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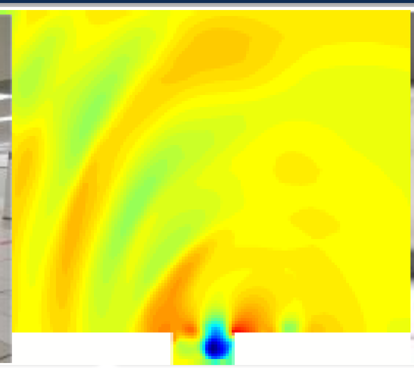

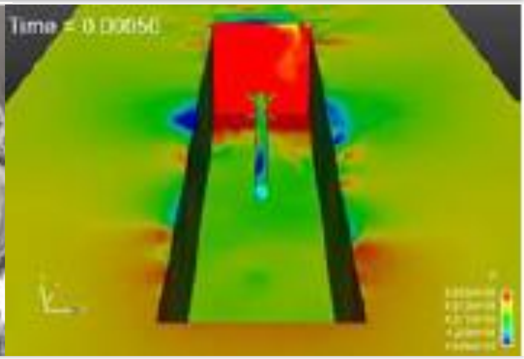

A minimal subspace rotation approach for obtaining stable & accurate low-order projection-based reduced order models for nonlinear compressible flow

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Outline

1. Motivation
2. Projection-based model order reduction
3. Accounting for modal truncation
    - Traditional linear eddy-viscosity approach
    - New proposed approach via subspace rotation
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    - High angle of attack laminar airfoil
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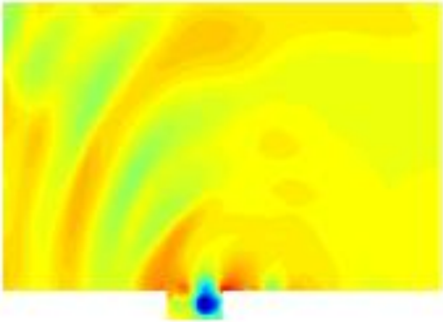
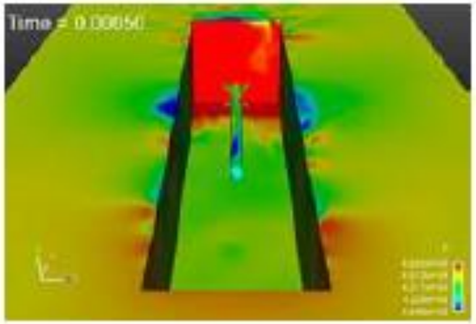
Targeted application: compressible fluid flow (e.g., captive-carry)





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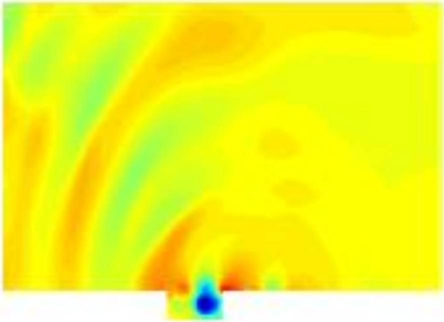

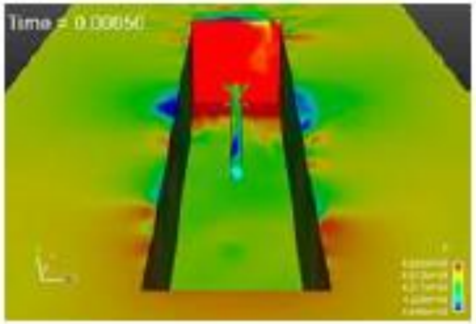

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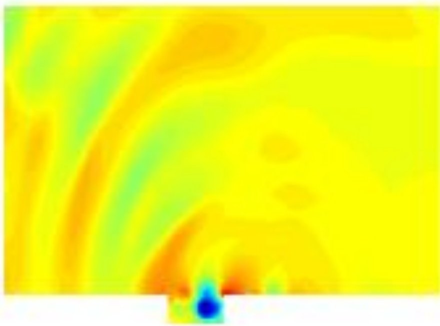

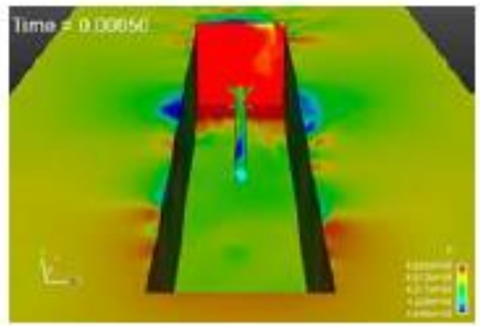

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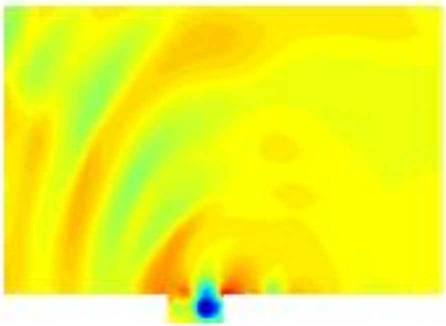

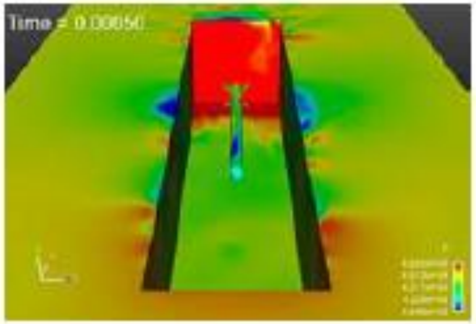

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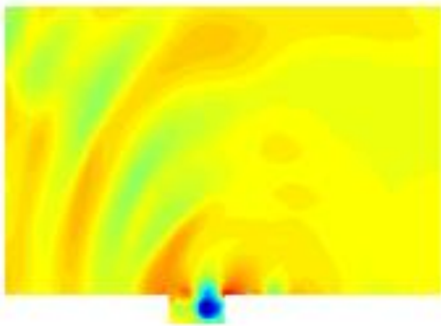

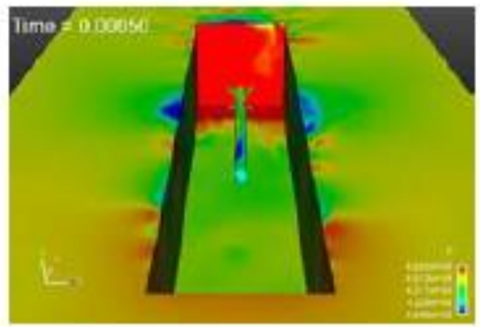

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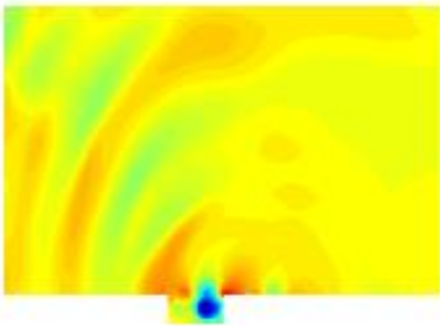

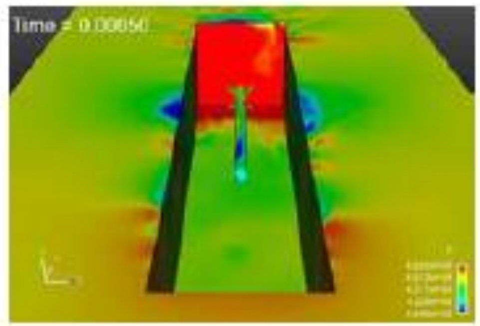

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MOR for <u>nonlinear</u>, <u>compressible</u> fluid flows is still in its infancy!

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Projection-based model order reduction

High-Fidelity CFD Simulations:

Snapshot 1

Snapshot 2

⋮

Snapshot K

Step 1

Fluid Modal Decomposition (POD):

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

Step 2

Galerkin Projection of Fluid PDEs:

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

Snapshot matrix: $\boldsymbol{X} = (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^K) \in \mathbb{R}^{NxK}$

SVD: $\boldsymbol{X} = \boldsymbol{U\Sigma V}^T$

Truncation: $\boldsymbol{U} \leftarrow (\boldsymbol{U}_1, \ldots, \boldsymbol{U}_n) = \boldsymbol{U}(:, 1\!:\!\boldsymbol{n})$

"Small" ROM ODE System:

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

N = # of dofs in high-fidelity simulation

K = # of snapshots

n = # of dofs in ROM

$(n << N, n << K)$

POD/Galerkin Method to Model Order Reduction

Projection-based model order reduction

Governing equations

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

[PDEs]

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

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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 $i = 1, \dots, n$.

Projection-based model order reduction

Summary of technical challenges

Projection-based MOR necessitates ***truncation.***

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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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  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* $\rightarrow$ 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., $\boldsymbol{U}_1, \boldsymbol{U}_2$, $\boldsymbol{U}_3$, $\boldsymbol{U}_4$, …
- *Proposed approach:* choose some higher order basis modes to increase dissipation, i.e., $\boldsymbol{U}_1, \boldsymbol{U}_2$, $\boldsymbol{U}_6$, $\boldsymbol{U}_8$, …

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

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

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.

Accounting for modal truncation

Goals of proposed new approach

Find $\boldsymbol{X}$ such that:

1. New modes $\widetilde{\boldsymbol{U}}$ remain *good approximations* of the flow.
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$$\begin{aligned}&\text{minimize}_{\boldsymbol{X}\in\mathcal{V}_{(n+p),n}} \quad f(\boldsymbol{X})\\ &\text{subject to} \quad g(\boldsymbol{X},\boldsymbol{L})=0\end{aligned}$$

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

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

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

Accounting for modal truncation

Objective function

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  - Minimize *subspace rotation*

$$\boxed{f(\boldsymbol{X}) = \left\|\boldsymbol{X} - \boldsymbol{I}_{(n+p),n}\right\|_F = -\mathrm{tr}\left(\boldsymbol{X}^T\boldsymbol{I}_{(n+p)\times n}\right)} \tag{6}$$

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  - Maximize resolved *turbulent kinetic energy (TKE)*

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

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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.

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

Accounting for modal truncation

Constraint

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

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

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

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  - η = 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*.
  - η = proxy for the balance between linear energy production and energy dissipation.
- Constraint comes from property that *averaged total power* $(= \mathrm{tr}(\boldsymbol{X}^T\boldsymbol{L}\boldsymbol{X}) +$ energy transfer) has to vanish.

Accounting for modal truncation

Minimal subspace rotation: trace minimization on Stiefel manifold

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

- $\eta \in \mathbb{R}$: 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.

Accounting for modal truncation

Remarks

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- Disadvantages of proposed approach:
  1. Off-line calibration of free parameter η is required.
  2. Stability cannot be proven like for incompressible case.

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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° $\Longrightarrow n = 4$ ROM (86% snapshot energy).

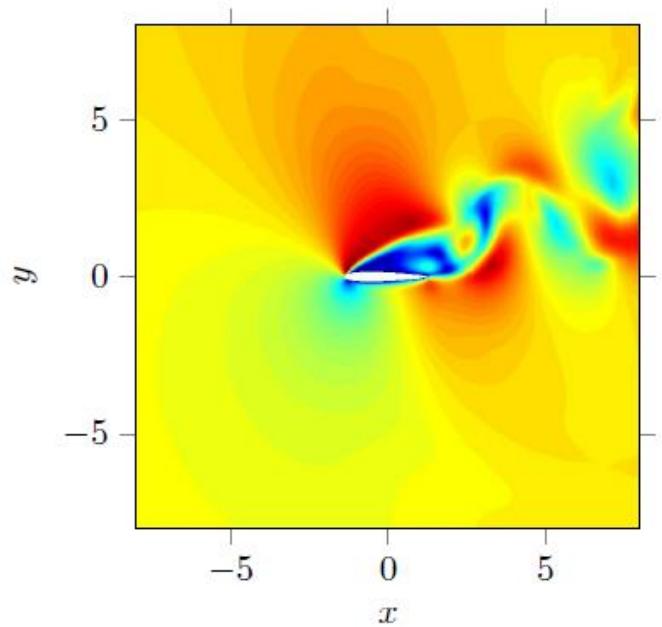

Figure 1: Contours of velocity magnitude at time of final snapshot.

Applications

High angle of attack laminar airfoil

- *Minimizing subspace rotation*:

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

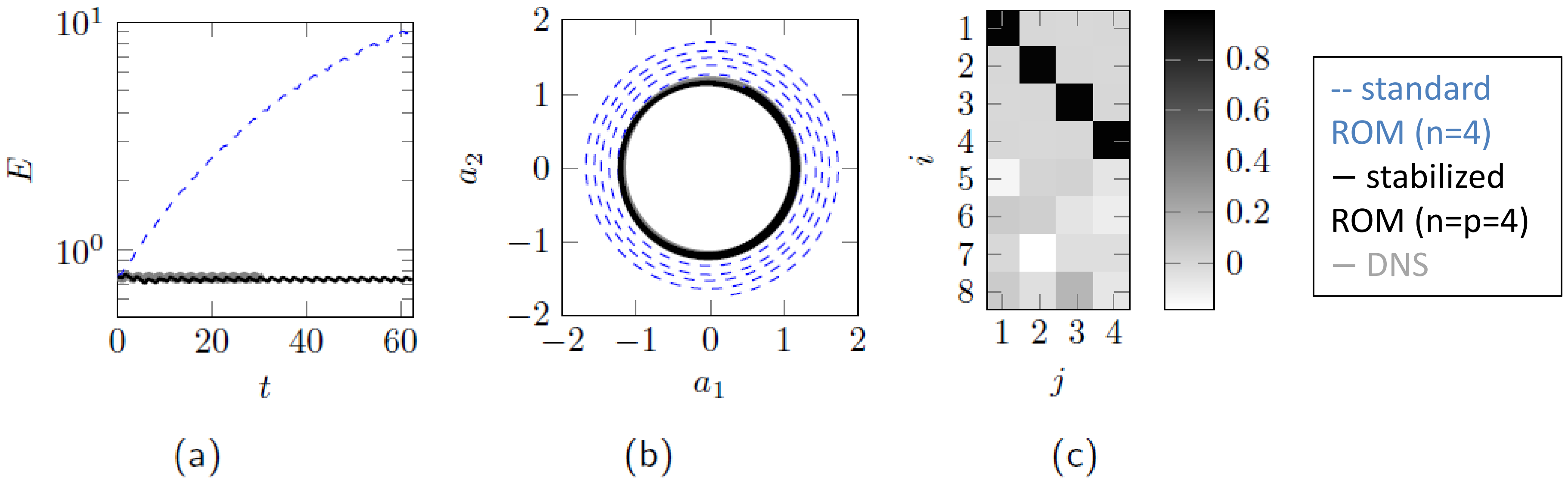

Figure 2: (a) evolution of modal energy, (b) phase plot of first and second temporal basis $a_1(t)$ and $a_2(t)$, (c) illustration of stabilizing rotation showing that rotation is small: $\frac{\left\|\boldsymbol{X}-\boldsymbol{I}_{(n+p),n}\right\|_F}{n} = 0.083, \boldsymbol{X} \approx \boldsymbol{I}_{(n+p),n}$

Applications

High angle of attack laminar airfoil

- *Minimizing subspace rotation*:

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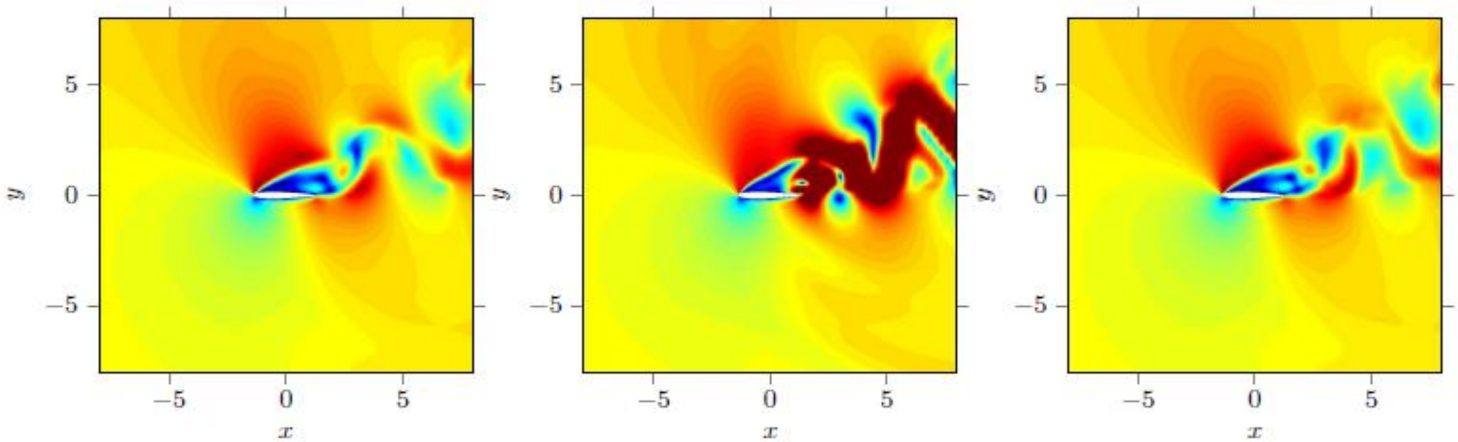

DNS

Standard ROM ($n = 4$)

Stabilized ROM ($n = p = 4$)

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).

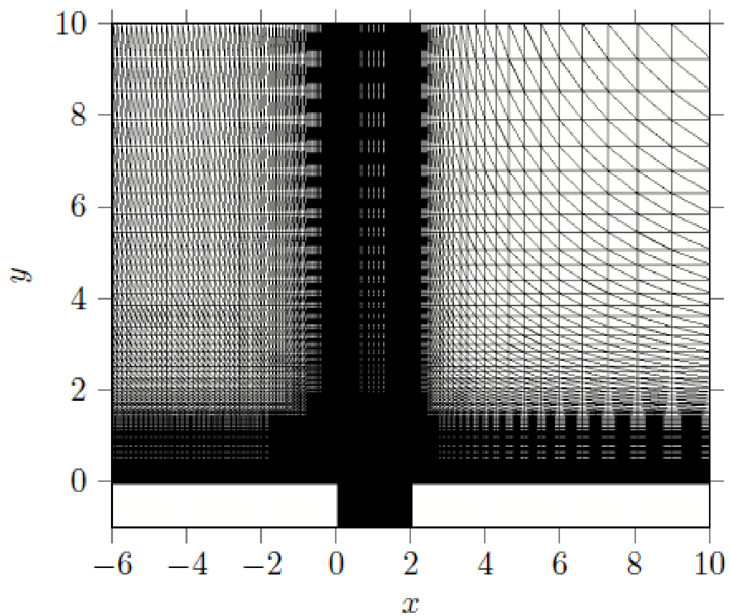


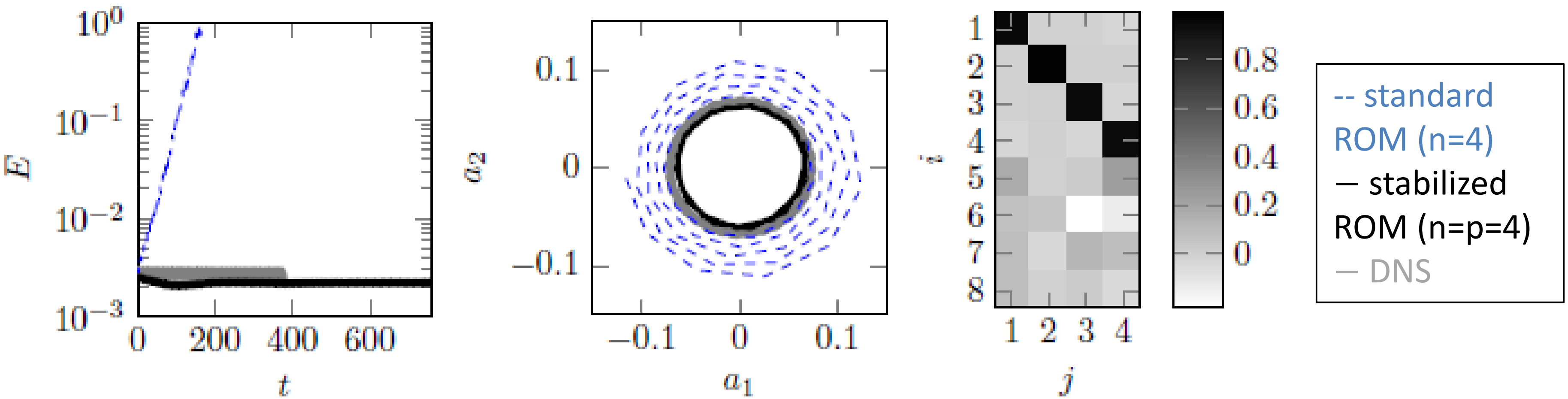
Figure 4: Domain and mesh for viscous channel driven cavity problem.

Applications

Channel driven cavity: low Reynolds number case

- *Minimizing subspace rotation:*

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



(a) (b) (c)

Figure 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: $\frac{\left\|\boldsymbol{X}-\boldsymbol{I}_{(n+p),n}\right\|_F}{n} = 0.188, \boldsymbol{X} \approx \boldsymbol{I}_{(n+p),n}$

Applications

Channel driven cavity: low Reynolds number case

- *Minimizing subspace rotation*:

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

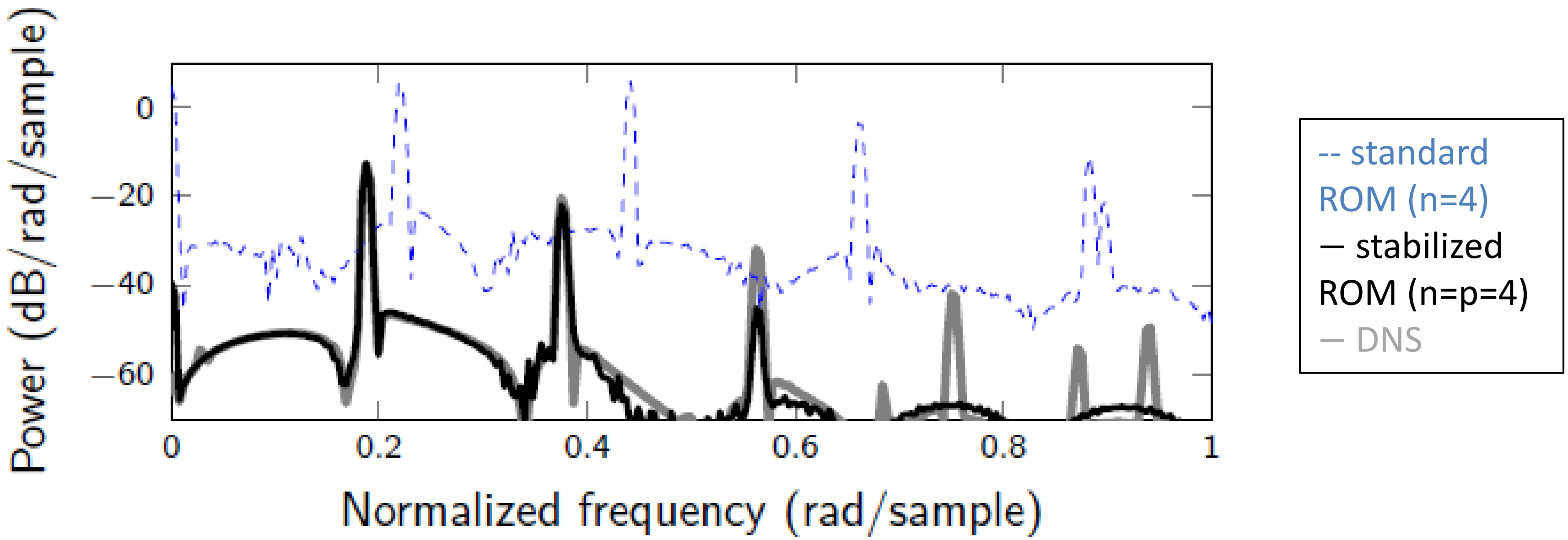


Figure 6: Pressure power spectral density (PSD) at location $\boldsymbol{x} = (2, -1)$; stabilized ROM minimizes subspace rotation.

Applications

Channel driven cavity: low Reynolds number case

- *Maximizing resolved TKE*:

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

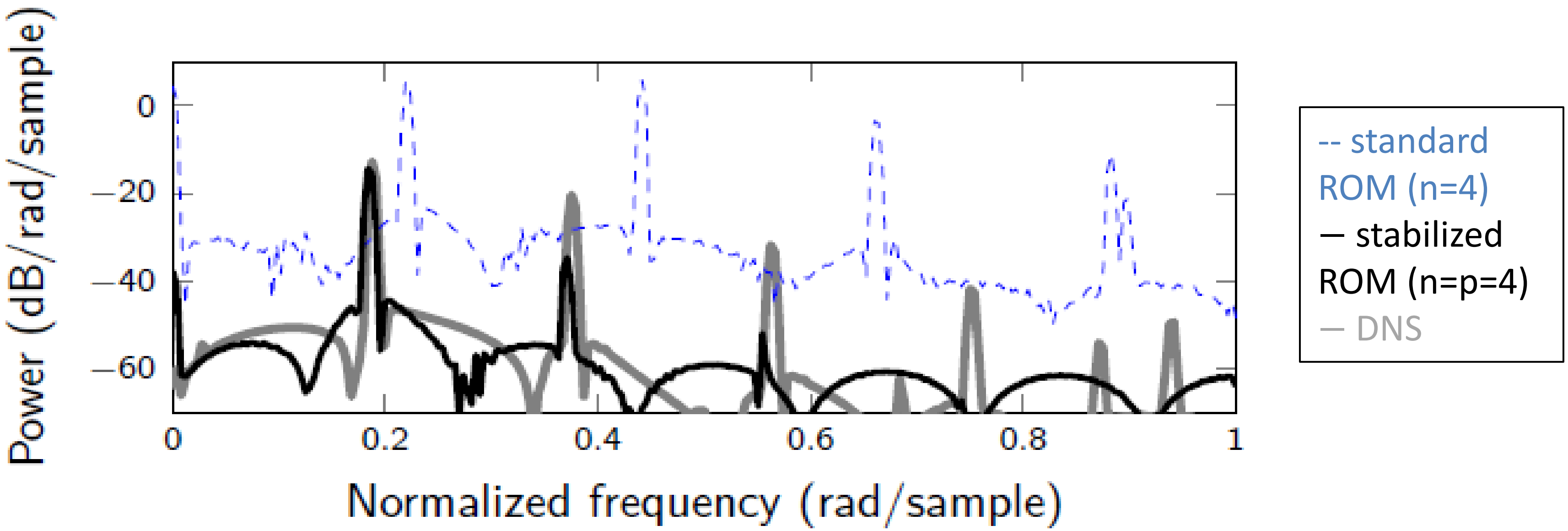


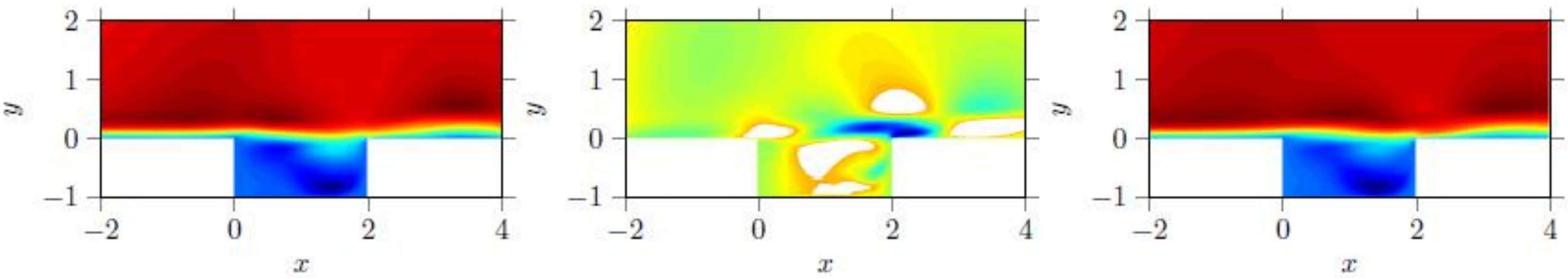
Figure 7: Pressure power spectral density (PSD) at location $\boldsymbol{x} = (2, -1)$; stabilized ROM maximizes resolved TKE.

Applications

Channel driven cavity: low Reynolds number case

- *Minimizing subspace rotation*:

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



DNS

Standard ROM ($n = 4$)

Stabilized ROM ($n = p = 4$)

Figure 8: Channel driven cavity 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).

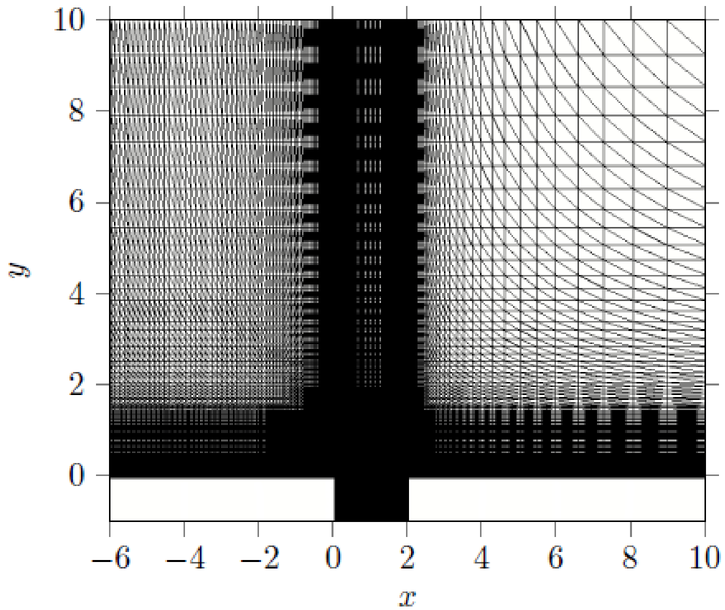

Figure 9: Domain and mesh for viscous channel driven cavity problem.

Applications

Channel driven cavity: moderate Reynolds number case

- *Minimizing subspace rotation*:

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

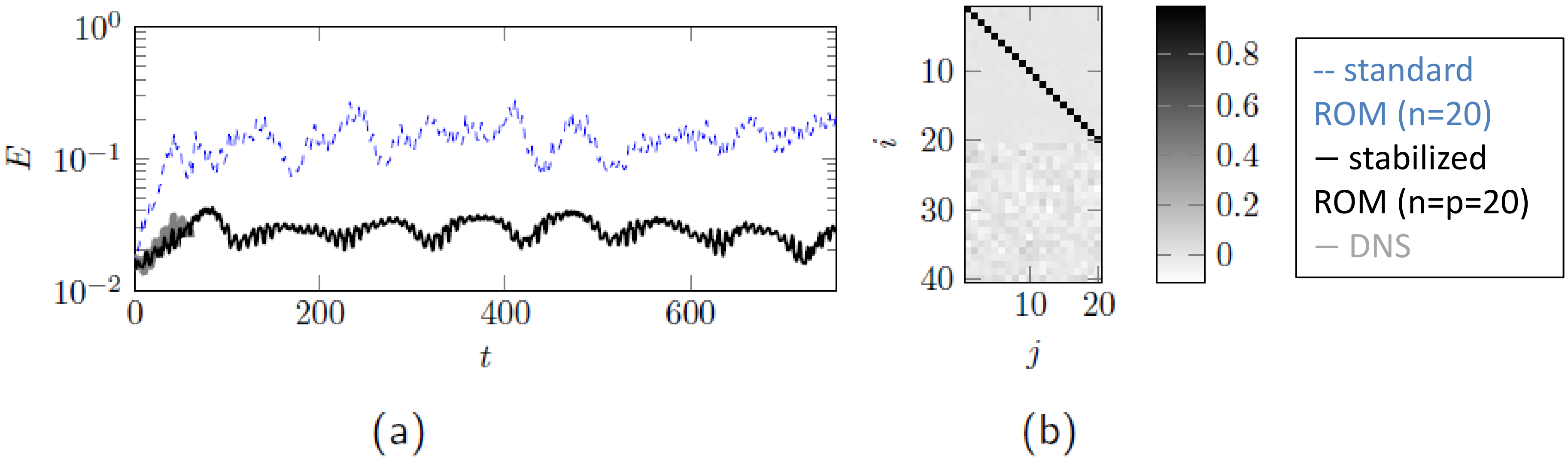

Figure 10: (a) evolution of modal energy, (b) illustration of stabilizing rotation showing that rotation is small: $\frac{\left\|\boldsymbol{X}-\boldsymbol{I}_{(n+p),n}\right\|_F}{n} = 0.038, \boldsymbol{X} \approx \boldsymbol{I}_{(n+p),n}$

Applications

Channel driven cavity: moderate Reynolds number case

- *Minimizing subspace rotation:*

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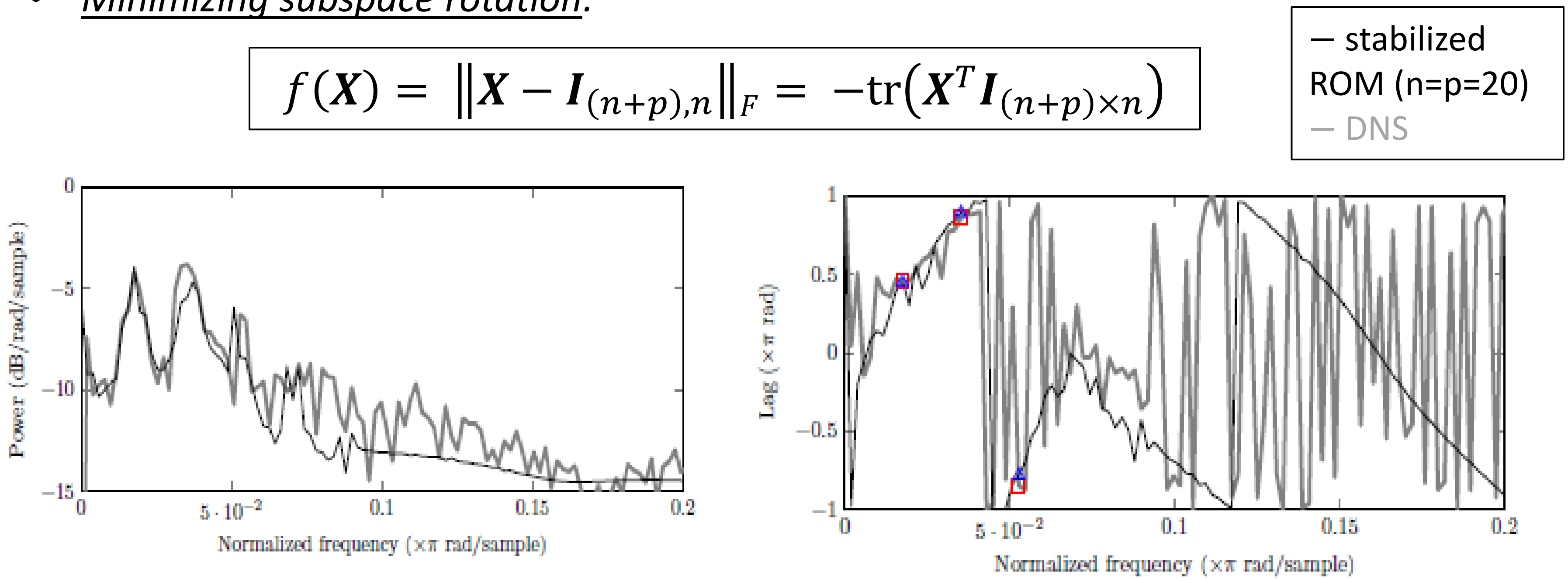

Figure 11: Pressure cross PSD of of $p(\boldsymbol{x}_1, t)$ and $p(\boldsymbol{x}_2, t)$ where $\boldsymbol{x}_1 = (2, -0.5)$, $\boldsymbol{x}_2 = (0, -0.5)$

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

Applications

Channel driven cavity: moderate Reynolds number case

- *Minimizing subspace rotation*:

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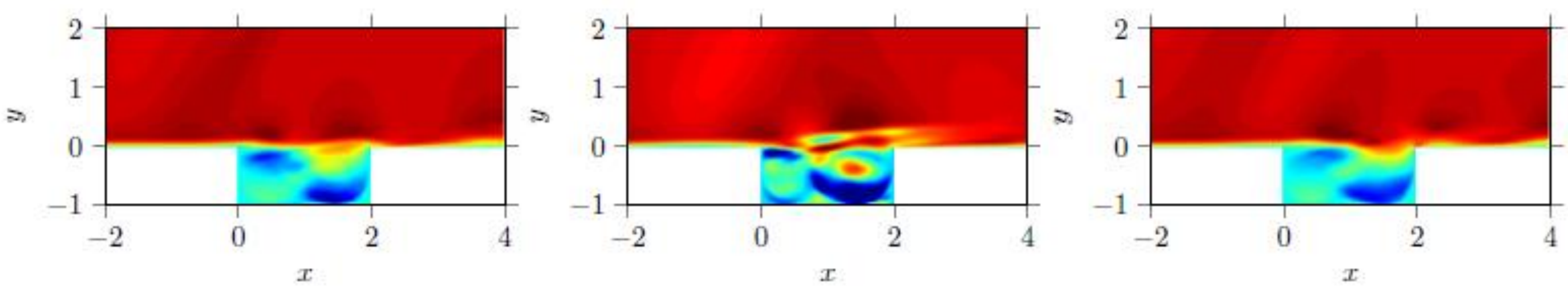

DNS

Standard ROM ($n = 20$)

Stabilized ROM ($n = p = 20$)

Figure 12: Channel driven cavity 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
	FOM # of DOF	360,000	288,250	243,750
offline	Time-integration of FOM	7.8 hrs	72 hrs	179 hrs
offline	Basis construction (size $n+p$ ROM)	0.16 hrs	0.88 hrs	3.44 hrs
offline	Galerkin projection (size $n+p$ ROM)	0.74 hrs	5.44 hrs	14.8 hrs
offline	Stabilization	28 sec	14 sec	170 sec
	ROM # of DOF	4	4	20
online	Time-integration of ROM	0.31 sec	0.16 sec	0.83 sec
	Online computational speed-up	9.1e4	1.6e6	7.8e5

* For minimizing subspace rotation.

Applications

Sandia National Laboratories

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- Significant *online computational speed-up*!

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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

- Application to *higher Reynolds number* problems.
- Extension of the proposed approach to problems with *generic nonlinearities*, where the ROM involves some form of hyper-reduction (e.g., DEIM, gappy POD).
- 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 $\eta^{(0)} = \mathrm{tr}(L(1:n, 1:n))$ ($\boldsymbol{X} = \boldsymbol{I}_{(n+p)\times n}$), 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:

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

  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 ϵ 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