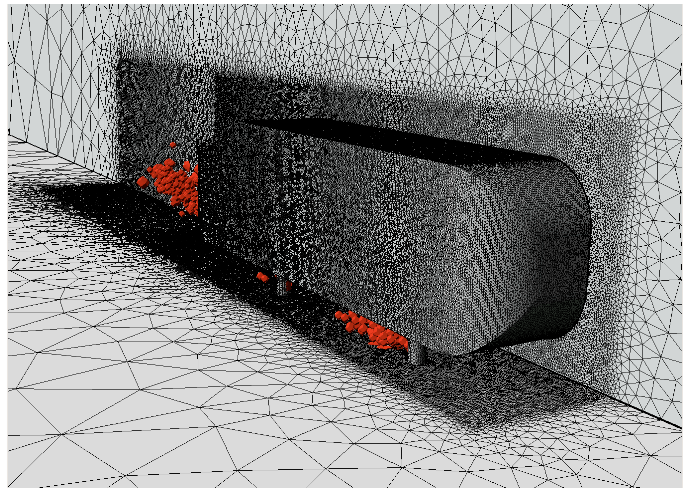
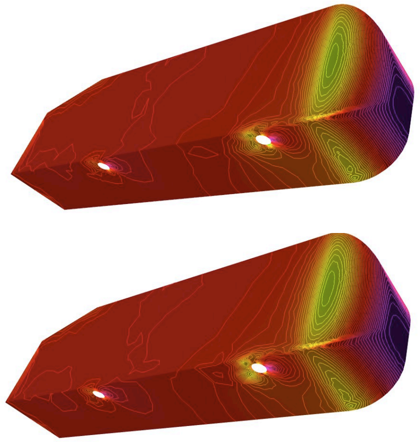
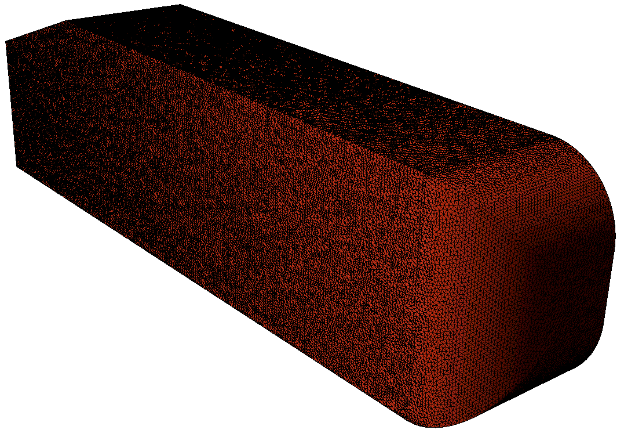
SAND2013-5024C

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







Kevin Carlberg*, Charbel Farhat#, Julien Cortial*, David Amsallem#

*Sandia National Laboratories

#Stanford University

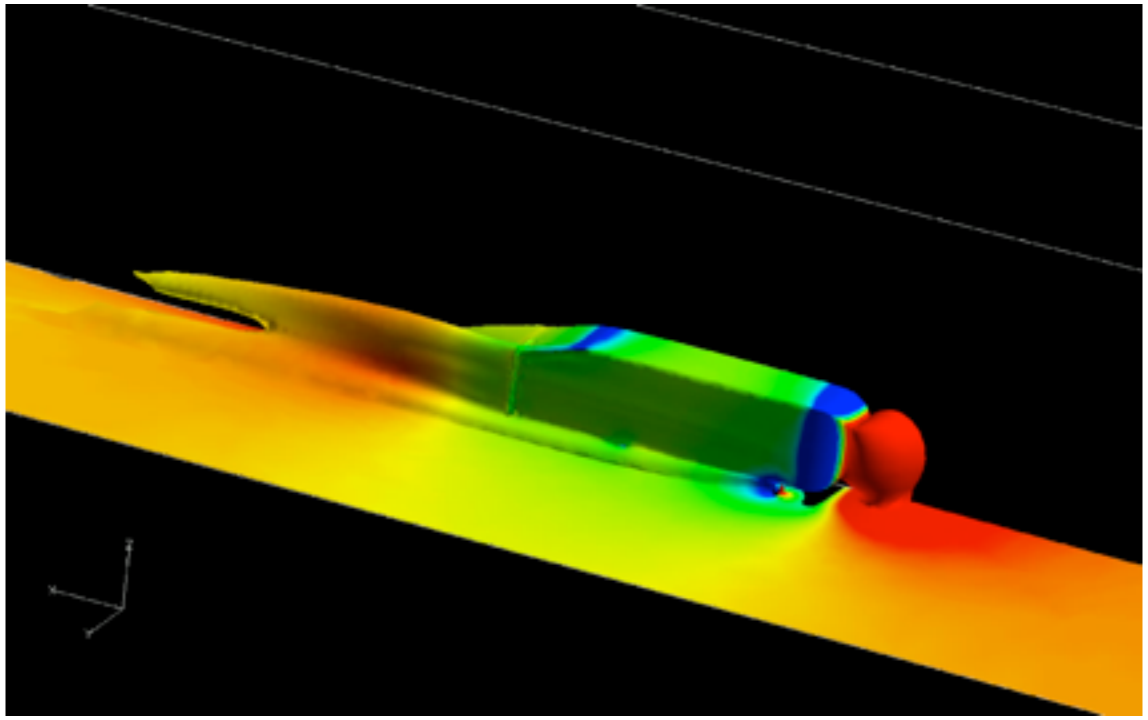
10th World Congress on Computational Mechanics

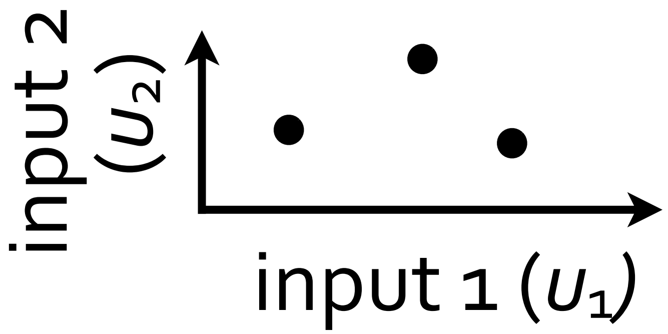
July 12, 2012

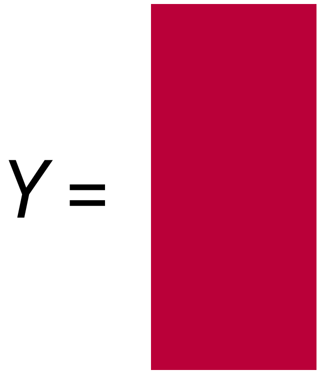
Summary

- **Goal**: practical model reduction for nonlinear ODEs
- **Problem**: POD–Galerkin often does not work
  - lacks *discrete optimality*
- **Idea**: GNAT model reduction
  - *discrete-optimal* approximations
  - effective 'sample mesh' implementation
  - works on large-scale problems

1. Collect snapshots of the state vector

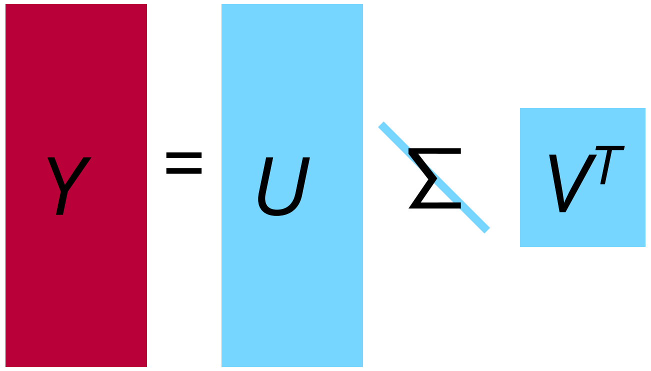




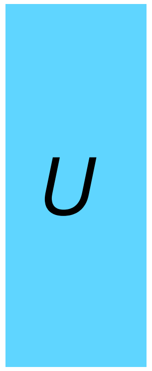


2. Compression

a. compute singular value decomposition



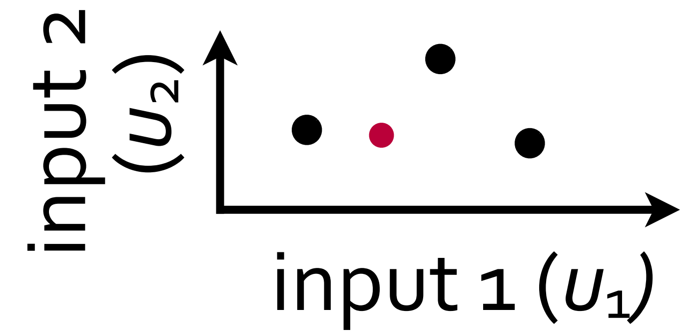
b. truncate



POD–Galerkin: online projection

Online

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



- Galerkin projection

<u>reduce # unknowns</u>

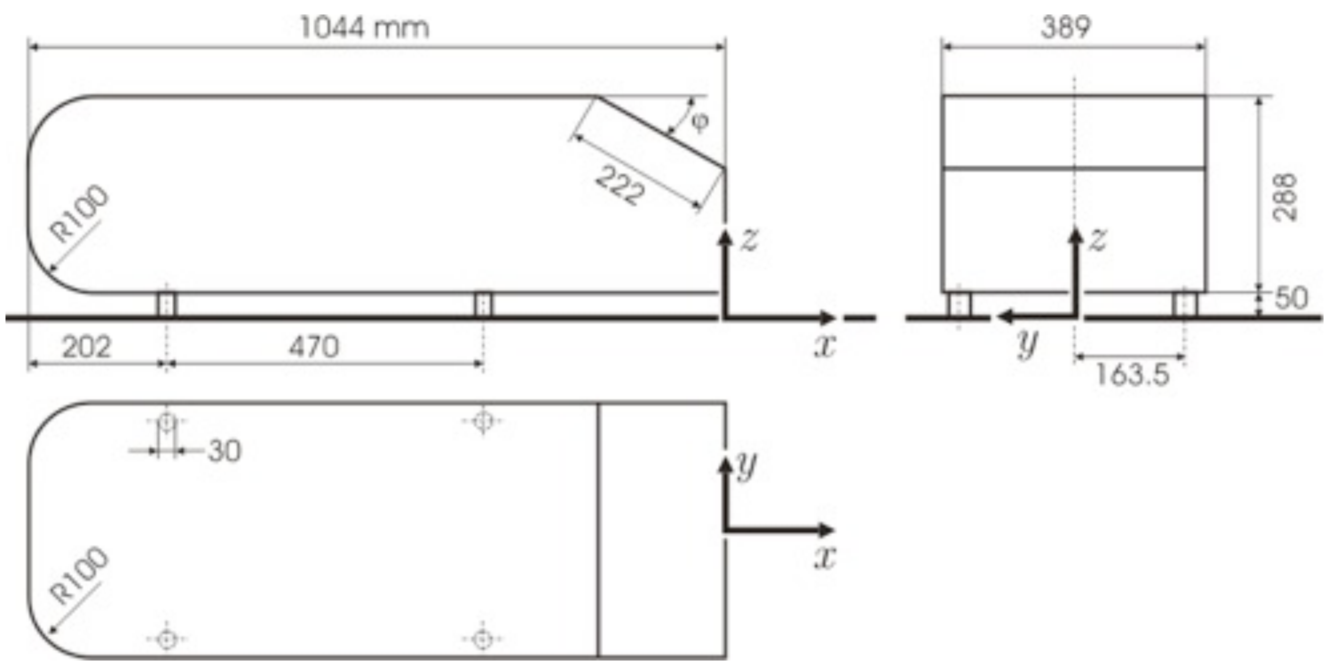
$$y \approx \Phi y_r$$

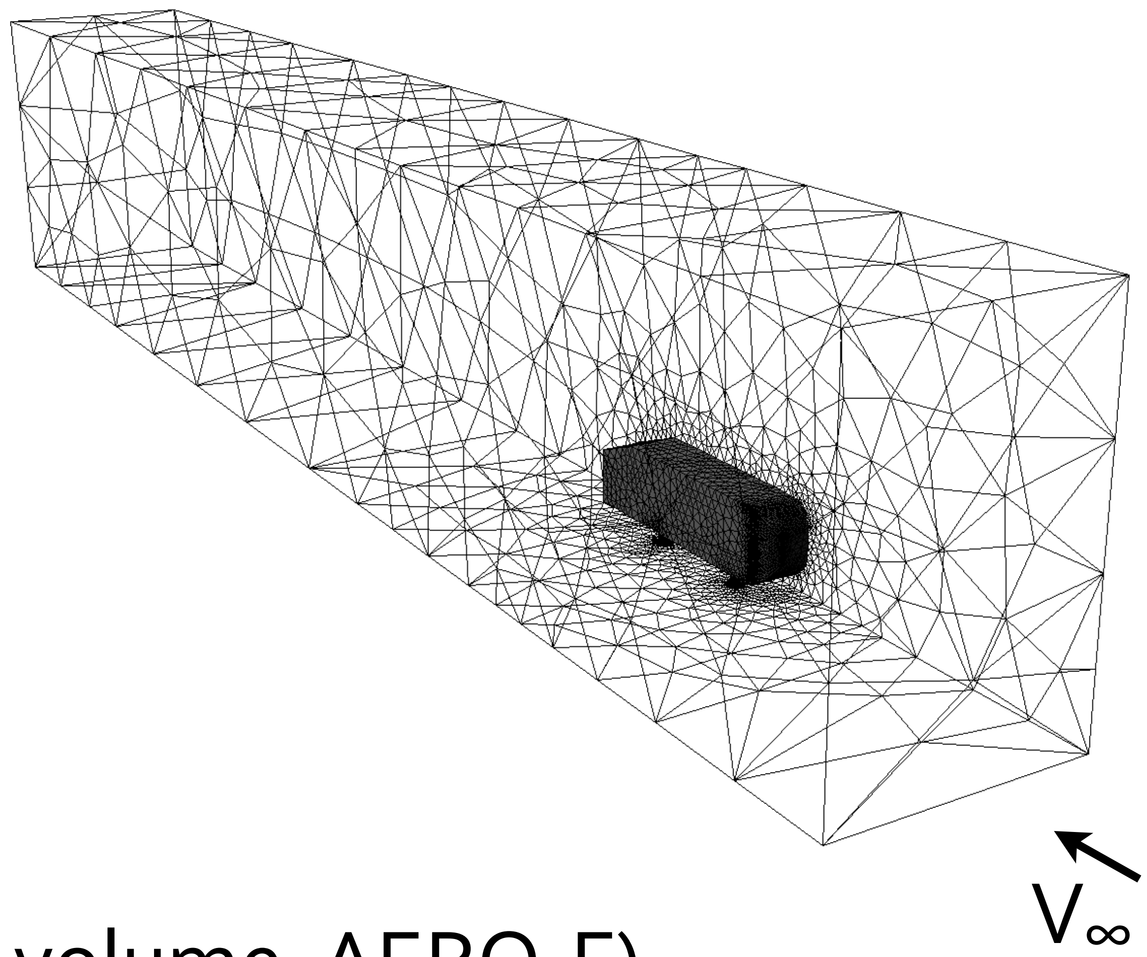
<u>reduce # equations</u>

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

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

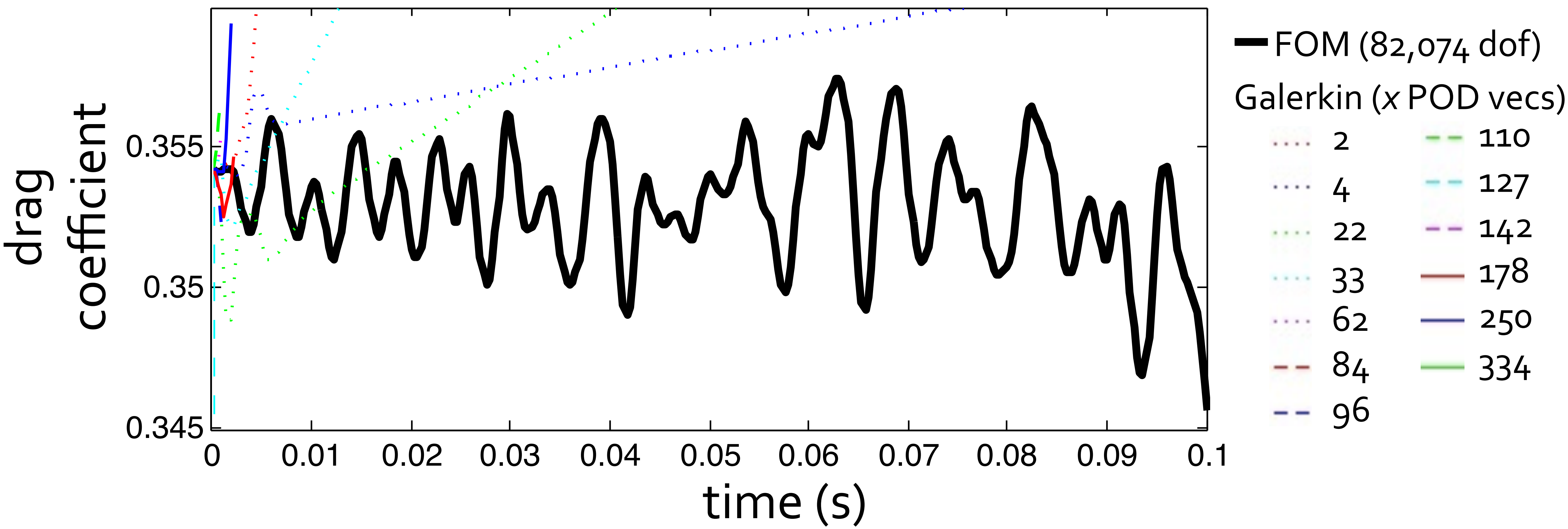
Benchmark: Ahmed body





- 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'

full-order model | **Galerkin ROM**

$$\begin{tikzcd}[column sep=huge, row sep=large]
a(v;x,t,u)=0 \arrow[d, "\textit{spatial discretization}"'] & \\
\dot{y}=f(y;t,u) \arrow[r, "\textit{Galerkin}", "\textit{projection}"'] \arrow[d, "\textit{implicit time integration}"'] & \boxed{\dot{y}_r=\Phi^T f(\Phi y_r;t,u)} \arrow[d, "\textit{implicit time integration}"] \\
R^n(y^n;u)=0 & \boxed{\Phi^T R^n(\Phi y_r^n;u)=0}
\end{tikzcd}$$

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

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

GNAT strategy

- Discrete-optimal approximations

offline

I. *Discrete* full-order model → snapshot collection → compression

reduce dimension

II. Minimum-residual ROM → snapshot collection → compression

reduce complexity

online

III. GNAT ROM

GNAT strategy

- Discrete-optimal approximations

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I. *Discrete* full-order model → snapshot collection → compression

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III. GNAT ROM

Minimum-residual ROM is discrete optimal

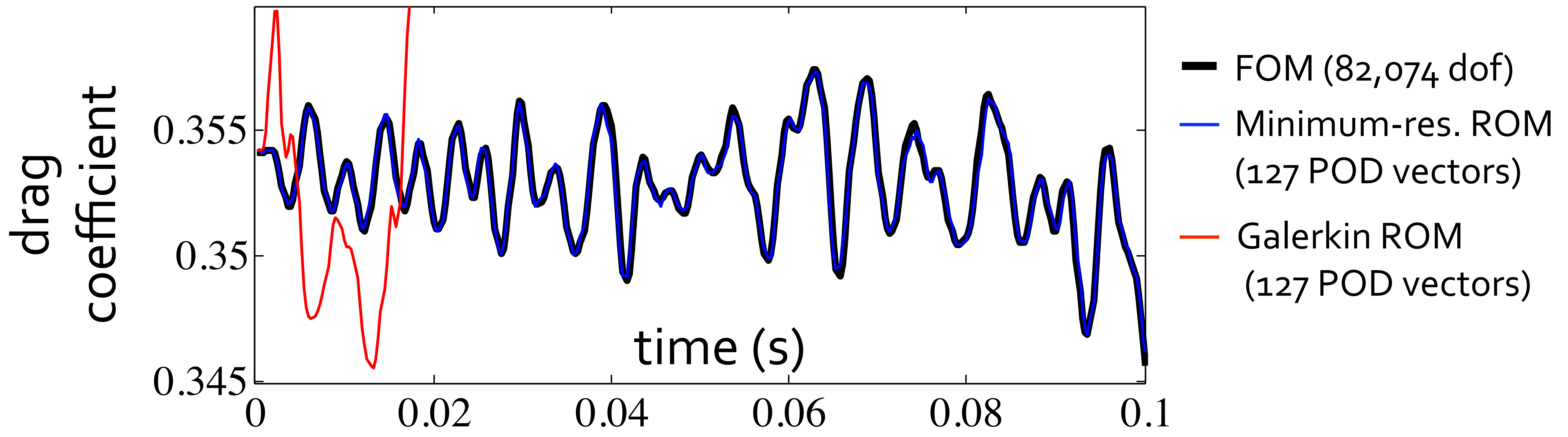
Minimum-residual ROM	full-order model	Galerkin ROM
	$a(v; x, t, u) = 0$	
	$\big\downarrow$ *spatial discretization*	
not defined	$\dot{y} = f(y; t, u)$ $\longrightarrow$	$\dot{y}_r = \Phi^T f(\Phi y_r; t, u)$
	$\big\downarrow$ *implicit time integration*	$\big\downarrow$
$y_r^n = \arg\min_x \|R^n(\Phi x; u)\|_2$ $\longleftarrow$	$R^n(y^n; u) = 0$	$\Phi^T R^n(\Phi y_r^n; u) = 0$

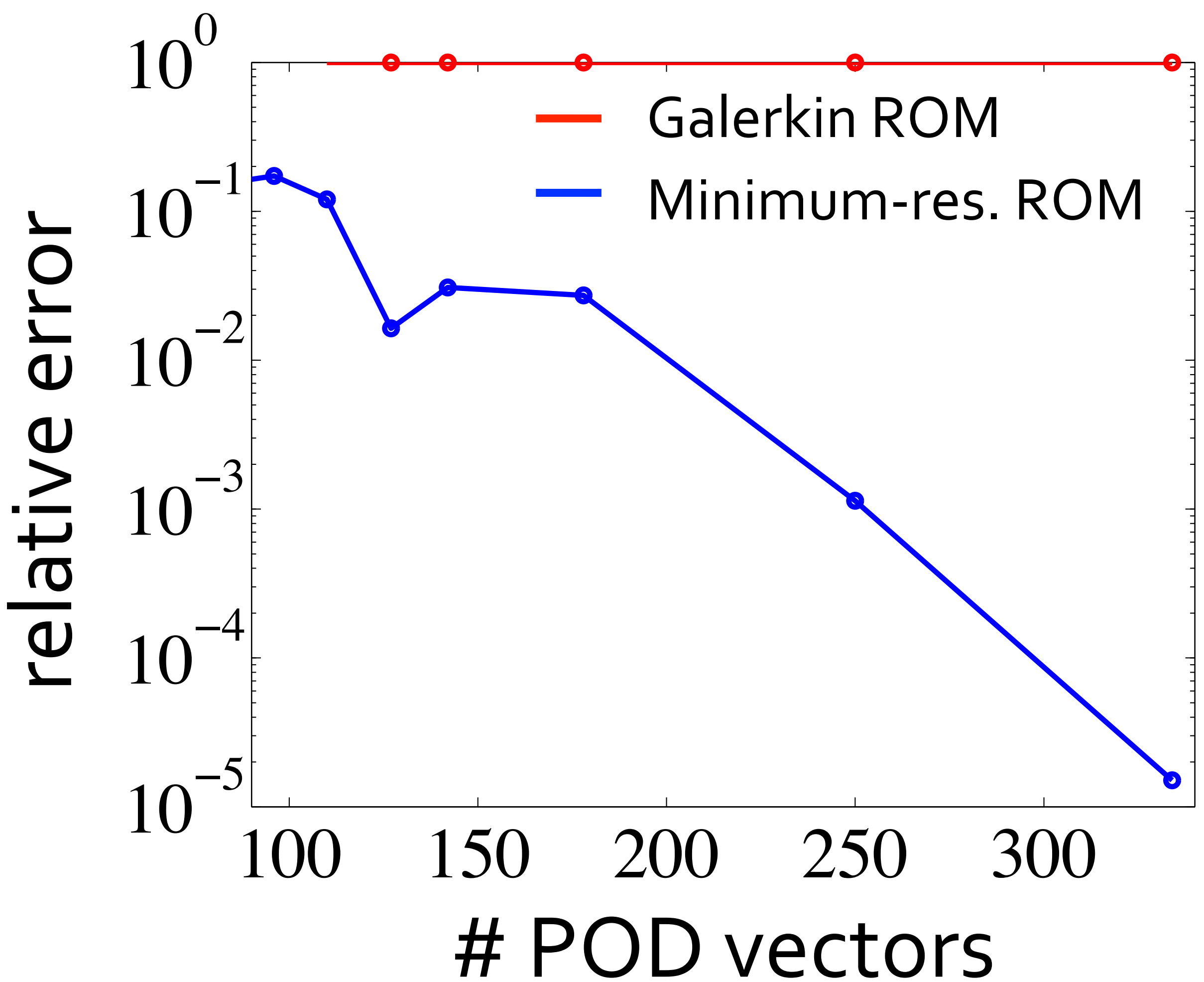
+ Discrete optimal

- 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





+ convergence in outputs

– Minimum-residual ROM slower if >33 POD vectors

GNAT strategy

offline

I. *Discrete* full-order model → snapshot collection → compression

reduce dimension

II. Minimum-residual ROM → snapshot collection → compression

reduce complexity

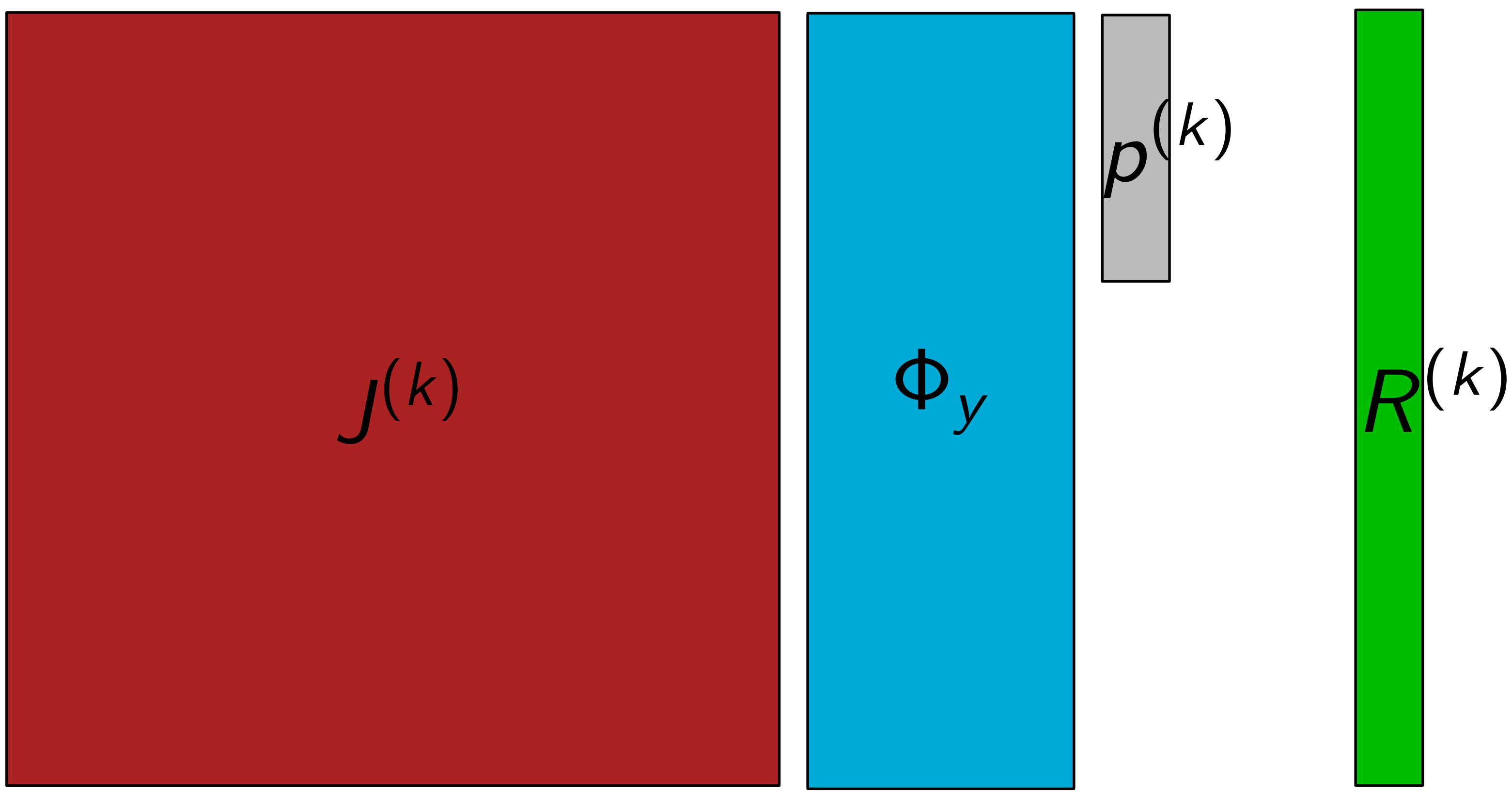
online

III. GNAT ROM

Gappy POD complexity reduction

- Minimum-residual ROM iterations are

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

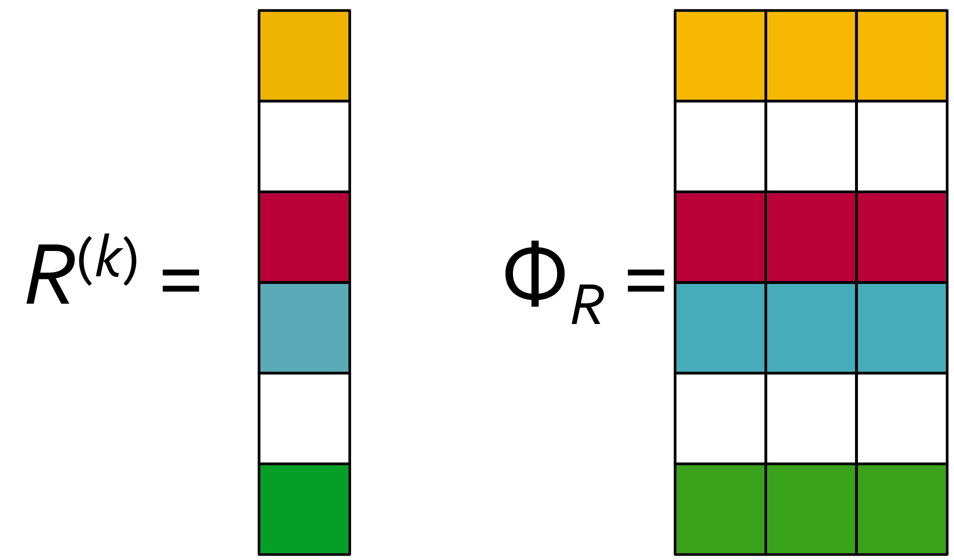


- Operation count scales with N

Gappy POD complexity reduction

- Goal: approximate $R^{(k)}$
- Given: i) basis Φ_R

  ii) a few sampled entries of $R^{(k)}$



[Everson & Sirovich, 1995]

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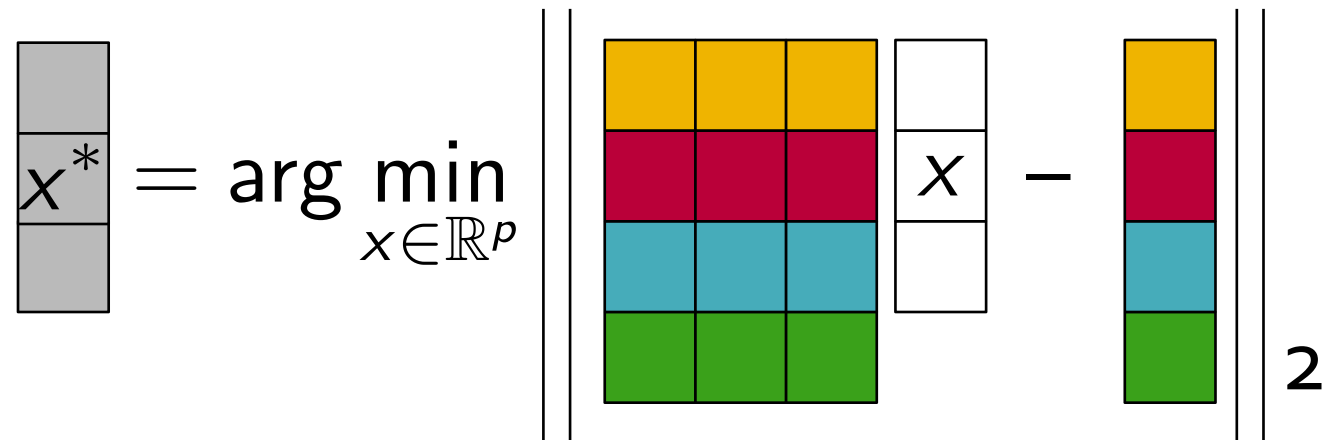
1. Least squares minimization on sampled entries



2. Reconstruct all entries: $\bar{R}^{(k)} = \Phi_R x^\star$

\+ Discrete optimality: $\bar{R}^{(k)} = \arg \min_{x \in \mathrm{range}(\Phi_R)} \|E^T(x - R^{(k)})\|_2$

\+ Complexity reduction: compute only a few entries of $R^{(k)}$

Gauss–Newton with Approximated Tensors (GNAT)

offline

I. *Discrete* full-order model → snapshot collection → compression

reduce dimension

II. Minimum-residual ROM → snapshot collection → compression

reduce complexity

online

III. GNAT ROM

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 $(y^0, \tilde{y}^1, \ldots, \tilde{y}^{n_t})$ is

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

Discrete optimality enables min. error bound

Proposition [Carlberg et al., 2012]

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

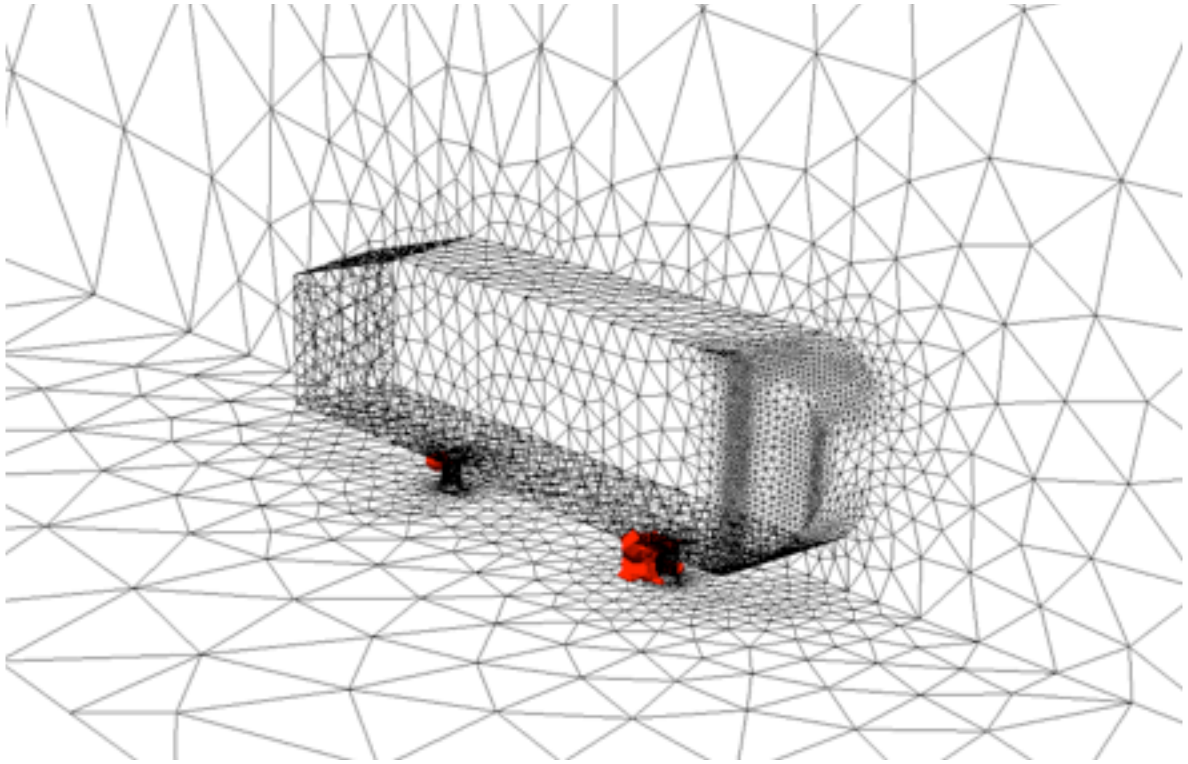
$$\|y^n - \tilde{y}^n\| \leq \sum_{k=0}^{n-1} a^k \boxed{b_{n-k}} \leq \sum_{k=0}^{n-1} a^k \boxed{c_{n-k}}$$

- a: inverse Lipschitz constant
- $b_n = \epsilon + \boxed{\|\tilde{R}^n(\tilde{y}^n; u)\|}$
- $c_n = \epsilon + \boxed{\|P\tilde{R}^n(\tilde{y}^n; u)\|} + \boxed{\|(I - P)\tilde{R}^n(\tilde{y}^n; u)\|}$
- $\tilde{R}$: residual for sequence $\{\tilde{y}^n\}$
- P : Gappy POD operator

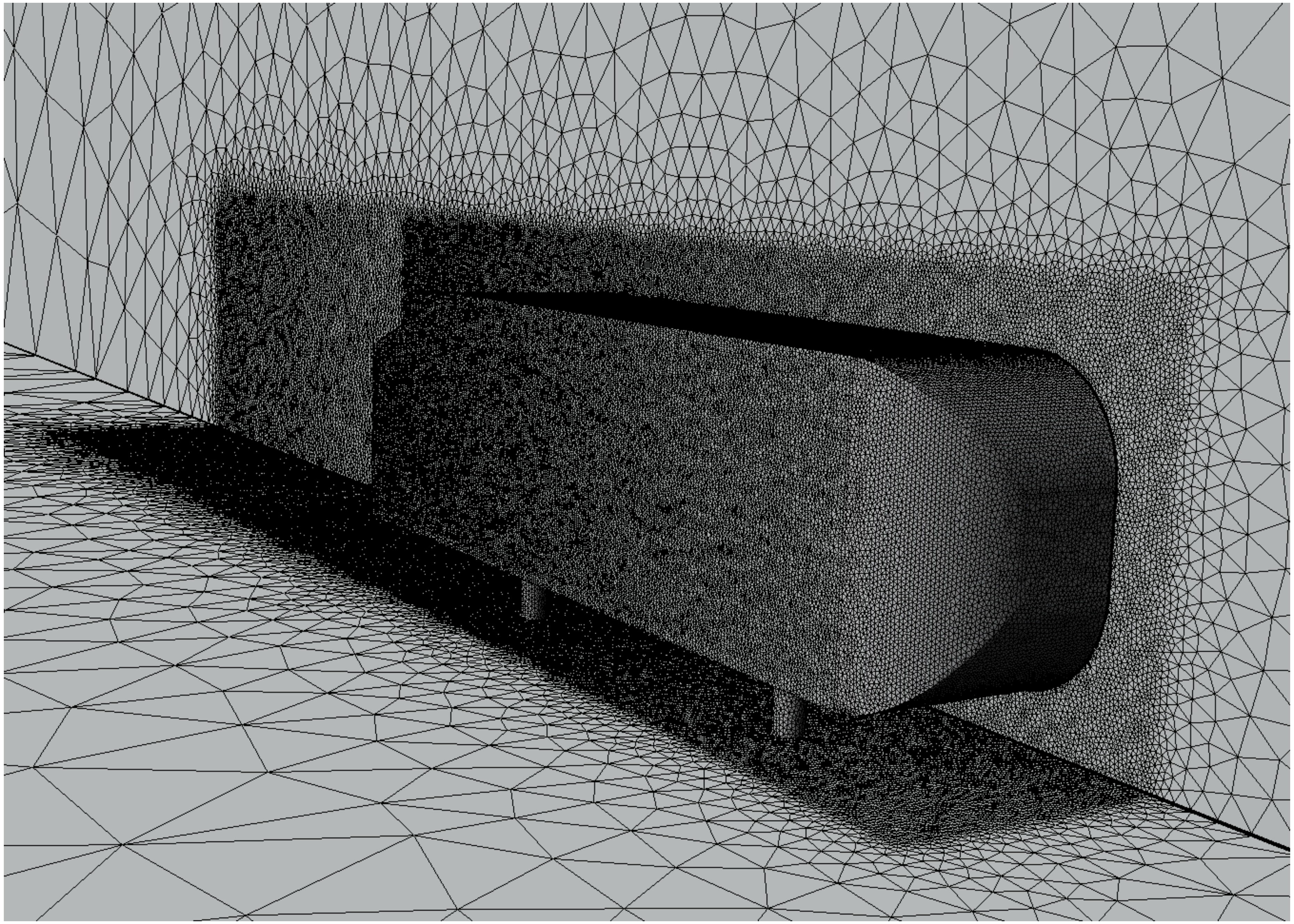
+ Minimum-residual ROM solutions minimize b_n
+ GNAT ROM solutions minimize $\|P\tilde{R}^n(\tilde{y}^n; u)\|$
+ sampling algorithm: heuristic for minimizing $\|(I - P)\tilde{R}^n(\tilde{y}^n; u)\|$
  - discrete optimality enables this!

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

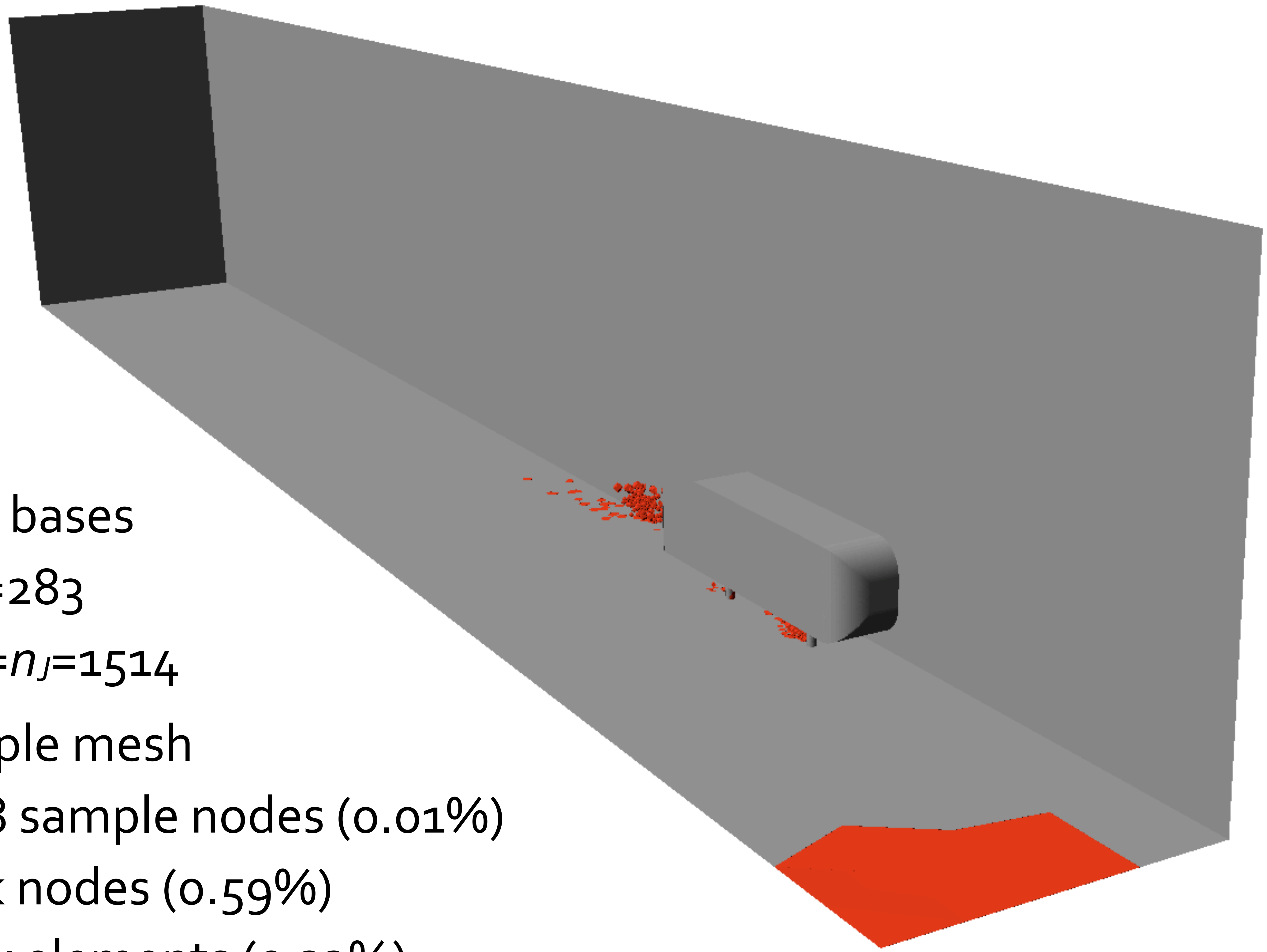


Example: Ahmed body (validated)



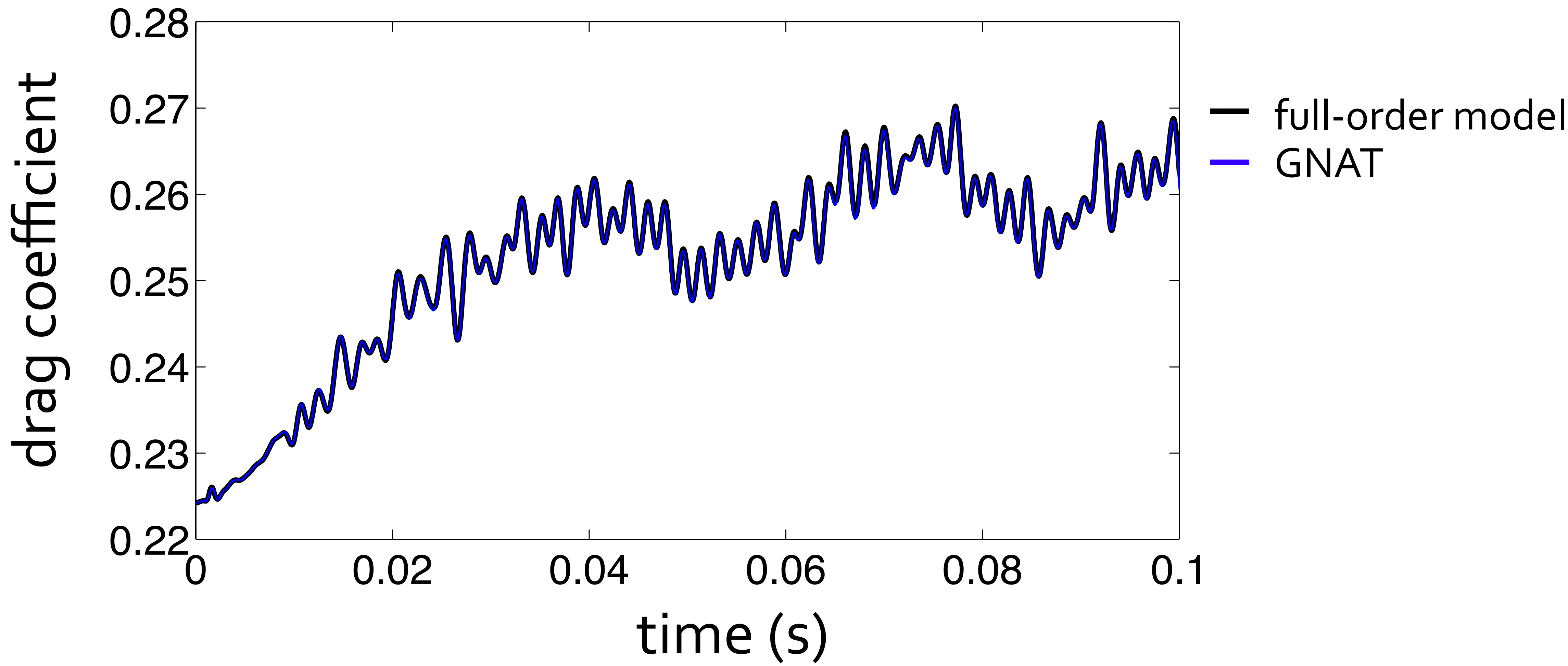
- 2.89×10^6 nodes, 1.70×10^7 tetrahedral volumes
- 1.73×10^7 degrees of freedom

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

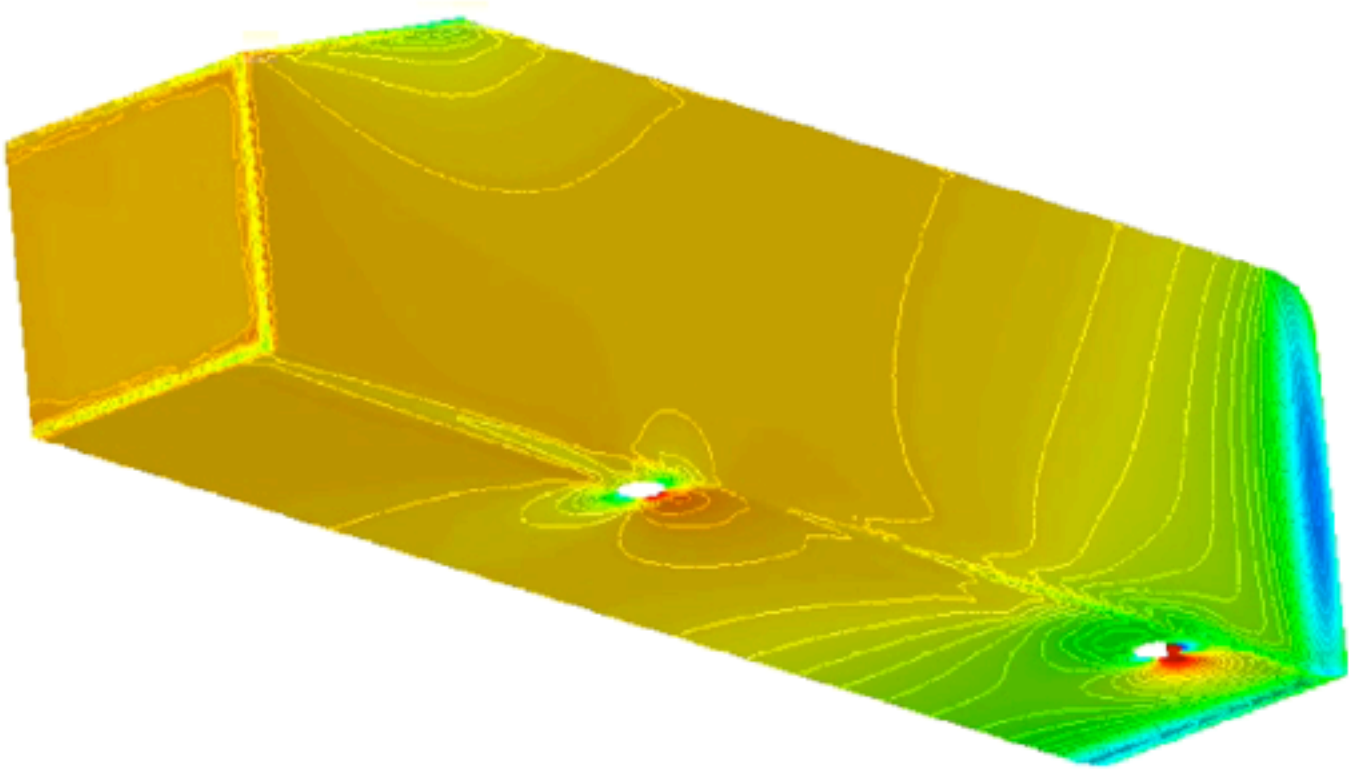


model	relative error	# cores	time, hours	speedup in cpu resources
FOM	-	512	13.3	-
GNAT	0.68%	4	3.88	438

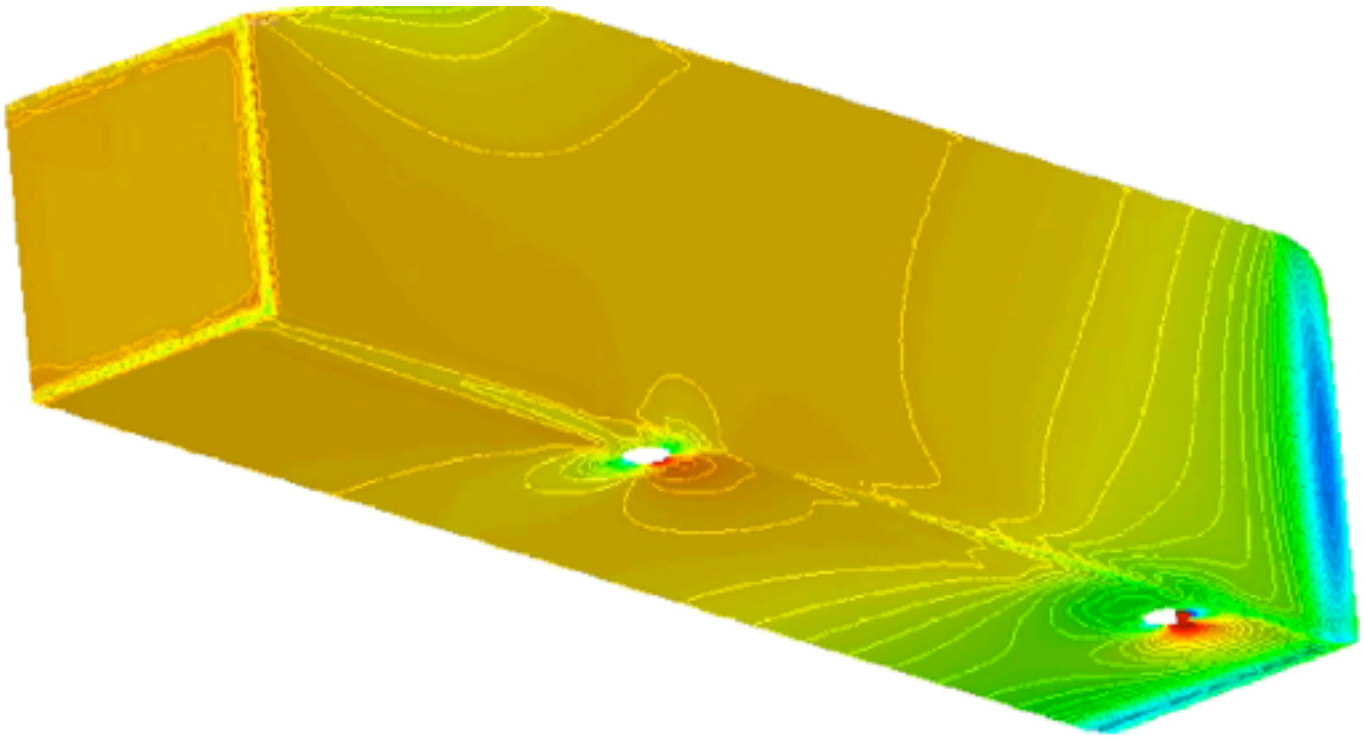
+ negligible error + wall-time decrease + supercomputer → desktop

GNAT results: accurate pressure contours

full-order model

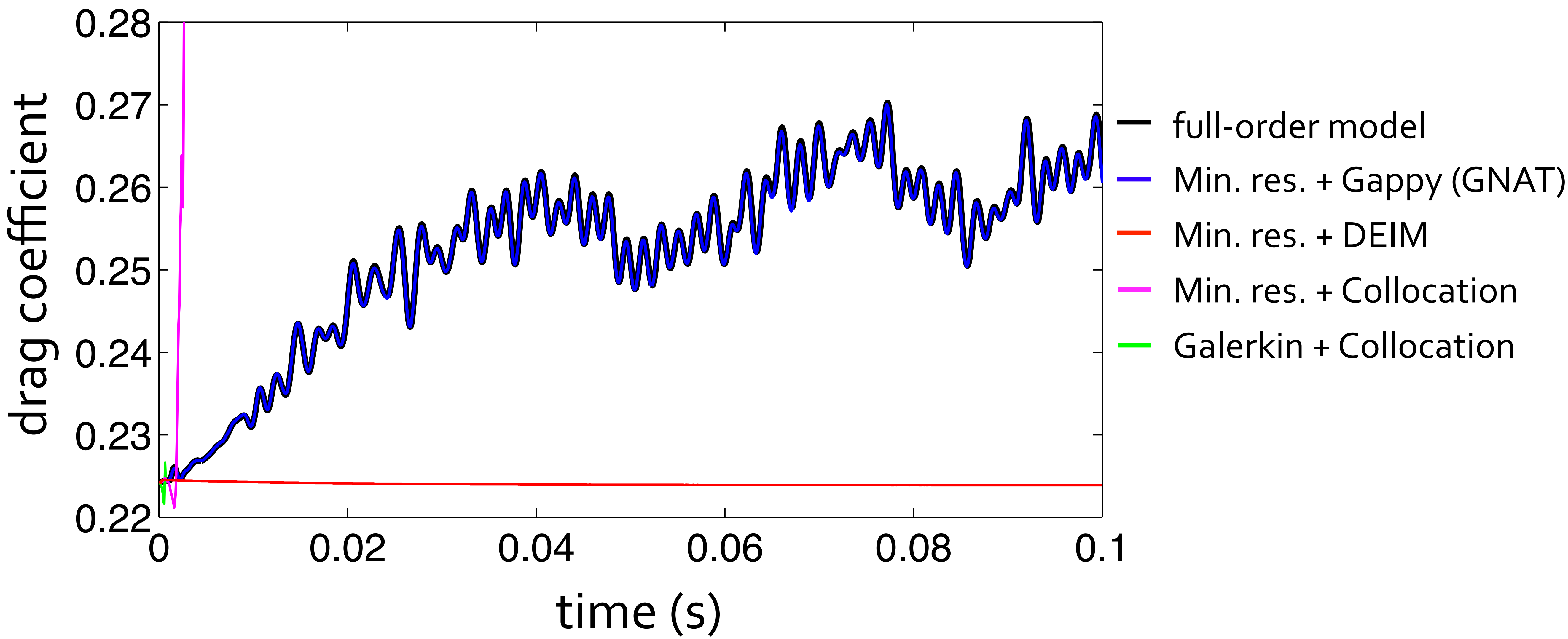


GNAT



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

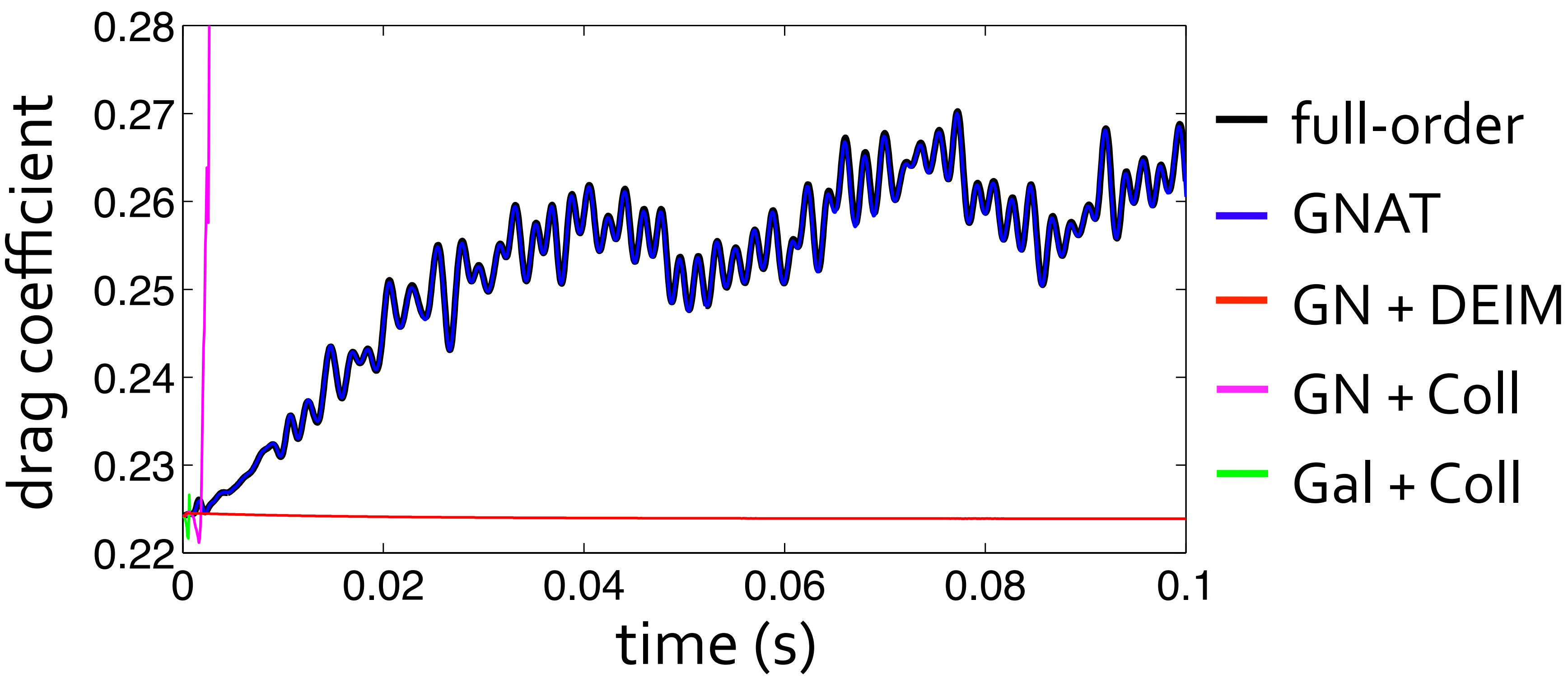
- GNAT method
  - discrete-optimal approximations
  - error bound justifies its design
- Sample mesh concept enables many fewer cores
  - supercomputer → desktop
- Ahmed body example
  - speedups over 400, error less than 1%
  - other model-reduction methods failed
- Key papers
  - K. Carlberg, C. Bou-Mosleh, 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 work @ Sandia

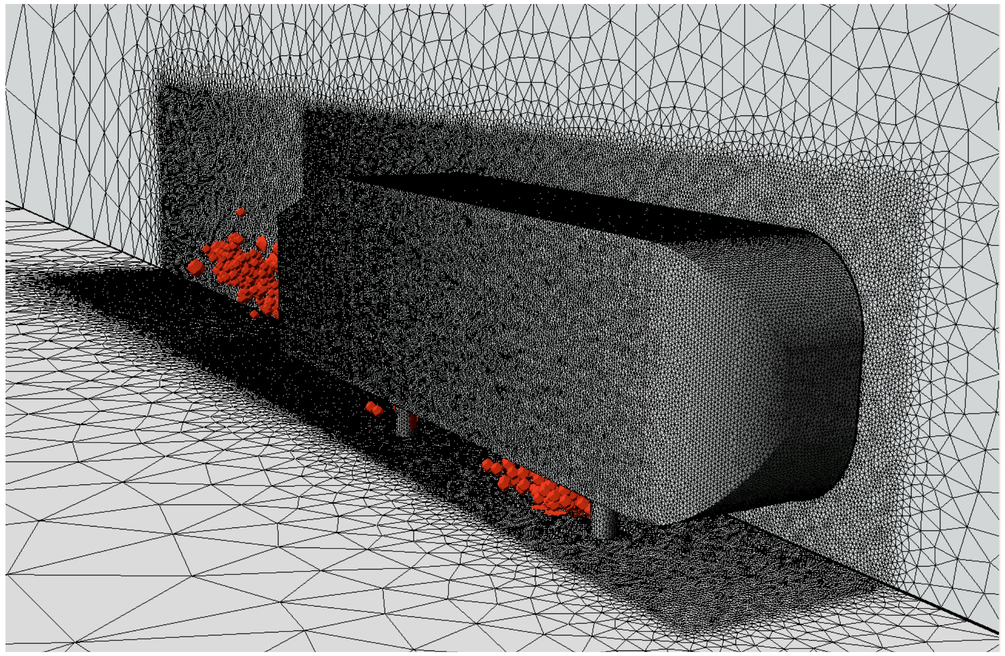
1. Preserve classical Hamiltonian/Lagrangian structure [Tuminaro, Boggs]
   - *Goal*: preserve key properties (e.g., energy conservation)
   - Structural dynamics, molecular dynamics
2. Decrease temporal complexity via forecasting [Ray, van Bloemen Waanders]
   - *Goal:* decrease wall-time for nonlinear 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

Questions?

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

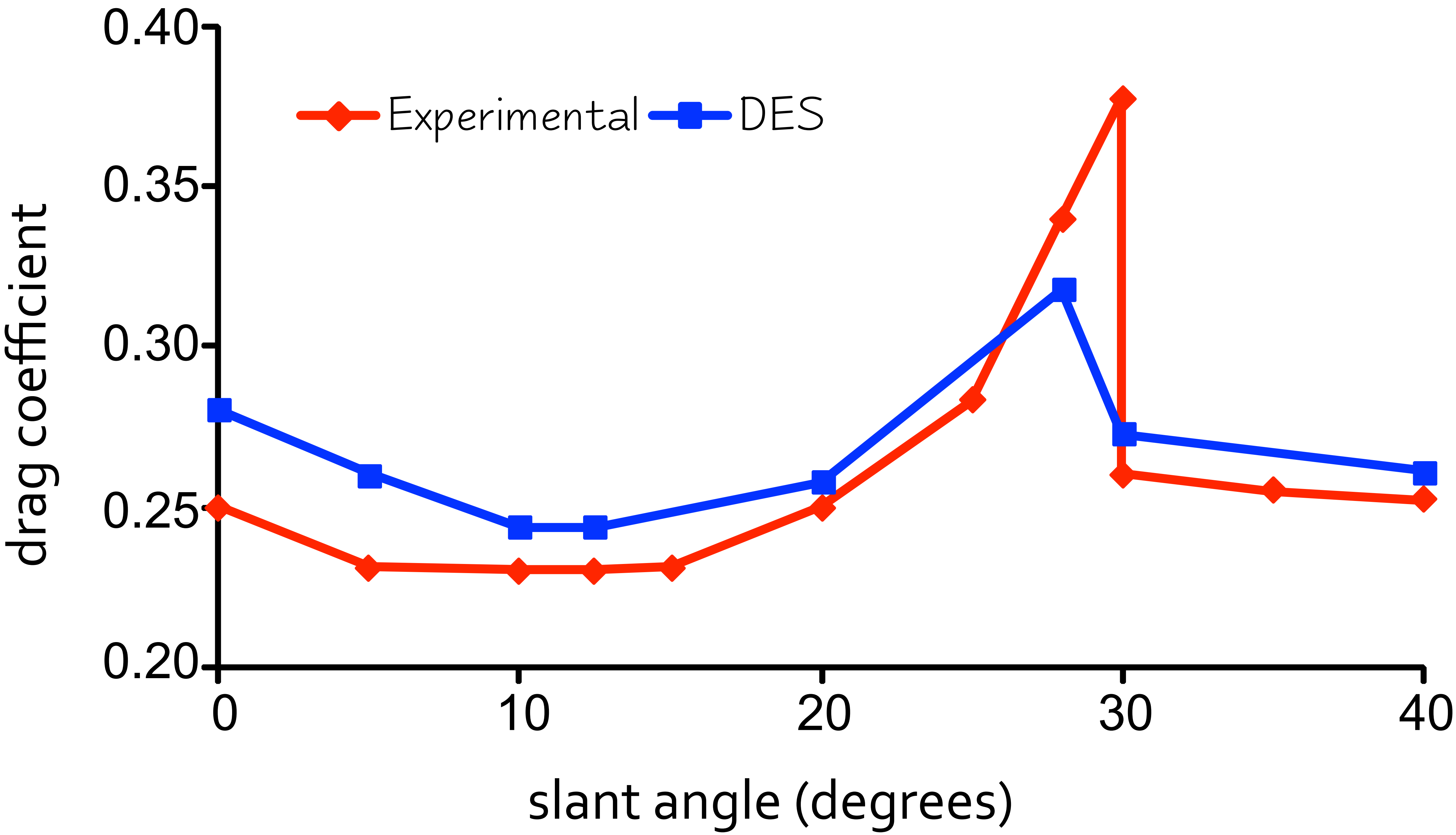


- Funding
  - NSF Graduate Fellowship
  - Toyota Motor Corporation
  - Army Research Laboratory
  - Truman Fellowship program*



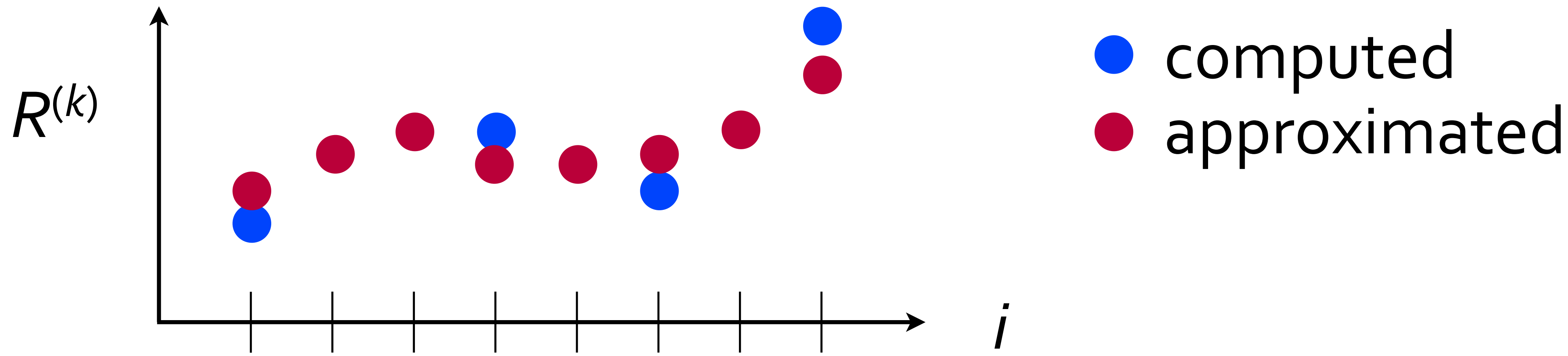
* Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

CFD model matches experiment well



Gappy POD complexity reduction [Everson & Sirovich, 1995]

- Goal: approximate the vector $R^{(k)}$
- Given: i) some computed entries of $R^{(k)}$
  ii) basis Φ_R
- Procedure: minimize least-squares error *at computed entries*



- Also apply to each column of $J^{(k)}\Phi$

+ Discrete optimality: least-squares fit of discrete nonlinear functions
+ Inexpensive: compute only a few entries of $R^{(k)}$