Stabilization and fine-tuning of projection-based reduced order models for compressible flow via minimal subspace rotation on the Stiefel manifold

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Outline

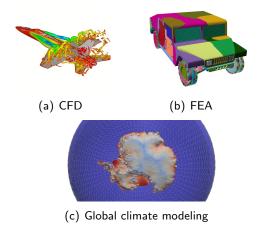
- 1. Motivation
- 2. Projection-based model order reduction
- 3. Accounting for modal truncation
 - 3.1 Traditional linear eddy-viscosity approach
 - 3.2 New proposed approach via subspace rotation
- 4. Applications
 - 4.1 High-angle of attack airfoil
 - 4.2 Low Reynolds number channel driven cavity
 - 4.3 Higher Reynolds number channel driven cavity
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Computational models of high-dimensional systems arise in a rich variety of engineering and scientific applications



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High-fidelity simulations remain prohibitive

- Computational costs still too high for parametric, time-critical and many-query applications (i.e., design, design optimization, control, UQ)
- Postprocessing/visualization difficulties
- → There are significant <u>scientific</u> and <u>engineering</u> benefits in developing and studying <u>low-dimensional</u> representations of high-dimensional systems that retain <u>physical fidelity</u> while substantially reducing the <u>size</u> and <u>cost</u> of the computational model

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Data-driven model order reduction (MOR)¹

- \rightarrow Underlying mathematical premises:
 - Compression: solution of governing parametric partial differential equation (PDE) or a coupled system of PDEs lies in a subspace of <u>significantly lower dimension</u>
 - Off-line training: subspace can be identified/learned off-line via training simulations and high-fidelity model can be reformulated with respect to this subspace
 - On-line prediction: identified parametric reduced-order models (ROMs) capable of providing new solutions at a <u>fraction</u> of the computational cost

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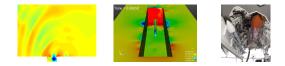
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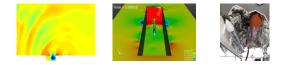
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Targeted application: compressible fluid flow (e.g., captive carry).



- Majority of MOR approaches in the literature for fluids are for incompressible flow.
- Some works on MOR for compressible flows:
 - Energy-based inner products: Rowley et al., 2004 (isentropic); Barone et al., 2009 (linear); Serre et. al, 2012 (linear); Kalashnikova et al., 2014 (nonlinear).
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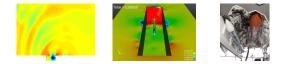


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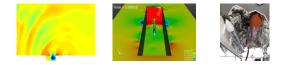
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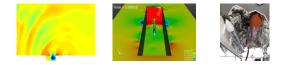
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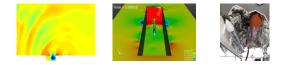
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Standard 3 step recipe

► Low-rank approximation of snapshot matrix *M* ∈ ℝ^{N×K} (Proper Orthogonal Decomposition, a.k.a., POD):

$$\min_{\boldsymbol{U}\in\mathbb{R}^{N\times n},\boldsymbol{V}\in\mathbb{R}^{n\times K}}\|\boldsymbol{M}-\boldsymbol{U}\boldsymbol{V}\|_{F}.$$
 (1)

Spectral discretization

$$\boldsymbol{u}(\boldsymbol{x},t) \approx \sum_{i=1}^{n} a_i(t) \boldsymbol{U}_i(\boldsymbol{x}).$$
 (2)

 Projection yields a small set of evolution equations for the mode coefficients a_i

$$\frac{d}{dt}a_i = f_i(\boldsymbol{a}). \tag{3}$$

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Governing equations

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

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

$$(4)$$

► For the compressible Navier-Stokes equations (4), Galerkin projection yields a system of *n* coupled quadratic ODEs

$$\frac{d\boldsymbol{a}}{dt} = \boldsymbol{C} + \boldsymbol{L}\boldsymbol{a} + \begin{bmatrix} \boldsymbol{a}^{\mathrm{T}} \boldsymbol{Q}^{(1)} \boldsymbol{a} & \boldsymbol{a}^{\mathrm{T}} \boldsymbol{Q}^{(2)} \boldsymbol{a} & \cdots & \boldsymbol{a}^{\mathrm{T}} \boldsymbol{Q}^{(n)} \boldsymbol{a} \end{bmatrix}^{\mathrm{T}} (5)$$

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

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Summary of technical challenges

- Projection-based MOR necessitates <u>truncation</u>.
- POD is, by definition and design, biased towards the large, energy producing scales of the flow (i.e., modes with large POD eigenvalues).
- Truncated/unresolved modes are negligible from a data compression point of view (i.e., small POD eigenvalues) but are crucial for the dynamical equations.
- For fluid flow applications, higher-order modes are associated with energy <u>dissipation</u> and thus, low-dimensional ROMs are often inaccurate and sometimes unstable.
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Traditional linear eddy-viscosity approach

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

$$\frac{d\boldsymbol{a}}{dt} = \boldsymbol{C} + (\boldsymbol{L} + \boldsymbol{L}_{\nu})\boldsymbol{a} + \begin{bmatrix} \boldsymbol{a}^{\mathrm{T}} \boldsymbol{Q}^{(1)} \boldsymbol{a} & \boldsymbol{a}^{\mathrm{T}} \boldsymbol{Q}^{(2)} \boldsymbol{a} & \cdots & \boldsymbol{a}^{\mathrm{T}} \boldsymbol{Q}^{(n)} \boldsymbol{a} \end{bmatrix}^{\mathrm{T}}$$

• L_{ν} is designed to decrease magnitude of positive eigenvalues and increase magnitude of negative eigenvalues of $L + L_{\nu}$ (for stability).

Disadvantages of this approach:

- Additional term destroys <u>consistency</u> between ROM and Navier-Stokes equations.
- Calibration necessary to derive optimal L_ν and optimal value is flow dependent.
- 3. Inherently a <u>linear</u> model \rightarrow cannot be expected to perform well for all classes of problems (e.g., nonlinear).

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Proposed new approach

- Instead of modeling truncation via additional linear term, model the truncation <u>a priori</u> by "rotating" the projection subspace into a more dissipative regime.
- ► Standard approach: retain only the most energetic POD modes, i.e., U₁, U₂, U₃, U₄...
- Proposed approach: choose some higher order basis to increase dissipation, i.e., U₁, U₂, U₆, U₈, ...
- That is, approximate the solution using a linear superposition of n + p (with p > 0) most energetic modes:

$$\tilde{\boldsymbol{U}}_{i} = \sum_{j=1}^{n+p} X_{ji} \boldsymbol{U}_{j} \quad i = 1, \cdots, n,$$
(6)

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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- Proposed approach: choose some higher order basis to increase dissipation, i.e., U₁, U₂, U₆, U₈, ...
- That is, approximate the solution using a linear superposition of n + p (with p > 0) most energetic modes:

$$\tilde{\boldsymbol{U}}_{i} = \sum_{j=1}^{n+p} X_{ji} \boldsymbol{U}_{j} \quad i = 1, \cdots, n,$$
(6)

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.

Balajewicz, Tezaur

Goals of proposed new approach:

Find **X** such that

- 1. New modes \widetilde{U} remain good approximations of the flow \rightarrow minimize the "rotation" angle, i.e. minimize $||\mathbf{X} \mathbf{I}_{(n+p),n}||_F$.
- 2. New modes produce stable and accurate ROMs \rightarrow ensure appropriate balance between energy production and energy dissipation.
- → Extension of earlier work for incompressible flow (Balajewicz et al., 2013) where it was shown that new POD modal basis is guaranteed to respect the power balance equation for the resolved turbulent kinetic energy and gives a <u>stable</u> ROM.

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Trace minimization on Stiefel manifold

$$\begin{array}{ll} \underset{\boldsymbol{X} \in \mathcal{V}_{(n+p),n}}{\text{minimize}} & -\operatorname{tr} \left(\boldsymbol{X}^{\mathrm{T}} \boldsymbol{I}_{(n+p) \times n} \right) \\ \text{subject to} & \operatorname{tr} \left(\boldsymbol{X}^{\mathrm{T}} \boldsymbol{L} \boldsymbol{X} \right) = \eta \end{array}$$
(7)

where $\eta \in \mathbb{R}$ and

$$\mathcal{V}_{(n+p),n} \in \{\boldsymbol{X} \in \mathbb{R}^{(n+p) \times n} : \boldsymbol{X}^{\mathrm{T}} \boldsymbol{X} = \boldsymbol{I}_{n}, \ p > 0\}.$$
(8)

 η is a proxy for the balance between energy production and energy dissipation (calculated iteratively using modal energy).

- Equation (7) is solved efficiently offline using method of Lagrange multipliers (Manopt MATLAB toolbox).
- Result is system of the form (5) with

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

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Stabilization algorithm: returns stabilizing rotation matrix X.

Inputs: Initial guess $\eta^{(0)} = \operatorname{tr}(L(1:n, 1:n))$ ($\mathbf{X} = \mathbf{I}_{(n+p) \times n}$), ROM size *n* and $p \ge 1$, 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:

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

Construct new Galerkin matrices using (9). 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 $||c_{1}^{(k)}|| < TOL$ $\mathbf{X} := \mathbf{X}^{(k)}$. terminate the algorithm.

end

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- Advantages of proposed approach:
 - Retains <u>consistency</u> between ROM and Navier-Stokes equations → no additional turbulence terms required.
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 - 3. Works with any basis and Petrov-Galerkin projection.
- Disadvantages of proposed approach:
 - 1. Off-line calibration of a free parameter η is required.
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High angle of attack laminar airfoil

 ▶ 2D flow around an inclined NACA0012 airfoil at Mach 0.7, Re = 500, Pr = 0.72, AOA = 20°, 1.25M DOFs ⇒ n = 4 ROM (86% snapshot energy).

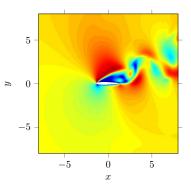


Figure 1: Contours of velocity magnitude at time of final snapshot.

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High angle of attack laminar airfoil

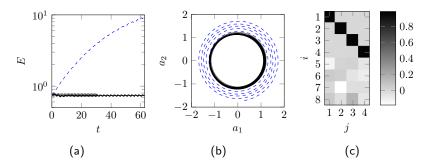


Figure 2: Nonlinear model reduction of the laminar airfoil. Evolution of modal energy (a), and phase plot of the first and second temporal basis, $a_1(t)$ and $a_2(t)$ (b); DNS (thick gray line), standard n = 4 ROM (dashed blue line), fine-tuned n, p = 4 ROM (solid black line). Stabilizing rotation matrix, X (c). Rotation is small: $||X - I_{(n+p) \times n}||_F/n = 0.083$, $X \approx I_{(n+p) \times n}$.

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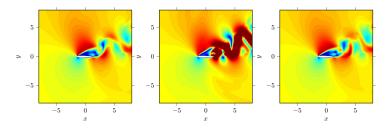


Figure 3: Snapshot of high angle of attack airfoil at final snapshot; contours of velocity magnitude. DNS (left), standard n = 4 ROM (middle), and fine-tuned n, p = 4 ROM (right)

Channel driven cavity: low Reynolds number case

► Flow over square cavity at Mach 0.6, Re = 1453.9, Pr = 0.72, 500K DOFs ⇒ n = 4 ROM (91% snapshot energy).

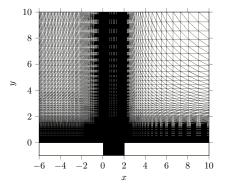


Figure 4: Domain and mesh for viscous channel driven cavity problem

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Channel driven cavity: low Reynolds number case

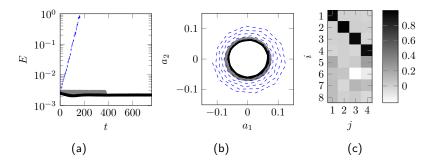


Figure 5: Nonlinear model reduction of channel drive cavity at Re \approx 1500. Evolution of modal energy (a) and phase plot of the first and second temporal basis, $a_1(t)$ and $a_2(t)$ (b); DNS (thick gray line), standard n = 4 ROM (dashed blue line), fine-tuned n, p = 4 ROM (solid black line). Stabilizing rotation matrix, **X** (c). Rotation is small: $||\mathbf{X} - \mathbf{I}_{(n+p) \times n}||_F / n = 0.118$, $\mathbf{X} \approx \mathbf{I}_{(n+p) \times n}$.

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Channel driven cavity: low Reynolds number case

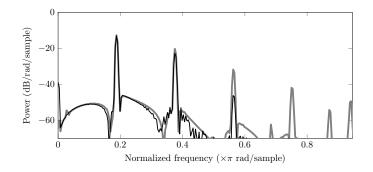


Figure 6: PSD of $p(\mathbf{x}, t)$ where x = (2, -1) of channel drive cavity Re \approx 1500. DNS (thick gray line), fine-tuned n, p = 4 ROM (black line)

Channel driven cavity: low Reynolds number case

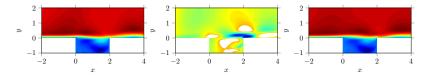


Figure 7: Snapshot of channel drive cavity $\text{Re} \approx 1500$; contours of *u*-velocity magnitude at the final snapshot. DNS (left), standard n = 4 ROM (middle) and fine-tuned n, p = 4 ROM (right)

Channel driven cavity: moderate Reynolds number case

▶ Flow over square cavity at Mach 0.6, Re = 5452.1, Pr = 0.72
 ⇒ n = 20 ROM (71% snapshot energy).

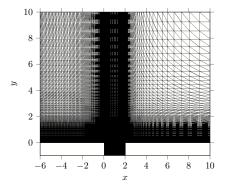


Figure 8: Domain and mesh for viscous channel driven cavity problem

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Channel driven cavity: moderate Reynolds number case

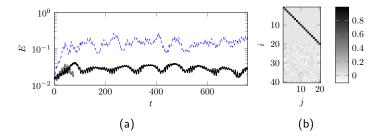


Figure 9: Nonlinear model reduction of channel drive cavity at Re \approx 5500. Evolution of modal energy (a); DNS (thick gray line), standard n = 20 ROM (dashed blue line), fine-tuned n, p = 20 ROM (solid black line). Stabilizing rotation matrix, **X** (b). Rotation is small: $||\mathbf{X} - \mathbf{I}_{(n+p) \times n}||_F / n = 0.038$, $\mathbf{X} \approx \mathbf{I}_{(n+p) \times n}$.

Channel driven cavity: moderate Reynolds number case

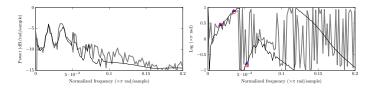


Figure 10: CPSD of $p(\mathbf{x}_1, t)$ and $p(\mathbf{x}_2, t)$ where $\mathbf{x}_1 = (2, -0.5)$ and $\mathbf{x}_2 = (0, -0.5)$ of channel driven cavity at $\text{Re} \approx 5500$. DNS (thick gray line), fine-tuned n, p = 20 ROM (black line)

- Power and phase lag at the fundamental frequency, and first two super harmonics are predicted accurately using the fine-tuned ROM.
- Phase lag at these three frequencies as predicted by the CFD and the fine-tuned ROM is identified by red squares and blue triangles, respectively.

Channel driven cavity: moderate Reynolds number case

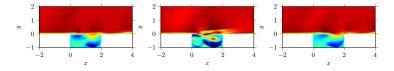


Figure 11: Snapshot of channel drive cavity $\text{Re} \approx 5500$; contours of *u*-velocity magnitude at the final snapshot. DNS (left), standard n = 20 ROM (middle), and fine-tuned n, p = 20 ROM (right)

Channel driven cavity: moderate Reynolds number case

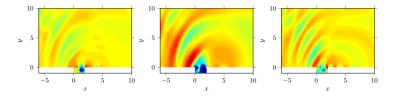


Figure 12: Snapshot of channel driven cavity $\text{Re} \approx 5500$; contours of pressure at the final snapshot. DNS (left), standard n = 20 ROM (middle), and fine-tuned n, p = 20 ROM (right)

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5. Conclusions and future work

- We have developed a non-intrusive approach for <u>stabilizing</u> and <u>fine-tuning</u> projection-based ROMs for compressible flows.
- The standard POD modes are <u>rotated</u> into a more dissipative regime to account for the dynamics in higher order modes truncated by the standard POD method.
- The new method is <u>consistent</u> and does not require addition of empirical turbulence model terms.
- Mathematically, the approach is formulated as a quadratic matrix program on the Stiefel manifold.
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- The method is demonstrated to deliver more <u>stable</u> and <u>accurate</u> ROMs on several applications.

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- Extension of the proposed approach to problems with <u>generic non-linearities</u>, where the ROM involves some form of hyper-reduction (e.g., DEIM, gappy POD).
- Extension of the method to predictive applications, e.g., problems with varying Reynolds number and geometry.
- Selecting different <u>goal-oriented</u> objectives and constraints in our optimization problem:

$$\begin{array}{ll} \underset{\boldsymbol{X} \in \mathcal{V}_{(n+p),n}}{\text{minimize}} & f(\boldsymbol{X}) \\ \text{subject to} & g(\boldsymbol{X}, \boldsymbol{L}) \end{array}$$
 (10)

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: $g = ||\mathbf{a}(t) \mathbf{a}^*(t)|| < \epsilon$

- Extension of the proposed approach to problems with <u>generic non-linearities</u>, where the ROM involves some form of hyper-reduction (e.g., DEIM, gappy POD).
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Balajewicz, Tezaur

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- ► Maximize *parametric robustness*:
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Maximize parametric robustness:

$$f = \sum_{i=1}^k \beta_i || \boldsymbol{U}^*(\mu_i) \boldsymbol{X} - \boldsymbol{U}^*(\mu_i) ||_{\boldsymbol{F}}.$$

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Thank you!

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