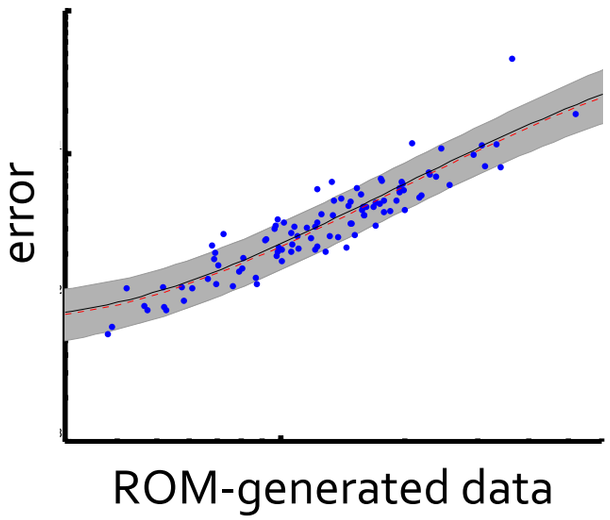
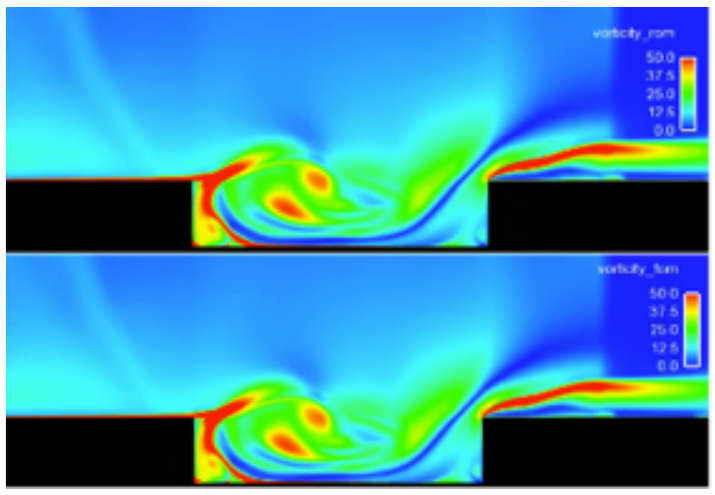
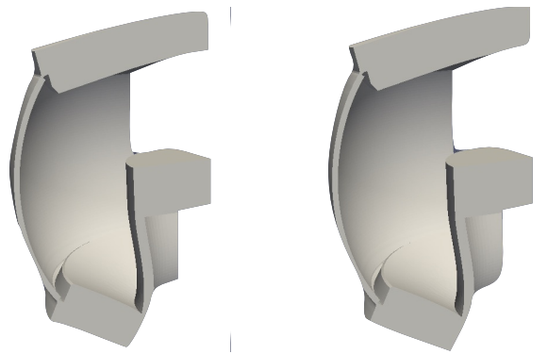
SAND2016-5525PE

Breaking computational barriers via nonlinear model reduction







Kevin Carlberg

CIS External Review

Sandia National Laboratories

June 7, 2016

Computational barrier

High-fidelity simulation

+ Indispensable in mission-critical applications
- *High fidelity*: large-scale nonlinear dynamical system models

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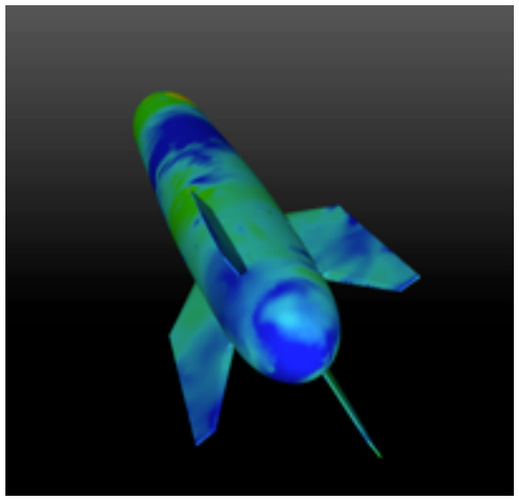

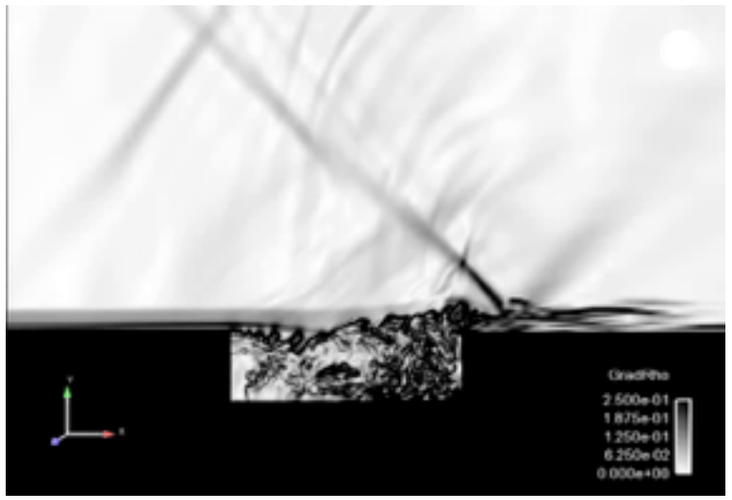

+ *Validated, predictive model:* matches experiment to within 5%
- *High simulation costs*: 6 weeks, 5000 cores

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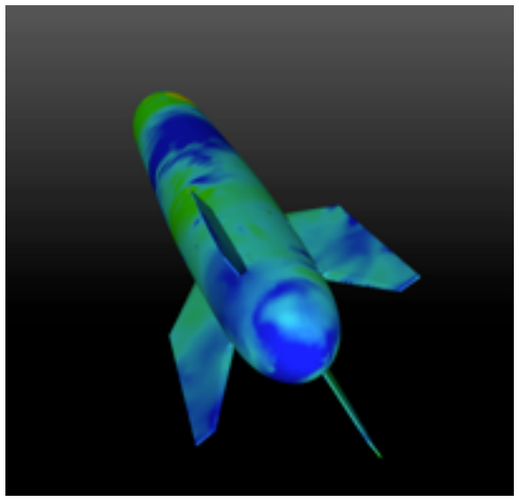

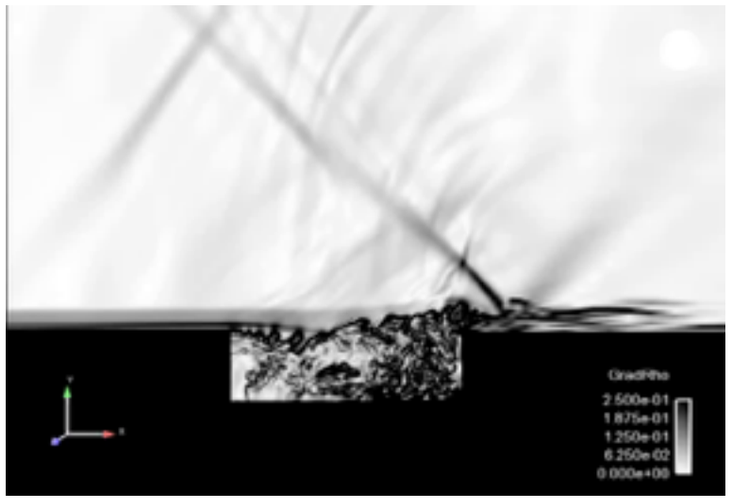

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barrier

Time-critical applications

◉ rapid design ◉ stochastic optimization ◉ uncertainty quantification

Model reduction

Goal: Exploit data to drastically reduce simulation costs

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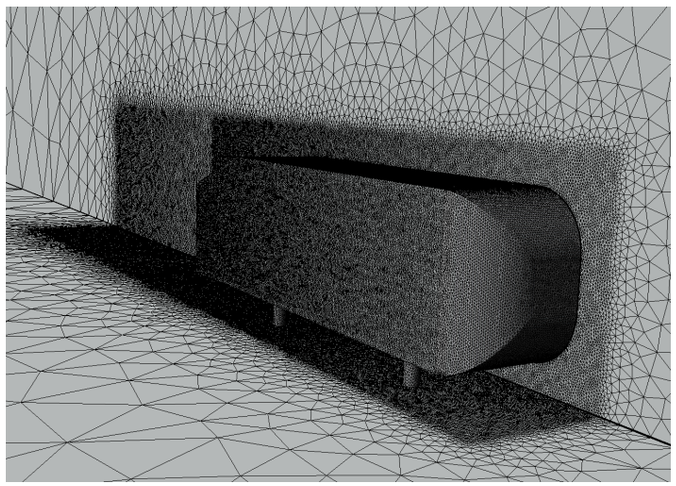
high-fidelity model



Model reduction

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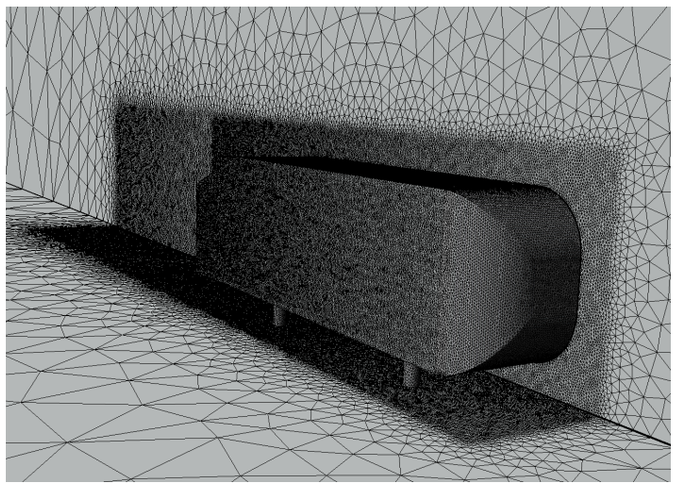
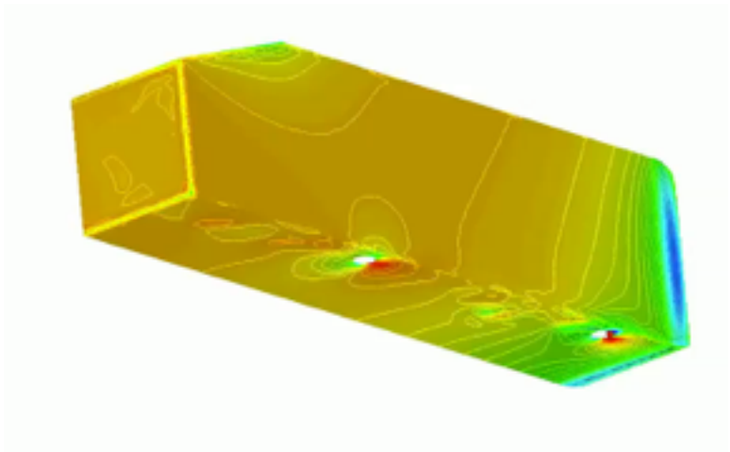
high-fidelity model → *analyses* → data





Model reduction

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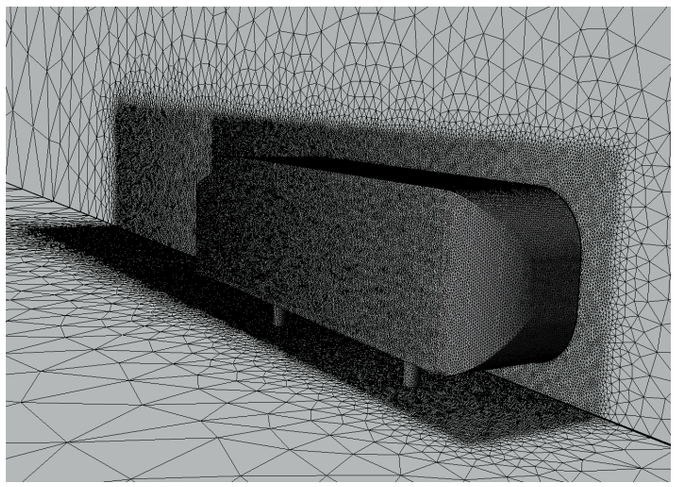
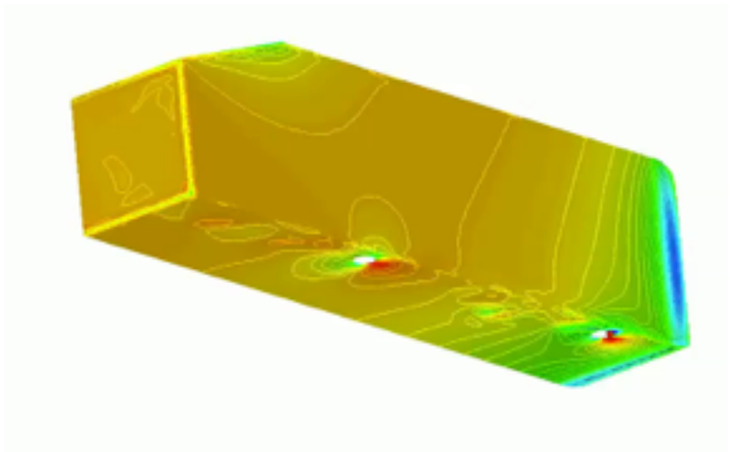
high-fidelity model → *analyses* → data → *machine learning* → • low-dim subspaces • index clusters • sample nodes





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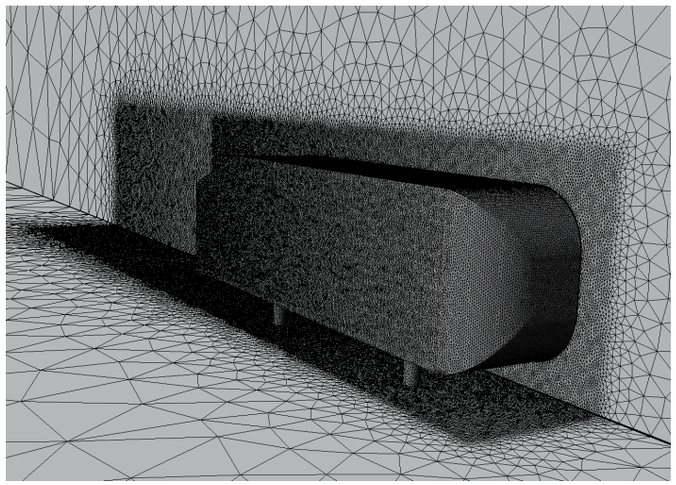
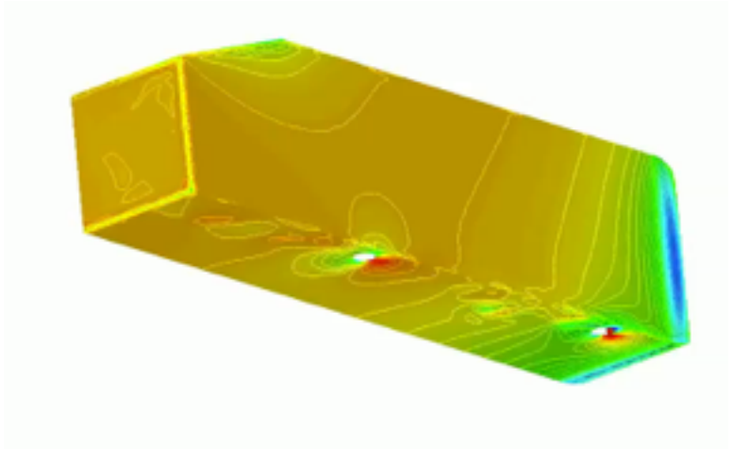
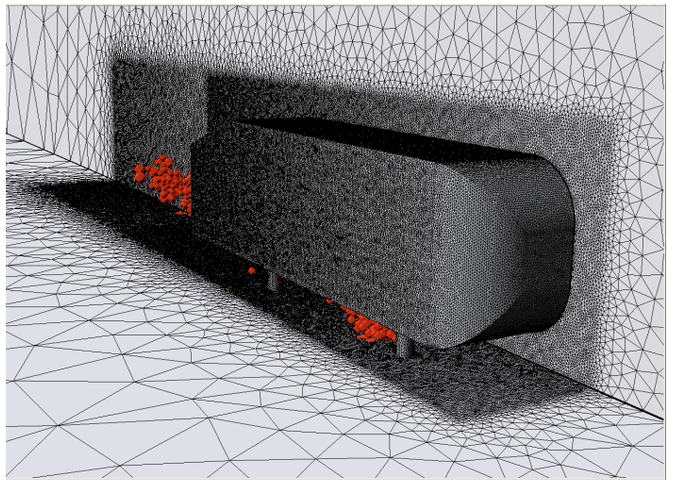
→ *model reduction* → reduced-order model (ROM)







ROM: state of the art

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- Linear time-invariant systems: mature [Antoulas, 2005]
  - Balanced truncation [Moore, 1981]
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  - Moment matching [Bai, 2002; Freund, 2003; Gallivan et al, 2004; Baur et al., 2001]
  - Loewner framework [Lefteriu and Antoulas, 2010; Ionita and Antoulas, 2014]
  - + *Reliable*: guaranteed stability, *a priori* error bounds
  - + *Certified*: sharp, computable *a posteriori* error bounds

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- Nonlinear dynamical systems: unproven
  - Proper orthogonal decomposition (POD)–Galerkin [Sirovich, 1987]
  - – *Not reliable*: often unstable and inaccurate
  - – *Not certified*: error bounds not sharp

Our research

Nonlinear model-reduction methods that are

accurate, *low cost*, *certified*, and *reliable*

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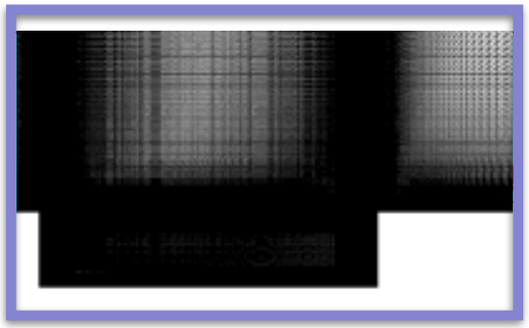
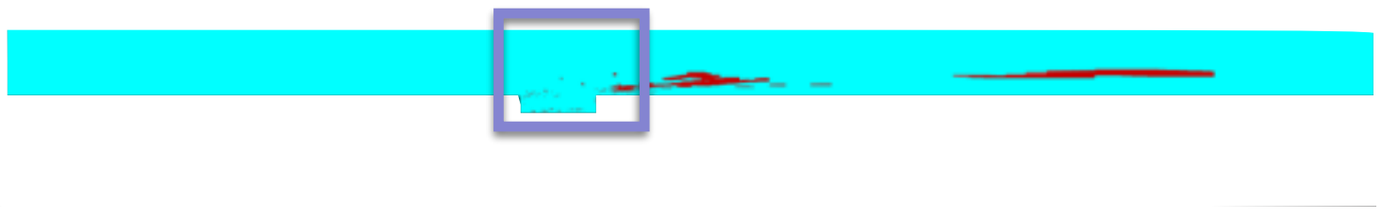
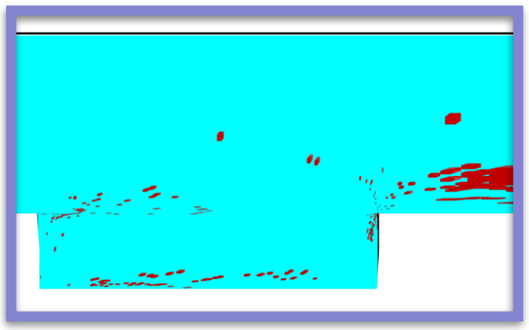
Captive-carry results



Captive-carry results

sample mesh





+ HPC on a laptop

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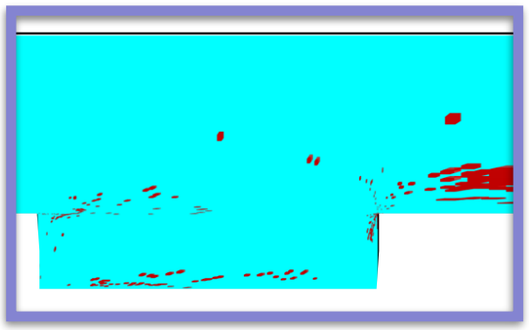


+ HPC on a laptop

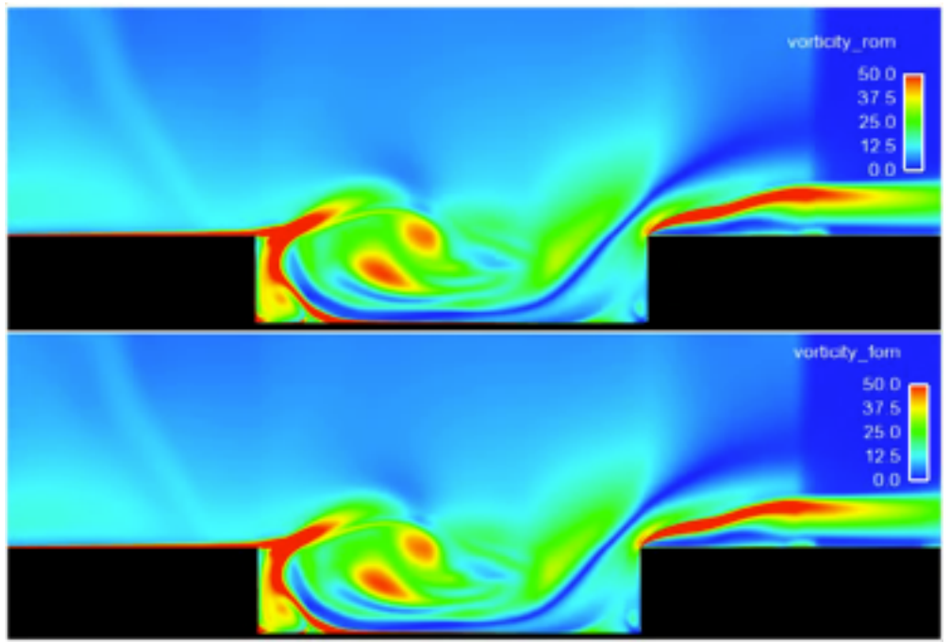
vorticity field | *pressure field*

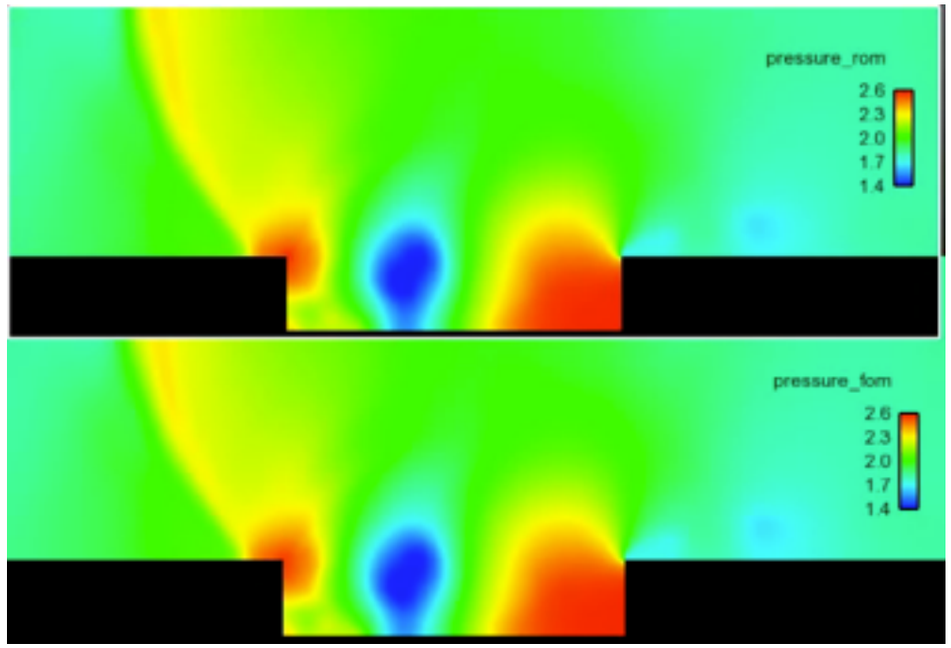
LSPG ROM

32 min, 2 cores

high-fidelity

5 hours, 48 cores





+ 229x savings in core–hours

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Nonlinear model-reduction methods that are
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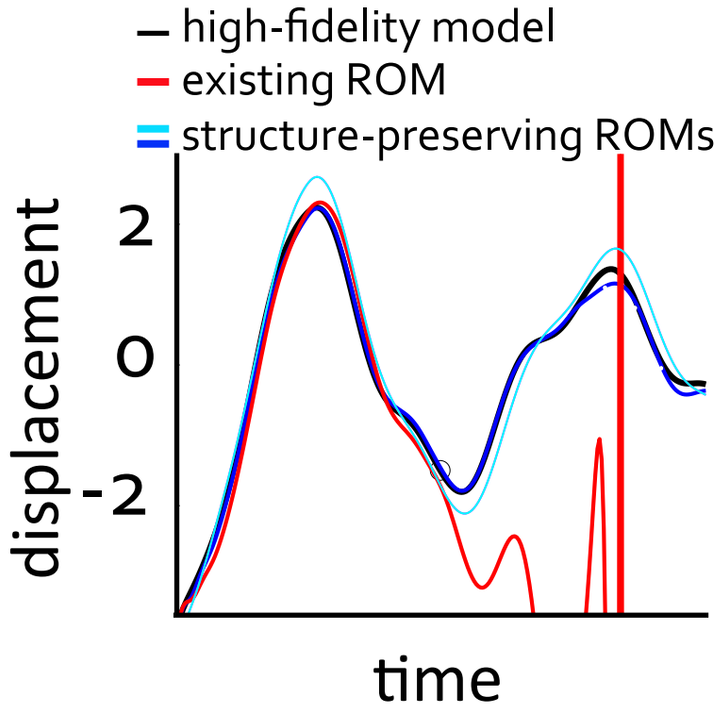

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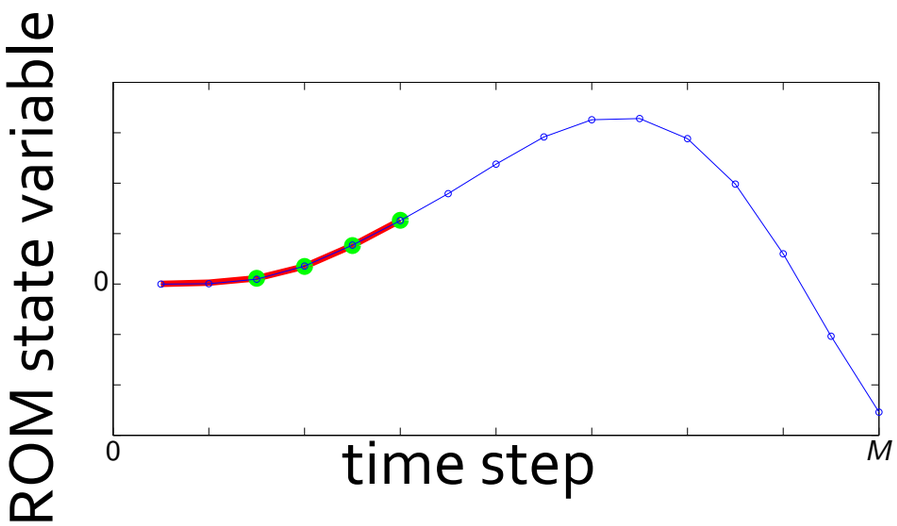

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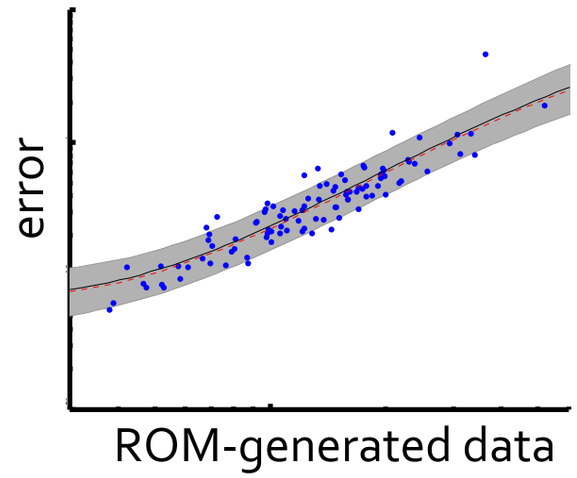
Statistical error modeling



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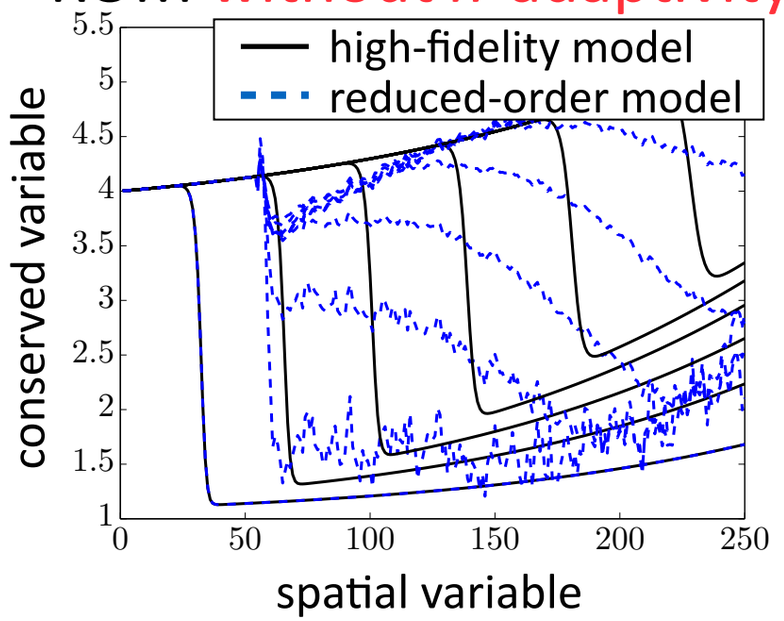
ROM without *h*-adaptivity



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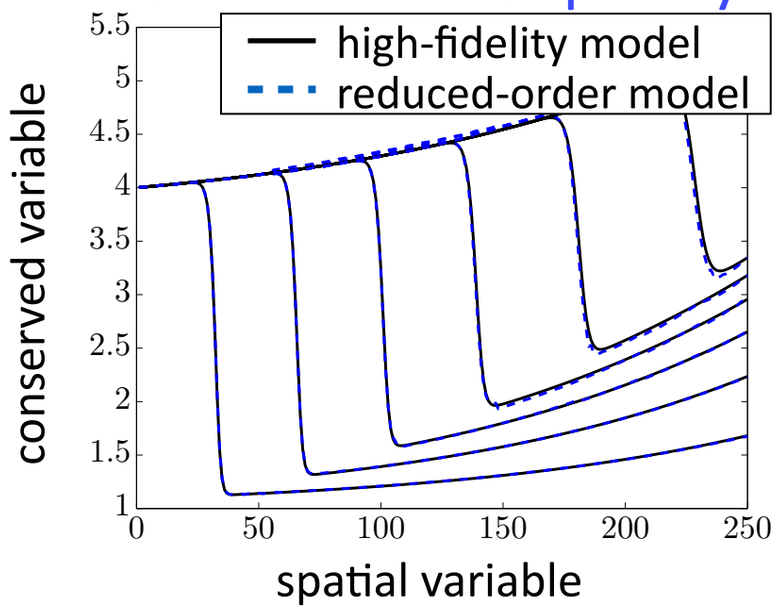

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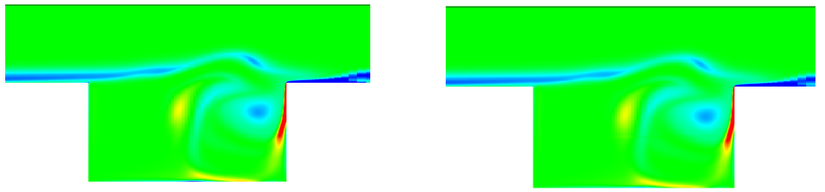
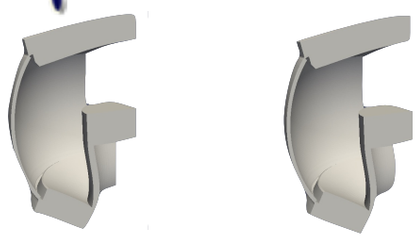
  - *A posteriori h*-refinement [C., 2015]
+ **HPC implementation**
  - Three computational-mechanics codes

SPARC — Sandia National Laboratories



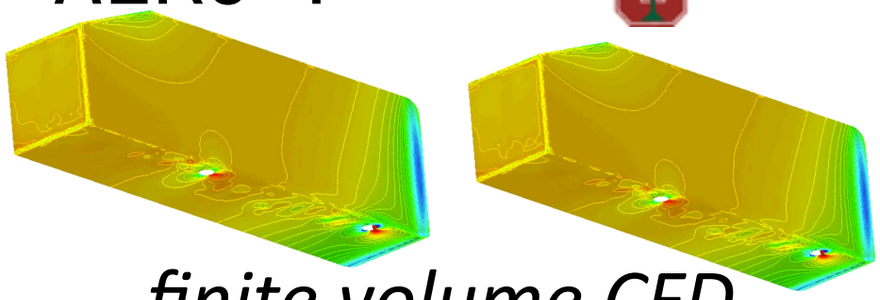
finite volume CFD

Albany — Sandia National Laboratories



finite element multiphysics

AERO–F



finite volume CFD

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$3.1M Funding

2011–2014 *LDRD: Truman Fellowship*
$260k/year
3 postdocs, 1 summer student

2014–present *NNSA/ASC/V&V: Fluid dynamics*
$250k/year
4 staff, 1 postdoc

2014–present *NNSA/ASC/V&V: Thermomechanics*
$425k/year
3 staff, 2 postdocs, 1 summer student

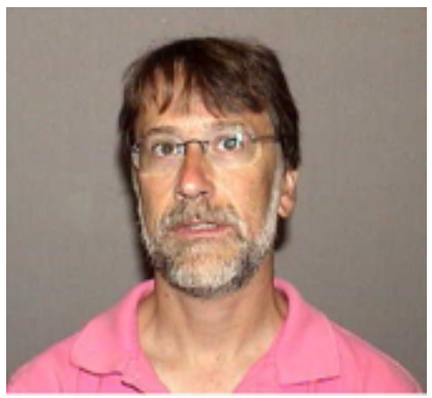
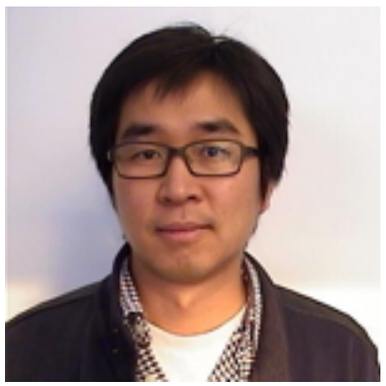
2014–present *NNSA/ASC/V&V: Nonlinear model reduction*
$200k/year
2 staff, 1 postdocs, 1 summer student

2015–present *LDRD: Model reduction in extreme-scale networks*
$500k/year
3 staff, 2 postdocs, 1 summer student

Interdisciplinary team

Computational mathematics



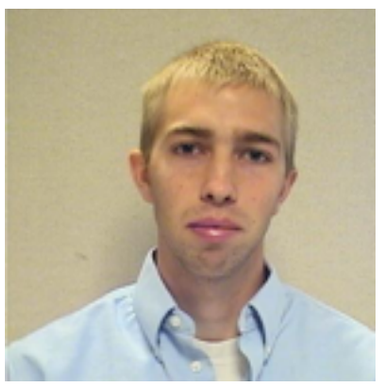
Fluid dynamics



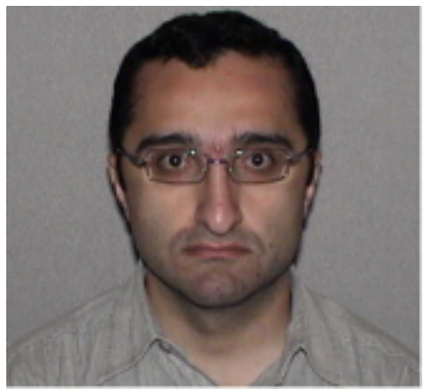
Optimization



Thermomechanics

Uncertainty Quantification




External collaborators

Faculty






UNIVERSITY of WASHINGTON

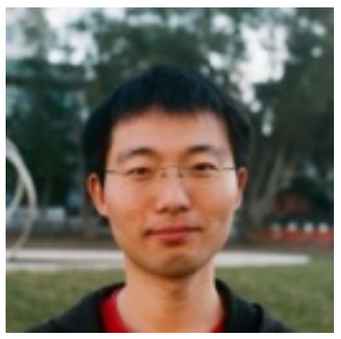
GEORGE MASON UNIVERSITY

Universität Stuttgart

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE







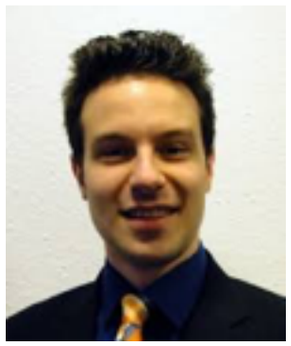

STANFORD UNIVERSITY

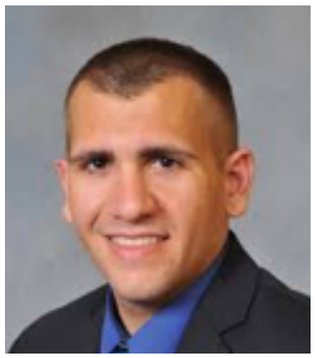
UNIVERSITY OF MARYLAND

BERKELEY LAB Lawrence Berkeley National Laboratory

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Students and Postdocs

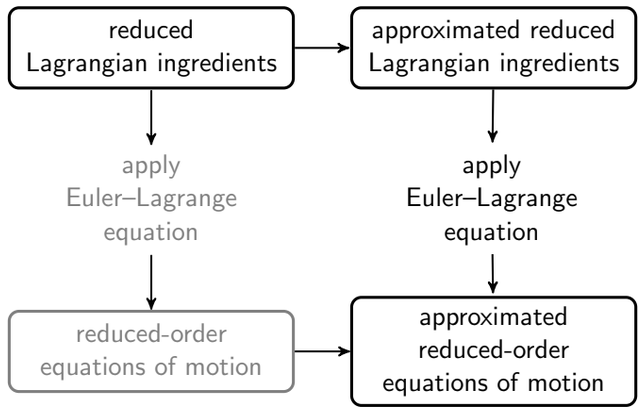



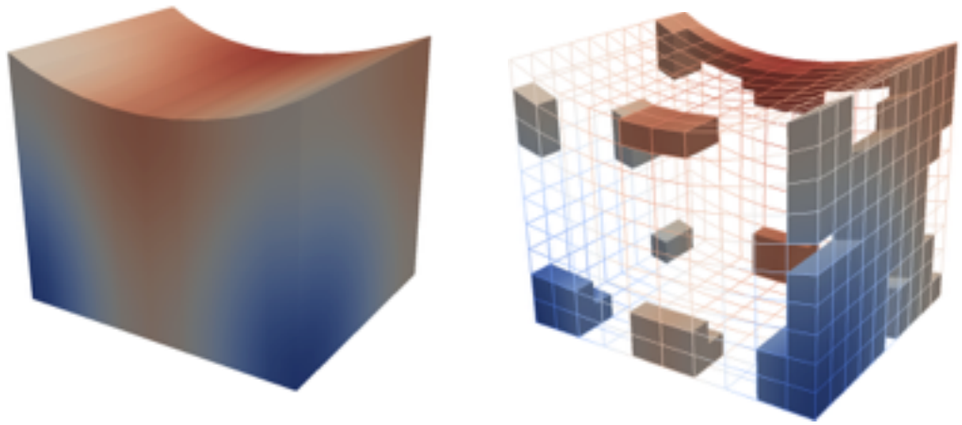


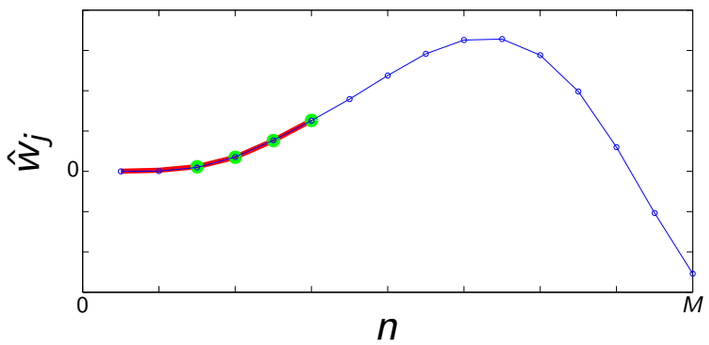

Summary

- 15 publications
  - *Featured article*, June 2015, SIAM J Sci Comput
  - *#1 most cited paper*, 2013, J Comput Phys
  - *#2 most cited paper*, 2011, Int J Numer Meth Eng
- 35 presentations
  - *Keynote lecture*: Model Order Reduction & Machine Learning, 2016
  - 13 invited talks (including MIT, Stanford, UC Berkeley, Cornell)
- Implementation in 3 HPC codes
- Team and funding
  - Span research and development spectrum
  - Range of real-world problems and applications
  - *Internal*: 13 staff, 6 postdocs
  - *External*: 13 faculty, 14 students/postdocs

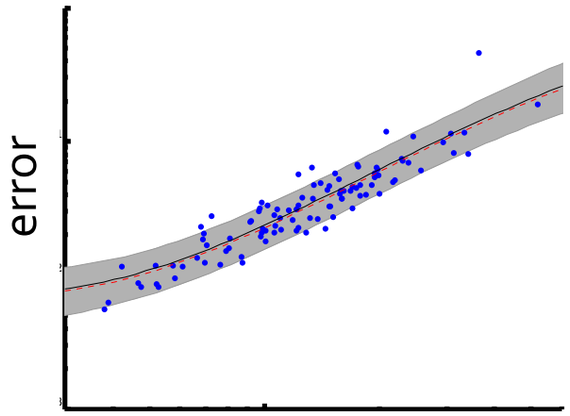
Questions?

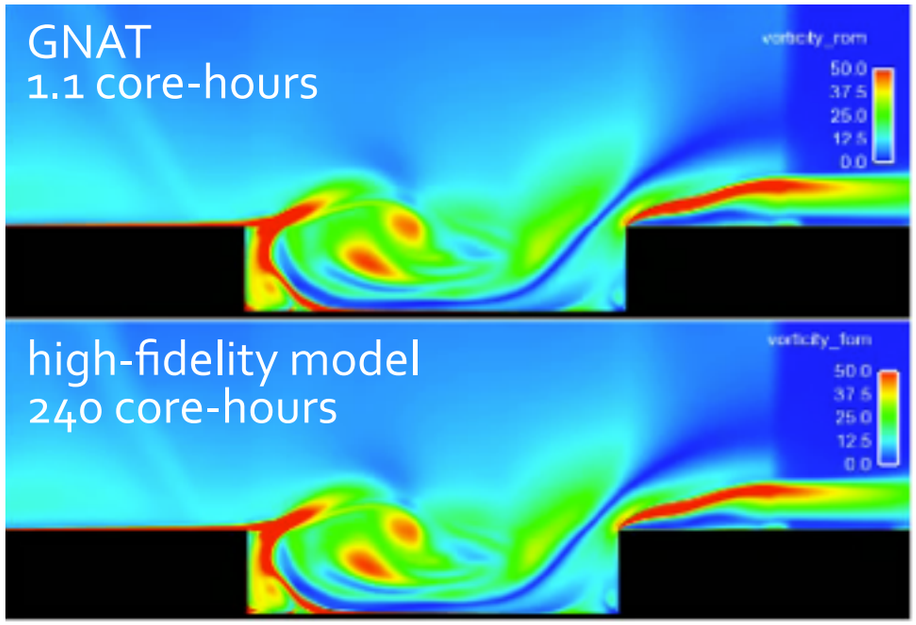




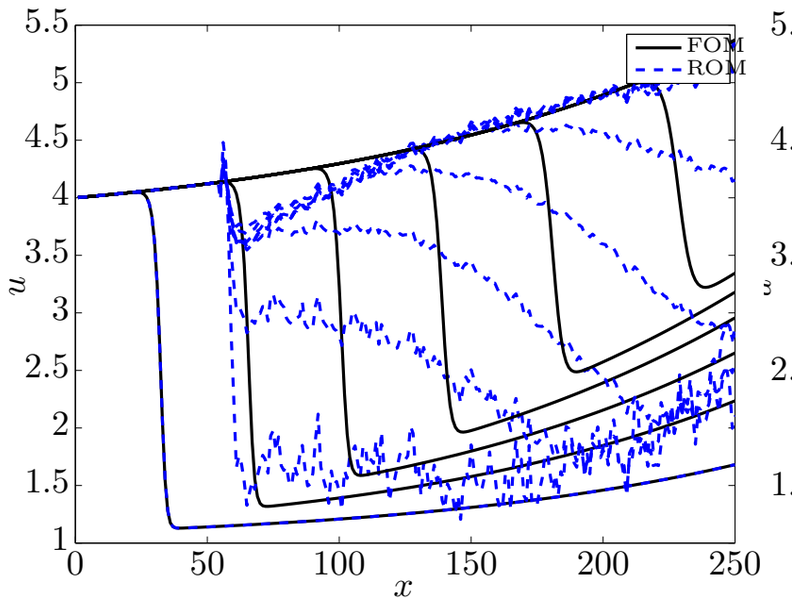


$\hat{w}_j$ so far; memory $\alpha = 4$; forecast





ROM



ROM **with *h*-adaptivity**