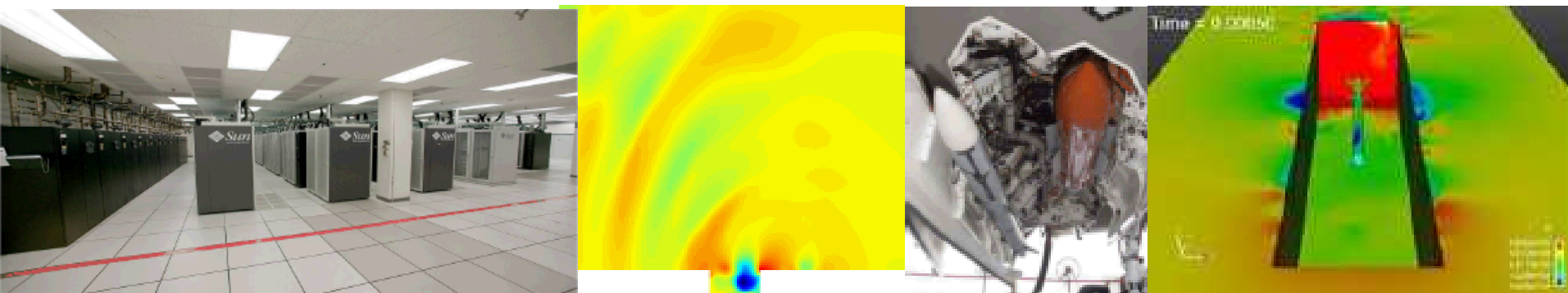


*Exceptional service in the national interest*



# A minimal subspace rotation approach for obtaining stable & accurate low-order projection-based reduced order models for nonlinear compressible flow

I. Tezaur<sup>1</sup>, M. Balajewicz<sup>2</sup>

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# Outline

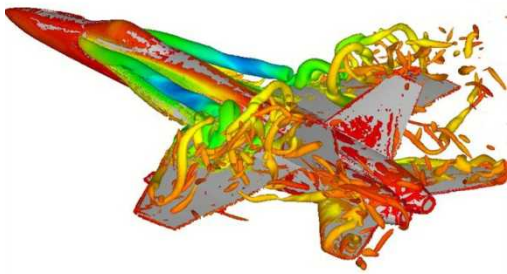
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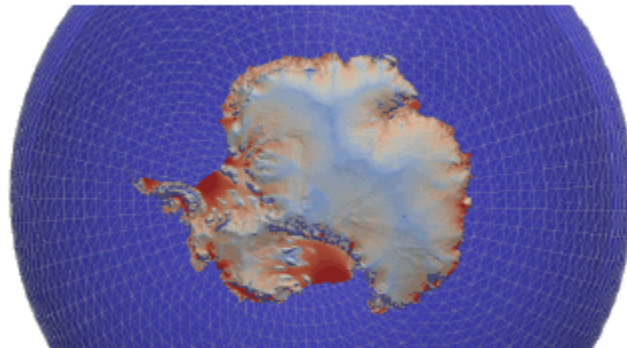
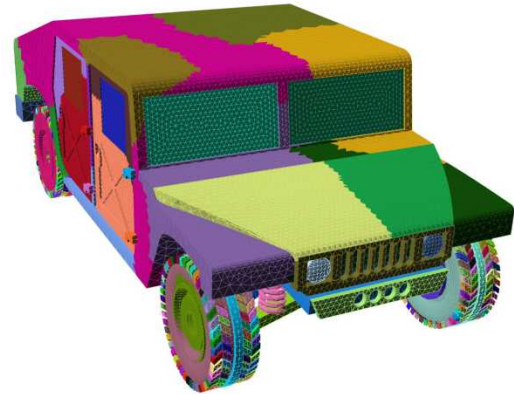
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# Motivation

**Computational models of high-dimensional systems arise in a rich variety of engineering and scientific applications**



Computational Fluid Dynamics (left)  
Finite Element Analysis (right)  
Climate Modeling (bottom)



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*“Purpose of computing is insight, not numbers.”*

- Richard Hamming, 1962

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# Projection-based model order reduction

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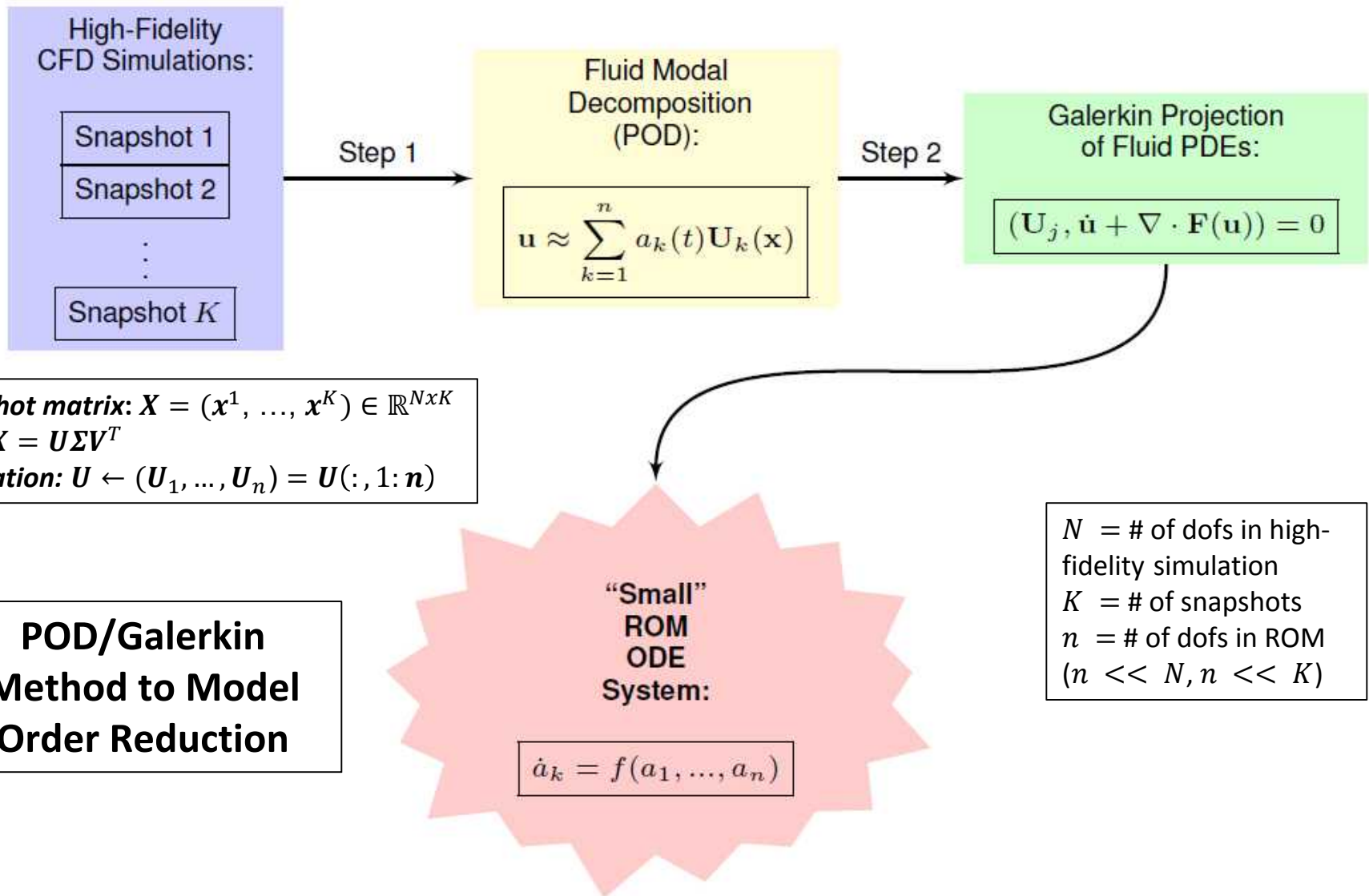
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3. **Online prediction:** identified parametric reduced order models (ROMs) capable of providing new solutions at a fraction of the computational cost.

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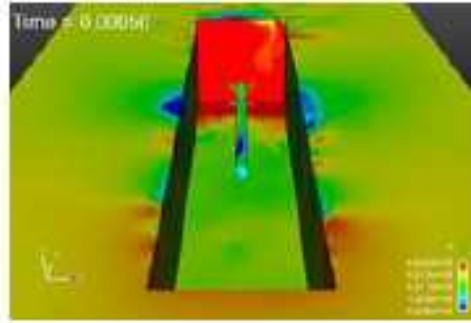
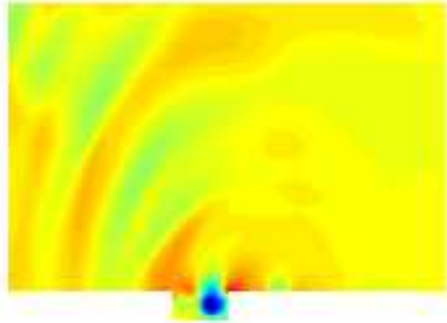
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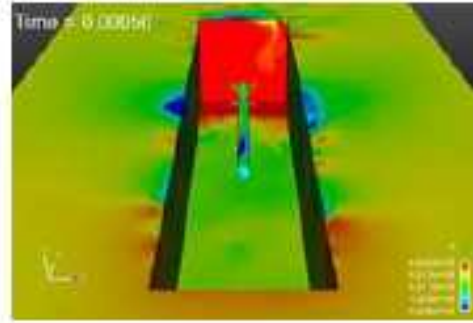
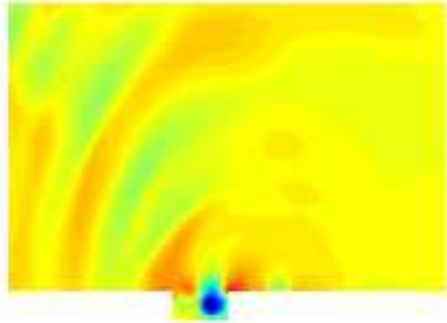
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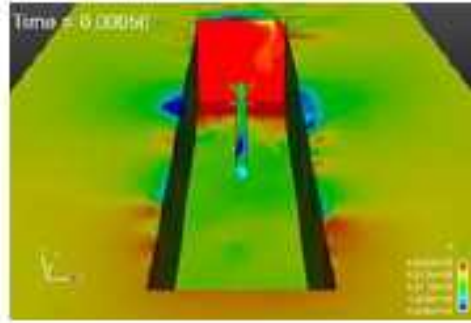
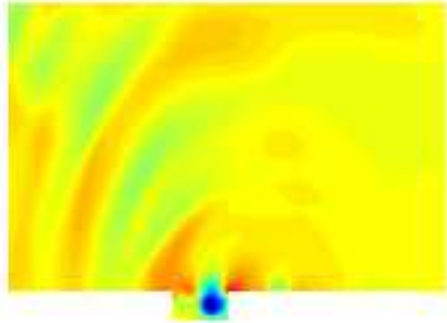
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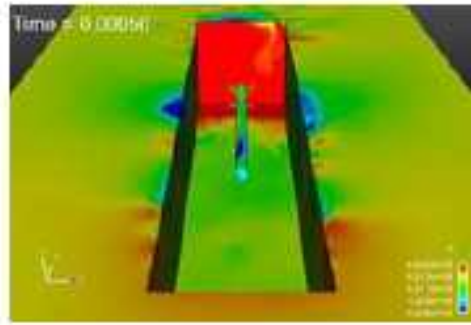
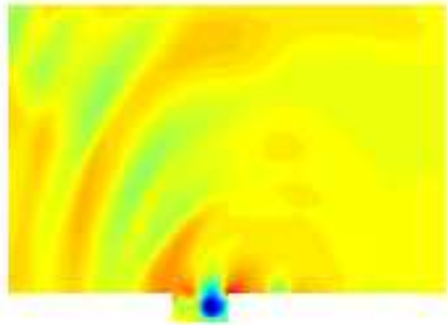
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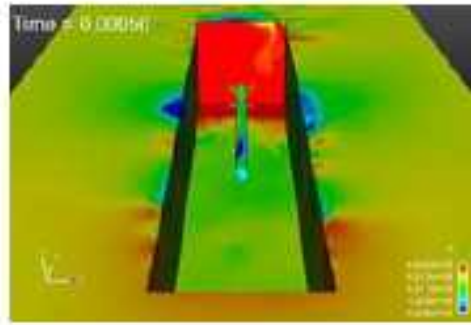
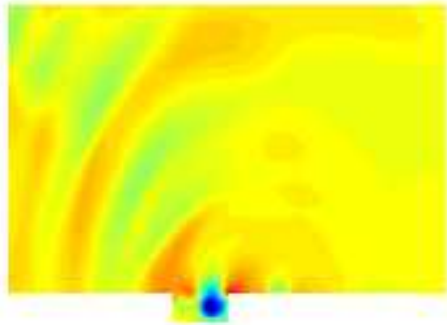
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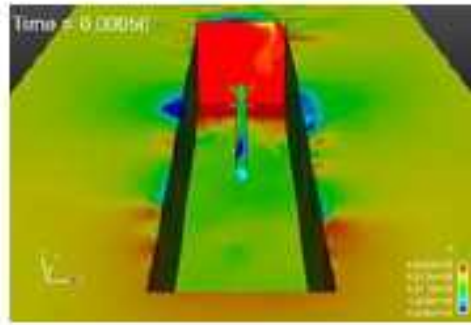
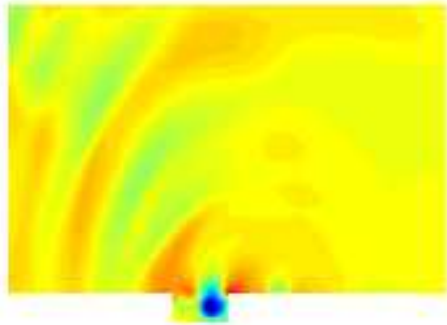
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**MOR for nonlinear, compressible fluid flows is still in its infancy!**

# Projection-based model order reduction

## Governing equations

- 3D compressible Navier-Stokes equations in primitive specific volume form:

[PDEs]

$$\begin{aligned} \zeta_{,t} + \zeta_{,j}u_j - \zeta u_{j,j} &= 0 \\ u_{i,t} + u_{i,j}u_j + \zeta p_{,i} - \frac{1}{Re}\zeta\tau_{ij,j} &= 0 \\ p_{,t} + u_jp_{,j} + \gamma u_{j,j}p - \left(\frac{\gamma}{PrRe}\right)(\kappa(p\zeta)_{,j})_{,j} - \left(\frac{\gamma-1}{Re}\right)u_{i,j}\tau_{ij} &= 0 \end{aligned} \tag{1}$$

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- Spectral discretization ( $\mathbf{q}(\mathbf{x}, t) \approx \sum_{i=1}^n a_i(t)\mathbf{U}_i(\mathbf{x})$ ) + Galerkin projection applied to (1) yields a system of  $n$  coupled quadratic ODEs:

[ROM]

$$\frac{d\mathbf{a}}{dt} = \mathbf{C} + \mathbf{L}\mathbf{a} + [\mathbf{a}^T \mathbf{Q}^{(1)} \mathbf{a} + \mathbf{a}^T \mathbf{Q}^{(2)} \mathbf{a} + \dots + \mathbf{a}^T \mathbf{Q}^{(n)} \mathbf{a}]^T\tag{2}$$

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



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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:

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  3. Inherently a linear model → cannot be expected to perform well for all classes of problems (e.g., nonlinear).

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### Illustrative example

- Standard approach: retain only the most energetic POD modes, i.e.,  $U_1, U_2, U_3, U_4, \dots$
- Proposed approach: choose some higher order basis modes to increase dissipation, i.e.,  $U_1, U_2, U_6, U_8, \dots$

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

$$\tilde{\mathbf{U}}_i = \sum_{j=1}^{n+p} X_{ij} \mathbf{U}_j, \quad i = 1, \dots, n, \quad (3)$$

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

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## Goals of proposed new approach

Find  $\mathbf{X}$  such that:

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where  $\mathcal{V}_{(n+p),n} \in \{\mathbf{X} \in \mathbb{R}^{(n+p) \times n} : \mathbf{X}^T \mathbf{X} = \mathbf{I}_n, p > 0\}$  is the Stiefel manifold.

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- Once  $\mathbf{X}$  is found, the result is a system of the form (2) with:

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

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- Maximize resolved turbulent kinetic energy (TKE)

$$f(\mathbf{X}) = -\|\boldsymbol{\Sigma} - \mathbf{X}\mathbf{X}^T \boldsymbol{\Sigma}\|_F \tag{7}$$

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$$f(\mathbf{X}) = \|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p) \times n}) \quad (6)$$

- Maximize resolved turbulent kinetic energy (TKE)

$$f(\mathbf{X}) = -\|\boldsymbol{\Sigma} - \mathbf{X}\mathbf{X}^T \boldsymbol{\Sigma}\|_F \quad (7)$$

- TKE objective (7) comes from earlier work (Balajewicz *et al.*, 2013) involving stabilization of incompressible flow ROMs.

# Accounting for modal truncation

## Objective Function

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

- We have considered two objectives  $f(\mathbf{X})$  in (5):

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- TKE objective (7) comes from earlier work (Balajewicz *et al.*, 2013) involving stabilization of incompressible flow ROMs.
- Numerical experiments reveal objective (6) produces better results than objective (7) for compressible flow.

# Accounting for modal truncation

## Constraint

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

- We use the traditional linear eddy-viscosity closure model ansatz for the constraint  $g(\mathbf{X}, \mathbf{L}) = 0$  in (5):

$$g(\mathbf{X}, \mathbf{L}) = \text{tr}(\mathbf{X}^T \mathbf{L} \mathbf{X}) - \eta \tag{8}$$

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  - $\eta$  = proxy for the balance between linear energy production and energy dissipation.

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- Specifically, constraint (8) involves overall balance between linear energy production and dissipation.
  - $\eta$  = proxy for the balance between linear energy production and energy dissipation.
- Constraint comes from property that averaged total power ( $= \text{tr}(\mathbf{X}^T \mathbf{L} \mathbf{X}) +$  energy transfer) has to vanish.

# Accounting for modal truncation

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

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

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

# Accounting for modal truncation

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Proposed approach may be interpreted as an *a priori consistent* formulation of the eddy-viscosity turbulence modeling approach.



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  2. Stability cannot be proven like for incompressible case.
  3. Uniqueness of solution to (5) is *not* guaranteed.



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  - Low Reynolds number channel driven cavity
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# Applications

## High angle of attack laminar airfoil

2D flow around an inclined NACA0012 airfoil at Mach 0.7,  
 $Re = 500$ ,  $Pr = 0.72$ ,  $AOA = 20^\circ \Rightarrow n = 4$  ROM (86% snapshot energy).

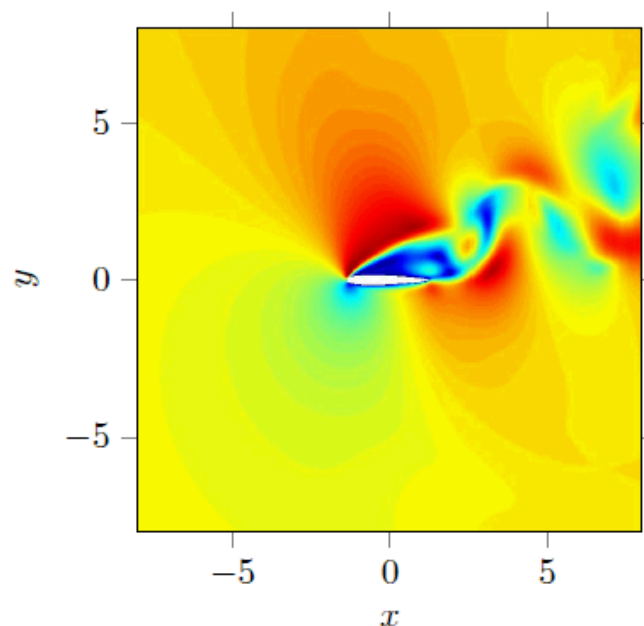


Figure 1: Contours of velocity magnitude at time of final snapshot.

# Applications

## High angle of attack laminar airfoil

- Minimizing subspace rotation:

$$f(\mathbf{X}) = \|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p) \times n})$$

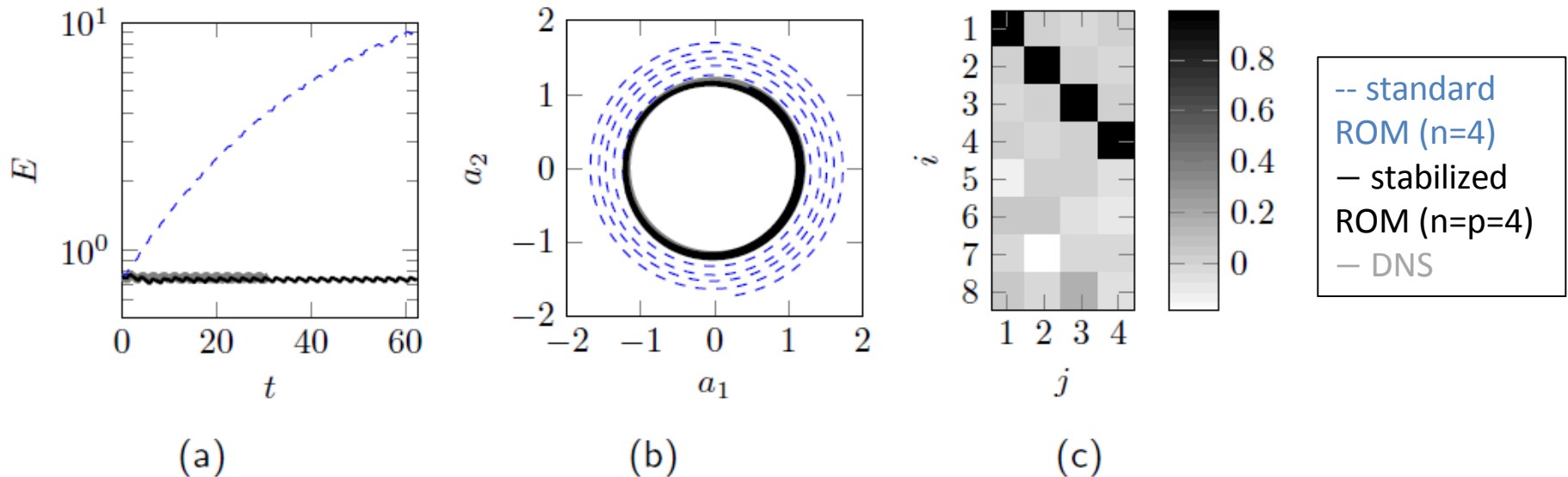


Figure 2: (a) evolution of modal energy, (b) phase plot of first and second temporal basis  $a_1(t)$  and  $a_2(t)$ , (c) illustration of stabilizing rotation showing that rotation is small:

$$\frac{\|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F}{n} = 0.083, \mathbf{X} \approx \mathbf{I}_{(n+p),n}$$

# Applications

## High angle of attack laminar airfoil

- Minimizing subspace rotation:

$$f(\mathbf{X}) = \|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p) \times n})$$

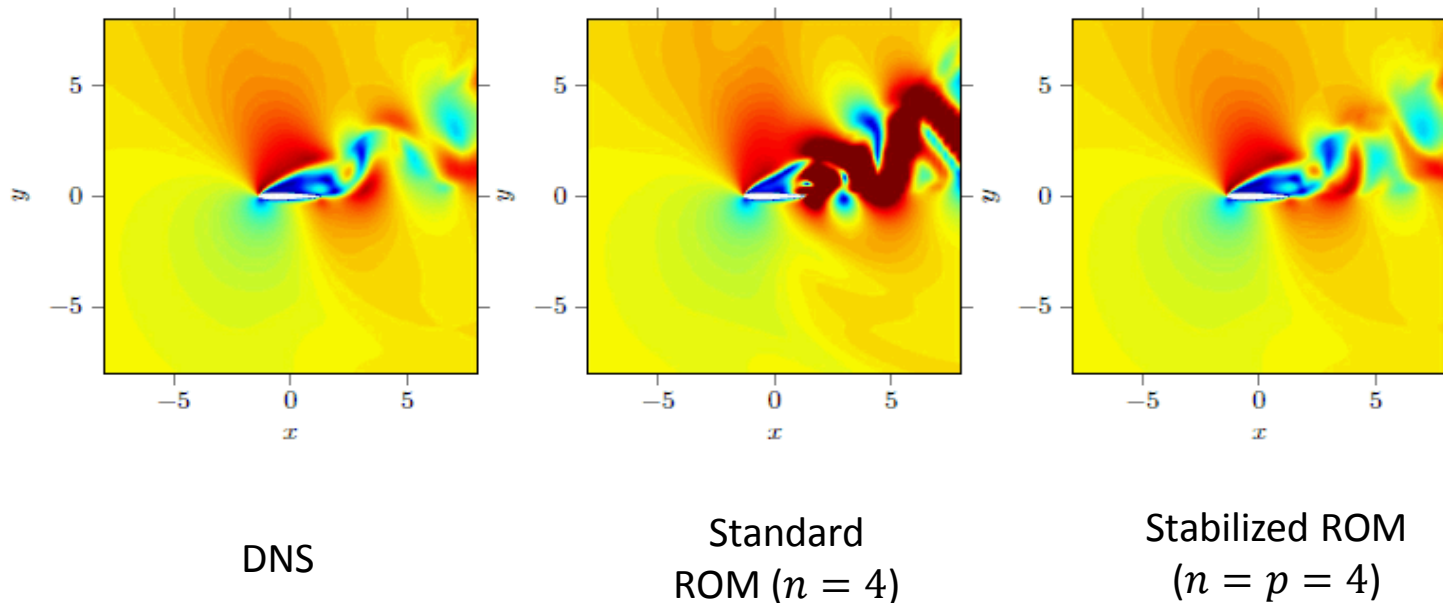


Figure 3: High angle of attack laminar airfoil contours of velocity magnitude at time of final snapshot.

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# Applications

## Channel driven cavity: low Reynolds number case

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

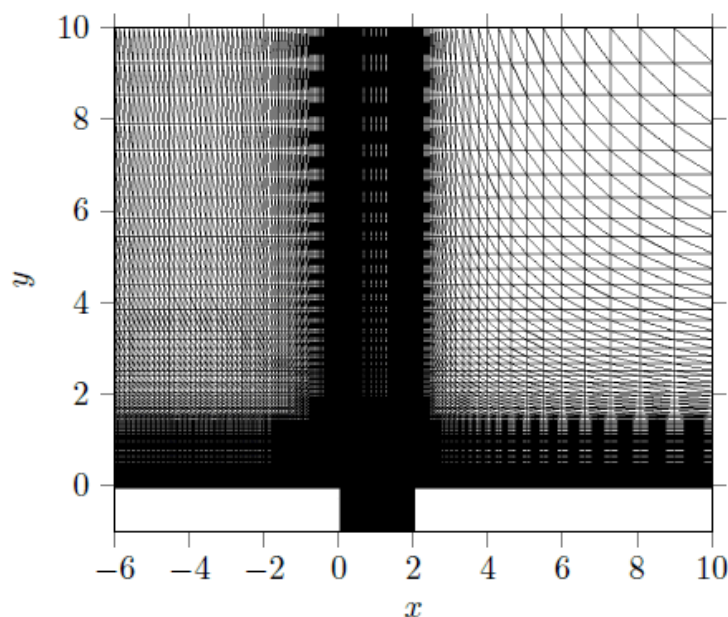


Figure 4: Domain and mesh for viscous channel driven cavity problem.

# Applications

## Channel driven cavity: low Reynolds number case

- Minimizing subspace rotation:

$$f(\mathbf{X}) = \|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p) \times n})$$

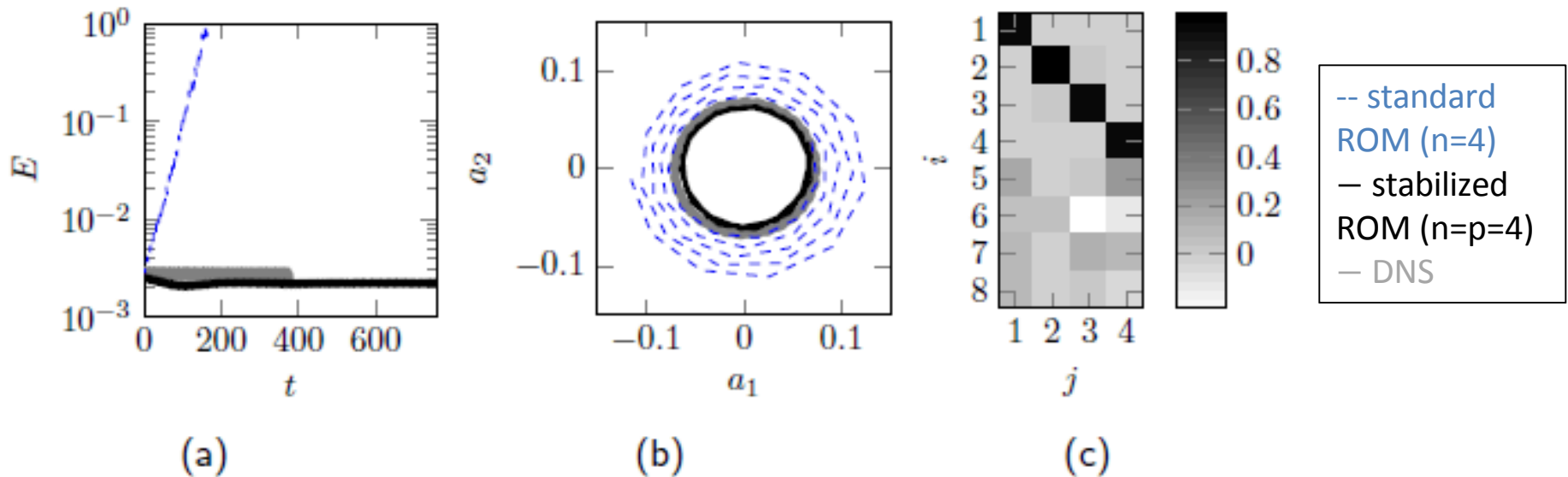


Figure 5: (a) evolution of modal energy, (b) phase plot of first and second temporal basis  $a_1(t)$  and  $a_2(t)$ , (c) illustration of stabilizing rotation showing that rotation is small:

$$\frac{\|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F}{n} = 0.188, \mathbf{X} \approx \mathbf{I}_{(n+p),n}$$



# Applications

## Channel driven cavity: low Reynolds number case

- Minimizing subspace rotation:

$$f(\mathbf{X}) = \|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p) \times n})$$

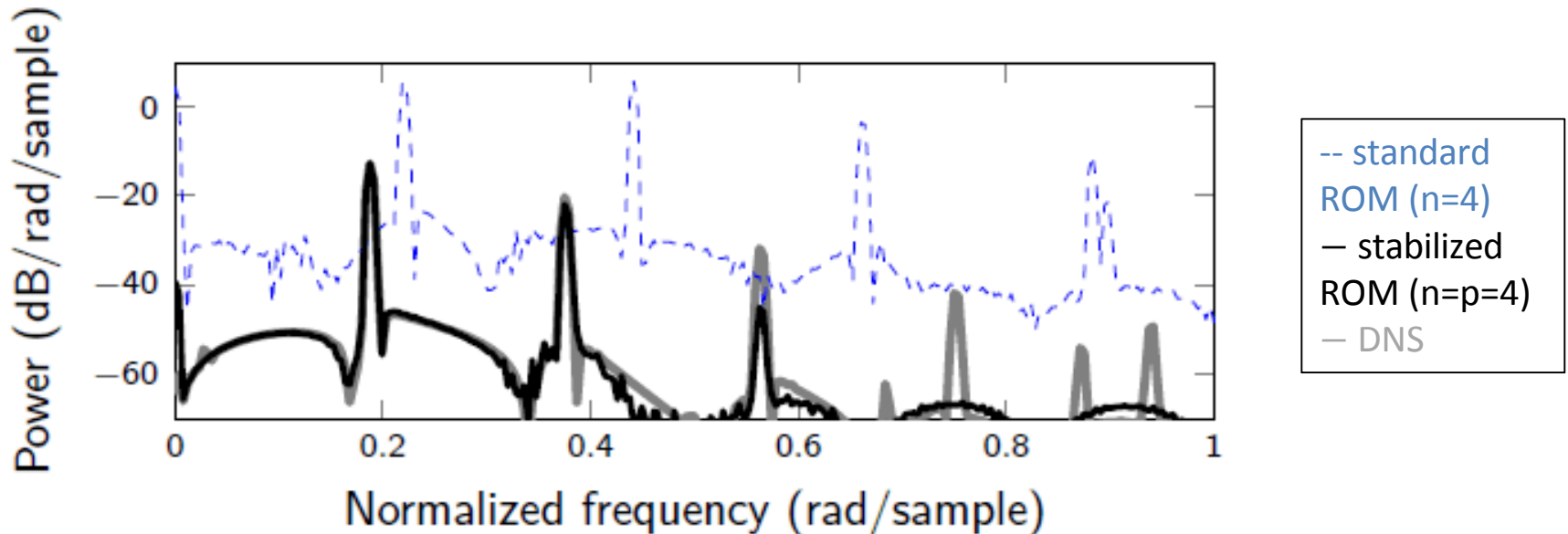


Figure 6: Pressure power spectral density (PSD) at location  $\mathbf{x} = (2, -1)$ ; stabilized ROM minimizes subspace rotation.

# Applications

## Channel driven cavity: low Reynolds number case

- Maximizing resolved TKE:

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

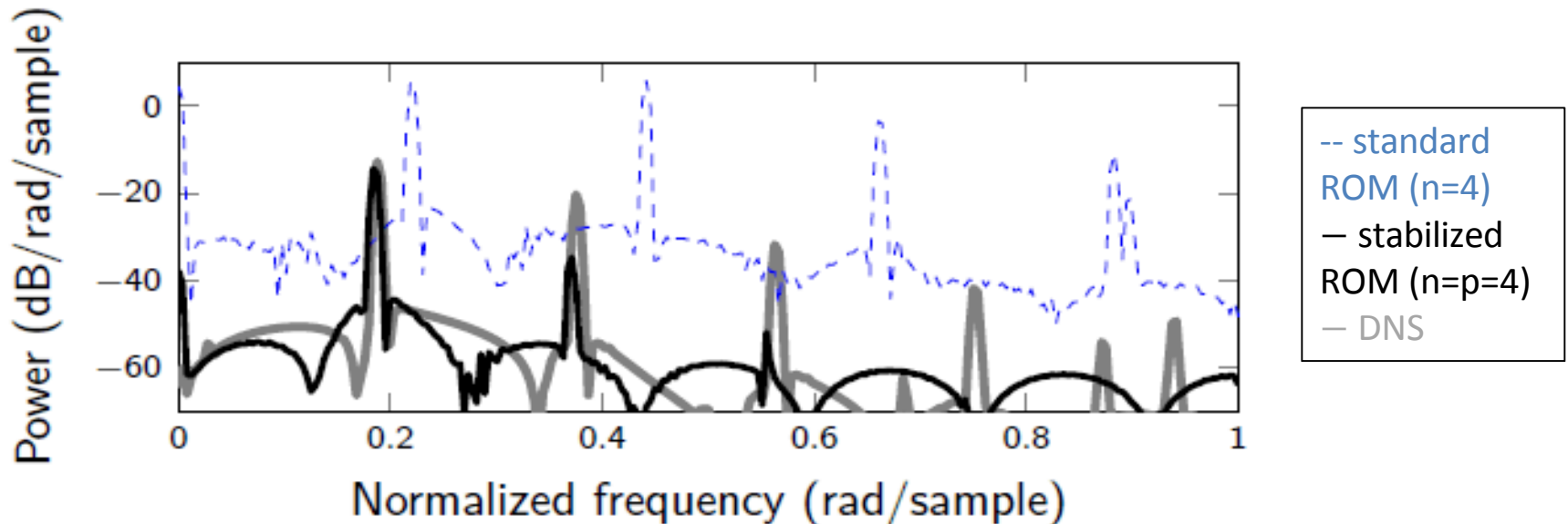


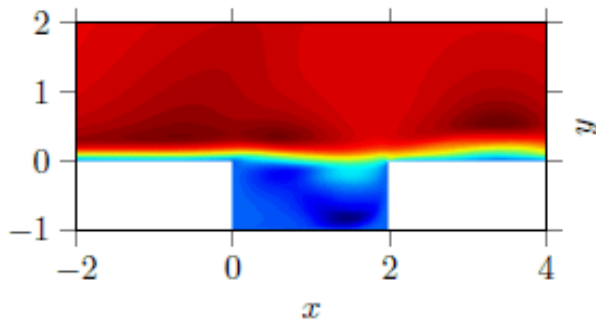
Figure 7: Pressure power spectral density (PSD) at location  $\mathbf{x} = (2, -1)$ ; stabilized ROM maximizes resolved TKE.

# Applications

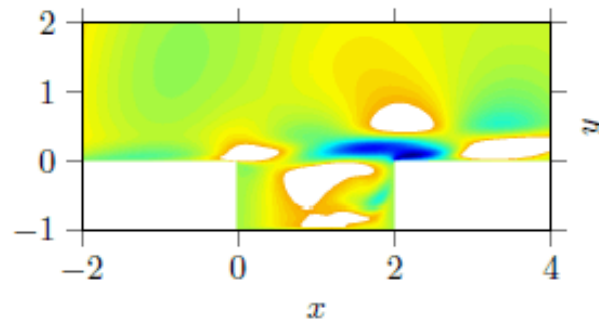
## Channel driven cavity: low Reynolds number case

- Minimizing subspace rotation:

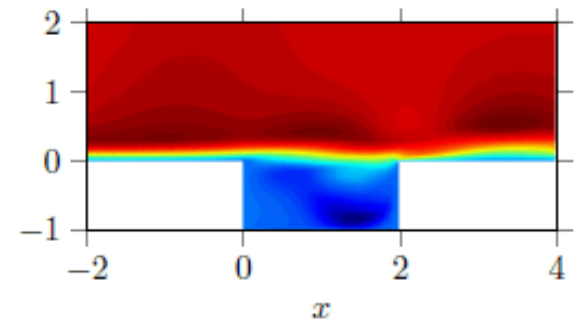
$$f(X) = \|X - I_{(n+p),n}\|_F = -\text{tr}(X^T I_{(n+p) \times n})$$



DNS



Standard  
ROM ( $n = 4$ )



Stabilized ROM  
( $n = p = 4$ )

Figure 8: Channel driven cavity  $\text{Re} \approx 1500$  contours of  $u$ -velocity at time of final snapshot.

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# Applications

## Channel driven cavity: moderate Reynolds number case

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

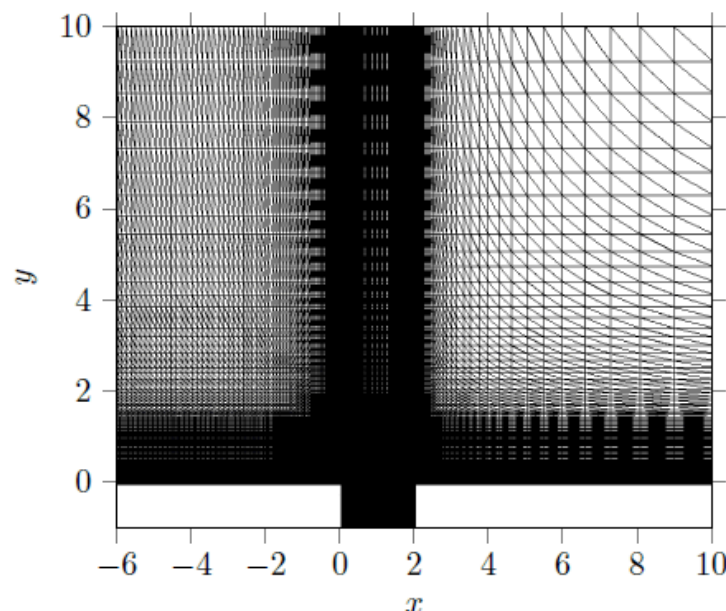


Figure 9: Domain and mesh for viscous channel driven cavity problem.

# Applications

## Channel driven cavity: moderate Reynolds number case

- Minimizing subspace rotation:

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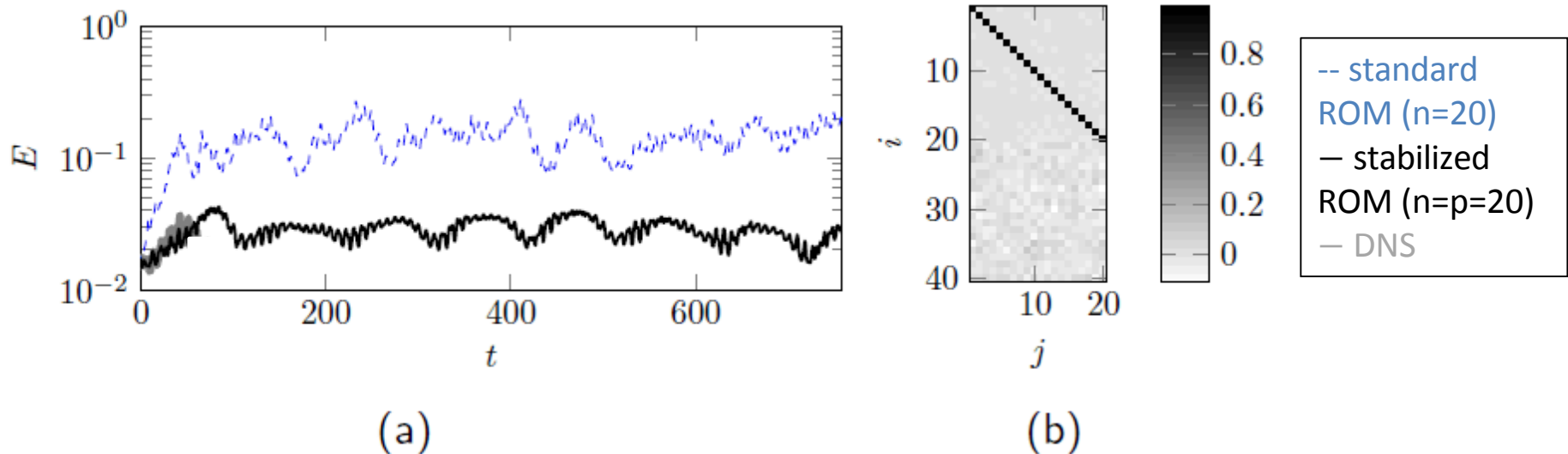


Figure 10: (a) evolution of modal energy, (b) illustration of stabilizing rotation showing that rotation is small:  $\frac{\|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F}{n} = 0.038, \mathbf{X} \approx \mathbf{I}_{(n+p),n}$

# Applications

## Channel driven cavity: moderate Reynolds number case

- Minimizing subspace rotation:

$$f(\mathbf{X}) = \|\mathbf{X} - \mathbf{I}_{(n+p),n}\|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p) \times n})$$

— stabilized  
ROM (n=p=20)  
— DNS

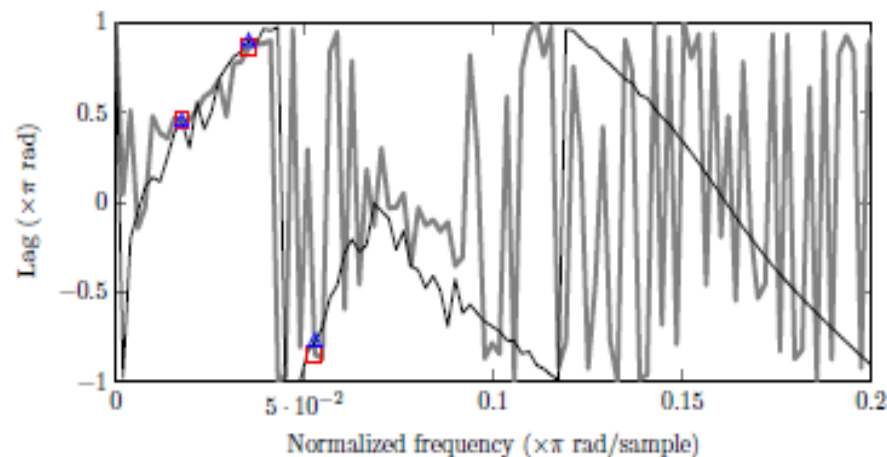
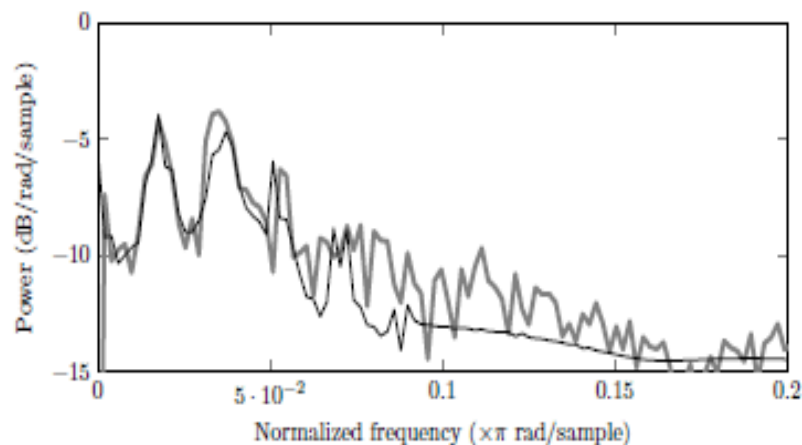


Figure 11: Pressure cross PSD of  $p(\mathbf{x}_1, t)$  and  $p(\mathbf{x}_2, t)$  where  $\mathbf{x}_1 = (2, -0.5)$ ,  $\mathbf{x}_2 = (0, -0.5)$

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

# Applications

## Channel driven cavity: moderate Reynolds number case

- Minimizing subspace rotation:

$$f(X) = \|X - I_{(n+p),n}\|_F = -\text{tr}(X^T I_{(n+p) \times n})$$

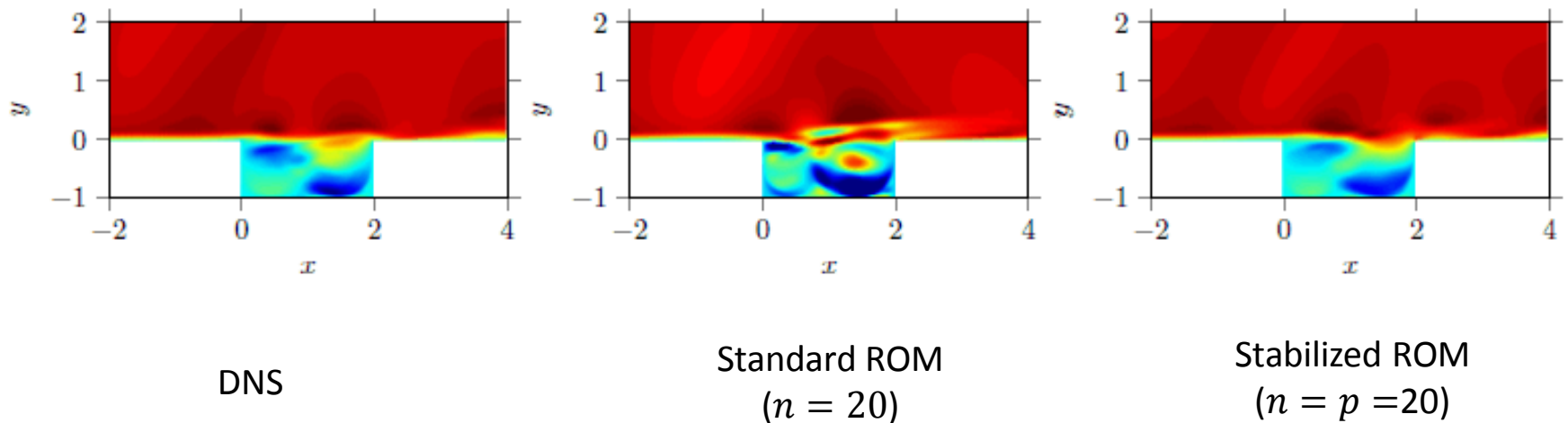


Figure 12: Channel driven cavity  $\text{Re} \approx 5500$  contours of  $u$ -velocity at time of final snapshot.



# Applications

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

Procedure		Airfoil	Low Re Cavity	Moderate Re Cavity
offline	FOM # of DOF	360,000	288,250	243,750
	Time-integration of FOM	7.8 hrs	72 hrs	179 hrs
	Basis construction (size $n + p$ ROM)	0.16 hrs	0.88 hrs	3.44 hrs
	Galerkin projection (size $n + p$ ROM)	0.74 hrs	5.44 hrs	14.8 hrs
	Stabilization	28 sec	14 sec	170 sec
online	ROM # of DOF	4	4	20
	Time-integration of ROM	0.31 sec	0.16 sec	0.83 sec
	Online computational speed-up	9.1e4	1.6e6	7.8e5

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# 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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# Future work

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- Selecting different goal-oriented objectives and constraints in our optimization problem:

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e.g.,

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

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# Appendix: Accounting for modal truncation

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

**Inputs:** Initial guess  $\eta^{(0)} = \text{tr}(\mathbf{L}(1:n, 1:n))$  ( $\mathbf{X} = \mathbf{I}_{(n+p) \times n}$ ), 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  $k = 0, \dots, k_{max}$

    Solve constrained optimization problem on Stiefel manifold:

$$\begin{aligned} & \underset{\mathbf{X}^{(k)} \in \mathcal{V}_{(n+p), n}}{\text{minimize}} && -\text{tr}(\mathbf{X}^{(k)\text{T}} \mathbf{I}_{(n+p) \times n}) \\ & \text{subject to} && \text{tr}(\mathbf{X}^{(k)\text{T}} \mathbf{L} \mathbf{X}^{(k)}) = \eta^{(k)}. \end{aligned}$$

    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  $\|c_1^{(k)}\| < TOL$

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

        terminate the algorithm.

    end

end