, and D. Amsallam. "The GNAT method for nonlinear model reduction: Effective implementation and application to computational fluid dynamics and turbulent flows," Journal of Computational Physics, Vol. 242, p. 623–647 (2013).

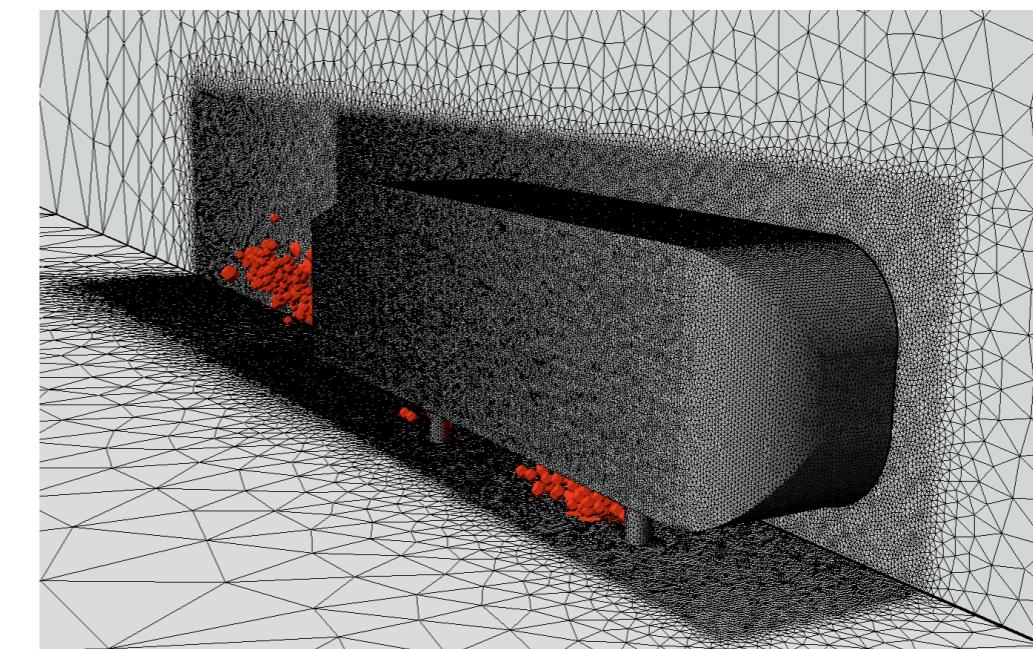
Current model-reduction @ Sandia

1. Preserve classical Hamiltonian/Lagrangian structure [Tuminaro, Boggs]
 - *Goal:* preserve key properties (e.g., energy conservation)
 - Structural dynamics, molecular dynamics
2. Decrease temporal complexity via forecasting [Ray, van Bloemen Waanders]
 - *Goal:* decrease wall-time for nonlinear ROM simulation
 - Exploit temporal data to reduce total # Newton its
3. Integrate ROMs within a UQ framework [Drohmann]
 - *Goal:* quantify epistemic uncertainty due to ROM
 - Error bounds (i.e., ‘certification’) not useful in UQ
4. ROM interface for Trilinos-based simulation codes [Cortial]
 - *Goal:* easily apply nonlinear ROM methods to codes
 - non-intrusive Trilinos-based ROM module

- Key collaborators
 - Charbel Farhat
 - Julien Cortial
 - David Amsallem



- Funding
 - NSF Graduate Fellowship
 - Toyota Motor Corporation
 - Army Research Laboratory
 - Truman Fellowship program*



* Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.