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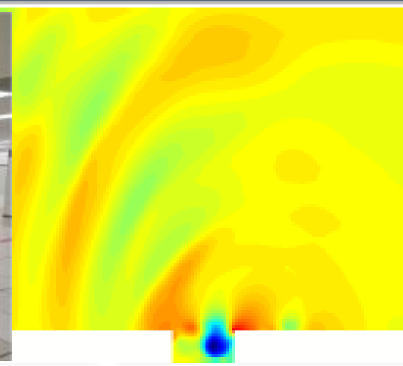

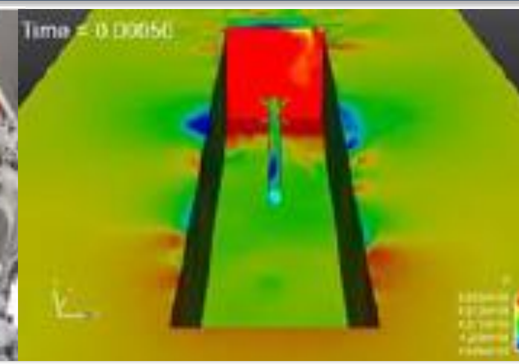

# A minimal subspace rotation approach for extreme model reduction in fluid mechanics

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Recent Developments MOR 2016    Paris, France    November 7-10, 2016

U.S. DEPARTMENT OF ENERGY    NNSA National Nuclear Security Administration

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SAND2016-10461C

# Outline

1. Introduction
   - Targeted application
   - POD/Galerkin approach to MOR
   - Extreme model reduction
   - Mode truncation instability in MOR
2. Accounting for modal truncation
   - Traditional linear eddy-viscosity approach
   - New proposed approach via subspace rotation
3. Applications
   - Low Reynolds (*Re*) number channel driven cavity
   - Moderate Reynolds (*Re*) number channel driven cavity
4. Extension to Least-Squares Petrov-Galerkin (LSPG) ROMs
5. Summary & future work

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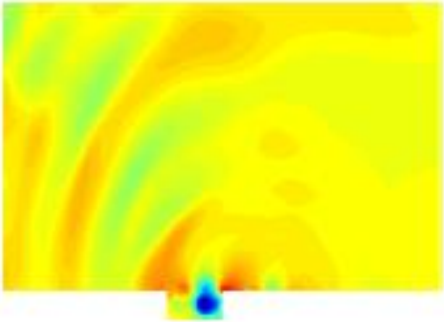

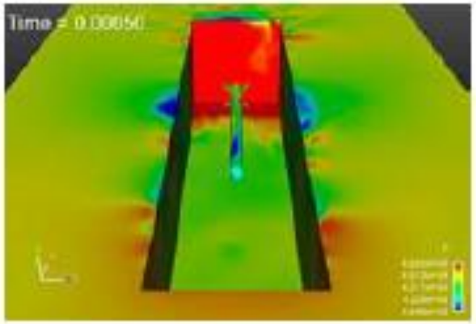

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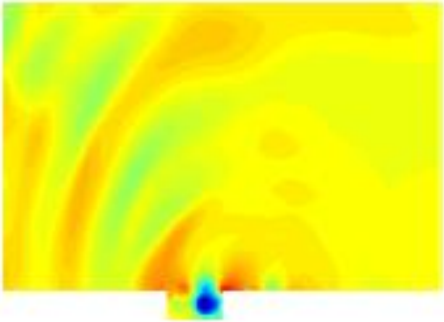

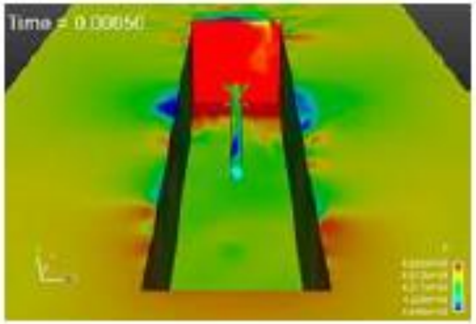

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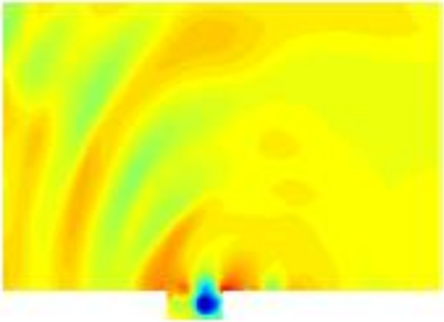
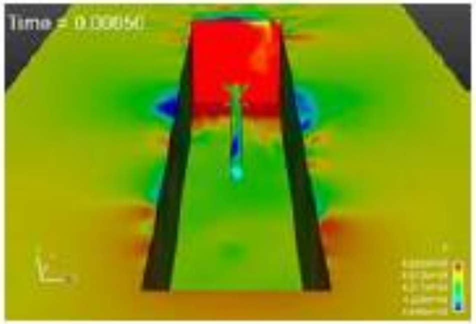


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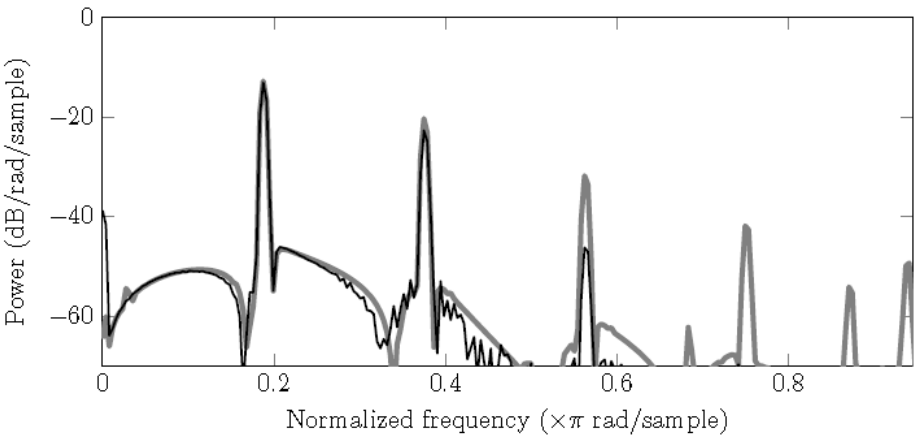

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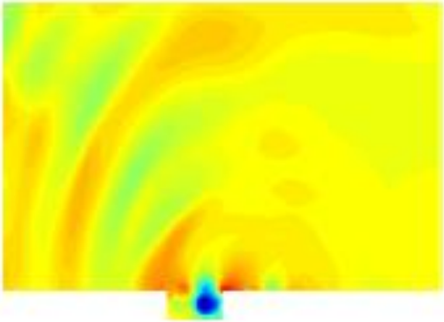

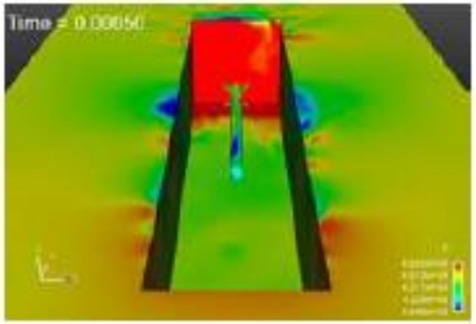


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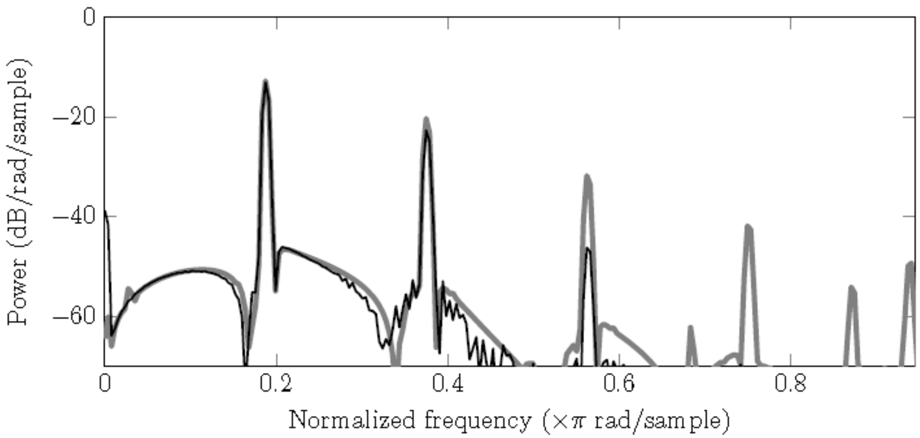



- <u>Secondary interest</u>: ROMs robust w.r.t. ***parameter changes*** (e.g., Reynolds, Mach number) for enabling ***uncertainty quantification***.

# POD/Galerkin Method to MOR

**High-Fidelity CFD Simulations:**

- Snapshot 1
- Snapshot 2
- ⋮
- Snapshot $K$

Step 1 →

**Fluid Modal Decomposition (POD):**

$$\boxed{\mathbf{u} \approx \sum_{k=1}^{n} a_k(t)\mathbf{U}_k(\mathbf{x})}$$

Step 2 →

**Galerkin Projection of Fluid PDEs:**

$$\boxed{(\mathbf{U}_j, \dot{\mathbf{u}} + \nabla \cdot \mathbf{F}(\mathbf{u})) = 0}$$

***Snapshot matrix***: $\boldsymbol{X} = (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^K) \in \mathbb{R}^{NxK}$
***SVD:*** $\boldsymbol{X} = \boldsymbol{U\Sigma V}^T$
***Truncation:*** $\boldsymbol{U} \leftarrow (\boldsymbol{U}_1, \ldots, \boldsymbol{U}_n) = \boldsymbol{U}(:, 1\!:\!n)$

**"Small" ROM ODE System:**

$$\boxed{\dot{a}_k = f(a_1, \ldots, a_n)}$$

$N$ = # of dofs in full order model (FOM)
$K$ = # of snapshots
$n$ = # of dofs in ROM
$(n << N, n << K)$

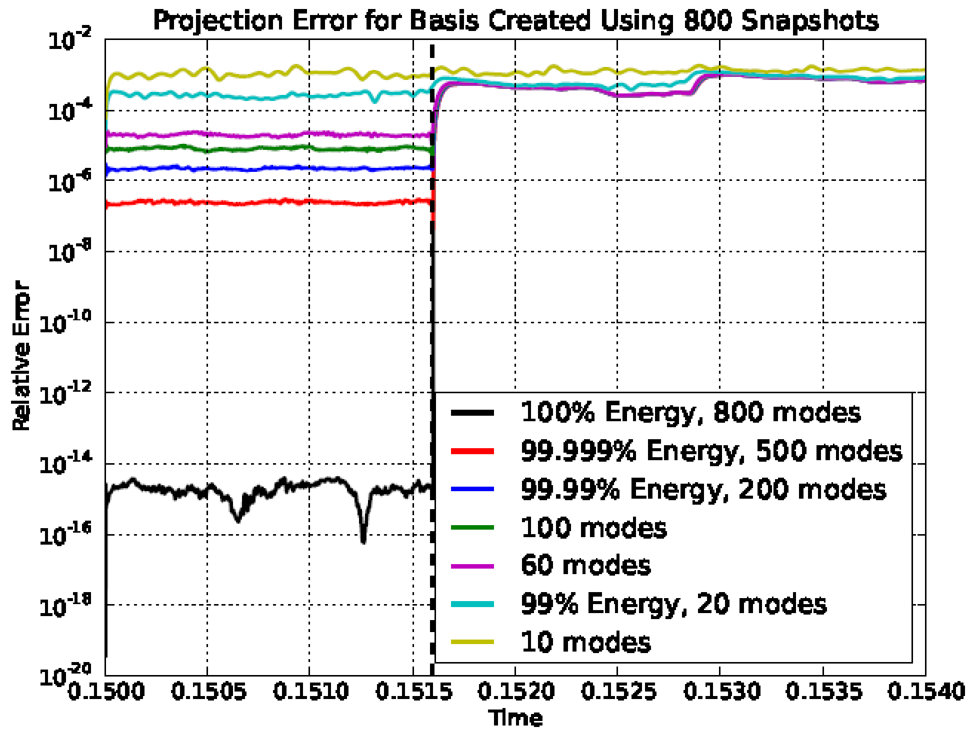
Our focus has been primarily on ***POD/Galerkin ROMs***

# Extreme Model Reduction

- Most realistic applications (e.g., high *Re* compressible cavity): basis that captures $>$***99% snapshot energy*** is required to accurately reproduce snapshots.
  - $\rightarrow$ leads to $n > O(1000)$ except for ***toy problems*** and/or ***low-fidelity*** models.

- Higher order modes are in general ***unreliable for prediction***, so including them in the basis is unlikely to improve the ***predictive*** capabilities of a ROM.

Figure (right) shows projection error for POD basis constructed using 800 snapshots for cavity problem. Dashed line = end of snapshot collection period.




We are looking for an approach that enables ***extreme model reduction***: ROM basis size is $O(10)$ or $O(100)$.

# 3D Compressible Navier-Stokes Equations

- We start with the 3D compressible Navier-Stokes equations in ***primitive specific volume form***:

[PDEs]

$$\begin{gathered}
\zeta_{,t} + \zeta_{,j} u_j - \zeta u_{j,j} = 0 \\
u_{i,t} + u_{i,j} u_j + \zeta p_{,i} - \frac{1}{Re} \zeta \tau_{ij,j} = 0 \\
p_{,t} + u_j p_{,j} + \gamma u_{j,j} p - \left(\frac{\gamma}{PrRe}\right) \left(\kappa (p\zeta)_{,j}\right)_{,j} - \left(\frac{\gamma - 1}{Re}\right) u_{i,j} \tau_{ij} = 0
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- Spectral discretization $\left(\boldsymbol{q}(\boldsymbol{x},t) \approx \sum_{i=1}^{n} a_i(t) \boldsymbol{U}_i(\boldsymbol{x})\right)$ + Galerkin projection applied to (1) yields a system of *$n$ coupled quadratic ODEs*:

[ROM]

$$\frac{d\boldsymbol{a}}{dt} = \boldsymbol{C} + \boldsymbol{L}\boldsymbol{a} + \left[\boldsymbol{a}^T \boldsymbol{Q}^{(1)} \boldsymbol{a} + \boldsymbol{a}^T \boldsymbol{Q}^{(2)} \boldsymbol{a} + \cdots + \boldsymbol{a}^T \boldsymbol{Q}^{(n)} \boldsymbol{a}\right]^T \tag{2}$$

where $\boldsymbol{C} \in \mathbb{R}^n, \boldsymbol{L} \in \mathbb{R}^{n \times n}$ and $\boldsymbol{Q}^{(i)} \in \mathbb{R}^{n \times n}$ for all $i = 1, \dots, n$.

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This talk focuses on remedying "***mode truncation instability***" problem for projection-based (POD/Galerkin) compressible flow ROMs.

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***Turbulence Modeling***
(traditional approach)

***Subspace Rotation***
(our approach)

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- Dissipative dynamics of truncated higher-order modes are modeled using an additional linear term:

$$\frac{d\boldsymbol{a}}{dt} = \boldsymbol{C} + \boldsymbol{L}\boldsymbol{a} + \left[\boldsymbol{a}^T \boldsymbol{Q}^{(1)} \boldsymbol{a} + \boldsymbol{a}^T \boldsymbol{Q}^{(2)} \boldsymbol{a} + \cdots + \boldsymbol{a}^T \boldsymbol{Q}^{(n)} \boldsymbol{a}\right]^T$$

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- Disadvantages of this approach:
  1. Additional term destroys *consistency* between ROM and Navier-Stokes equations.
  2. Calibration is necessary to derive optimal $\boldsymbol{L}_\nu$ and optimal value is *flow dependent*.
  3. Inherently a *linear model* → cannot be expected to perform well for all classes of problems (e.g., nonlinear).

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Instead of modeling truncation via additional linear term, model the truncation *a priori* by "rotating" the projection subspace into a more dissipative regime

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**Illustrative example**

- *Standard approach:* retain only the most energetic POD modes, i.e., $\boldsymbol{U}_1, \boldsymbol{U}_2$, $\boldsymbol{U}_3$.
- *Proposed approach:* add some higher order basis modes to increase dissipation, i.e., $a_1\boldsymbol{U}_1 + b_1\boldsymbol{U}_6 + c_1\boldsymbol{U}_8, a_2\boldsymbol{U}_2 + b_2\boldsymbol{U}_{11} + c_2\boldsymbol{U}_{18}, a_3\boldsymbol{U}_3 + b_3\boldsymbol{U}_{21} + c_3\boldsymbol{U}_{28}$

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- *More generally:* approximate the solution using a linear superposition of $n + p$ (with $p > 0$) most energetic modes:

$$\widetilde{\boldsymbol{U}}_i = \sum_{j=1}^{n+p} X_{ij}\, \boldsymbol{U}_j, \quad i = 1, \dots, n, \tag{3}$$

where $\boldsymbol{X} \in \mathbb{R}^{(n+p)\times n}$ is an orthonormal ($\boldsymbol{X}^T\boldsymbol{X} = \boldsymbol{I}_{n\times n}$) "rotation" matrix.

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- Once $\boldsymbol{X}$ is found, the result is a system of the form:

$$\frac{d\boldsymbol{a}}{dt} = \boldsymbol{C} + \boldsymbol{L}\boldsymbol{a} + \left[\boldsymbol{a}^T \boldsymbol{Q}^{(1)} \boldsymbol{a} + \boldsymbol{a}^T \boldsymbol{Q}^{(2)} \boldsymbol{a} + \cdots + \boldsymbol{a}^T \boldsymbol{Q}^{(n)} \boldsymbol{a}\right]^T$$

with:

$$Q^{(i)}{}_{jk} \leftarrow \sum_{s,q,r=1}^{n+p} X_{si} Q^{(s)}{}_{qr} X_{qr} X_{rk}, \quad \boldsymbol{L} \leftarrow \boldsymbol{X}^T \boldsymbol{L} \boldsymbol{X}, \quad \boldsymbol{C} \leftarrow \boldsymbol{X}^T \boldsymbol{C}^* \qquad (4)$$

# Objective function

$$\begin{aligned} &\text{minimize}_{\boldsymbol{X} \in \mathcal{V}_{(n+p),n}} \ f(\boldsymbol{X}) \\ &\text{subject to} \quad g(\boldsymbol{X}, \boldsymbol{L}) = 0 \end{aligned} \tag{5}$$

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- TKE objective (7) comes from earlier work (Balajewicz *et al.,* 2013) involving stabilization of incompressible flow ROMs
  - POD modes associated with low KE are important *dynamically* even though they contribute little to overall energy of the fluid flow.

* In (7), $\boldsymbol{\Sigma}$ denotes the square of second moments of ROM modal coefficients (Balajewicz et al., 2013).

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- Numerical experiments reveal objective (6) produces better results than objective (7) for compressible flow.

# Constraint

$$\begin{aligned} &\text{minimize}_{\boldsymbol{X}\in\mathcal{V}_{(n+p),n}} \quad f(\boldsymbol{X}) \\ &\text{subject to} \quad g(\boldsymbol{X},\boldsymbol{L}) = 0 \end{aligned} \tag{5}$$

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$$\boxed{g(\boldsymbol{X}, \boldsymbol{L}) = \mathrm{tr}(\boldsymbol{X}^T \boldsymbol{L} \boldsymbol{X}) - \eta} \tag{8}$$

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- Constraint comes from property that *averaged total power* (= $\mathrm{tr}(\boldsymbol{X}^T\boldsymbol{L}\boldsymbol{X})$ + energy transfer) has to vanish.

# Optimization problem summary

**Minimal subspace rotation:** trace minimization on Stiefel manifold

$$\begin{aligned} &\text{minimize}_{\boldsymbol{X} \in \mathcal{V}_{(n+p),n}} && -\mathrm{tr}\left(\boldsymbol{X}^T \boldsymbol{I}_{(n+p)\times n}\right) \\ &\text{subject to} && \mathrm{tr}(\boldsymbol{X}^T \boldsymbol{L} \boldsymbol{X}) = \eta \end{aligned} \tag{9}$$

- $\eta \in \mathbb{R}$: proxy for the balance between linear energy production and energy dissipation (calculated iteratively using modal energy).
- $\mathcal{V}_{(n+p),n} \in \left\{\boldsymbol{X} \in \mathbb{R}^{(n+p)\times n} : \boldsymbol{X}^T\boldsymbol{X} = \boldsymbol{I}_n, p > 0\right\}$ is the *Stiefel manifold*.
- Equation (9) is solved efficiently offline using the method of Lagrange multipliers (`Manopt MATLAB toolbox`).
- See (Balajewicz, Tezaur, Dowell, 2016) and Appendix slide for Algorithm.

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- Disadvantages of proposed approach:

    1. Off-line calibration of free parameter $\eta$ is required.
    2. Stability cannot be proven like for incompressible case.

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# Low *Re* Channel Driven Cavity

Flow over square cavity at Mach 0.6, Re = 1453.9, Pr = 0.72 ⇒ $n = 4$ ROM (91% snapshot energy).

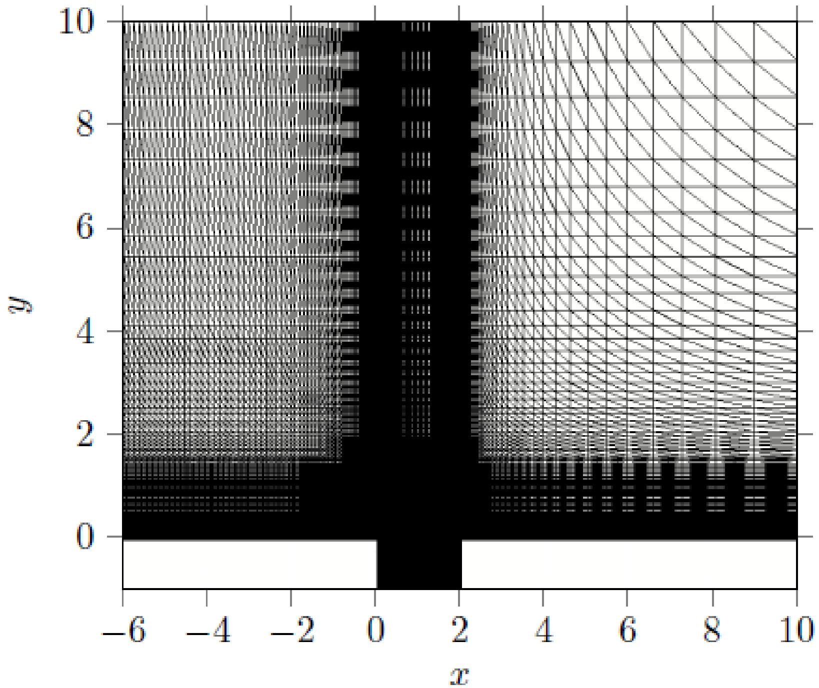
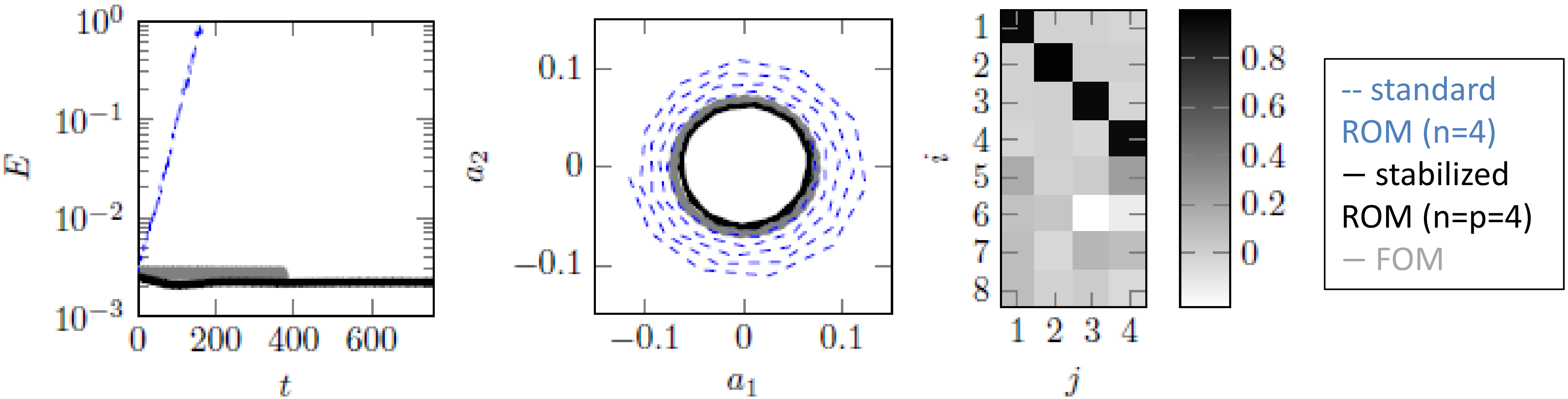



Figure 1: Domain and mesh for viscous channel driven cavity problem.

# Low *Re* Channel Driven Cavity

- *Minimizing subspace rotation:*

$$\boxed{f(\boldsymbol{X}) = \left\|\boldsymbol{X} - \boldsymbol{I}_{(n+p),n}\right\|_F = -\mathrm{tr}\left(\boldsymbol{X}^T \boldsymbol{I}_{(n+p)\times n}\right)}$$




(a) (b) (c)

Figure 2: (a) evolution of modal energy, (b) phase plot of first and second temporal basis $a_1(t)$ and $a_2(t)$, (c) illustration of stabilizing rotation showing that rotation is small: $\frac{\|\boldsymbol{X}-\boldsymbol{I}_{(n+p),n}\|_F}{n} = 0.188, \boldsymbol{X} \approx \boldsymbol{I}_{(n+p),n}$

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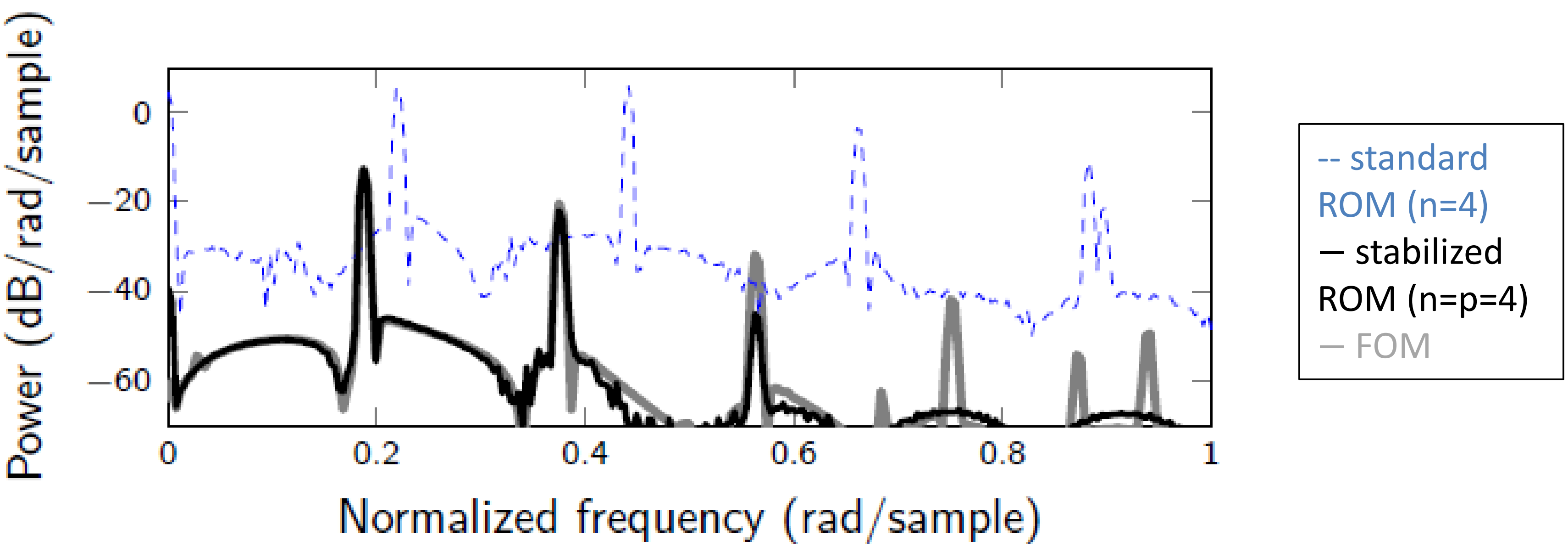


Figure 3: Pressure power spectral density (PSD) at location $\boldsymbol{x} = (2, -1)$; stabilized ROM minimizes subspace rotation.

# Low *Re* Channel Driven Cavity

- <u>*Maximizing resolved TKE*</u>*:*

$$\boxed{f(\boldsymbol{X}) = -||\boldsymbol{\Sigma} - \boldsymbol{X}\boldsymbol{X}^T\boldsymbol{\Sigma}||_F}$$

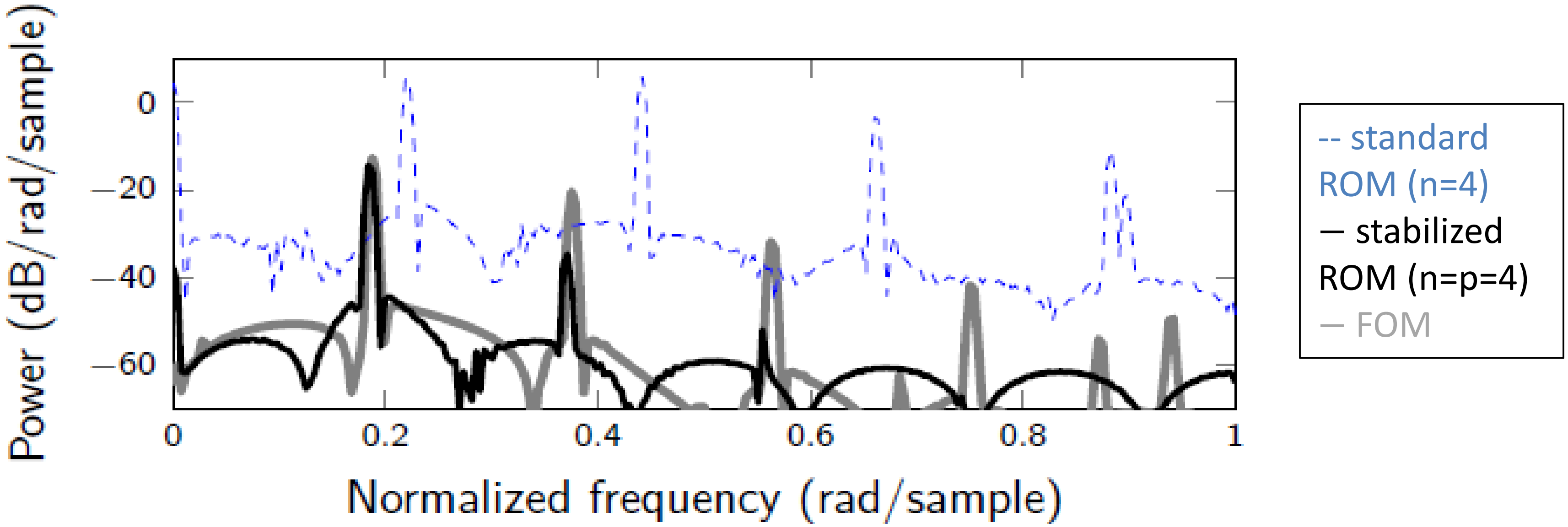


Figure 4: Pressure power spectral density (PSD) at location $\boldsymbol{x} = (2, -1)$; stabilized ROM maximizes resolved TKE.

# Low *Re* Channel Driven Cavity

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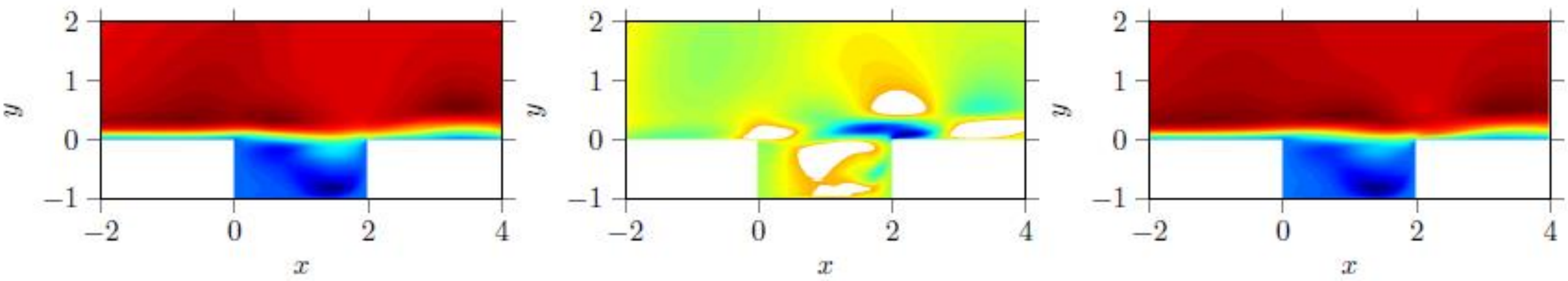


FOM

Standard ROM ($n = 4$)

Stabilized ROM ($n = p = 4$)

Figure 5: Channel driven cavity Re ≈ 1500 contours of $u$-velocity at time of final snapshot.

# Moderate *Re* Channel Driven Cavity

Flow over square cavity at Mach 0.6, Re = 5452.1, Pr = 0.72 ⇒ $n = 20$ ROM (71.8% snapshot energy).

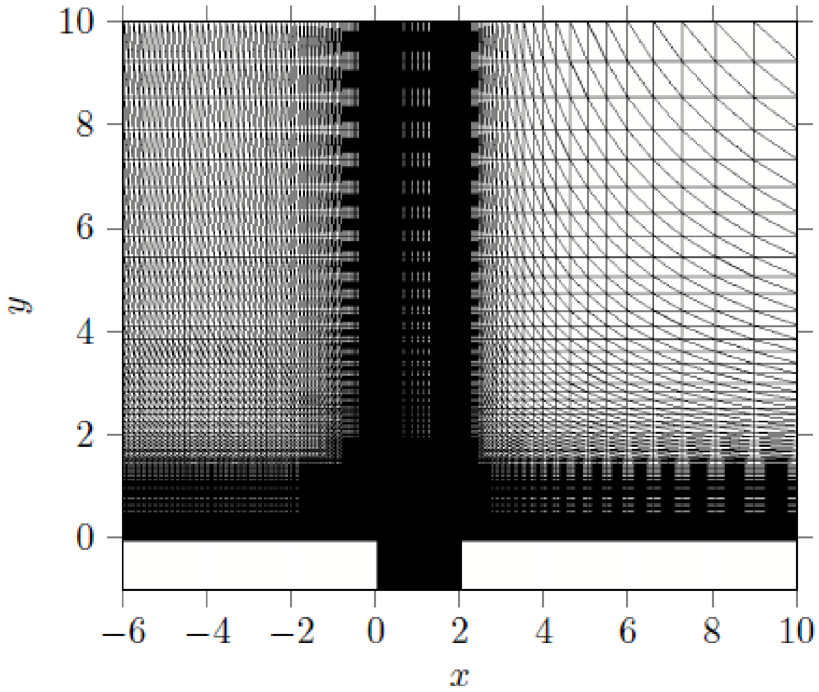


Figure 6: Domain and mesh for viscous channel driven cavity problem.

# Moderate *Re* Channel Driven Cavity

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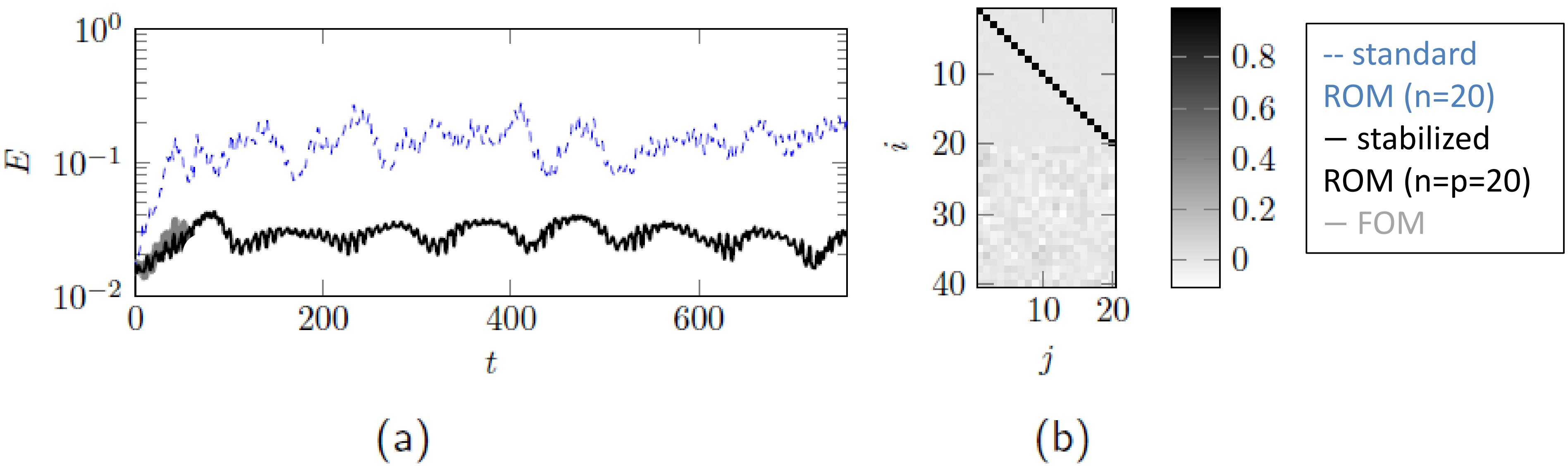


Figure 7: (a) evolution of modal energy, (b) illustration of stabilizing rotation showing that rotation is small: $\frac{\left\|\boldsymbol{X}-\boldsymbol{I}_{(n+p),n}\right\|_F}{n} = 0.038, \boldsymbol{X} \approx \boldsymbol{I}_{(n+p),n}$

# Moderate *Re* Channel Driven Cavity

- *Minimizing subspace rotation:*

$$\boxed{f(\boldsymbol{X}) = \left\|\boldsymbol{X} - \boldsymbol{I}_{(n+p),n}\right\|_F = -\mathrm{tr}\left(\boldsymbol{X}^T \boldsymbol{I}_{(n+p)\times n}\right)}$$

— stabilized ROM (n=p=20)
— FOM

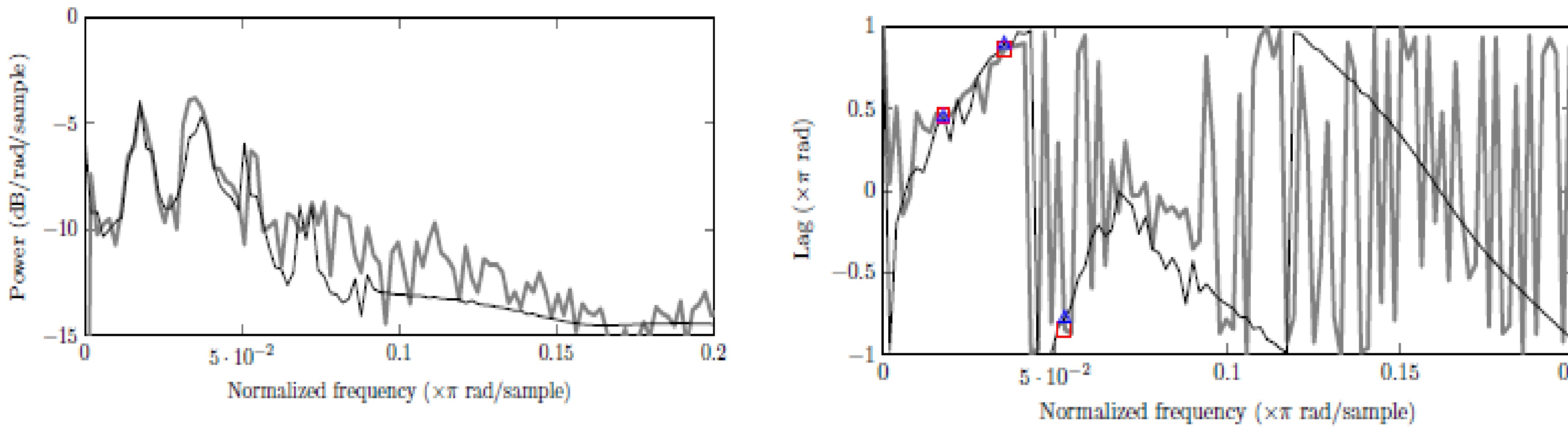


Figure 8: Pressure cross PSD of of $p(\boldsymbol{x}_1, t)$ and $p(\boldsymbol{x}_2, t)$ where $\boldsymbol{x}_1 = (2, -0.5)$, $\boldsymbol{x}_2 = (0, -0.5)$

Power and phase lag at fundamental frequency, and first two super harmonics are predicted accurately using the fine-tuned ROM ($\Delta$ = stabilized ROM, $\square$ = FOM)

# Moderate *Re* Channel Driven Cavity

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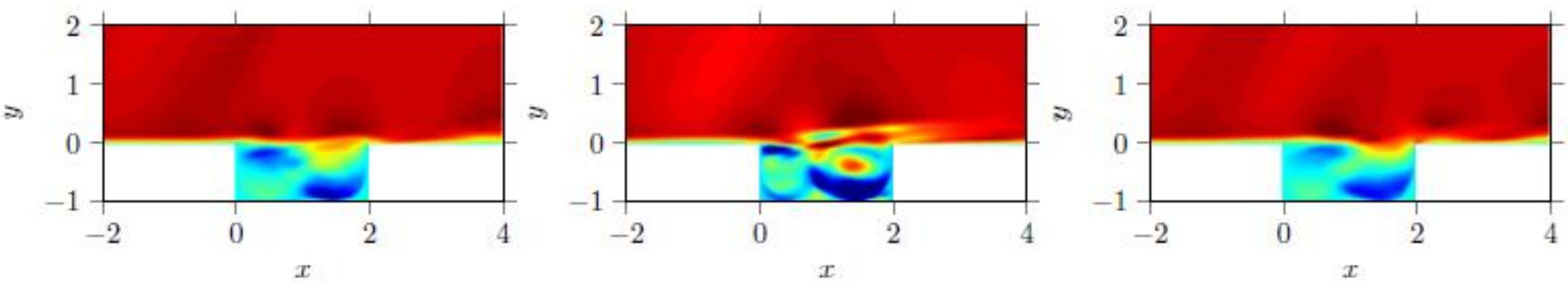


FOM

Standard ROM
($n = 20$)

Stabilized ROM
($n = p =$20)

Figure 9: Channel driven cavity Re ≈ 5500 contours of $u$-velocity at time of final snapshot.

# CPU times (CPU-hours) for offline and online computations*

| | Procedure | Low Re Cavity | Moderate Re Cavity |
|---|---|---|---|
| | FOM # of DOF | 288,250 | 243,750 |
| offline | Time-integration of FOM | 72 hrs | 179 hrs |
| offline | Basis construction (size $n + p$ ROM) | 0.88 hrs | 3.44 hrs |
| offline | Galerkin projection (size $n + p$ ROM) | 5.44 hrs | 14.8 hrs |
| offline | Stabilization | 14 sec | 170 sec |
| | ROM # of DOF | 4 | 20 |
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  → Nevertheless, ***low-dimensional*** LSPG ROMs can benefit from basis stabilization.

# Stabilization of Inviscid Pulse in Uniform Flow Low Order LSPG ROM

**Preliminary Workflow**

1. Run LSPG ROM in SPARC $\rightarrow$ output POD basis.
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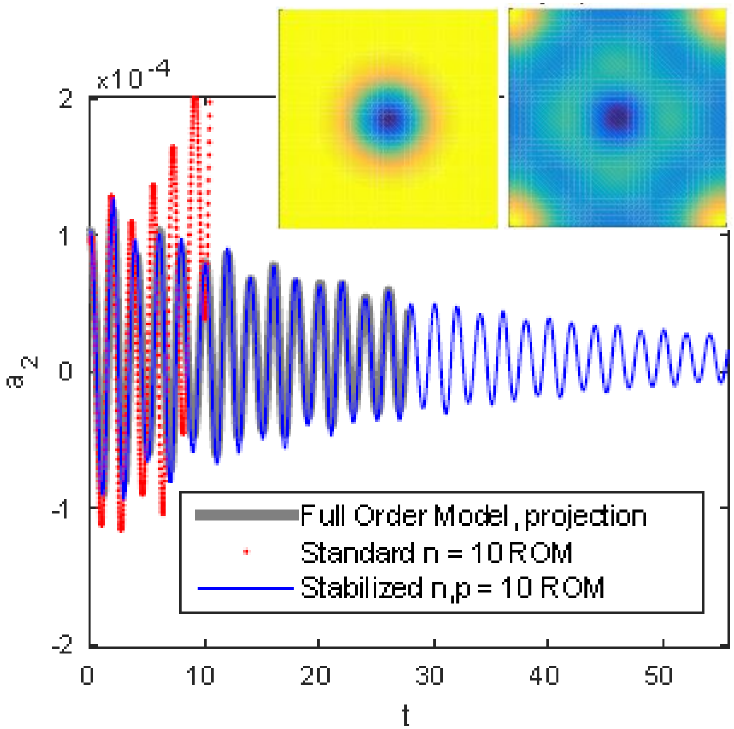


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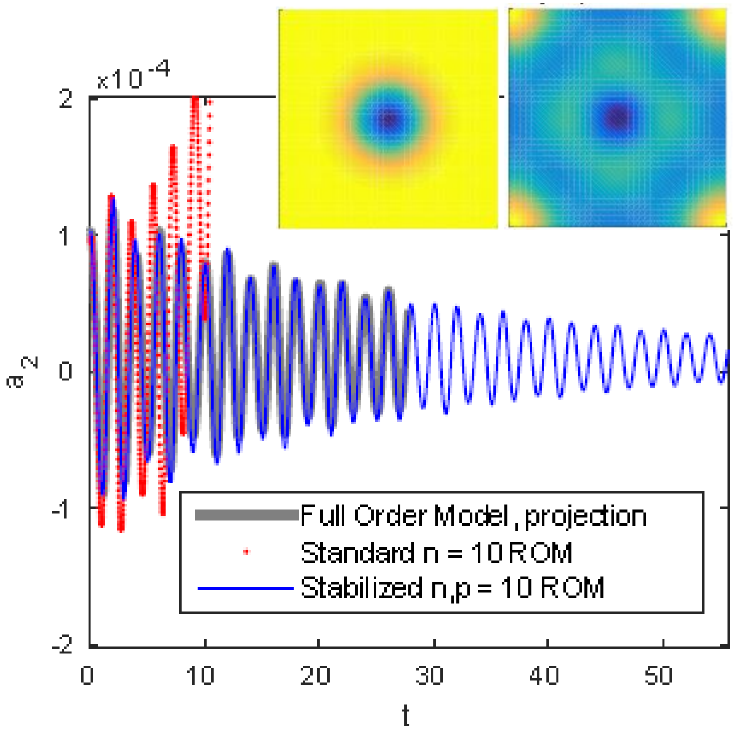


- Figure (left) shows ***generalized coordinates*** for mode 2 compared to FOM projection.
- Our approach effectively ***stabilizes*** LSPG ROM.
- Preliminary approach needs improvement, as there are ***inconsistencies*** between SPARC and Spirit codes.

We are currently working on extending our stabilization/enhancement approach to ROMs with ***generic nonlinearities***.

# Outline

1. Introduction
   - Targeted application
   - POD/Galerkin approach to MOR
   - Extreme model reduction
   - Mode truncation instability in MOR
2. Accounting for modal truncation
   - Traditional linear eddy-viscosity approach
   - New proposed approach via subspace rotation
3. Applications
   - Low Reynolds (*Re*) number channel driven cavity
   - Moderate Reynolds (*Re*) number channel driven cavity
4. Extension to Least-Squares Petrov-Galerkin (LSPG) ROMs
5. **Summary & future work**

# Summary

- We have developed a non-intrusive approach for *stabilizing* and *fine-tuning* projection-based ROMs for compressible flows.
- The standard POD modes are *"rotated"* into a more dissipative regime to account for the dynamics in the higher order modes truncated by the standard POD method.
- The new approach is *consistent* and does not require the addition of empirical turbulence model terms unlike traditional approaches.
- Mathematically, the approach is formulated as a *quadratic matrix program* on the Stiefel manifold.
- The constrained minimization problem is solved *offline* and *small* enough to be solved in MATLAB.
- The method is demonstrated on several compressible flow problems and shown to deliver *stable* and *accurate* ROMs.

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- Extension of the method to *minimal-residual-based* nonlinear ROMs.
- Extension of the method to *predictive applications*, e.g., problems with varying Reynolds number and/or Mach number.
- Selecting different *goal-oriented* objectives and constraints in our optimization problem:

$$\boxed{\begin{array}{ll} \text{minimize}_{\boldsymbol{X}\in\mathcal{V}_{(n+p),n}} & f(\boldsymbol{X}) \\ \text{subject to} & g(\boldsymbol{X},\boldsymbol{L}) = 0 \end{array}}$$

e.g.,

- Maximize parametric robustness: $f = \sum_{i=1}^{k} \beta_i \|\boldsymbol{U}^*(\mu_i)\boldsymbol{X} - \boldsymbol{U}^*(\mu_i)\|_F$.
- ODE constraints: $g = \|\boldsymbol{a}(t) - \boldsymbol{a}^*(t)\|$.

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# Appendix: Accounting for modal truncation

**Stabilization algorithm:** returns stabilizing rotation matrix $\boldsymbol{X}$.

**Inputs:** Initial guess $\eta^{(0)} = \text{tr}(L(1:n, 1:n))$ ($\boldsymbol{X} = \boldsymbol{I}_{(n+p)\times n}$), ROM size $n$ and $p \geq 1$, ROM matrices associated with the first $n+p$ most energetic POD modes, convergence tolerance $TOL$, maximum number of iterations $k_{max}$.

for $k = 0, \cdots, k_{max}$

Solve constrained optimization problem on Stiefel manifold:

$$\underset{\boldsymbol{X}^{(k)} \in \mathcal{V}_{(n+p),n}}{\text{minimize}} \quad -\operatorname{tr}\left(\boldsymbol{X}^{(k)\mathrm{T}} \boldsymbol{I}_{(n+p)\times n}\right)$$

$$\text{subject to} \quad \operatorname{tr}(\boldsymbol{X}^{(k)\mathrm{T}} \boldsymbol{L} \boldsymbol{X}^{(k)}) = \eta^{(k)}.$$

Construct new Galerkin matrices using (4).

Integrate numerically new Galerkin system.

Calculate "modal energy" $E(t)^{(k)} = \sum_i^n (a(t)_i^{(k)})^2$.

Perform linear fit of temporal data $E(t)^{(k)} \approx c_1^{(k)} t + c_0^{(k)}$, where $c_1^{(k)}$ =energy growth.

Calculate $\epsilon$ such that $c_1^{(k)}(\epsilon) = 0$ (no energy growth) using root-finding algorithm.

Perform update $\eta^{(k+1)} = \eta^{(k)} + \epsilon$.

if $||c_1^{(k)}|| < TOL$

$\boldsymbol{X} := \boldsymbol{X}^{(k)}$.

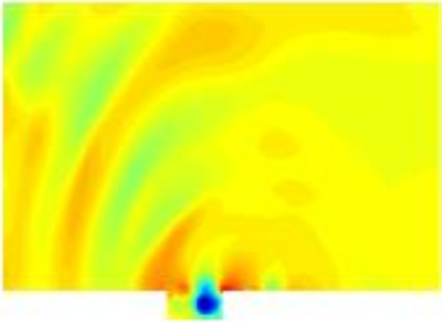
terminate the algorithm.

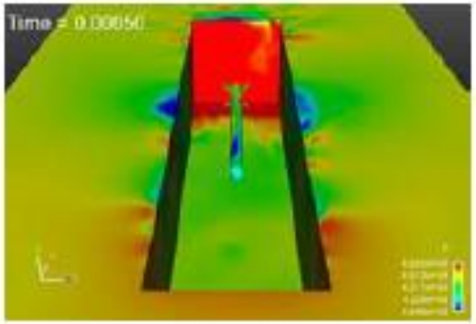
end

end

# Targeted Application: Compressible Flow

- We are interested in the ***compressible captive-carry problem***.





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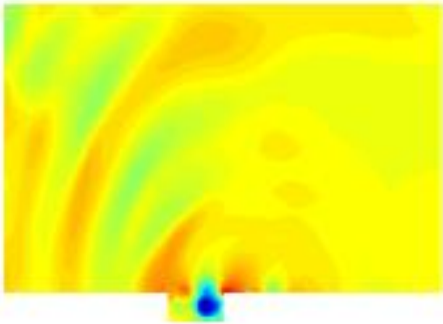

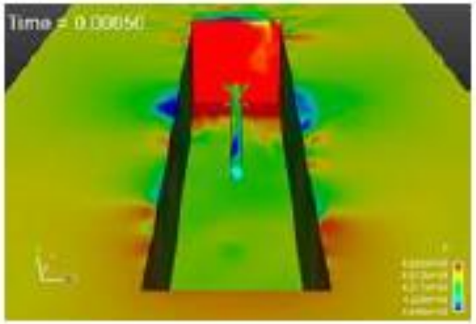


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- Desired numerical properties of ROMs:
  - ***Consistency*** (w.r.t. the continuous PDEs).
  - ***Stability:*** if full order model (FOM) is stable, ROM should be stable.
  - ***Convergence:*** requires consistency and stability.
  - ***Accuracy*** (w.r.t. FOM).
  - ***Efficiency***.
  - ***Robustness*** (w.r.t. time or parameter changes).

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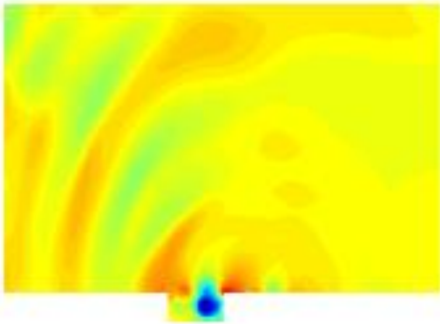

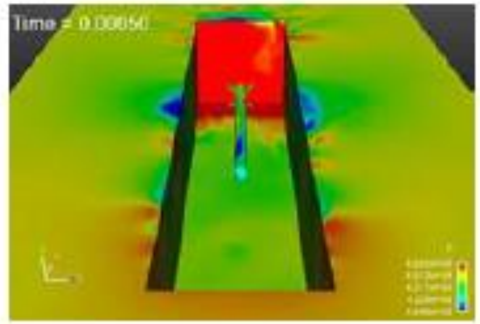

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Stability can be a real problem for compressible flow ROMs!