Reduced-Order Models of Fluids

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Overview

POD  Sensitivity Analysis

Collaborators

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Objective:

Replace current “well mixed,” “node” models with reduced-order models to facilitate analysis, optimization and/or control.

Models may include parameters, such as

- model coefficients
- initial conditions
- boundary conditions
- shape

Need to work for moderately turbulent flows. (Zhu Wang’s talk)

Need to improve accuracy of models over parameter ranges.
Outline

- Review of POD/Galerkin
- Alternate Basis Selection Methods
- Sensitivity analysis
  - to generate bases at new parameter values
Proper Orthogonal Decomposition

Given data $y(\cdot, t) \in \mathcal{H}$ and $t \in [0, T]$, find $\phi(\cdot) \in \mathcal{H}$ such that

$$\phi(\cdot) \text{ solves } \max_{\|\hat{\phi}\|=1} \frac{1}{T} \int_0^T |\langle y(\cdot, t), \hat{\phi}(\cdot) \rangle|^2 dt.$$ 

Necessary Conditions ($L^2$)

Let $R^s(x, \bar{x}) \equiv \frac{1}{T} \int_0^T y(x, t)y^*(\bar{x}, t) \, dt$ then $\phi(\cdot)$ is a solution to the eigenvalue problem

$$\int_{\Omega} R^s(x, \bar{x}) \phi(\bar{x}) \, d\bar{x} = \lambda \phi(x).$$
Proper Orthogonal Decomposition

Given data \( y(\cdot, t) \in \mathcal{H} \) and \( t \in [0, T] \), find \( \phi(\cdot) \in \mathcal{H} \) such that

\[
\phi(\cdot) \text{ solves } \max_{\|\hat{\phi}\|=1} \frac{1}{T} \int_{0}^{T} \left| \langle y(\cdot, t), \hat{\phi}(\cdot) \rangle \right|^2 \, dt.
\]

Necessary Conditions (\( L^2 \))

Let \( R^s(x, \bar{x}) \equiv \frac{1}{T} \int_{0}^{T} y(x, t)y^*(\bar{x}, t) \, dt \) then \( \phi(\cdot) \) is a solution to the eigenvalue problem

\[
\int_{\Omega} R^s(x, \bar{x})\phi(\bar{x}) \, d\bar{x} = \lambda \phi(x).
\]
Keep dominant $r$ vectors using heuristic.
The POD basis maintains linear properties.

Define

$$\mathbf{u}'(x, t) = \mathbf{U}(x) + \sum_{j=1}^{r} \phi_j(x) a_j(t).$$

Substitute into the weak form of the partial differential equations to obtain $r$-dimensional dynamical system for $\mathbf{a}$. 
Example: Navier-Stokes Equations

\[
\begin{align*}
    \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \nabla \cdot \left[ \nu \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right] \\
    \nabla \cdot \mathbf{u} &= 0
\end{align*}
\]

Reduced-Order Model

\[ \dot{\mathbf{a}} = \mathbf{b} + \mathbf{Aa} + \mathbf{a}^T \mathbf{B} \mathbf{a} \]

where \( \mathbf{B} \) is a tensor and \( a_i(0) = \langle \mathbf{u}(0, \cdot) - \mathbf{U}(\cdot), \phi_i(\cdot) \rangle, \quad i = 1, \ldots, r \).

Integrate to find \( \mathbf{a} \), then reconstruct \( \mathbf{u}^r \).

Flow past a square cylinder, \( Re = 100 \quad (\nu = 1/100) \ldots \)
Flow Past a Square Cylinder
Figure: POD functions: Steamwise Component

(a) $\phi^u_1$

(b) $\phi^u_2$

(c) $\phi^u_3$

(d) $\phi^u_4$
Figure: First 20 values of the POD spectrum for the baseline flow.
POD Accuracy

Figure: Accuracy of the ROM for the Baseline Flow, $Re = 100$
Limitations of the Basis

(a) $\text{Re} = 99.50 \ (0.5\%)$
(b) $\text{Re} = 95.24 \ (5\%)$
(c) $\text{Re} = 90.91 \ (10\%)$

Figure: Relative errors in reduced-order models using POD basis
Limitations of POD/Galerkin

Accuracy of the Basis
Basis is only as good as the data it is constructed from.
- optimization
- selection of time intervals
- parametric derivatives of the data

Accounting for Discarded Modes
Especially important for turbulent flows
- add stabilization terms
- use LES closure models to close the POD model
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"Definition" of Sensitivity Analysis

Quantify the dependence of parameters on flow variables using the Implicit Function Theorem

Let

\[ s_u \equiv \frac{\partial u}{\partial \nu} \quad \text{and} \quad s_p \equiv \frac{\partial p}{\partial \nu}. \]

\[
\dot{s}_u + s_u \cdot \nabla u + u \cdot \nabla s_u = -\nabla s_p + \nabla \cdot \left[ \nu \left( \nabla s + \nabla s^T \right) \right] + \nabla \cdot \left[ \nu' \left( \nabla u + \nabla u^T \right) \right] 
\]

\[ \nabla \cdot s_u = 0 \]

with \( s(x, 0) = 0, \ s(\cdot, t)|_{\Gamma_w} = 0 \) and \( \tau(s) \cdot \hat{n} = 0 \) at \( \Gamma_{\text{out}} \).
Sensitivity of the POD Basis

POD Eigenvalue Problem

\[ \int_{\Omega} R^s(x, \bar{x}) \phi(\bar{x}) \, d\bar{x} = \lambda \phi(x) \]

Solve for pairs \( \lambda \) and \( \phi(\cdot) \).

Implicit differentiation wrt \( \nu \)

\[ \int_{\Omega} R^s_{\nu}(x, \bar{x}) \phi(\bar{x}) + R^s(x, \bar{x}) \phi_{\nu}(\bar{x}) \, d\bar{x} = \lambda_{\nu} \phi(x) + \lambda \phi_{\nu}(x) \]

Solve for pairs \( \lambda_{\nu} \) and \( \phi_{\nu}(\cdot) \).
Sensitivity of the POD Basis

POD Eigenvalue Problem

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Solve for pairs \( \lambda \) and \( \phi(\cdot) \).

Implicit differentiation wrt \( \nu \)

\[ \int_\Omega R^s_{\nu}(x, \bar{x}) \phi(\bar{x}) + R^s(x, \bar{x}) \phi_{\nu}(\bar{x}) \, d\bar{x} = \lambda_{\nu} \phi(x) + \lambda \phi_{\nu}(x) \]

Solve for pairs \( \lambda_{\nu} \) and \( \phi_{\nu}(\cdot) \).
Solution by finite element discretization

\[ R^S_\nu \phi + R^S \phi_\nu = \lambda_\nu M \phi + \lambda M \phi_\nu \]

Solution

\[ \lambda_\nu = \frac{\phi^T R^S_\nu \phi}{\phi^T M \phi} = \phi^T R^S_\nu \phi \]

and

\[ (R^S - \lambda M) \phi_\nu = - (R^S_\nu - \lambda_\nu M) \phi \]

\[ R^S_\nu = M \left( Y_\nu Y^T + YY^T \right) M. \]
Extrapolated Basis

Idea

Use

$$\phi^i(x; \nu + \Delta \nu) \approx \phi^i(x; \nu) + \Delta \nu \phi^i_{\nu}(x; \nu)$$

as a basis for the flow at $\nu \equiv \nu + \Delta \nu$.

$$u^r(x, t; \nu) \approx U + \Delta \nu U_{\nu} + \sum_{j=1}^{r} \left( \phi^j(x; \nu) + \Delta \nu \phi^j_{\nu}(x; \nu) \right) a^j(t).$$
Since
\[ u^r(x, t; \nu) = \sum_{j=1}^{r} \phi_j(x; \nu) a_j(t) \]
we have
\[ u^r_{\nu}(x, t; \nu) = \sum_{j=1}^{r} \left( \phi_j(x; \nu) a_j(t) + \phi_j(x; \nu) a_j(\nu)(t) \right). \]

Idea
\[ u^r(x, t; \tilde{\nu}) \approx \sum_{j=1}^{r} \phi_j a_j + \Delta \nu \left[ \sum_{j=1}^{r} \phi_j a_j + \phi_j a_j(\nu) \right] \]
\[ = \sum_{j=1}^{r} \left[ \phi_j + \Delta \nu \phi_j \right] a_j + \Delta \nu \sum_{j=1}^{r} \left[ \phi_j \right] a_j(\nu) \]

Use both \( \phi_j \) and \( \phi_j \nu \) (and add \( U + \Delta \nu U_\nu \)).
Example: Navier-Stokes, $Re = 100$

(a) $\phi^1_{\nu}$

(b) $\phi^2_{\nu}$

(c) $\phi^3_{\nu}$

(d) $\phi^4_{\nu}$
Sensitivity of the POD Basis (not in the POD)

(a) $\phi_1^{\nu}$

(b) $\phi_2^{\nu}$

(c) $\phi_3^{\nu}$

(d) $\phi_4^{\nu}$
Relative errors in Reduced-Order Models

Figure: \[ \frac{\Delta v}{v_0} = 0.5\% \text{ (Re} = 99.50) \]
Relative errors in Reduced-Order Models

Figure: \[ \frac{\Delta \nu}{\nu_0} = 5\% \text{ (Re} = 95.24) \]
Relative errors in Reduced-Order Models

\[ \frac{\Delta \nu}{\nu_0} = 10\% \ (\text{Re} = 90.91) \]

Figure: [\( \frac{\Delta \nu}{\nu_0} = 10\% \ (\text{Re} = 90.91) \)]
Strouhal Number versus Reynolds Number

![Graph showing Strouhal Number versus Reynolds Number with lines and markers for different models: DNS, DNS-1st order from baseline, ROM - baseline POD, ROM - extrapolated POD, ROM - expanded POD.](image_url)
Comparison of Model Components to DNS Data (dashed)
$Re = 111$: Expanded Basis Model

Comparison of Model Components to DNS Data (dashed)
Re = 150: Baseline Model

Comparison of Model Components to DNS Data (dashed)
Comparison of Model Components to DNS Data (dashed)
Vertical Velocity Max/Min at Downstream Point
In the POD Sensitivity Problem...

\[ R_s^\ell \phi + R^S \phi_\ell = \lambda_\ell M \phi + \lambda M_\ell \phi + \lambda M \phi_\ell \]

Solve for pairs \( \lambda_\ell \) and \( \phi_\ell(\cdot) \).

We now need Lagrangian derivatives.
Lagrangian Derivatives

Figure: Mapping from the physical domain to the reference domain

\[ \chi^\alpha : \Omega_\alpha \longrightarrow \Omega_0 \]
\[ x(\alpha) \longmapsto \chi^\alpha(x(\alpha); \alpha) = \xi. \]

\[ G^\alpha : \Omega_0 \longrightarrow \Omega_\alpha \]
\[ \xi \longmapsto G^\alpha(\xi; \alpha) = x(\alpha). \]
Rotation of Cylinder
Mesh Warping

Figure: Nominal Mesh: $\alpha = 0^\circ$

Figure: $\alpha = -22.5^\circ$
Mesh Warping

Figure: Nominal Mesh: $\alpha = 0^\circ$

Figure: $\alpha = 22.5^\circ$
POD Spectra

\[ \lambda_q \]

\[ 10^4 \]

\[ 10^2 \]

\[ 10^0 \]

\[ 10^{-2} \]

\[ 10^{-4} \]

\[ 10^{-6} \]

\[ 10^{-8} \]

\[ q \]

\[ \alpha = 22.5 \text{ deg.} \]

\[ \alpha = 0 \text{ deg.} \]

\[ \alpha = -22.5 \text{ deg.} \]
POD Basis Functions

(a) Streamwise component of $\phi_1$
(b) Normal component of $\phi_1$
(c) Streamwise component of $\phi_2$
(d) Normal component of $\phi_2$
POD Basis Sensitivity Functions

(a) Streamwise component of $\phi_1^*$
(b) Normal component of $\phi_1^*$
(c) Streamwise component of $\phi_2^*$
(d) Normal component of $\phi_2^*$
Error in ROM

(a) Projection on the perturbed data for $q = 6$

(b) ROM for $q = 6$
Error in ROM

(c) Projection on the perturbed data for $q = 12$

(d) ROM for $q = 12$
Boussinesq CFD: $Re = 4.9 \times 10^4$, $Gr = 7.4 \times 10^7$
Boussinesq ROM: \( \mathbf{u} \) Modes

First two velocity modes
First two temperature modes
a Coefficient Phase Portraits
b Coefficient Phase Portraits

Graphs showing the phase portraits of coefficients $b_2$, $b_3$, $b_4$, and $b_2$.
Boussinesq ROM: $Re = 6800, Gr = 10^7$

DNS

POD

Mixing Length
Work in Progress

- Hermite interpolation
- Boundary conditions
- Other strategies for using sensitivity information
- Application to methods other than POD
- Coupling multiple room models


