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
4. Applications
   • High angle of attack laminar airfoil
   • Low Reynolds number channel driven cavity
   • Moderate Reynolds number channel driven cavity
5. Summary
6. Future work
7. References
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Targeted application: compressible fluid flow (e.g., captive-carry)
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- Majority of fluid MOR approaches in the literature are for *incompressible* flow.
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- There has been some on MOR for **compressible flows**.
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  - **Energy-based inner products:** Rowley *et al.*, 2004 (isentropic); Barone *et al.*, 2007 (linear); Serre *et al.*, 2012 (linear); Kalashnikova *et al.*, 2014 (nonlinear).
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  - Energy-based inner products: Rowley et al., 2004 (isentropic); Barone et al., 2007 (linear); Serre et al., 2012 (linear); Kalashnikova et al., 2014 (nonlinear).
  - GNAT method/Petrov-Galerkin projection: Carlberg et al., 2014 (nonlinear).
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MOR for **nonlinear, compressible** fluid flows is still in its infancy!
**Projection-based model order reduction**

**High-Fidelity CFD Simulations:**
- Snapshot 1
- Snapshot 2
- ... (Snapshot K)

**Step 1:**
- **Fluid Modal Decomposition (POD):**
  \[ u \approx \sum_{k=1}^{n} a_k(t) U_k(x) \]

**Step 2:**
- **Galerkin Projection of Fluid PDEs:**
  \[ (U_j, \dot{u} + \nabla \cdot F(u)) = 0 \]

**POD/Galerkin Method to Model Order Reduction**

**Snapshot matrix:** \( X = (x^1, ..., x^K) \in \mathbb{R}^{N \times K} \)

**SVD:** \( X = U \Sigma V^T \)

**Truncation:** \( U \leftarrow (U_1, ..., U_n) = U(:, 1:n) \)

**“Small” ROM ODE System:**
\[ \dot{a}_k = f(a_1, ..., a_n) \]

**POD/Galerkin Method to Model Order Reduction**

- \( N \) = # of dofs in high-fidelity simulation
- \( K \) = # of snapshots
- \( n \) = # of dofs in ROM
  \( n \ll N, n \ll K \)
Projection-based model order reduction

Governing equations

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

\[
\begin{align*}
\frac{\partial \zeta}{\partial t} + \zeta \frac{\partial u_j}{\partial x} - \zeta u_{j,j} &= 0 \\
\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_j}{\partial x} + \zeta p_i - \frac{1}{Re} \zeta \tau_{ij,j} &= 0 \\
\frac{\partial p}{\partial t} + u_j p_j + \gamma u_j \frac{\partial p}{\partial x} - \left( \frac{\gamma}{PrRe} \right) \left( \kappa(p\zeta)_j \right)_j - \left( \frac{\gamma - 1}{Re} \right) u_{i,j} \tau_{ij} &= 0
\end{align*}
\]
Projection-based model order reduction

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\begin{align*}
\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}{Pr Re} \right) (\kappa(p \zeta), j), j - \left( \frac{\gamma - 1}{Re} \right) u_{i,j} \tau_{ij} &= 0
\end{align*}
\]  

(PDEs)

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

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

(ROM)

where \( C \in \mathbb{R}^n, L \in \mathbb{R}^{n \times n} \) and \( Q^{(i)} \in \mathbb{R}^{n \times n} \) for all \( i = 1, \ldots, n \).
Projection-based model order reduction

Summary of technical challenges

Projection-based MOR necessitates *truncation*. 
Projection-based model order reduction

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Projection-based MOR necessitates **truncation**.

- POD is, by definition and design, biased towards the **large, energy producing** scales of the flow (i.e., modes with large POD eigenvalues).
Projection-based model order reduction

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Projection-based MOR necessitates *truncation*.

- 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 form a *data compression* point of view (i.e., small POD eigenvalues) but are crucial for the *dynamical equations*.
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- 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 **dissipation** $\Rightarrow$ low-dimensional ROMs are often **inaccurate** and sometimes **unstable**.
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For a ROM to be stable and accurate, the truncated/unresolved subspace must be accounted for.
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- POD is, by definition and design, biased towards the \textit{large, energy producing} scales of the flow (i.e., modes with large POD eigenvalues).
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For a ROM to be stable and accurate, the \textit{truncated/unresolved subspace} must be accounted for.

\begin{itemize}
  \item \textbf{Turbulence Modeling} (traditional approach)
  \item \textbf{Subspace Rotation} (our approach)
\end{itemize}
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Accounting for modal truncation

Traditional linear eddy-viscosity approach

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

\[
\frac{d\mathbf{a}}{dt} = \mathbf{C} + L\mathbf{a} + \left[ a^T Q^{(1)} a + a^T Q^{(2)} a + \cdots + a^T Q^{(n)} a \right]^T
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\frac{da}{dt} = C + (L + L_v)a + [a^T Q^{(1)}a + a^T Q^{(2)}a + \cdots + a^T Q^{(n)}a]^T
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• \(L_\nu\) is designed to decrease magnitude of positive eigenvalues and increase magnitude of negative eigenvalues of \(L + L_\nu\) (for stability).
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• **Disadvantages of this approach:**
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  2. Calibration is necessary to derive optimal \( L_\nu \) and optimal value is \textit{flow dependent}.
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• \(L_\nu\) is designed to decrease magnitude of positive eigenvalues and increase magnitude of negative eigenvalues of \(L + L_\nu\) (for stability).

• Disadvantages of this approach:
  1. Additional term destroys consistency between ROM and Navier-Stokes equations.
  2. Calibration is necessary to derive optimal \(L_\nu\) 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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Accounting for modal truncation

Proposed new approach

Instead of modeling truncation via additional linear term, model the truncation \textit{a priori} by “rotating” the projection subspace into a more dissipative regime
Accounting for modal truncation

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Instead of modeling truncation via additional linear term, model the truncation \textit{a priori} by “rotating” the projection subspace into a more dissipative regime.

**Illustrative example**

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

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

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

$$
\bar{U}_i = \sum_{j=1}^{n+p} X_{ij} U_j, \quad i = 1, \ldots, n,
$$

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

\begin{equation}
(3)
\end{equation}
Accounting for modal truncation

Goals of proposed new approach

Find $X$ such that:
1. New modes $\tilde{U}$ remain good approximations of the flow.
2. New modes produce stable and accurate ROMs.
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Find $X$ such that:

1. New modes $\tilde{U}$ remain *good approximations* of the flow.
2. New modes produce *stable* and *accurate* ROMs.

• We formulate and solve a *constrained optimization problem* for $X$:

$$\text{minimize}_{X \in \mathcal{V}_{(n+p),n}} f(X)$$

subject to $g(X, L) = 0$

where $\mathcal{V}_{(n+p),n} \in \{X \in \mathbb{R}^{(n+p) \times n}: X^T X = I_n, p > 0\}$ is the *Stiefel manifold*. 
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$$\begin{align*}
\text{minimize} & \quad f(X) \\
\text{subject to} & \quad g(X, L) = 0
\end{align*}$$

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

• Once $X$ is found, the result is a system of the form (2) with:

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

Objective function

\[
\begin{align*}
\text{minimize}_{X \in V_{(n+p),n}} & \quad f(X) \\
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\end{align*}
\]  

(5)

• We have considered two objectives \( f(X) \) in (5):
Accounting for modal truncation

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• We have considered two objectives \( f(X) \) in (5):
  
  • Minimize \textit{subspace rotation}

\[
\begin{align*}
f(X) &= \|X - I_{(n+p),n}\|_F = -\text{tr}(X^T I_{(n+p) \times n})
\end{align*}
\] (6)
Accounting for modal truncation

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\end{align*}
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\[
f(\mathbf{X}) = \| \mathbf{X} - \mathbf{I}_{(n+p),n} \|_F = -\text{tr}(\mathbf{X}^T \mathbf{I}_{(n+p)\times n})
\]

(6)

• Maximize resolved \textit{turbulent kinetic energy (TKE)}

\[
f(\mathbf{X}) = -\| \mathbf{\Sigma} - \mathbf{X} \mathbf{X}^T \mathbf{\Sigma} \|_F
\]

(7)
Accounting for modal truncation

Objective function

\[ \text{minimize}_{X \in V_{(n+p),n}} f(X) \]
\[ \text{subject to } g(X, L) = 0 \]

- We have considered two objectives \( f(X) \) in (5):
  - Minimize \textit{subspace rotation}
    \[ f(X) = \| X - I_{(n+p),n} \|_F = -\text{tr}(X^T I_{(n+p)\times n}) \] (6)
  - Maximize resolved \textit{turbulent kinetic energy (TKE)}
    \[ f(X) = -\| \Sigma - XX^T \Sigma \|_F \] (7)

- 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 \textit{dynamically} even though they contribute little to overall energy of the fluid flow.
Accounting for modal truncation

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• We have considered two objectives \( f(X) \) in (5):

  • Minimize *subspace rotation*

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

(6)

• Maximize resolved *turbulent kinetic energy (TKE)*

\[
f(X) = -\|\Sigma - XX^T \Sigma\|_F
\]

(7)

• Numerical experiments reveal objective (6) produces better results than objective (7) for compressible flow.
Accounting for modal truncation

Constraint

\[
\begin{align*}
\text{minimize}_{X \in \mathcal{V}_{(n+p),n}} & \quad f(X) \\
\text{subject to} & \quad g(X, L) = 0
\end{align*}
\]  

(5)

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

\[
g(X, L) = \text{tr}(X^T LX) - \eta
\]  

(8)
Accounting for modal truncation

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- Specifically, constraint (8) involves overall balance between \textit{linear energy production} and \textit{dissipation}.
  - \(\eta\) = 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* \( (= \text{tr}(X^T LX) + \text{energy transfer}) \) has to vanish.
Accounting for modal truncation

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

\[
\begin{align*}
\text{minimize } & \quad x \in \mathcal{V}_{(n+p),n} - \text{tr}(X^T I_{(n+p)\times n}) \\
\text{subject to } & \quad \text{tr}(X^T LX) = \eta
\end{align*}
\]  

(9)

- \( \eta \in \mathbb{R} \): proxy for the balance between linear energy production and energy dissipation (calculated iteratively using modal energy).

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

- Equation (9) is solved efficiently offline using the method of Lagrange multipliers (*Manopt MATLAB* toolbox).

- See (Balajewicz, Tezaur, Dowell, 2016) and Appendix slide for Algorithm.
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  2. Stability cannot be proven like for incompressible case.
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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° \( \Rightarrow n = 4 \) 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:**

\[
f(X) = \left\| X - I_{(n+p),n} \right\|_F = -\text{tr}(X^TI_{(n+p)\times n})
\]

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:

\[
\frac{\left\| X - I_{(n+p),n} \right\|_F}{n} = 0.083, \quad X \approx I_{(n+p),n}
\]
Applications

High angle of attack laminar airfoil

- **Minimizing subspace rotation:**

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

**Figure 3:** High angle of attack laminar airfoil contours of velocity magnitude at time of final snapshot.
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
   - **Low Reynolds number channel driven cavity**
   - Moderate Reynolds number channel driven cavity
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Channel driven cavity: low Reynolds number case

Flow over square cavity at Mach 0.6, Re = 1453.9, Pr = 0.72
⇒ 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**:

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

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: 
\[
\frac{\|X - I_{(n+p),n}\|_F}{n} = 0.188, \ X \approx I_{(n+p),n}
\]
Applications

Channel driven cavity: low Reynolds number case

- Minimizing subspace rotation:

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

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

Channel driven cavity: low Reynolds number case

- Maximizing resolved TKE:

\[ f(X) = -||\Sigma - XX^T\Sigma||_F \]

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

Channel driven cavity: low Reynolds number case

- *Minimizing subspace rotation:*

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

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

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

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

Channel driven cavity: moderate Reynolds number case

- **Minimizing subspace rotation:**

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

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

Channel driven cavity: moderate Reynolds number case

- *Minimizing subspace rotation:*

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

Figure 11: Pressure cross PSD of \(p(x_1, t)\) and \(p(x_2, t)\) where \(x_1 = (2, -0.5)\), \(x_2 = (0, -0.5)\)

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

<table>
<thead>
<tr>
<th>Procedure</th>
<th>Airfoil</th>
<th>Low Re Cavity</th>
<th>Moderate Re Cavity</th>
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</thead>
<tbody>
<tr>
<td>FOM # of DOF</td>
<td>360,000</td>
<td>288,250</td>
<td>243,750</td>
</tr>
<tr>
<td>Time-integration of FOM</td>
<td>7.8 hrs</td>
<td>72 hrs</td>
<td>179 hrs</td>
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<tr>
<td>Basis construction (size (n + p) ROM)</td>
<td>0.16 hrs</td>
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<tr>
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<tr>
<td>Stabilization</td>
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<td>14 sec</td>
<td>170 sec</td>
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<tr>
<td>ROM # of DOF</td>
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* For minimizing subspace rotation.
Applications

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- Stabilization is *fast* ($O$(sec) or $O$(min)).

* For minimizing subspace rotation.
Applications

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- Stabilization is **fast** ($O(\text{sec})$ or $O(\text{min})$).
- Significant **online computational speed-up**!

* For minimizing subspace rotation.
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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:

\[
\begin{align*}
\text{minimize} & \quad \mathbf{X} \in V_{(n+p),n} \quad f(\mathbf{X}) \\
\text{subject to} & \quad g(\mathbf{X}, \mathbf{L}) = 0
\end{align*}
\]
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 $X$.

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

Solve constrained optimization problem on Stiefel manifold:

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

Construct new Galerkin matrices using (4).
Integrate numerically new Galerkin system.
Calculate “modal energy” $E(t)^{(k)} = \sum_i \eta_i (a(t_i)^{(k)})^2$.
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 $||c_1^{(k)}|| < TOL$

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

terminate the algorithm.

end