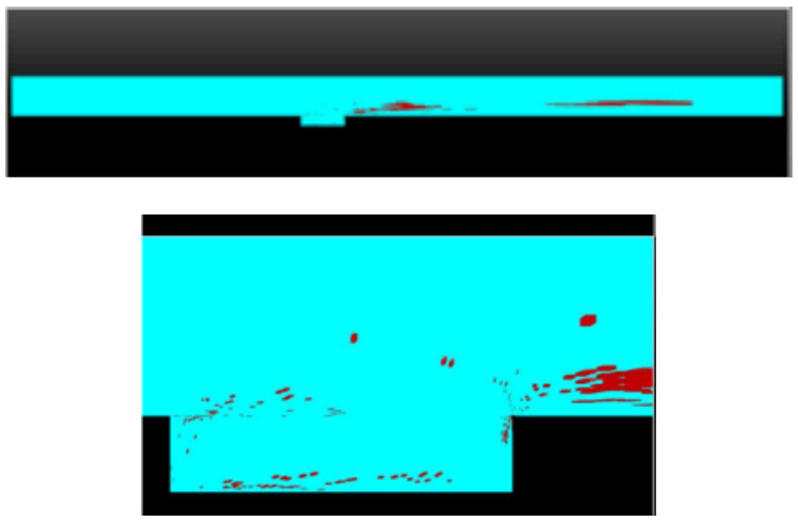
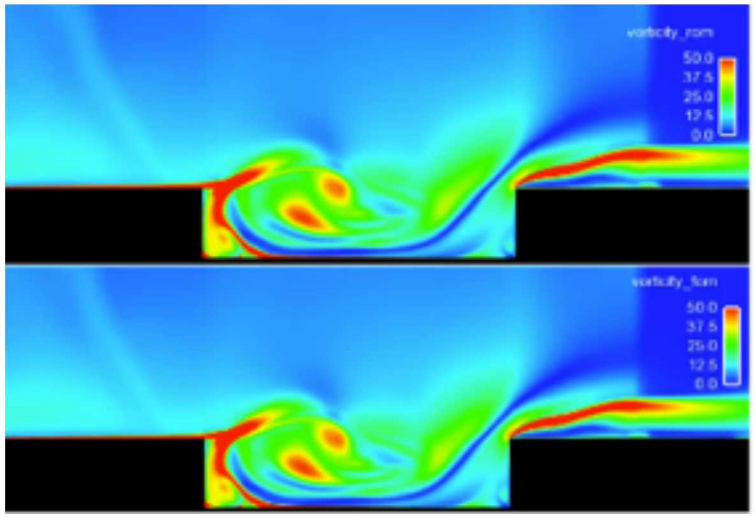
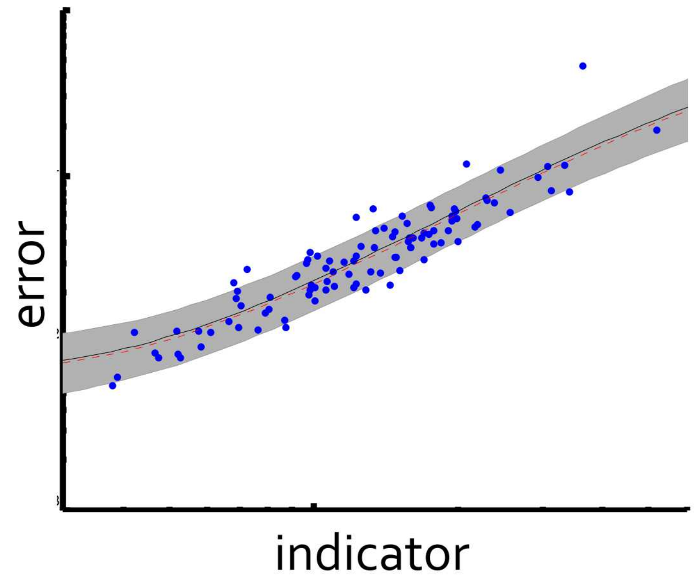
SAND2015-7787PE

Reduced-order models

Fancy emulators







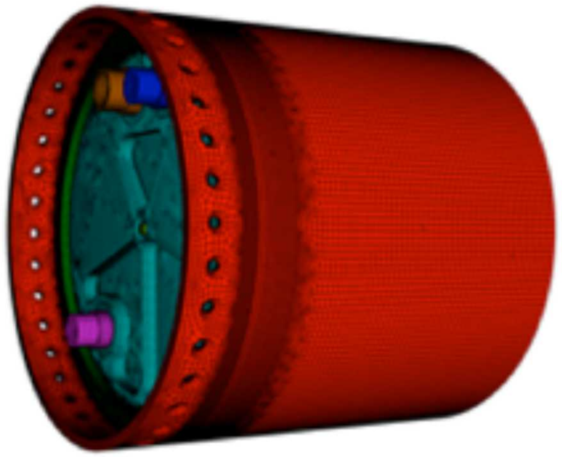
Kevin Carlberg

Durham University visit

July 23, 2015

Computational barrier

High-fidelity simulation

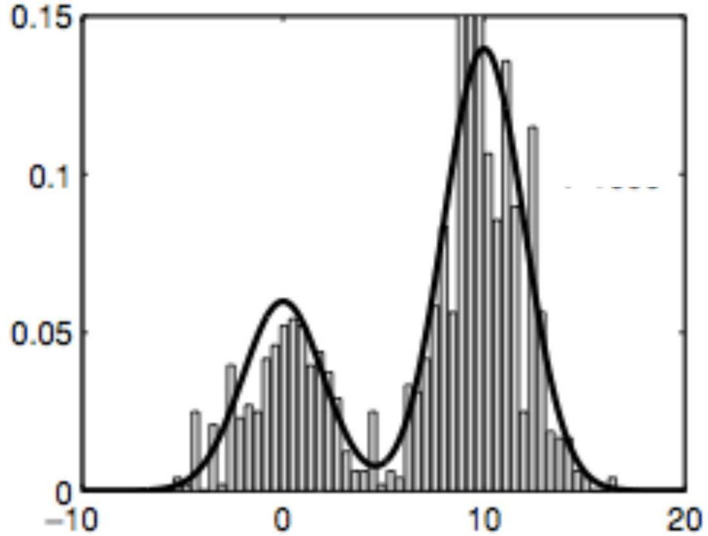


+ An indispensible tool
- Very high computational cost

barrier

Time-critical applications

Many query



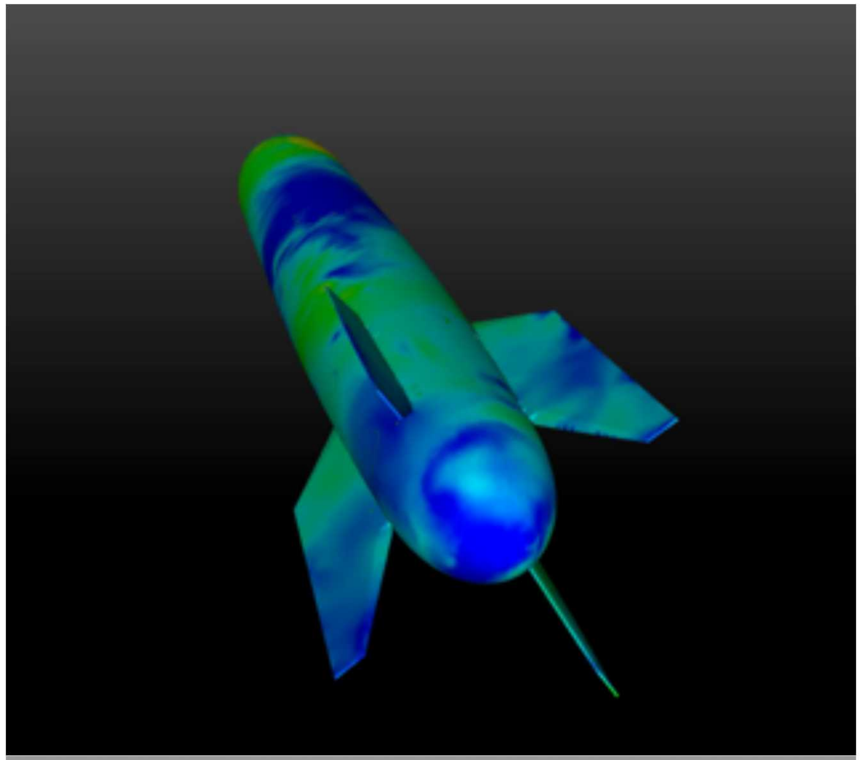
Source: Andrieu et al., 2003

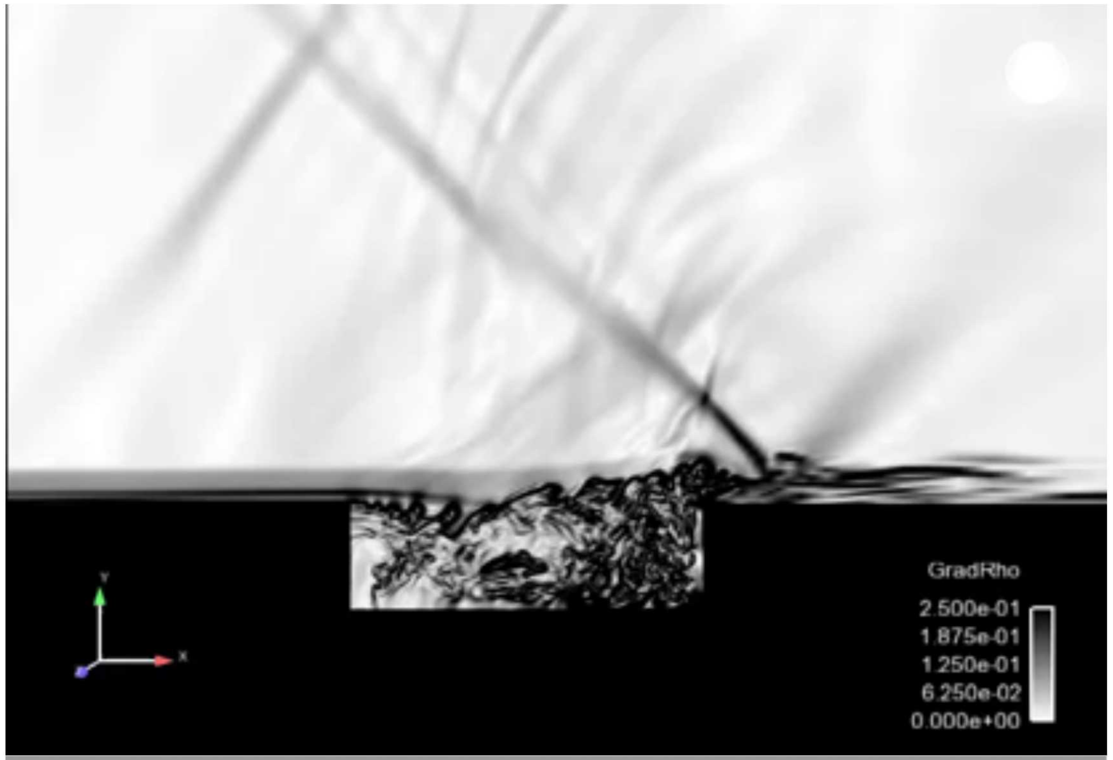
Near real-time

Source: National Power Grid Simulation Capability: Needs and Issues

Objective: break barrier

Captive carriage for B-61 LEP





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

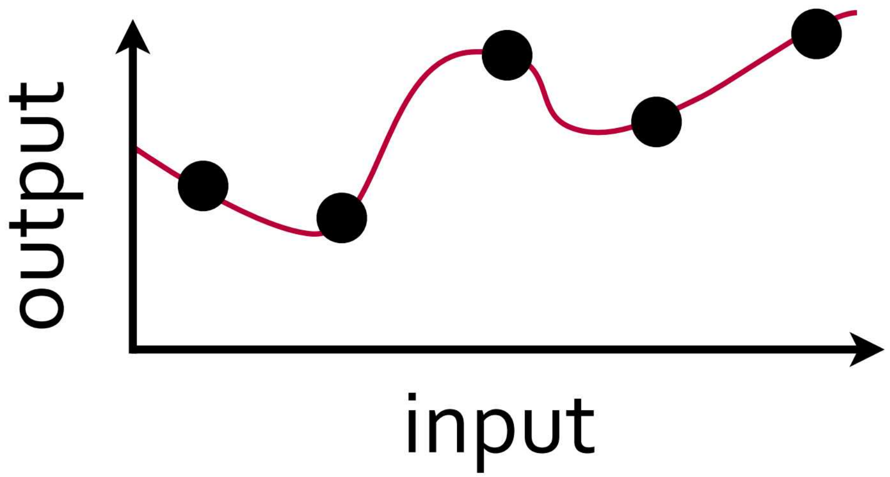
barrier

- Design engineers require faster simulations
- Uncertainty quantification (UQ)

Surrogate modeling taxonomy

inputs (u) → surrogate model → outputs (z)

1) **Data fits/emulators**

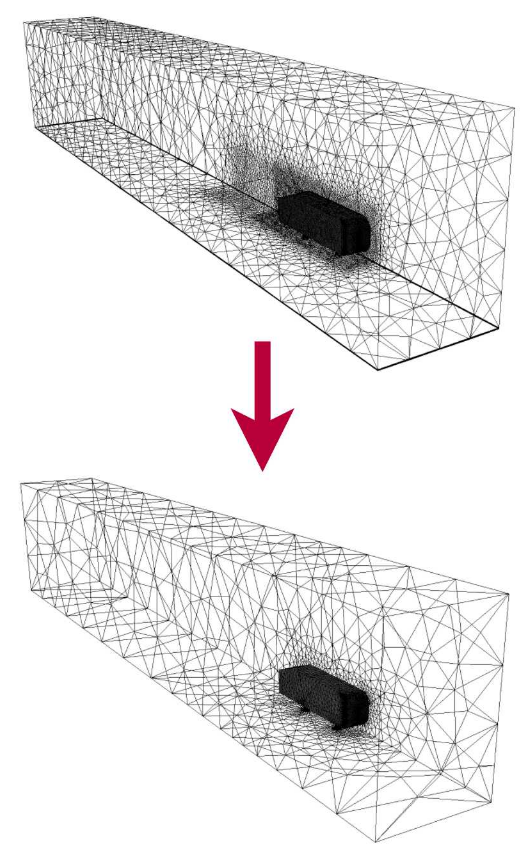


\+ black box

\+ high speedups

– no physical insight

2) **Coarsened physics**

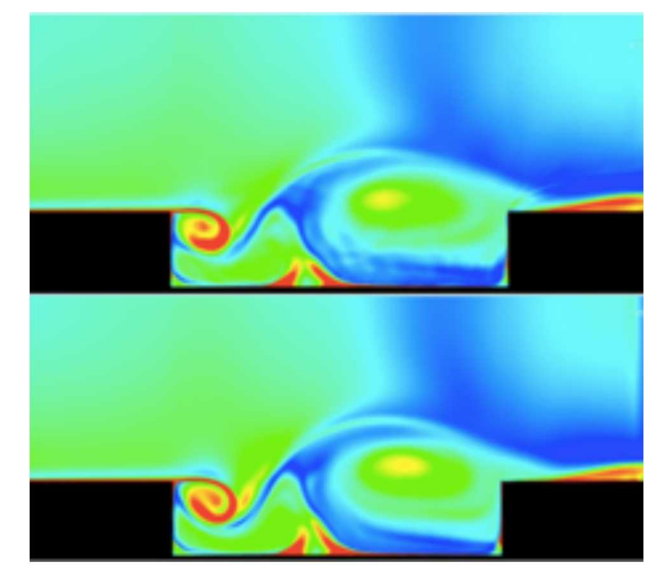


\+ existing codes

\+ physical insight

– low speedups

2) **Reduced-order models (ROMs)**



\+ physical insight

\+ high speedups

– unproven for nonlinear systems

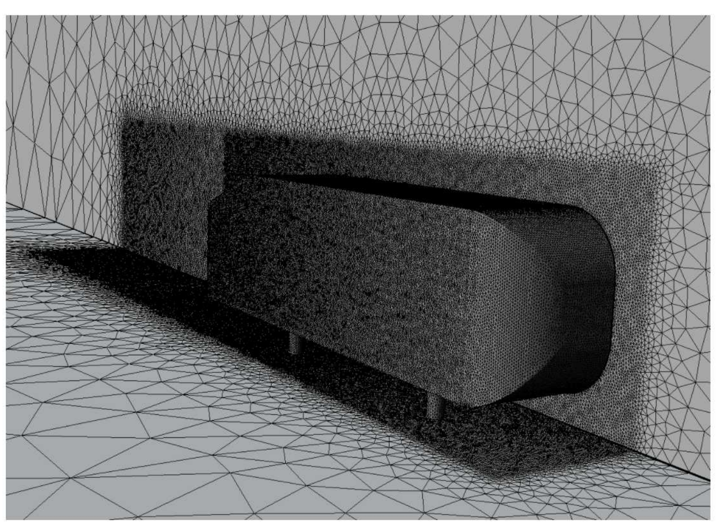
ROM = Data Science + Modeling & Simulation

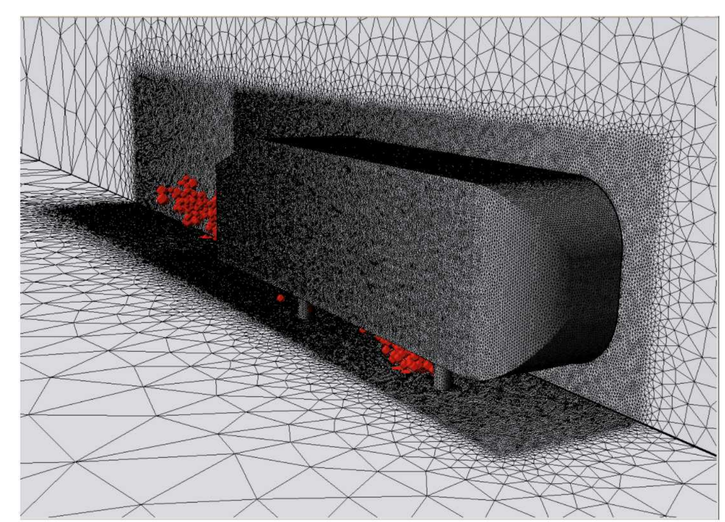
Goal: Exploit structure in data to drastically reduce simulation costs

High-fidelity model → Simulation → *data* → Machine learning →

- *low-dim structure*
- *index clusters*
- *sample nodes*

High-fidelity model + ML outputs → Model reduction → *Reduced-order model (ROM)*





The GNAT method

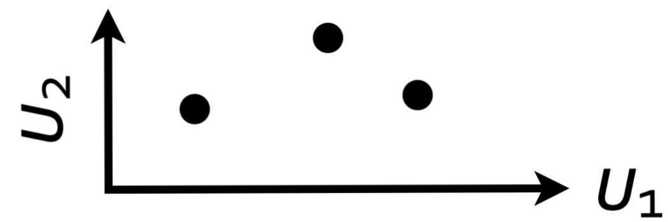
ROM: state of the art

- Linear systems: mature
  - linear time-invariant systems
    [Book: Antoulas, 2005; Willcox & Peraire, 2002; Rowley, 2005]
  - elliptic & parabolic equations
    [Book: Patera & Rozza, 2006; Veroy et al., 2003; Grepl et al., 2005]

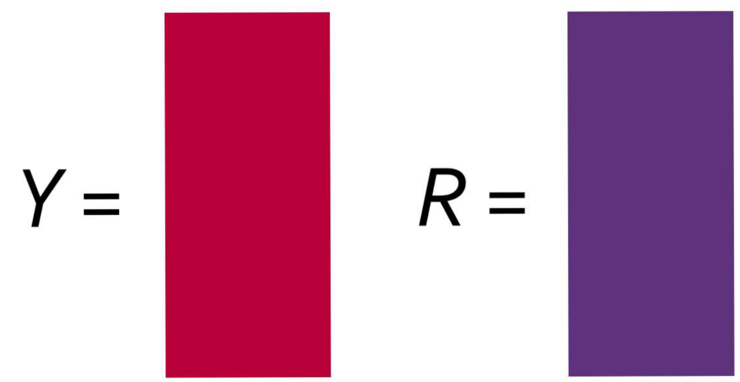
- Nonlinear systems: unproven
  - Proper Orthogonal Decomposition (POD)–Galerkin
    [Sirovich, 1987; Lall et al., 2002; Barrault et al., 2007; Chatarantabut & Sorensen, 2010]
    − lacks **discrete optimality**
  - Gauss–Newton with approximated tensors (GNAT)
    [Carlberg, Bou-Mosleh, Farhat, 2011]
    + exhibits **discrete optimality**

GNAT: *data collection*

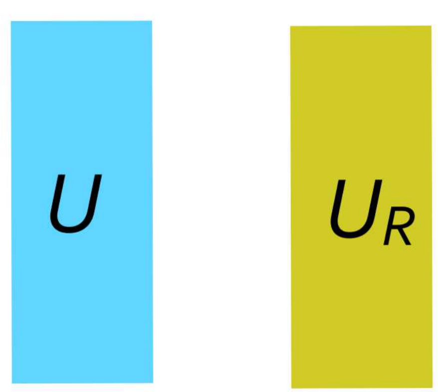
high-fidelity model: $R^n(y^n; u) = 0$

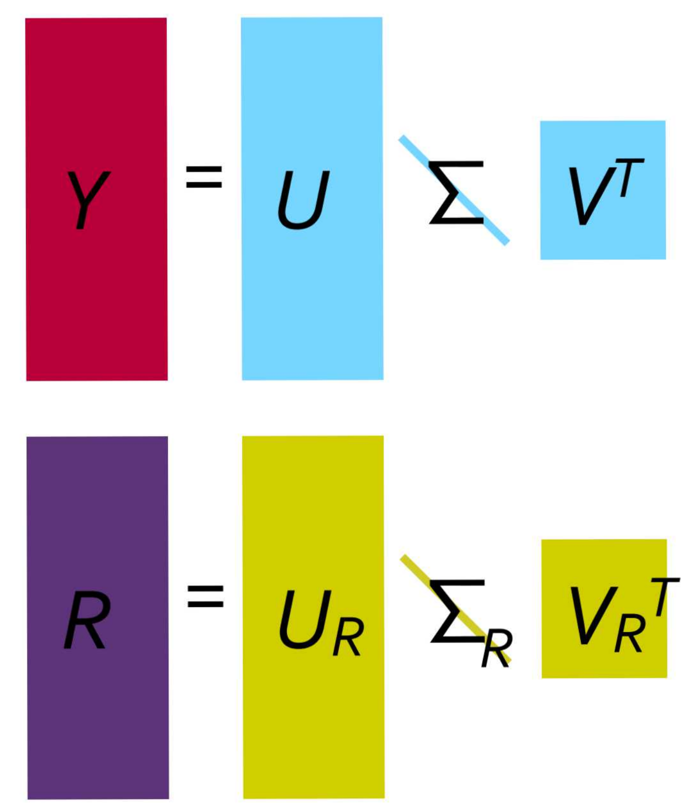


1. Collect solution and residual ‘snapshots’



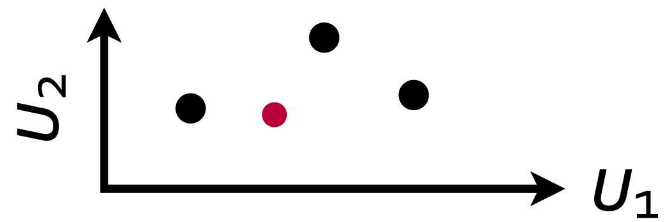
2. Compression
   - compute singular value decomposition
   - truncate





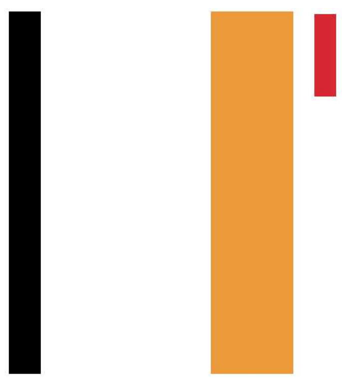
GNAT: *online*

high-fidelity model: $R^n(y^n; u) = 0$



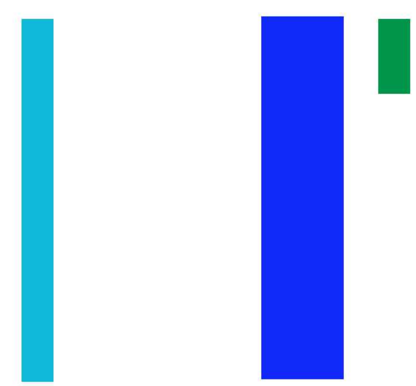
<u>approximate solution</u>

$$y^n \approx \Phi y_r^n$$



<u>approximate residual</u>

$$R^n \approx \Phi_R R_r^n$$



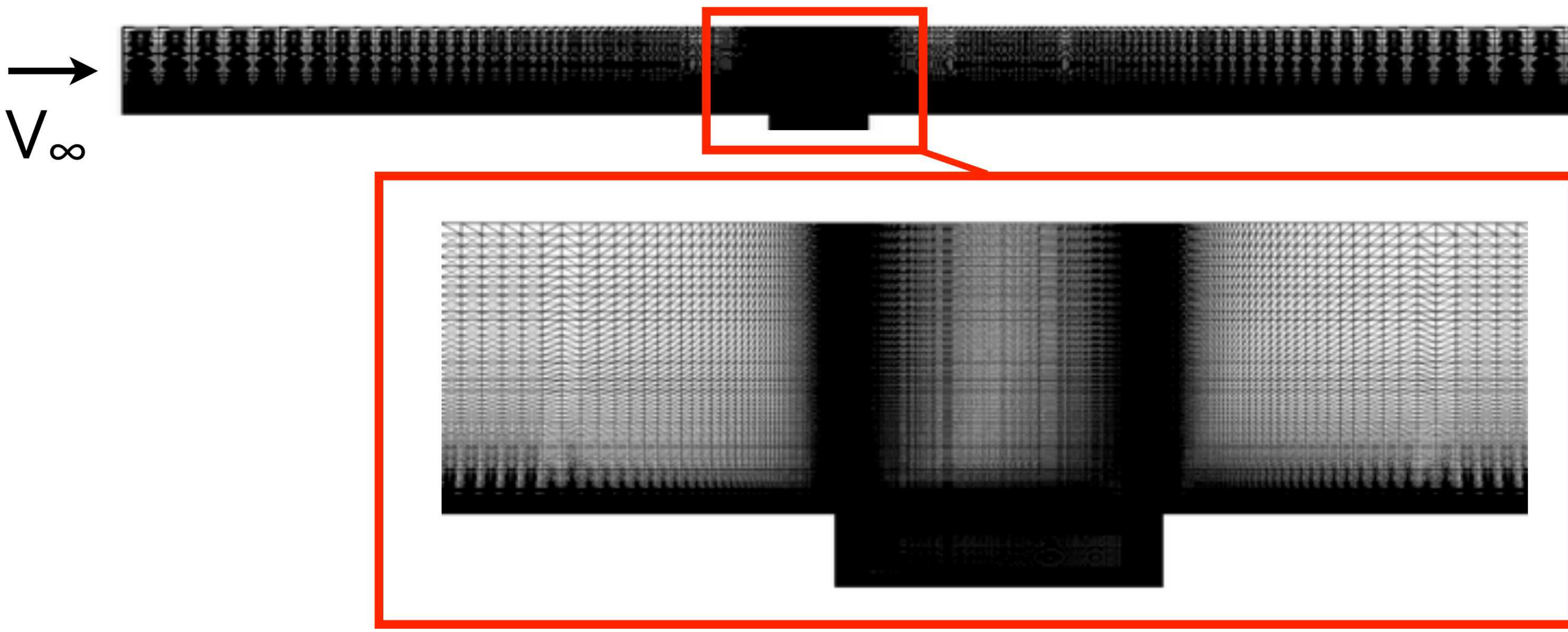
<u>minimize *approximated* residual</u>

$$\underset{y_r^n}{\text{minimize}} \| R_r^n(\Phi y_r^n; u) \|_2^2$$

\+ cheap

\+ discrete optimality

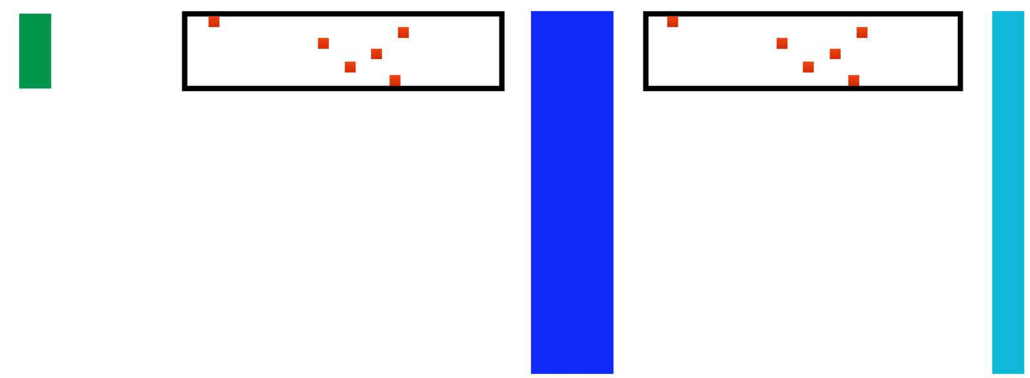
Cavity flow for captive carriage

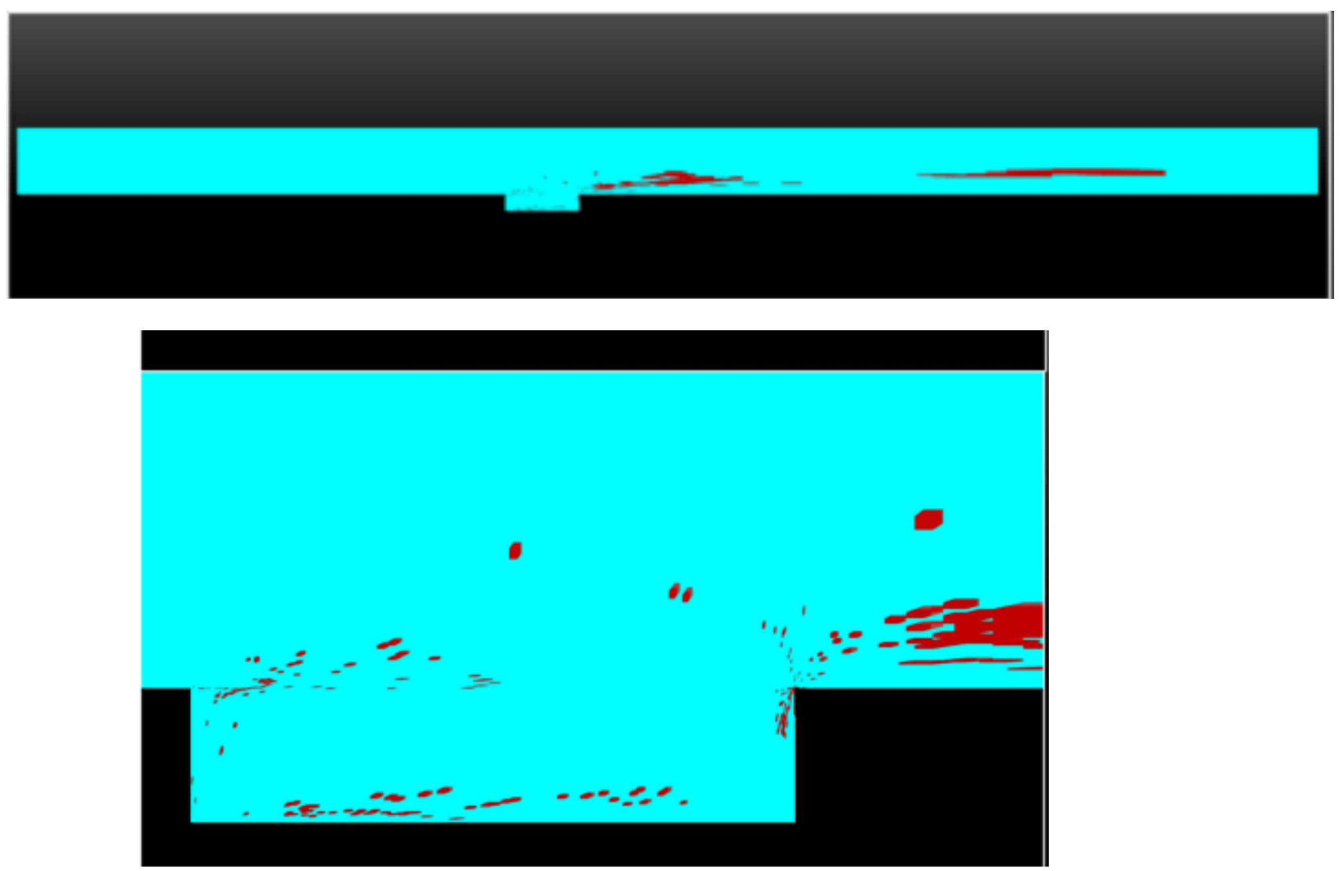


- High-fidelity model
  - Compressible Navier–Stokes
  - Finite-volume discretization
  - DES turbulence model
  - Re = 6.30×10^6
  - $M_\infty = 0.6$
  - 1.2 million degrees of freedom
- GNAT ROM
  - 179 degrees of freedom

GNAT sample mesh

$$R_r^n = (P\Phi_R)^+ P R^n$$





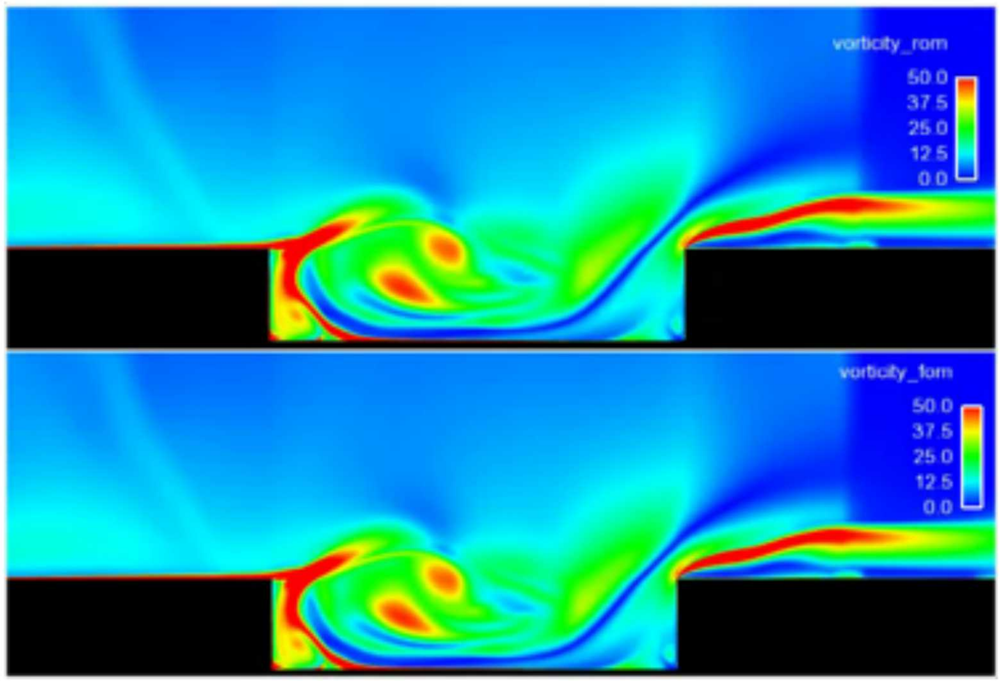
+ Enables ROM to run on far fewer cores

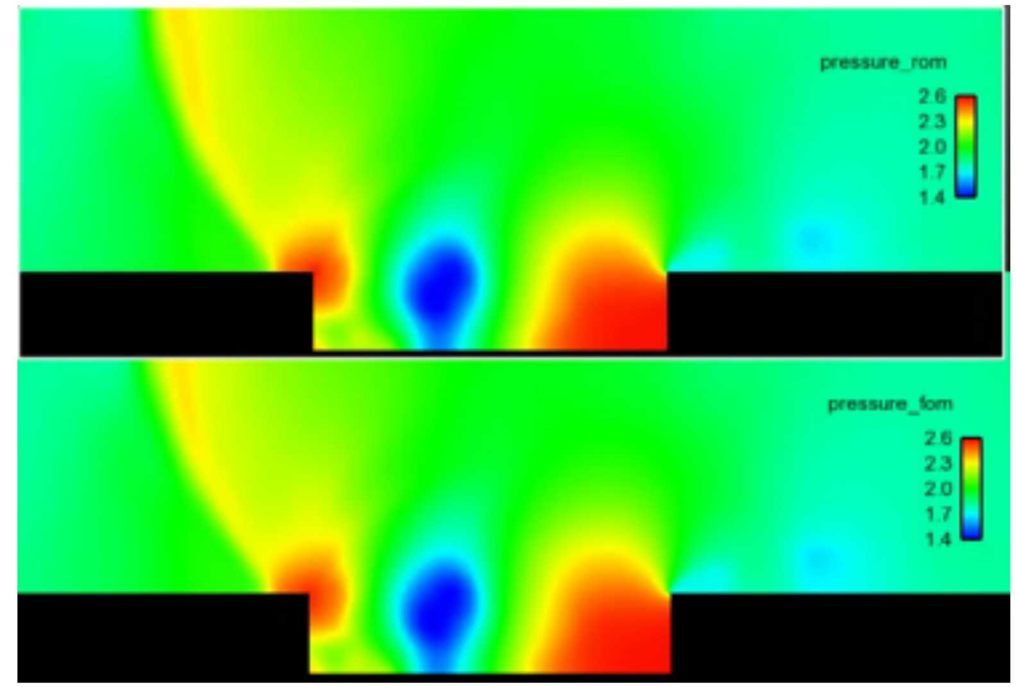
Cavity-flow results

vorticity field | pressure field

GNAT ROM

high-fidelity model





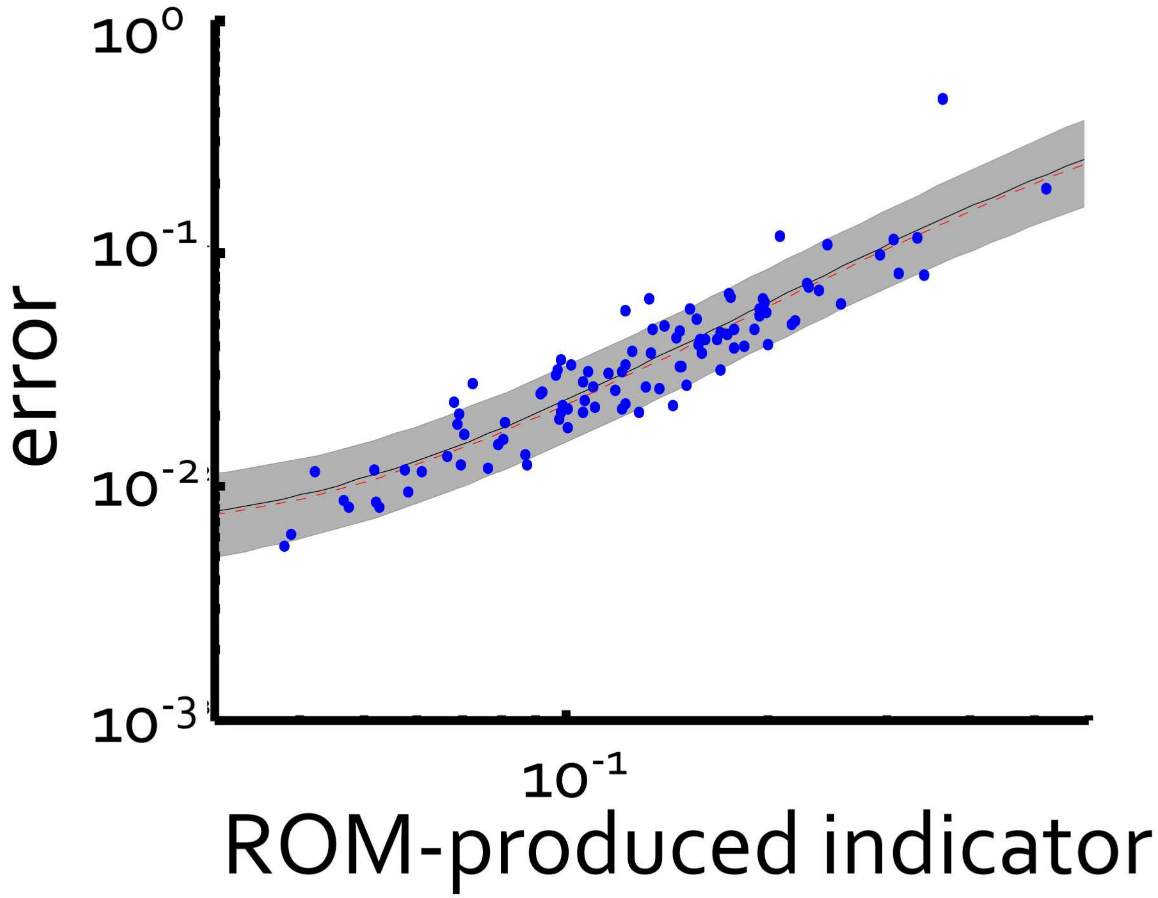
model	wall time	# cores	CPU savings
GNAT ROM	32 minutes	2	**229**
FOM	5 hours	48	1

Error models

Sandia National Laboratories

Statistical error model

- **Motivation**: UQ demands error statistics, not error bounds
- **Discovery**: simple relationship: ROM-produced indicators & errors



- **Idea**: generate a stochastic-process statistical error model
  - quantifies ROM-induced uncertainty
  - 10x accuracy improvement
- **Breakthrough**: 'glue' connecting ROMs and UQ
- **Publication**: Drohmann and Carlberg, *SIAM JUQ*, 2014.

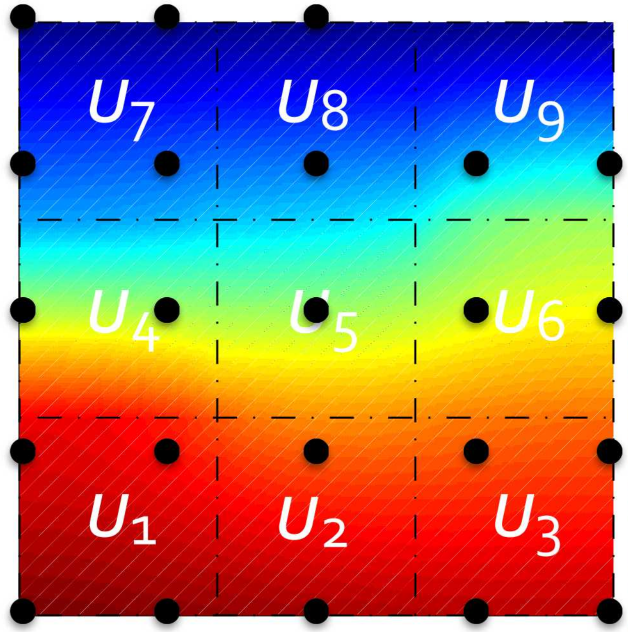
Bayesian inference

inputs u $\longrightarrow$ $\boxed{\text{high-fidelity model / ROM} + \delta}$ $\longrightarrow$ outputs z

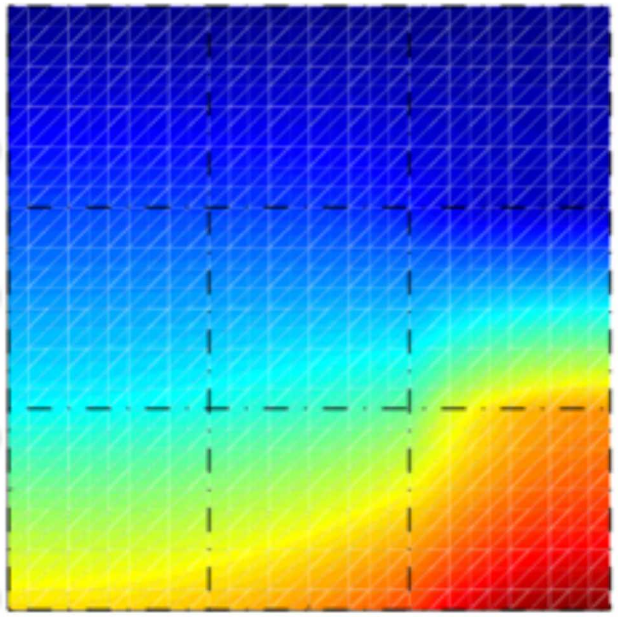
$$P(u|\bar{z}) \propto P(\bar{z}|u)P(u)$$

- Prior: $P(u)$
- Likelihood: $P(\bar{z}|u) \sim \mathcal{N}(z(u), \sigma^2 I)$
  - requires expensive high-fidelity simulations
- common approach: set $P(\bar{z}|u) \sim \mathcal{N}(z_{\mathrm{ROM}}(u), \sigma^2 I)$
  - \+ cheap
  - \- neglects ROM error
- **Idea**: set $P(\bar{z}|u) \sim \mathcal{N}(z_{\mathrm{ROM}}(u) + \mathrm{E}\left[\delta(u)\right], \sigma^2 I + \mathrm{var}[\delta(u)])$
  - statistical error model $\delta(u)$

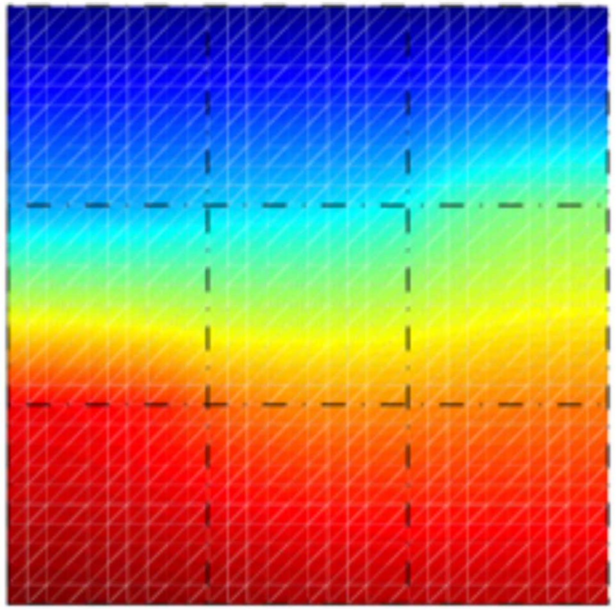
Bayesian inference



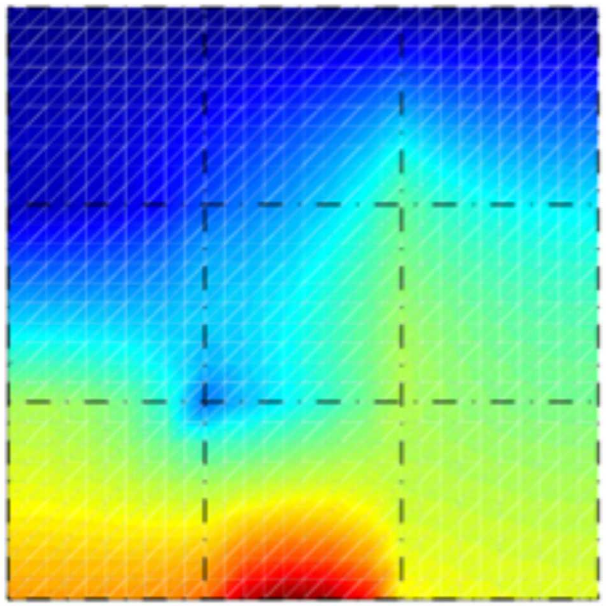
true distribution



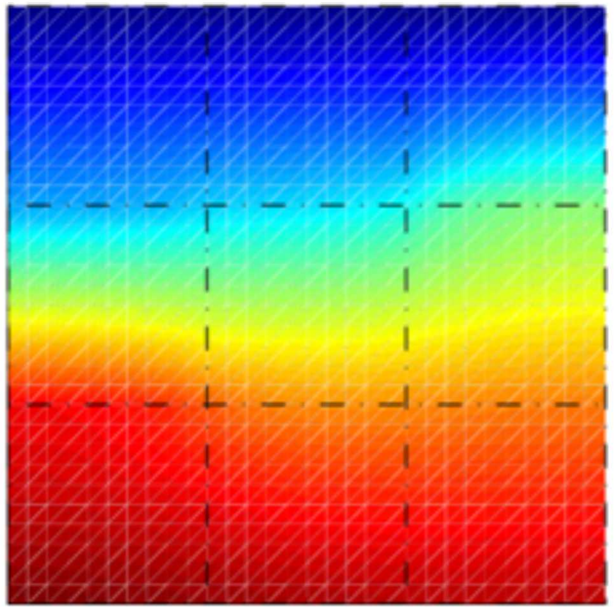
prior mean



full-order model



ROM



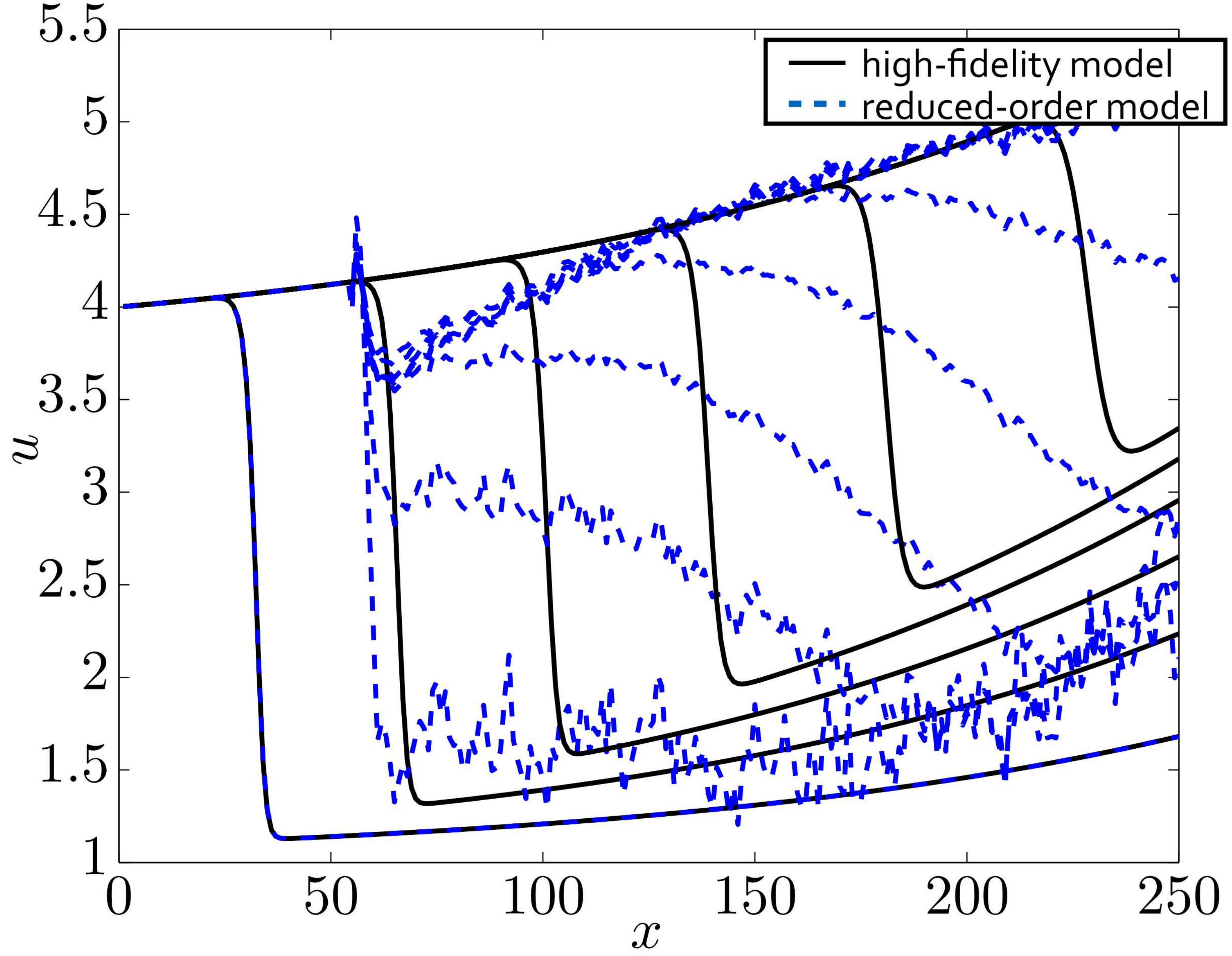
ROM $+\ \delta$

- **Result**: fast + rigorous ROMs in data assimilation
- **Publication:** Carlberg, Lu, Morzfeld, *in preparation*, 2014.

Overcoming insufficient training data

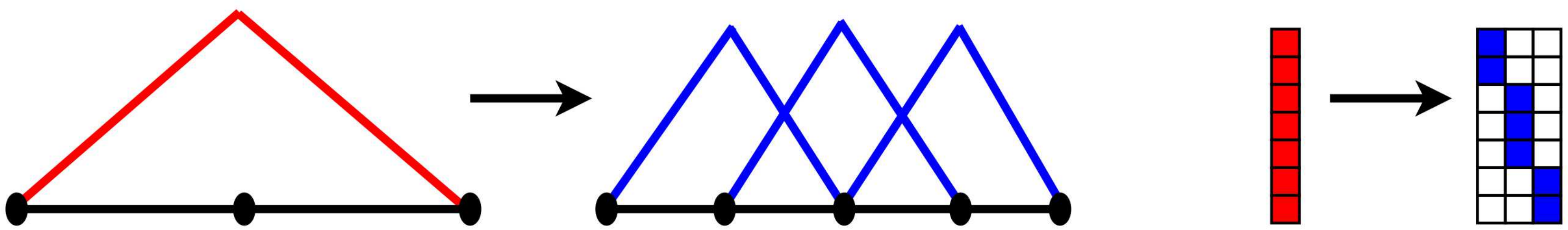
Overcome insufficient data

- **Motivation**: ROM relies heavily on 'data relevance' $y^n \approx \Phi y_r^n$
- **Example**: inviscid Burgers equation
  - *Data collection*: 0 to 2.5 seconds
  - *Prediction*: 0 to 50 seconds



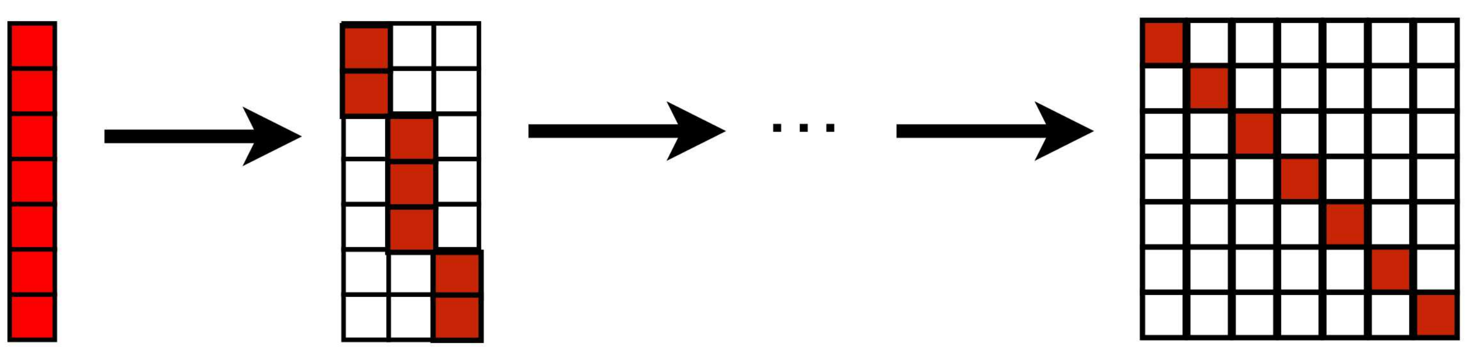
Overcome insufficient data

- **Idea**: ROM analog to *adaptive mesh refinement*
  - 'Split' basis vectors

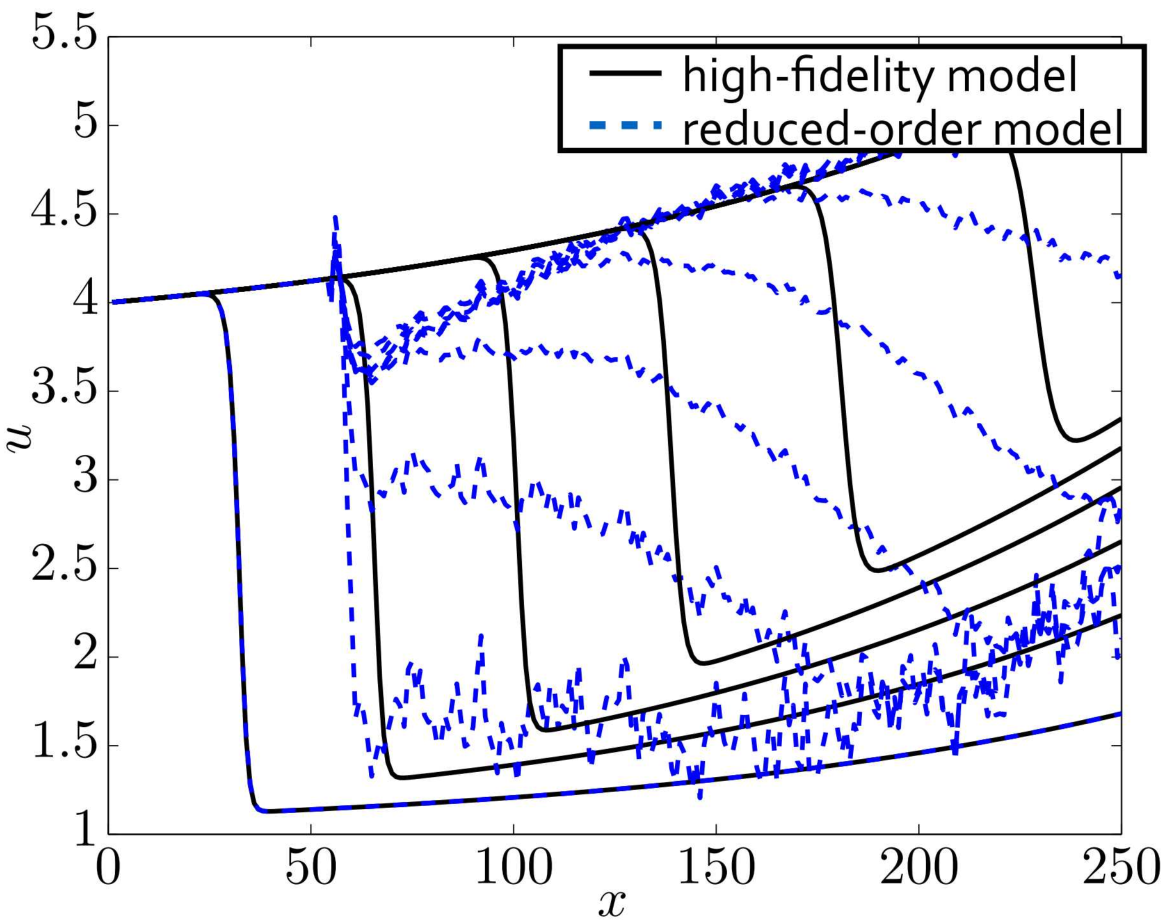


finite element h-refinement *ROM h-refinement*

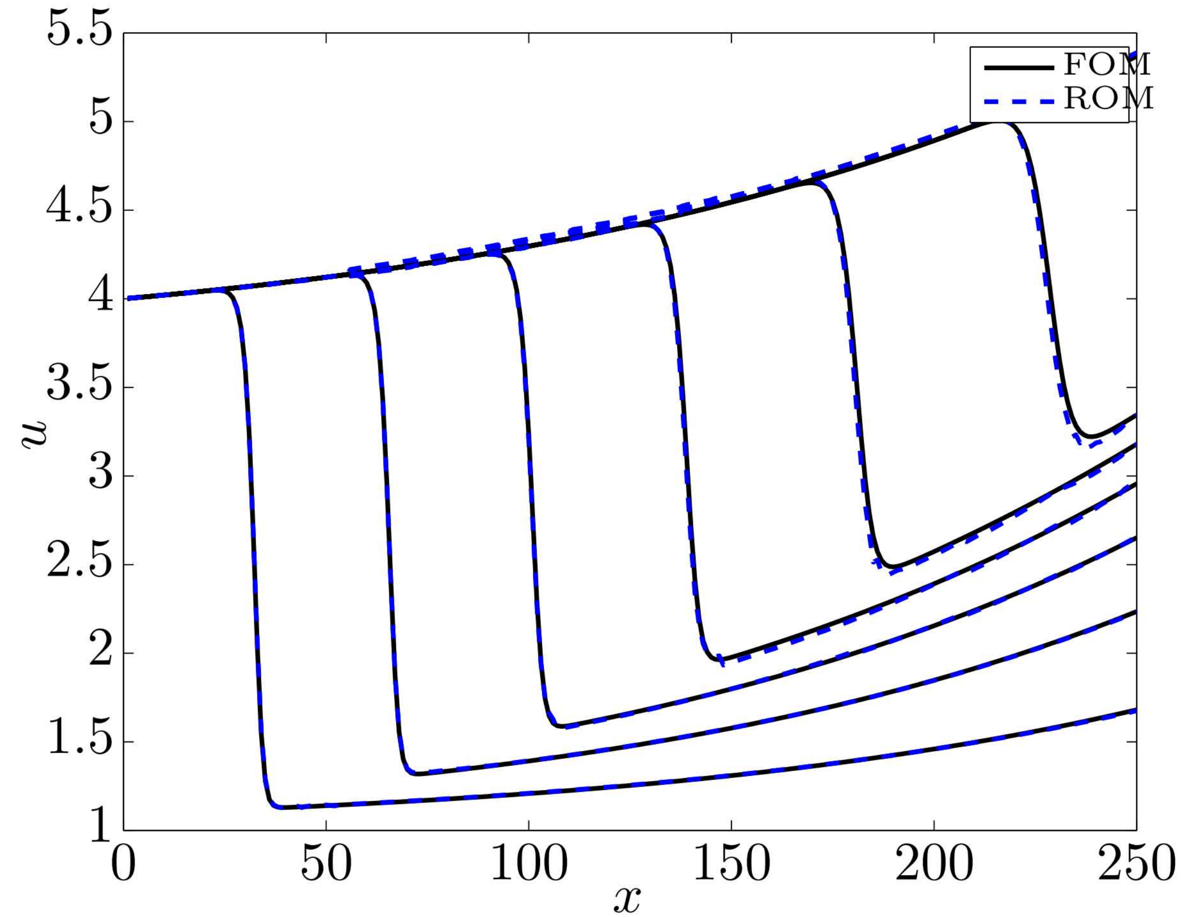
  - ROM converges to the high-fidelity model



Example: inviscid Burgers' equation



ROM

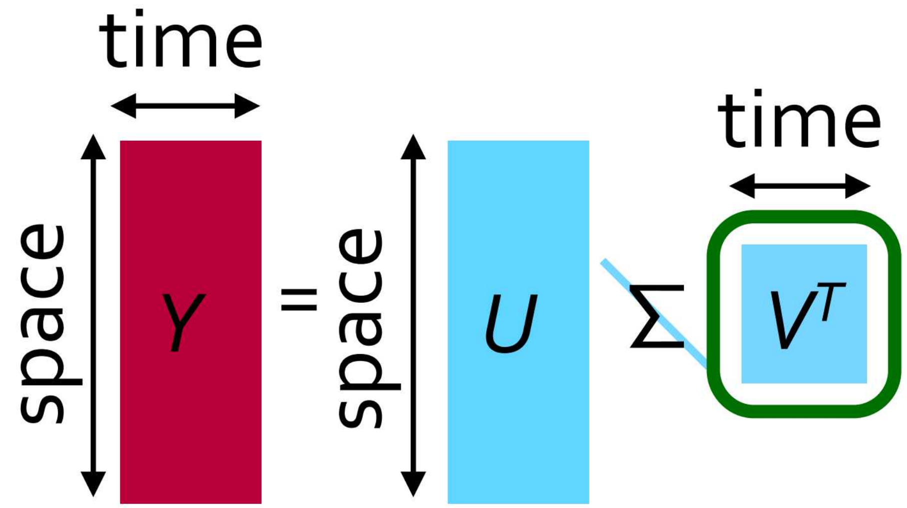


ROM **with *h*-adaptivity**

- **Breakthrough**: ROMs can be always used safely
- **Publication:** Carlberg, *Int J Numer Meth Eng*, 2014.

Leveraging temporal data

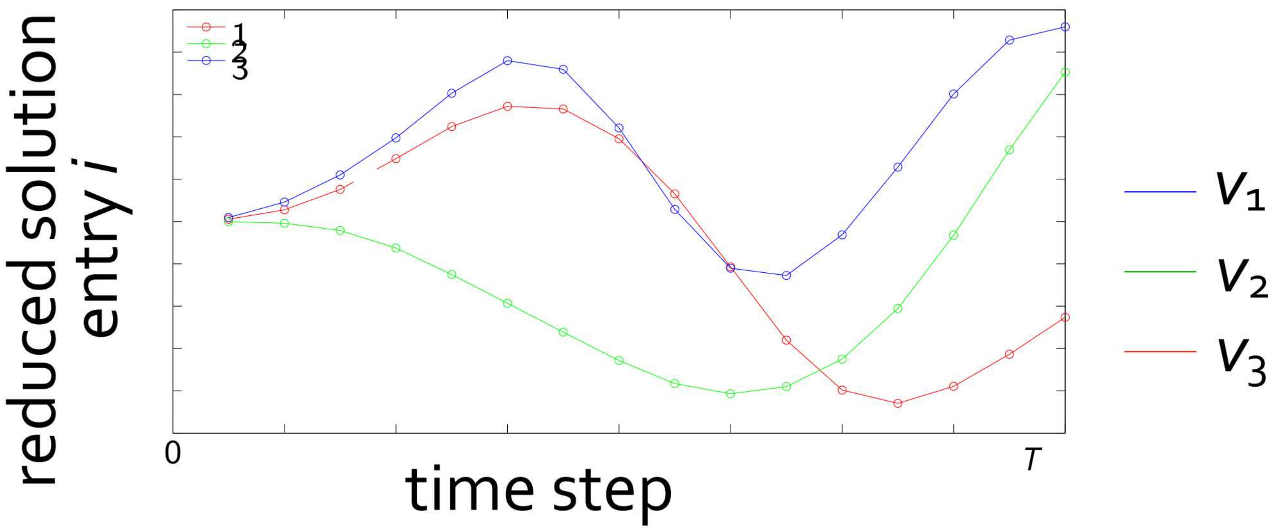
Leverage temporal data



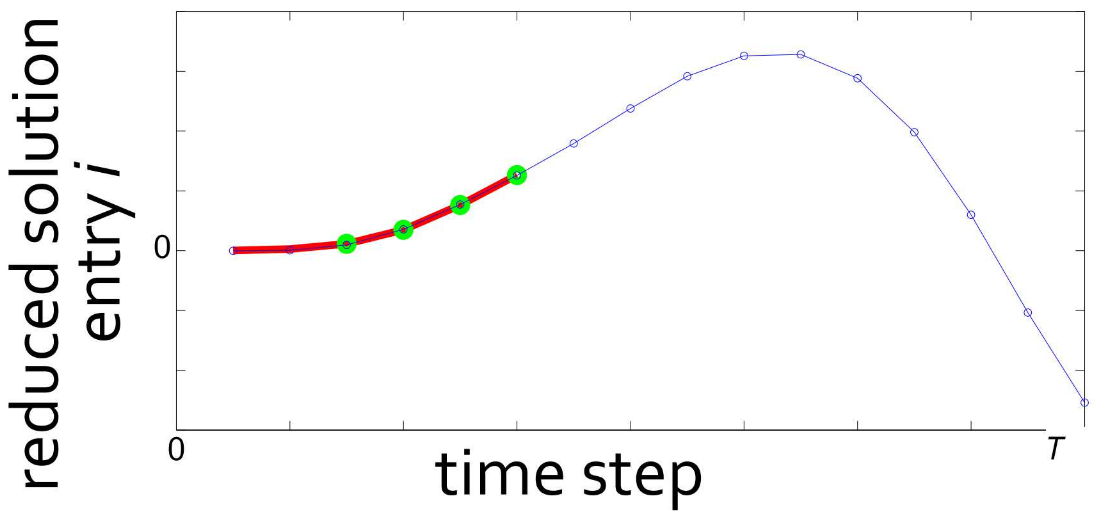
- **Motivation**: can we exploit temporal simulation data?

Leverage temporal data

- Interpret V as a low-dimensional *time-evolution* basis



- *Online:* 1) forecast the reduced solution using low-dim basis



2) use prediction as an initial guess for Newton solver

- **Results:** reduce ROM simulation time by 30% with no accuracy loss
- **Publication:** Carlberg, Ray, van Bloemen Waanders, *CMAME, 2014.*

Software

Razor

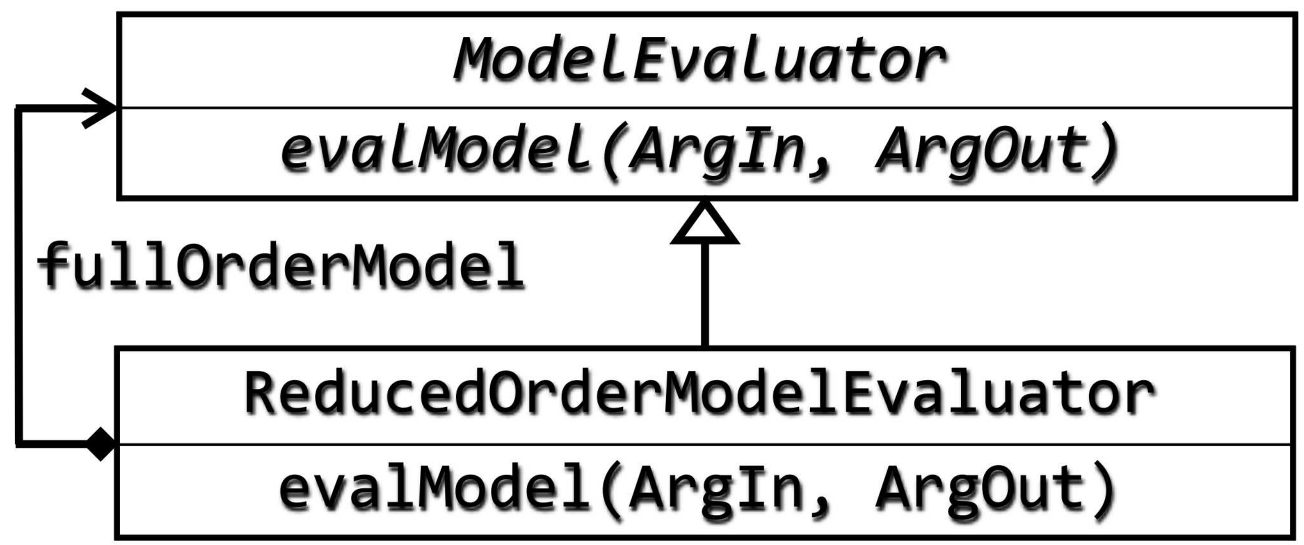
- **Motivation**: easily deploy ROMs on Sandia applications
- **Design principles**
  - Minimally intrusive
  - Trilinos-based library

$$R(y; t, u) = 0$$

$$\underset{y_r}{\text{minimize}} \| R(\Phi y_r; t, u) \|_2^2$$

$$\Leftrightarrow$$

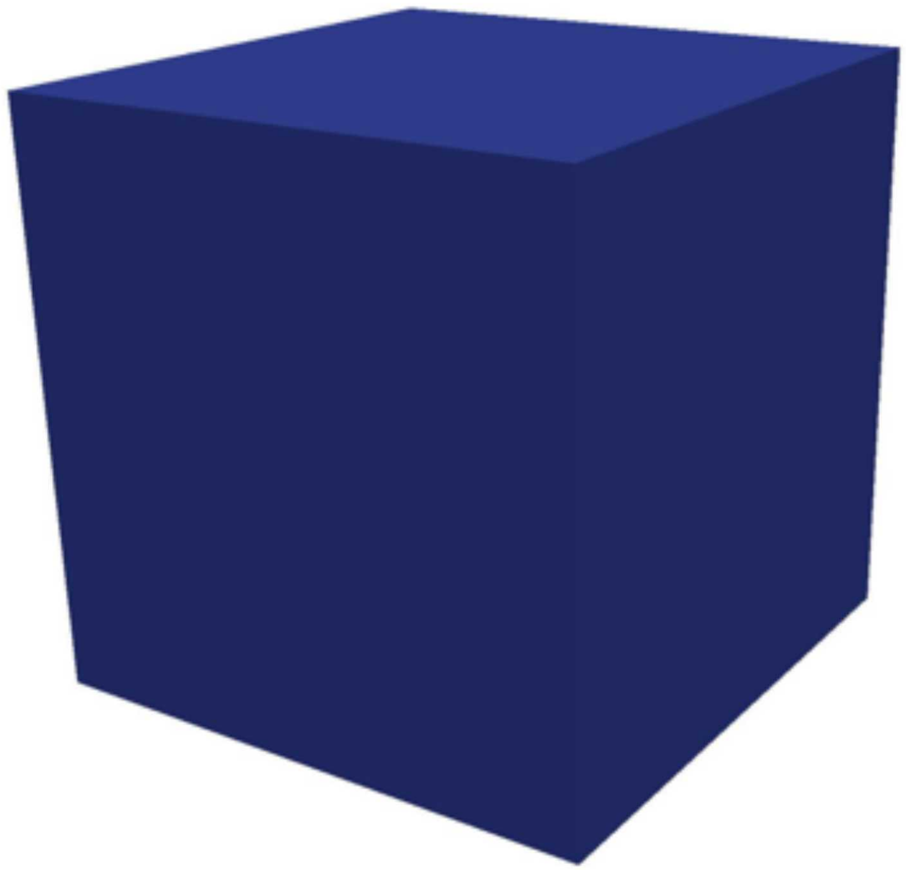
$$R_r(y_r; t, u) = 0$$

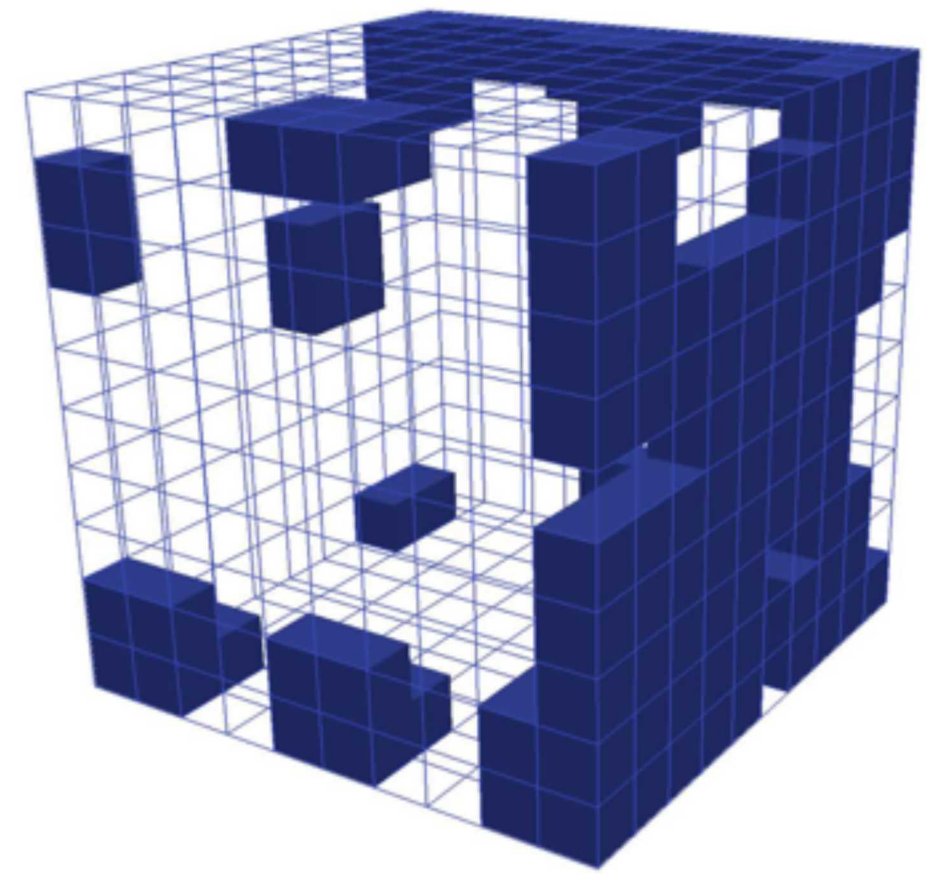


- **Current status:** loosely coupled module in Albany

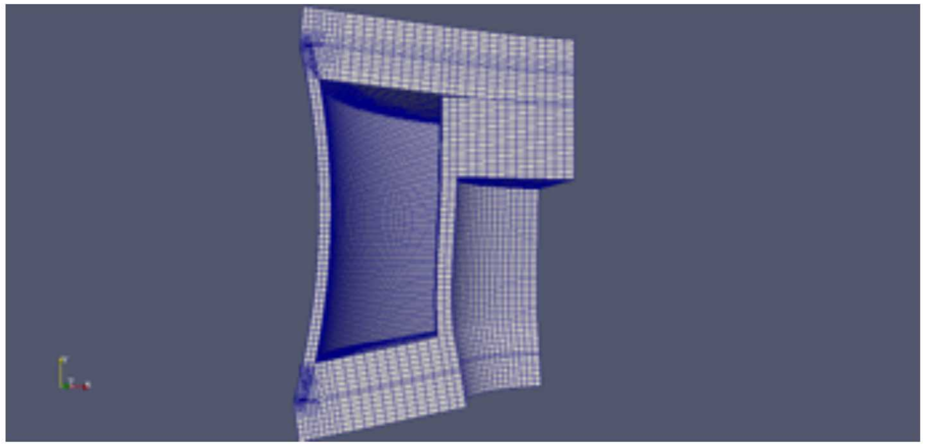
Razor

- **Application**: Thermal/mechanical response

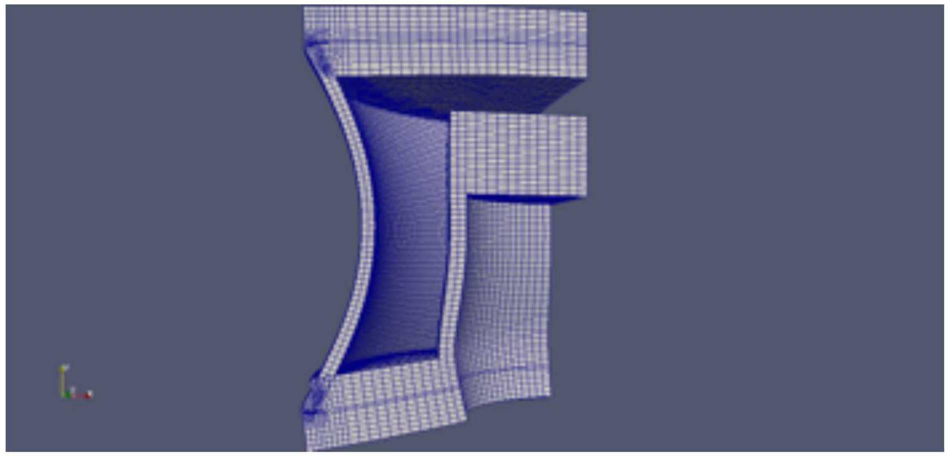




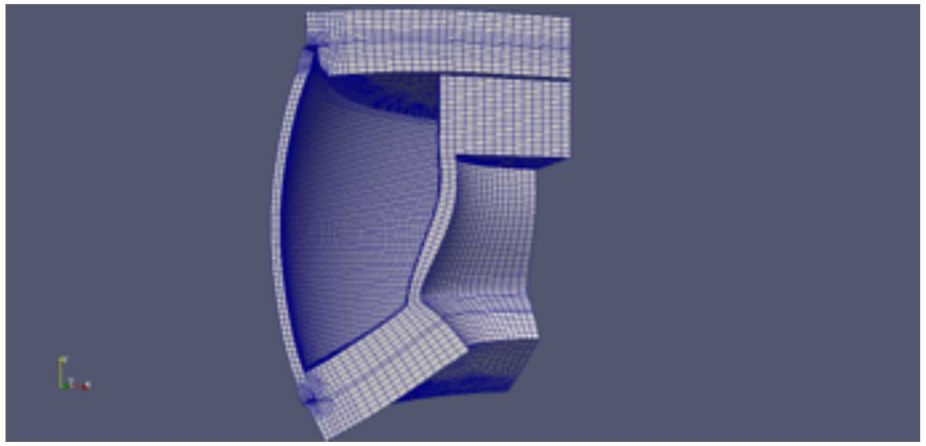
- Full-order model
  - 5324 degrees of freedom
- ROM
  - 15 degrees of freedom
  - cpu savings factor = 12.5



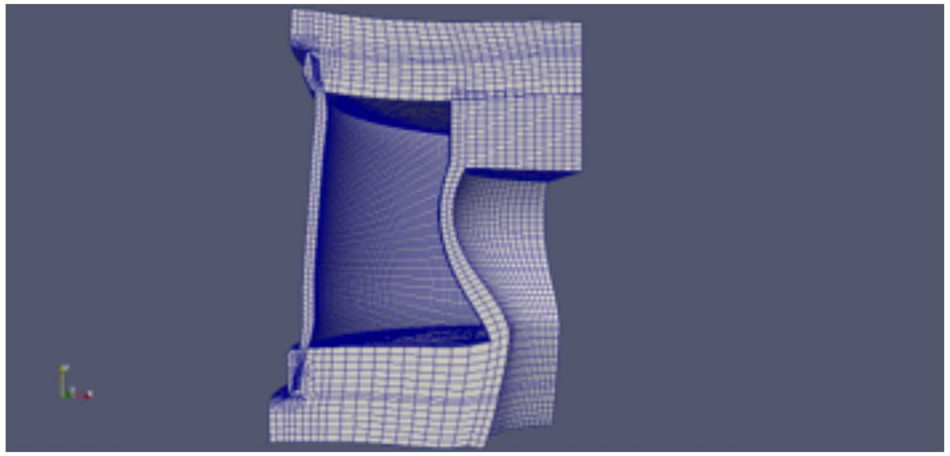
POD mode 1



POD mode 2

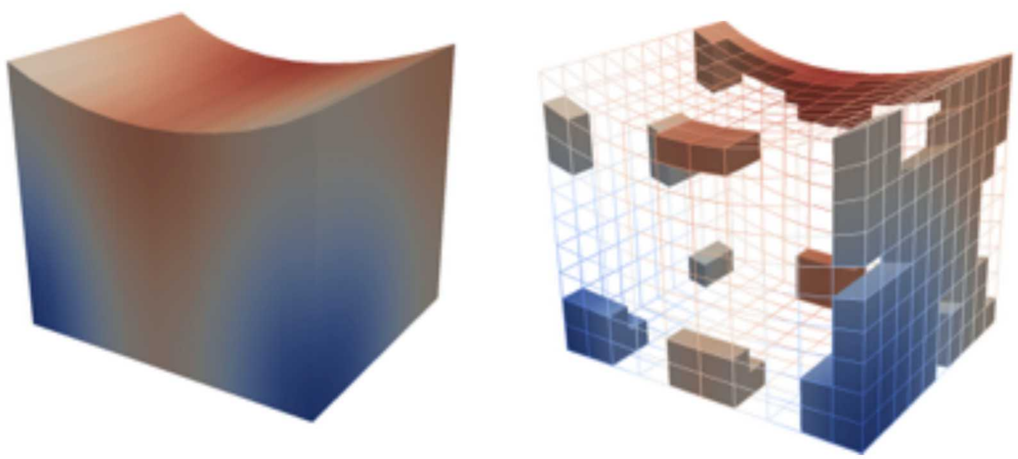


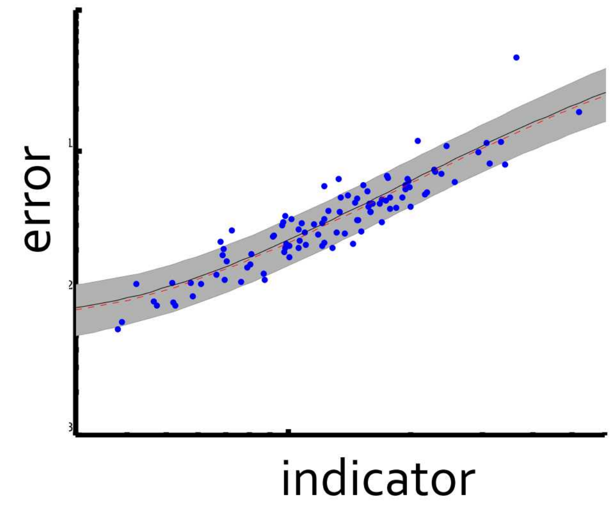
POD mode 3

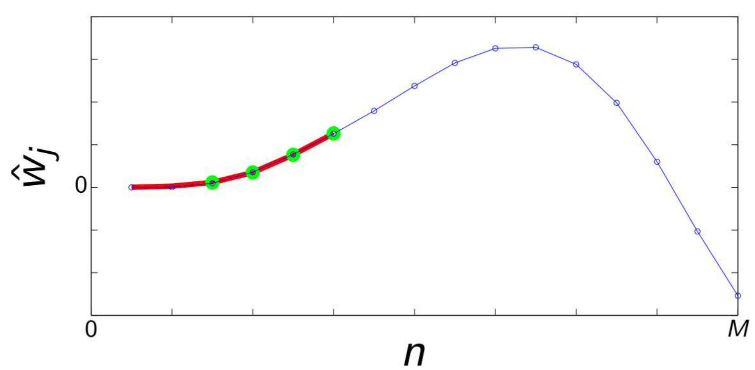


POD mode 4

Questions?







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