Energy-Stable Galerkin Reduced Order Models for Nonlinear Compressible Flow

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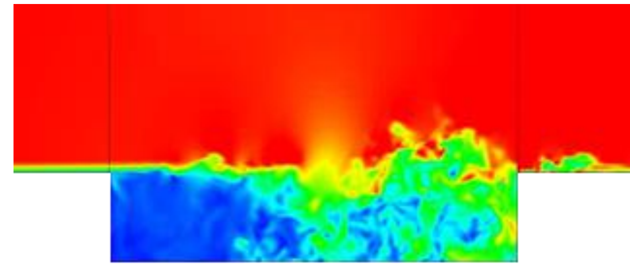
Motivation

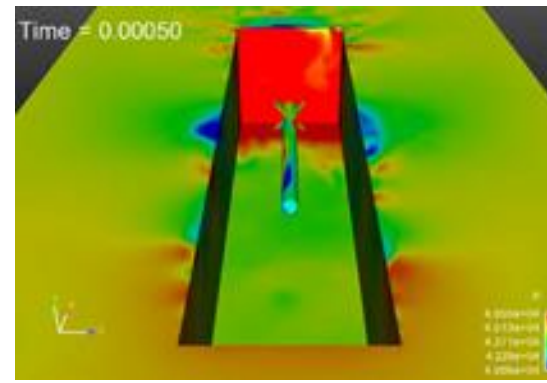
- Despite improved algorithms and powerful supercomputers, **“high-fidelity” models** are often too expensive for use in a design or analysis setting.

- ***Targeted application area in which this situation arises:*** compressible cavity flow problem.

→ **Large Eddy Simulations (LES)** with very fine meshes and long times are required to predict accurately dynamic pressure loads in cavity.

These simulations take ***weeks*** even when run in parallel on state-of-the-art supercomputers!





Proper Orthogonal Decomposition (POD)/ Galerkin Method to Model Reduction

High-Fidelity Simulations:

- Snapshot 1
- Snapshot 2
- ⋮
- Snapshot K

Step 1 →

Modal Decomposition (POD):

$$\boxed{\mathbf{x}(t) \approx \mathbf{\Phi}_M \mathbf{x}_M(t)}$$

Step 2 →

Galerkin Projection of LTI FOM:

$$\boxed{\mathbf{\Phi}_M^T \left[\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)\right]}$$

- ***Snapshot matrix***: $\boldsymbol{X} = (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^K) \in \mathbb{R}^{NxK}$
- ***SVD:*** $\boldsymbol{X} = \boldsymbol{U\Sigma V}^T$
- ***Truncation:*** $\boldsymbol{\Phi}_M = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_M) = \boldsymbol{U}(:, 1{:}\,M)$

N = # of dofs in high-fidelity simulation
K = # of snapshots
M = # of dofs in ROM
$(M << N, M << K)$

"Small" ROM LTI System:

$$\boxed{\begin{array}{lcl} \dot{\mathbf{x}}_M(t) & = & \mathbf{\Phi}_M^T \mathbf{A} \mathbf{\Phi}_M \mathbf{x}_M(t) + \mathbf{\Phi}_M^T \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}_M(t) & = & \mathbf{C}\mathbf{\Phi}_M \mathbf{x}_M(t) \end{array}}$$

Discrete vs. Continuous Galerkin Projection

Discrete Projection

Governing PDEs
$\dot{\boldsymbol{q}} = \mathcal{L}\boldsymbol{q}$

CFD model
$\dot{\boldsymbol{q}}_N = \boldsymbol{A}_N \boldsymbol{q}_N$

Discrete modal basis $\boldsymbol{\Phi}$

Projection of CFD model (matrix operation)

ROM
$\dot{\boldsymbol{a}}_M = \boldsymbol{\Phi}^T \boldsymbol{A}_N \boldsymbol{\Phi} \boldsymbol{a}_M$

This talk focuses on

If PDEs are linear or have polynomial non-linearities, projection can be calculated in **offline stage** of MOR.

Continuous Projection

Governing PDEs
$\dot{\boldsymbol{q}} = \mathcal{L}\boldsymbol{q}$

CFD model
$\dot{\boldsymbol{q}}_N = \boldsymbol{A}_N \boldsymbol{q}_N$

Continuous modal basis* $\boldsymbol{\phi}_j(\boldsymbol{x})$

Projection of governing PDEs (numerical integration)

ROM
$\dot{a}_j = (\boldsymbol{\phi}_j, \mathcal{L}\boldsymbol{\phi}_k) a_k$

* Continuous functions space is defined using finite elements.

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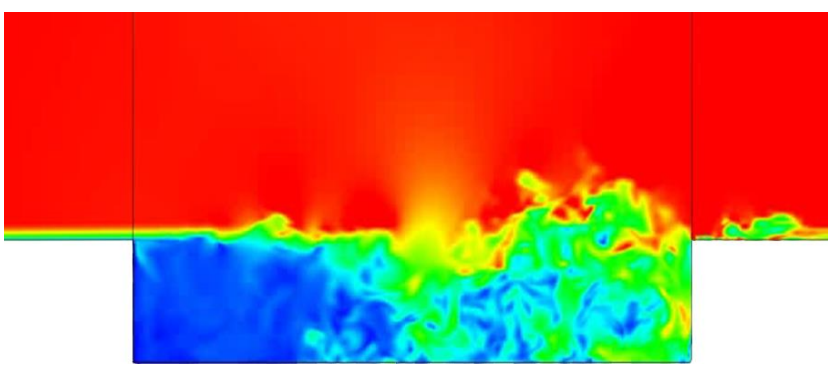
Stability Issues of POD/Galerkin ROMs

Full Order Model (FOM)	**Reduced Order Model (ROM)**
$\dot{\boldsymbol{q}}(t) = \mathcal{L}\boldsymbol{q}(t) + \mathcal{N}(\boldsymbol{q}(t))$	$\dot{\boldsymbol{q}}_M(t) = \boldsymbol{A}_M\boldsymbol{q}_M(t) + \boldsymbol{N}_M(\boldsymbol{q}_M(t))$

Problem: FOM stable $\nRightarrow$ ROM stable!

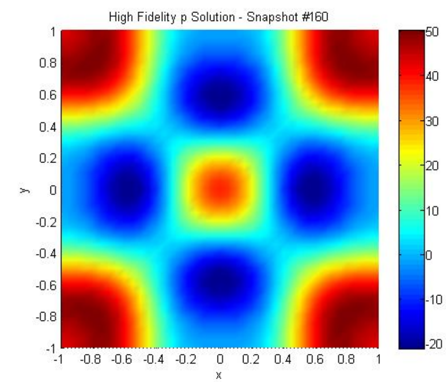
- There is no *a priori* stability guarantee for POD/Galerkin ROMs.
- Stability of a ROM is commonly evaluated *a posteriori* – **RISKY!**
- Instability of POD/Galerkin ROMs is a **real** problem in some applications…

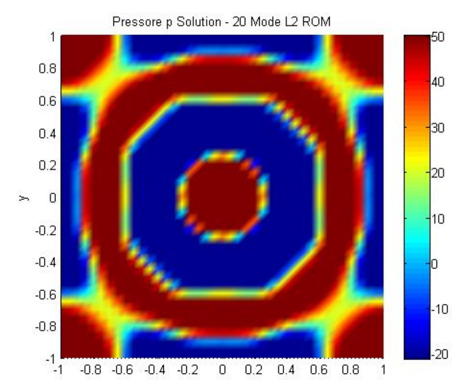


…e.g., compressible flows, high-Reynolds number flows.

Top right: FOM

Bottom right: ROM





Energy-Stability

- **Practical Definition:** Numerical solution does not "blow up" in finite time.
- **More Precise Definition:** Numerical discretization does not introduce any spurious instabilities inconsistent with natural instability modes supported by the governing continuous PDEs.

Numerical solutions must maintain proper **energy balance**.

- Stability of ROM is intimately tied to choice of **inner product** for the Galerkin projection.
- Stability-preserving inner product derived using the **energy method**:
  - Bounds numerical solution energy in a physical way.
  - Borrowed from spectral methods community.
  - Analysis is straightforward for ROMs constructed via **continuous projection.**

Practical implication of energy-stability analysis:
energy inner product ensures that any "bad" modes will not introduce spurious non-physical numerical instabilities into the Galerkin approximation.

Linearized Compressible Flow Equations

Energy-Stability for Linearized PDEs:
FOM linearly stable ⇒ ROM built in energy inner product linearly stable ($Re(\lambda) < 0$)
(WCCM X talk and paper: Kalashnikova & Arunajatesan, 2012).

Linearized compressible Euler/Navier-Stokes equations are appropriate when a compressible fluid system can be described by small-amplitude perturbations about a steady-state mean flow.

- Linearization of full compressible Euler/Navier-Stokes equations obtained as follows:

1. Decompose fluid field as **steady mean** plus **unsteady fluctuation**

$$\boldsymbol{q}(\boldsymbol{x},t) = \overline{\boldsymbol{q}}(\boldsymbol{x}) + \boldsymbol{q}'(\boldsymbol{x},t)$$

2. Linearize full nonlinear compressible Navier-Stokes equations around steady mean to yield **linear hyperbolic/incompletely parabolic** system

$$\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial xi} + \frac{\partial}{\partial xj}\left[\boldsymbol{K}_{ij}(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial xi}\right] = \boldsymbol{0}$$

Energy-Stable ROMs for Linearized Compressible Flow

Linearized compressible Euler/Navier-Stokes equations are **symmetrizable** (Barone & Kalashnikova, 2009; Kalashnikova & Arunajatesan, 2012).

- There exists a symmetric positive definite matrix $\boldsymbol{H} \equiv \boldsymbol{H}(\overline{\boldsymbol{q}})$ (system "**symmetrizer**") s.t.:
  - The convective flux matrices $\boldsymbol{H}\boldsymbol{A}_i$ are symmetric
  - The following augmented viscosity matrix is symmetric positive semi-definite

$$\boldsymbol{K}^s = \begin{pmatrix} \boldsymbol{HK}_{11} & \boldsymbol{HK}_{12} & \boldsymbol{HK}_{13} \\ \boldsymbol{HK}_{21} & \boldsymbol{HK}_{22} & \boldsymbol{HK}_{23} \\ \boldsymbol{HK}_{31} & \boldsymbol{HK}_{32} & \boldsymbol{HK}_{33} \end{pmatrix}$$

Symmetry Inner Product (weighted L^2 inner product):

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{\boldsymbol{H}} = \int_{\Omega} \boldsymbol{q}_1 \boldsymbol{H} \boldsymbol{q}_2 d\Omega$$

- If ROM is built in **symmetry inner product**, Galerkin approximation will satisfy the same energy expression as continuous PDEs:

$$\left|\left|\boldsymbol{q}'_M(\boldsymbol{x},t)\right|\right|_{\boldsymbol{H}} \leq e^{\beta t}\left|\left|\boldsymbol{q}'_M(\boldsymbol{x},0)\right|\right|_{\boldsymbol{H}} \quad (\Rightarrow \frac{dE_M}{dt} \leq 0 \text{ for uniform base flow})$$

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Symmetrizers for Several Hyperbolic/ Incompletely Parabolic Systems

- ***Wave equation:*** $\ddot{u} = a^2 \frac{\partial^2 u}{\partial x^2}$ or $\dot{\boldsymbol{q}} = \boldsymbol{A}\frac{\partial \boldsymbol{q}}{\partial x}$ where $\boldsymbol{q} = \left(\dot{u}, \frac{\partial u}{\partial x}\right)$ $\Rightarrow \boldsymbol{H} = \begin{pmatrix} 1 & 0 \\ 0 & a^2 \end{pmatrix}$

- ***Linearized shallow water equations:*** $\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial xi} = \boldsymbol{0}$ $\Rightarrow \boldsymbol{H} = \begin{pmatrix} \bar{\phi} & 0 & 0 \\ 0 & \bar{\phi} & 0 \\ 0 & 0 & 1 \end{pmatrix}$

- ***Linearized compressible Euler:*** $\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial xi} = \boldsymbol{0}$ $\Rightarrow \boldsymbol{H} = \begin{pmatrix} \bar{\rho} & 0 & 0 \\ 0 & \alpha^2\gamma\bar{\rho}^2\bar{p} & \bar{\rho}\alpha^2 \\ 0 & 0 & \frac{(1+\alpha^2)}{\gamma\bar{p}} \end{pmatrix}$

- ***Linearized compressible Navier-Stokes:*** $\dot{\boldsymbol{q}}' + \boldsymbol{A}_i(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial xi} + \frac{\partial}{\partial xj}\left[\boldsymbol{K}_{ij}(\overline{\boldsymbol{q}})\frac{\partial \boldsymbol{q}'}{\partial xi}\right] = \boldsymbol{0}$

$$\Rightarrow \boldsymbol{H} = \begin{pmatrix} \bar{\rho} & 0 & 0 \\ 0 & \frac{\bar{\rho}R}{\overline{\overline{T}}(\gamma-1)} & 0 \\ 0 & 0 & \frac{R\bar{T}}{\bar{\rho}} \end{pmatrix}$$

- Barone & Kalashnikova, *JCP*, 2009.
- Kalashnikova & Arunajatesan, *WCCM X*, 2012.
- Kalashnikova *et al.*, *SAND report*, 2014.

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Continuous Projection Implementation: "Spirit" Code

"Spirit" ROM Code = 3D parallel C++ POD/Galerkin test-bed ROM code that uses data-structures and eigensolvers from **Trilinos** to build energy-stable ROMs for compressible flow problems
→ stand-alone code that can be synchronized with any high-fidelity code!

- POD modes defined using piecewise smooth finite elements.
- Gauss quadrature rules of sufficient accuracy are used to compute exactly inner products with the help of the `libmesh` library.
- Physics in Spirit:
  - ***Linearized compressible Euler*** (L^2, energy inner product).
  - ***Linearized compressible Navier-Stokes*** (L^2, energy inner product).
  - ***Nonlinear isentropic compressible Navier-Stokes*** (L^2, stagnation energy, stagnation enthalpy inner product).
  - ***Nonlinear compressible Navier-Stokes*** (L^2, energy inner product).

First, testing of ROMs for these physics

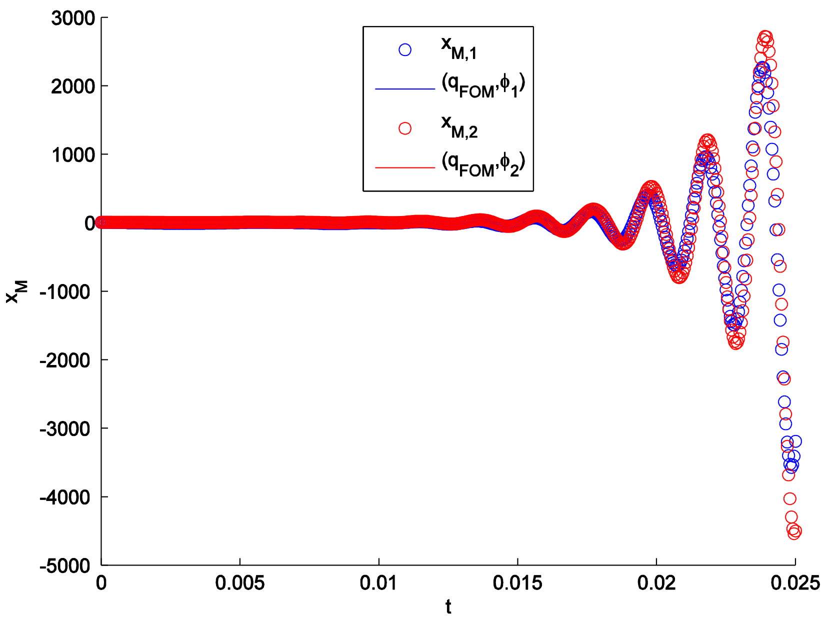
"SIGMA CFD" High-Fidelity Code = Sandia in-house finite volume flow solver derived from LESLIE3D (Genin & Menon, 2010), an LES flow solver originally developed in the Computational Combustion Laboratory at Georgia Tech.

Numerical Experiment: 2D Inviscid Pressure Pulse

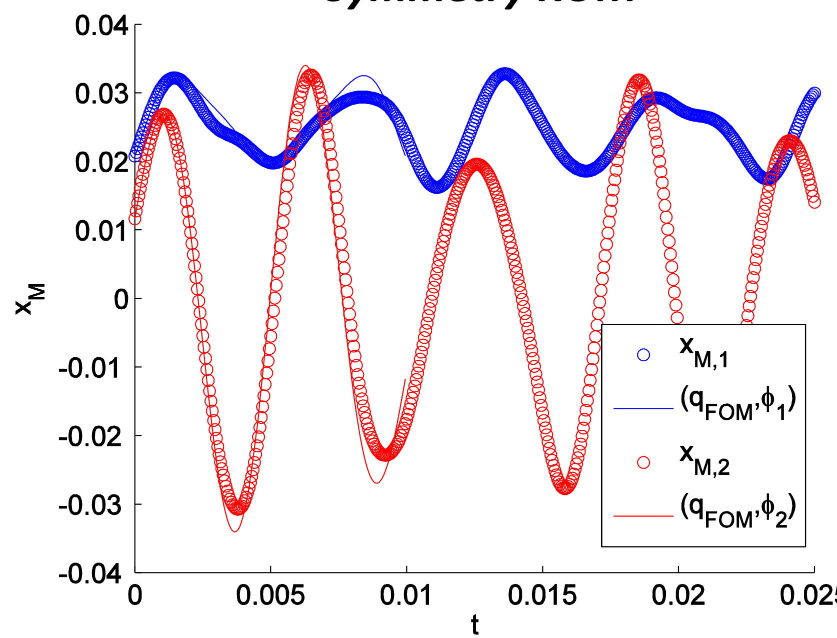
- Inviscid pulse in a uniform base flow (linear dynamics).
- High-fidelity simulation run on mesh with 3362 nodes, up to time $t = 0.01$ seconds.
- 200 snapshots of solution used to construct $M = 20$ mode ROM in L^2 and symmetry inner products.

$x_{M,i}(t)$ vs. $(\boldsymbol{q}'_{CFD}, \boldsymbol{\phi}_i)$ for $i = 1,2$

L^2 ROM



Symmetry ROM



Numerical Experiment: 2D Inviscid Pressure Pulse (cont'd)

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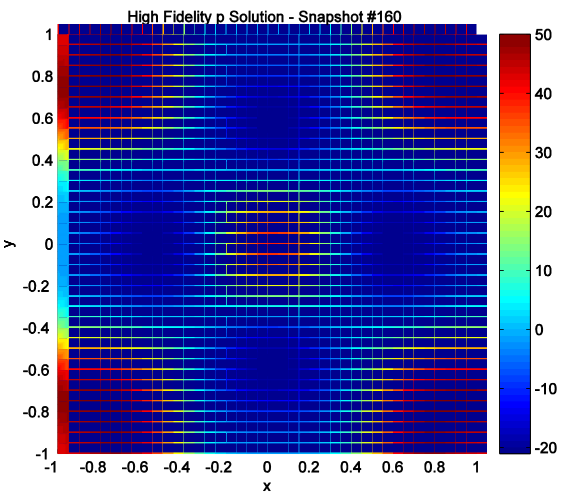
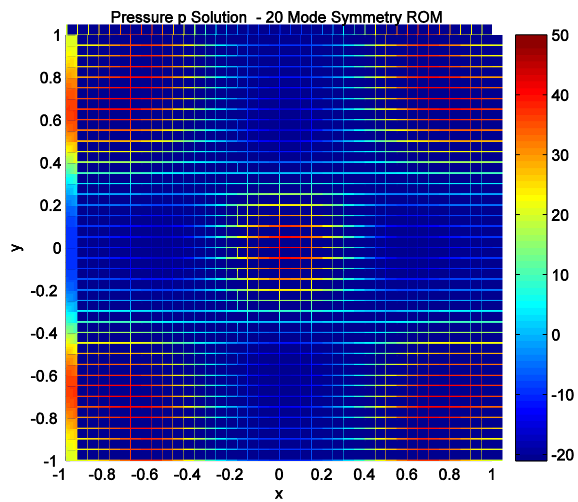
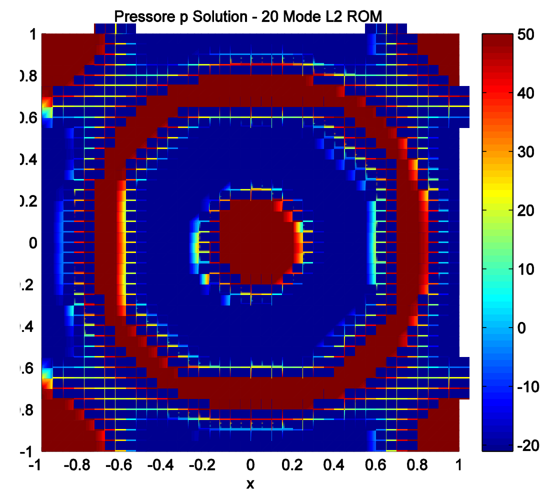
p': High-fidelity



p': Symmetry ROM



p': L^2 ROM



time of snapshot 160

Nonlinear Compressible Flow Equations

Energy-Stability for Nonlinear PDEs:
ROM built in energy inner product will preserve stability of an equilibrium point at 0 for the governing nonlinear system of PDEs (Rowley, 2004; Kalashnikova *et al., 2014*).

- Compressible isentropic Navier-Stokes equations (cold flows, moderate Mach #):

$$\frac{Dh}{Dt} + (\gamma - 1)h\nabla \cdot \boldsymbol{u} = 0$$
$$\frac{D\boldsymbol{u}}{Dt} + \nabla h - \frac{1}{Re}\Delta \boldsymbol{u} = \boldsymbol{0}$$

h = enthalpy
$\boldsymbol{u}$ = velocity vector
ρ = density
T = temperature
$\boldsymbol{\tau}$ = viscous stress tensor

- Full compressible Navier-Stokes equations:

$$\rho\frac{D\boldsymbol{u}}{Dt} + \frac{1}{\gamma M^2}\nabla(\rho T) - \frac{1}{Re}\nabla \cdot \boldsymbol{\tau} = \boldsymbol{0}$$
$$\frac{D\rho}{Dt} + \rho\nabla \cdot \boldsymbol{u} = 0$$
$$\rho\frac{DT}{Dt} + (\gamma - 1)\rho T\nabla \cdot \boldsymbol{u} - \frac{\gamma}{PrRe}\nabla \cdot (\kappa\nabla T) - \left(\frac{\gamma(\gamma - 1)M^2}{Re}\right)\nabla\boldsymbol{u} \cdot \boldsymbol{\tau} = 0$$

Energy-Stable ROMs for Nonlinear Compressible Flow (Isentropic NS)

In (Rowley, 2004), Rowley *et al.* showed that energy inner product for the compressible isentropic Navier-Stokes equations can be defined following a transformation of these equations.

- Transformed compressible isentropic Navier-Stokes equations:

$$\begin{aligned} \frac{Dc}{Dt} + \frac{\gamma-1}{2} c\nabla \cdot \boldsymbol{u} &= 0 \\ \frac{D\boldsymbol{u}}{Dt} + \frac{2}{\gamma-1} c\nabla c - \frac{1}{Re}\Delta \boldsymbol{u} &= \boldsymbol{0} \end{aligned}$$

c = speed of sound $(c^2 = (\gamma-1)h)$
$\boldsymbol{u}$ = velocity

- Family of inner products:

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_\alpha = \int_\Omega \left(\boldsymbol{u}_1 \cdot \boldsymbol{u}_2 + \frac{2\alpha}{\gamma-1} c_1 c_2 \right) d\Omega$$

$$\alpha = \begin{cases} 1 \Rightarrow ||\boldsymbol{q}||_\alpha = \text{stagnation enthalpy} \\ \frac{1}{\gamma} \Rightarrow ||\boldsymbol{q}||_\alpha = \text{stagnation energy} \end{cases}$$

If Galerkin projection step of model reduction is performed in α inner product, then the Galerkin projection will **preserve the stability of an equilibrium point at the origin** (Rowley, 2004).

Energy-Stable ROMs for Nonlinear Compressible Flow (Full NS)

Present work extends ideas in (Rowley, 2004) to **full compressible Navier-Stokes equations**.
Requirement: *transformation/inner product yields PDEs with only polynomial non-linearities.*

- First, full compressible Navier-Stokes equations are **transformed** into the following variables:

$$a = \sqrt{\rho}, \quad \boldsymbol{b} = a\boldsymbol{u}, \quad d = ae$$

e =internal energy

- Next, the following **"total energy"** inner product is defined:

$$(\boldsymbol{q}_1, \boldsymbol{q}_2)_{TE} = \int_{\Omega} (\boldsymbol{b}_1 \cdot \boldsymbol{b}_2 + a_1 d_2 + a_2 d_1) d\Omega$$

→ Norm induced by total energy inner product is the total energy of the fluid system:

$$||\boldsymbol{q}||_{TE} = \int_{\Omega} \left(\rho e + \frac{1}{2} \rho u i u_i \right) d\Omega$$

If Galerkin projection step of model reduction is performed in total energy inner product, then the Galerkin projection will **preserve the stability of an equilibrium point at the origin** (Kalashnikova *et al.*, 2014)

☺ Transformed equations have only **polynomial non-linearities** (projection of which can be computed in offline stage of MOR and stored).

☹ Transformation introduces **higher order polynomial** non-linearities.

☺ Efficiency of online stage of MOR can be recovered using **interpolation** (e.g., DEIM, gappy POD).

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Numerical Experiment: Viscous Laminar Cavity

- Viscous cavity problem at $M = 0.6$, $Re = 1500$ (laminar regime).
- **High-fidelity simulation**: DNS based on full nonlinear compressible Navier-Stokes equations with 99,408 nodes (right).
- 500 snapshots collected, every $\Delta t_{snap} = 1 \times 10^{-4}$ seconds.
- Snapshots used to construct $M = 5$ mode ROM for nonlinear compressible Navier-Stokes equations in $\boldsymbol{L^2}$ **and total energy inner products**.
- $M = 5$ mode POD bases capture $\approx$ 99% of snapshot energy.

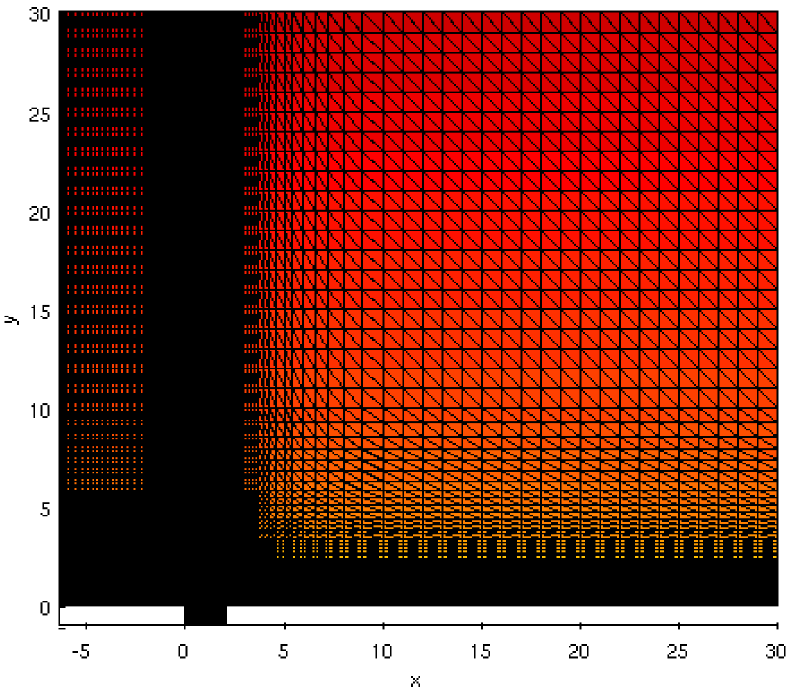
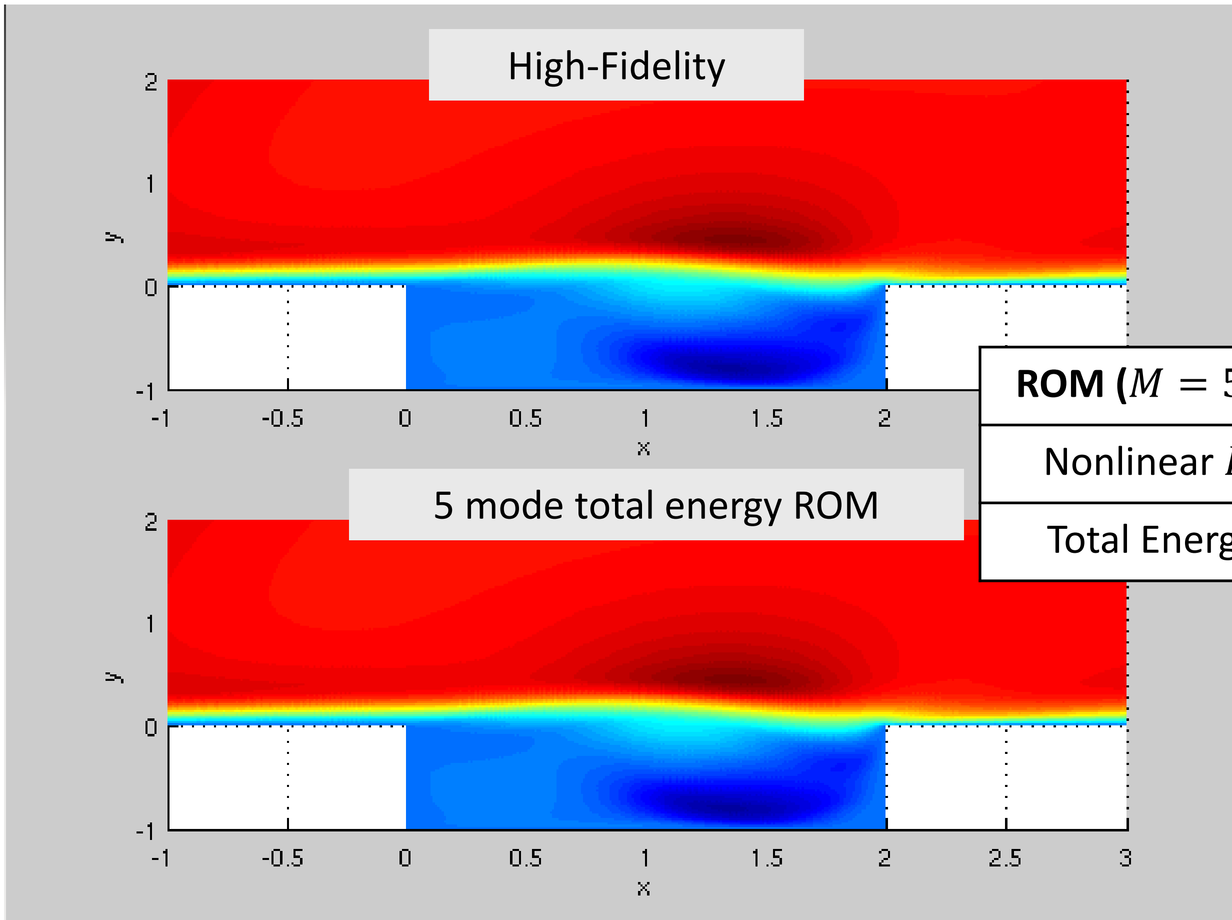


Figure above: viscous laminar cavity problem domain/mesh.

Numerical Experiment: Viscous Laminar Cavity (cont'd)



- L^2 ROM exhibited instability for for $M > 5$ modes.

ROM ($M = 5$ modes)	**Error (L^2 norm)**
Nonlinear L^2 ROM	NaN
Total Energy ROM	5.52×10^{-2}

- In contrast, total energy ROM remained stable and agreed well with high-fidelity solution!

Figure above: u-component of velocity as a function of time t

Summary & Future Work

- A Galerkin model reduction approach in which the ***continuous*** equations are projected onto the basis modes in a continuous inner product is proposed.

- It is shown that the choice of inner product for the Galerkin projection step is crucial to stability of the ROM.
  - For ***linearized compressible flow***, Galerkin projection in the "symmetry" inner product leads to a ROM that is energy-stable for any choice of basis.
  - For ***nonlinear compressible flow***, an inner product that induces the total energy of the fluid system is developed. A ROM constructed in this inner product will preserve the stability of an equilibrium point at 0 for the system.

- Results are promising for a nonlinear problem involving ***compressible viscous laminar flow*** over an open cavity: a total energy ROM remains stable whereas an L^2 ROM exhibits an instability.

<u>Ongoing/Future Work</u>

- Improve efficiency of nonlinear total energy ROMs through interpolation (e.g., DEIM, gappy POD)
- Studies of predictive capabilities of ROMs (robustness w.r.t. parameter changes).

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LDRD
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Thank You! Questions?

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Some references on these ideas:

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