Covariance balancing model reduction

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ICERM: Computational Learning for Model Reduction

PRINCETON UNIVERSITY

Projection methods

Start with a "full-order model"

$$\dot{x} = f(x, u)$$
$$y = g(x, u)$$

where $x \in \mathbb{R}^n$ is the state, u is an input, and y is an output.

Consider two r-dimensional subspaces of $\mathbb{R}^n$:

- Trial subspace $\mathcal{V} = \text{Range}(V)$
- Test subspace $\mathcal{W} = \text{Range}(W)$, $W^T V = I_r$

Reduced-order model (Petrov-Galerkin):

$$\dot{z} = W^T f(Vz, u)$$
$$y = g(Vz, u)$$

where $x = Vz$, $z \in \mathbb{R}^r$.

Reduced-order model

Reduced-order model is

$$\dot{z} = W^T f(Vz, u)$$
$$y = g(Vz, u)$$

Question: How should we choose V, W?

Can we do better than PCA?

Outline

Balanced truncation for linear systems

Covariance balancing reduction for nonlinear systems

Trajectory-based optimization of subspaces

Examples

Extensions using operator inference

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Overview of balanced truncation

- Consider a linear system with state x, a control input u and output y:

$$\dot{x} = Ax + Bu$$
$$y = Cx$$

- We wish to determine a model with approximately the same input-output behavior, but smaller state dimension.
- Balanced truncation[1] is an excellent method for this
  - A priori error bound, close to the smallest possible
  - Computationally tractable, even for high-dimensional systems[2]

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[1] BC Moore, IEEE Trans. Automat. Control, 1981

[2] Antoulas, 2005; Rowley, IJBC, 2005

ODE example

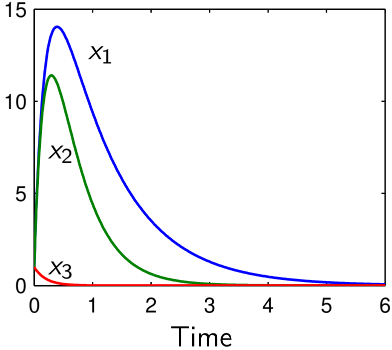
Consider the following ODE

$$\begin{aligned}
\dot{x}_1 &= -x_1 + 100x_3 + u \\
\dot{x}_2 &= -2x_2 + 100x_3 + u \\
\dot{x}_3 &= -5x_3 + u \\
y &= x_1 + x_2 + x_3
\end{aligned}$$

- u is the "input" (forcing term)
- y is the "output" (what we wish to capture with our model)
- Is there a 2-state model with nearly the same input-output behavior?

ODE response to an impulse

Consider the response to an impulsive input $u(t) = \delta(t)$
We're interested in modeling $y = x_1 + x_2 + x_3$



The state x_3 decays quickly, so we might think we can neglect it in a reduced-order model.

Naive reduced-order model

If we set $x_3 = 0$, the model becomes

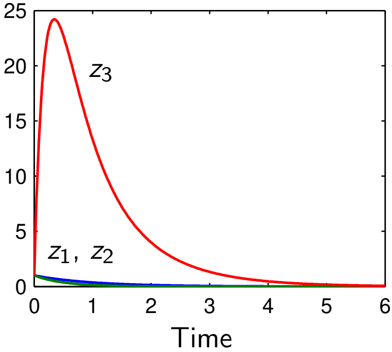
$$\begin{aligned}\dot{x}_1 &= -x_1 + u \\ \dot{x}_2 &= -2x_2 + u \\ y &= x_1 + x_2\end{aligned}$$

The impulse response decays monotonically (no transient growth)!
Clearly not a good model. What went wrong?

Look at sensitivity: adjoint system

The sensitivity of the output $y(t)$ to perturbations in the initial states are given by solving an adjoint system:

$$D_{x(0)}y(t) = (z_1(t), z_2(t), z_3(t))$$



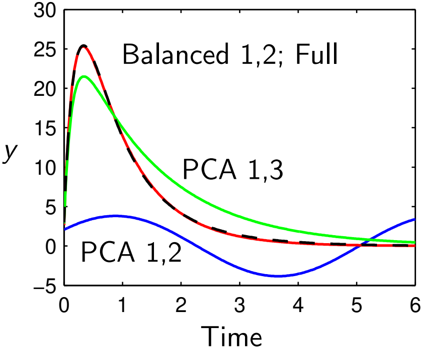
- The output is much more sensitive to perturbations in x_3 than to x_1 and x_2.
- But we neglected x_3 because it had small energy.

Balanced truncation

- Balanced truncation incorporates this sensitivity in an elegant and natural way.

Results for the ODE example

Impulse response for the projection onto two states:



- The first two PCA modes contain 99.97% of the energy, but projection onto these modes gives a poor model.
- Balanced truncation to two states matches the full model nearly perfectly.

What is balanced truncation doing?

- Most controllable states are those that are most easily excited by the input u.
  Quantified by a symmetric positive-definite matrix W_c:

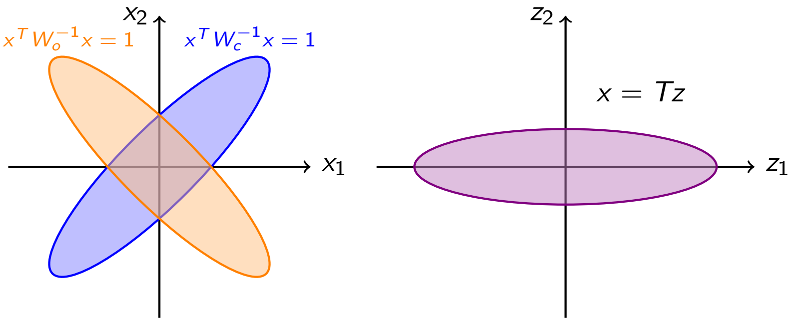
$$\text{Controllability}(x) = x^T W_c x$$

- Most observable states are those that excite the largest future outputs (with no input, $u = 0$).
  Quantified by a symmetric positive-definite matrix W_o:

$$\text{Observability}(x) = x^T W_o x$$

- Theorem: there is a change of coordinates in which W_c and W_o are equal and diagonal (under mild assumptions).
- Balanced truncation: change to these coordinates, and truncate the states that are least controllable/observable.

Geometric picture



An error bound

- Factor the controllability and observability matrices as

$$W_c = XX^T, \qquad W_o = YY^T$$

- Can prove that the error[3] between the full model and the reduced-order model with r states has a bound:

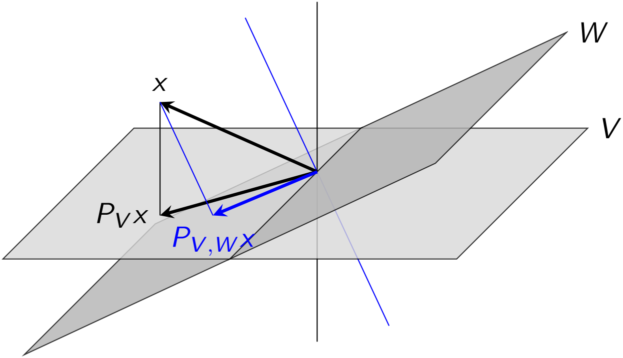
$$\text{Error} \leq 2(\sigma_{r+1} + \cdots + \sigma_n),$$

where σ_k are the singular values of $Y^T X$.

[3] in the operator norm induced by the 2-norm on signals

Balanced truncation as a projection of dynamics

- For a linear system, balanced truncation determines two subspaces, V and W



Summary of balanced truncation

- Effectively balances energy and sensitivity, and gives reduced-order models that are provably close to optimal
- Often significantly outperforms PCA, especially for "non-normal" systems with large transient energy growth
- Computationally tractable, even for high-dimensional systems
- Applies only to linear systems

Outline

Acknowledgements

Graduate students

- Sam Otto (Asst. Prof., Cornell)
- Alberto Padovan (Postdoc, UIUC)

Balancing for nonlinear systems

- We would like to find reduced-order models of a nonlinear system

$$x(t+1) = f(x(t), u(t))$$
$$y(t) = g(x(t))$$

- For linear systems, there are good methods (e.g., balanced truncation, H_2 optimal reduction)
- For nonlinear systems, the situation is much worse: available methods are
  - computationally intractable for high-dimensional systems
  - valid only in the neighborhood of an equilibrium point

Which coordinates should be retained?

- For now, we ignore the input:

$$
\begin{aligned}
x(t+1) &= f(x(t)) \\
y(t) &= g(x(t))
\end{aligned}
$$

- Consider a map from the current state x_0 to future outputs y, defined by

$$F(x_0) = (y(0), \ldots, y(L))$$

- A good set of coordinates $z = W^T x$ will allow us to approximate

$$F(x_0) \approx \tilde{F}(z_0)$$

Coordinates from projections

- Suppose V, W are $n \times r$ matrices such that $W^T V = I$. We have the decomposition

$$x = Vz + x_2, \qquad z = W^T x$$

- Given z, the optimal estimate for $F(x)$ (in the mean-square sense) is given by averaging over x_2:

$$\tilde{F}(z) = \mathbb{E}\big[F(Vz + x_2)\big]$$

- For a good estimate, want two things:
  - x_2 should have small variance
  - F should not be sensitive to variations in x_2.

Quantifying variance and sensitivity

- Variance is quantified using the state covariance

$$W_x = \mathbb{E}[xx^T].$$

- Sensitivity of F is quantified using the gradient covariance

$$W_g = \mathbb{E}\big[\nabla F(x) \nabla F(x)^T\big], \qquad \nabla F(x) = DF(x)^T$$

- Idea: change to coordinates in which W_x and W_g are equal and diagonal, and then truncate directions in which there is least variance and sensitivity.
- Observation: this is just like balanced truncation, with the covariance matrices W_x and W_g playing the role of controllability and observability.

Determining the optimal projection

- The covariance matrix W_x is easy to approximate by sampling
- The gradient covariance matrix W_g may be approximated by sampling an adjoint system
- Given these samples, the rank-r projection that balances these matrices is easily computed using singular value decomposition

We call this method Covariance Balancing Reduction using Adjoint Snapshots (CoBRAS) [4]

[4] SE Otto, A Padovan, and CW Rowley, SIAM J Scientific Computing, 45(5):A2325–A2355, 2023

An error bound

- Factor the covariance matrices as $W_x = XX^T$, $W_g = YY^T$
- Can prove that when x has Gaussian distribution,

$$\mathbb{E}\left[\|F(x) - \tilde{F}(Px)\|^2\right] \leq \sigma_{r+1}^2 + \cdots + \sigma_n^2,$$

where σ_k are the singular values of $Y^T X$.

Kernel method

- There is also a generalization of this to nonlinear projections, using a kernel method
- Lift the state and gradient vectors into a reproducing kernel Hilbert space (RKHS)
- Compute inner products implicitly via the kernel
- This allows us to extract rich nonlinear features from the system

Outline

Optimizing subspaces

- We can determine an even better choice of subspaces for projection by an iterative optimization

Trajectory-based optimization

- Consider observations $\{y_0, \dots, y_{L-1}\}$ along a trajectory from the full model.
- For given subspaces V and W, compute the corresponding observations $\{\hat{y}_0, \dots, \hat{y}_{L-1}\}$ from the reduced-order model.
- Let $L_y : \mathbb{R}^{\dim y} \to [0, \infty)$ be a smooth loss function for the predicted system outputs. We'd like to minimize

$$J(V, W) = \frac{1}{L} \sum_{l=0}^{L-1} L_y(\hat{y}_l - y_l).$$

- But we need to ensure that the subspace pairs (V, W) satisfy the non-orthogonality condition, so we introduce a regularization $\rho(V, W)$ that enforces this constraint, and define the objective

$$\boxed{J(V, W) = \frac{1}{L} \sum_{l=0}^{L-1} L_y(\hat{y}_l - y_l) + \gamma \rho(V, W).}$$

The overall method

We call this method Trajectory-based Optimization for Oblique Projection (TrOOP)

Solution of the optimization problem

- One optimizes over a manifold (two copies of the Grassmann manifold) using a geometric conjugate gradient algorithm [5] [6]
- The gradient is computed using an adjoint sensitivity method.
- This entails solving a linear ODE with the same dimension as the reduced-order model backwards in time.

[5] Absil et al., "Optimization Algorithms on Matrix Manifolds", 2008

[6] H. Sato, "A Dai–Yuan-type Riemannian conjugate gradient method with the weak Wolfe conditions", 2016

Outline

Two methods

We've described two different methods:

- Covariance Balanced Reduction using Adjoint Snapshots (CoBRAS)
- Trajectory-based Optimization for Oblique Projection (TrOOP)

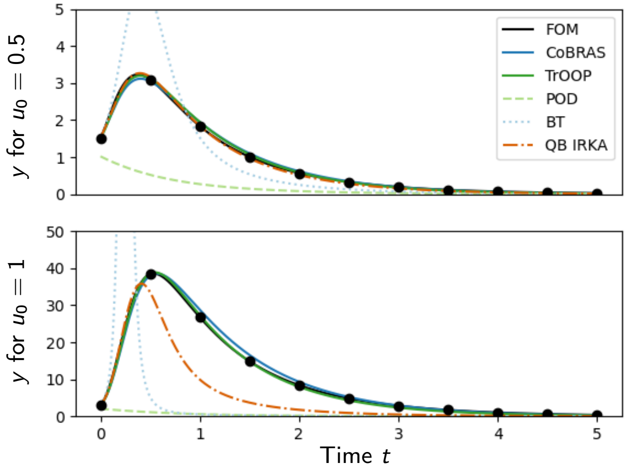
In practice, we can use CoBRAS to provide an initial guess for the optimization problem in TrOOP.

A challenging model problem

$$
\begin{aligned}
\dot{x}_1 &= -x_1 + 20x_1x_3 + u \\
\dot{x}_2 &= -2x_2 + 20x_2x_3 + u \\
\dot{x}_3 &= -5x_3 + u \\
y &= x_1 + x_2 + x_3,
\end{aligned}
$$

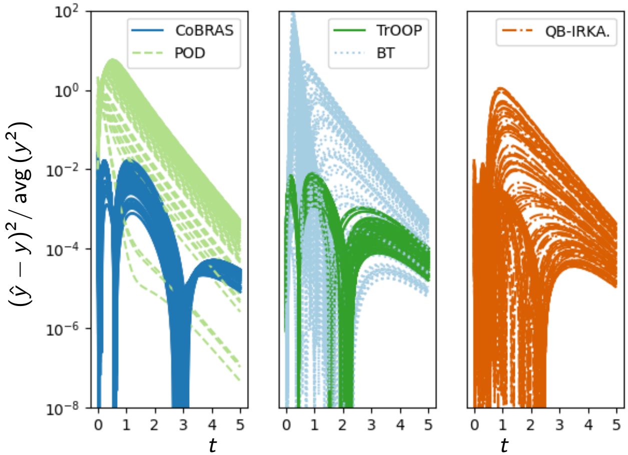
- The state x_3 is dynamically important, but remains small compared with x_1 and x_2 due to its fast decay rate.
- The linearized dynamics do not capture the system's behavior away from the origin, which exhibits transient growth.
- We seek 2-dimensional reduced-order models.

Training trajectories



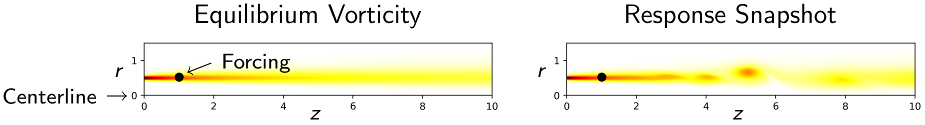
The training data consists of 22 sample points (black dots), from trajectories with impulsive inputs $u(t) = u_0\delta(t)$, with $u_0 = 0.5$ and 1.0.

Testing performance



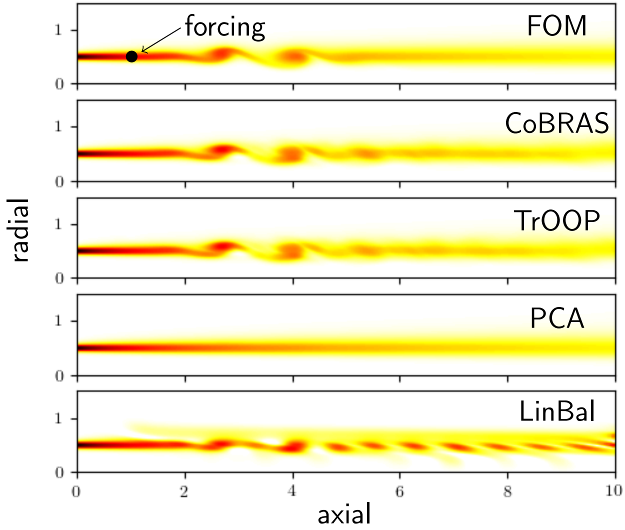
We tested our optimized Petrov-Galerkin model on 100 nonlinear impulse response trajectories with magnitudes drawn uniformly at random from the interval $[0, 1]$.

Axisymmetric jet flow example

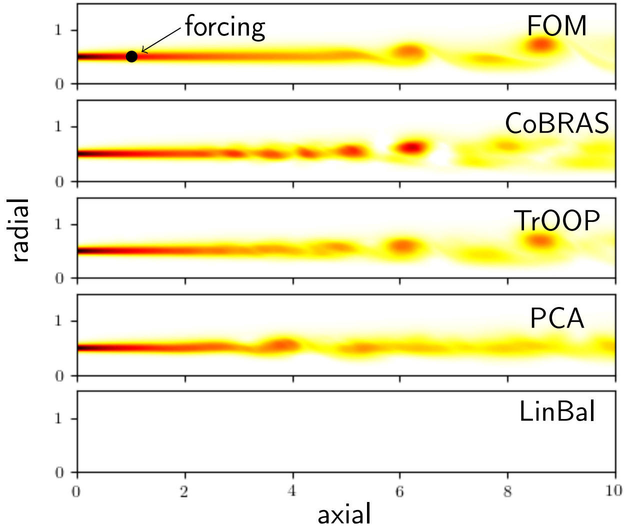


- Incompressible, axisymmetric jet flow
- Reynolds number 1000
- Full model: 100,000 states
- Actuation: body force in radial direction
- We seek 40-dimensional reduced order models capable of predicting the impulse response of the flow for a range of impulse amplitudes

Vorticity predictions for jet flow, $t = 5$

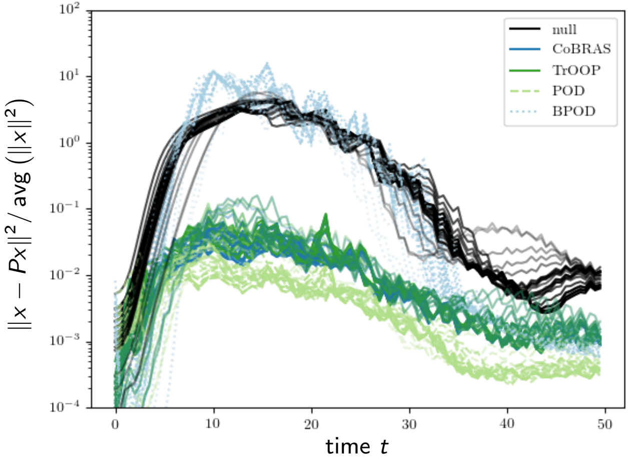


Vorticity predictions for jet flow, $t = 20$



Projection error

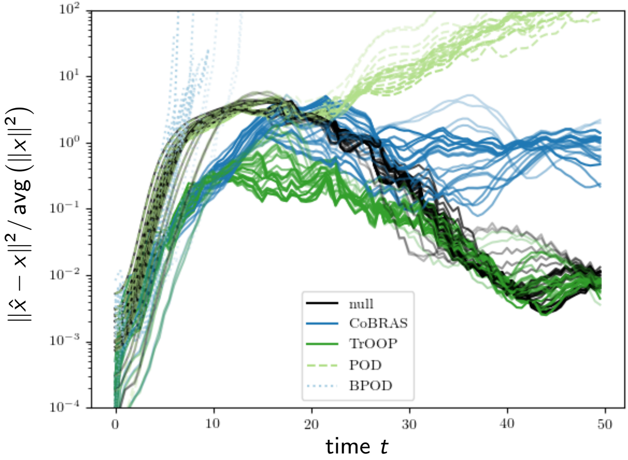
Project each testing trajectory onto 40-dimensional subspace.
The "null" projection means $Px = 0$.



PCA has the best projection error (as it must)

Forecasting error

Now, consider forecasting using the reduced-order model



CoBRAS and TrOOP both significantly outperform other methods, and PCA is no better than the "null" model.

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Extensions using operator inference

Drawbacks

- Some drawbacks of these approaches:
  - They are intrusive: require knowledge of the full model
  - The require adjoint simulations, which may not be available

Recent work by Alberto Padovan addresses both of these, using operator inference.

Leveraging operator inference

An exciting recent paper (arXiv:2401.01290):

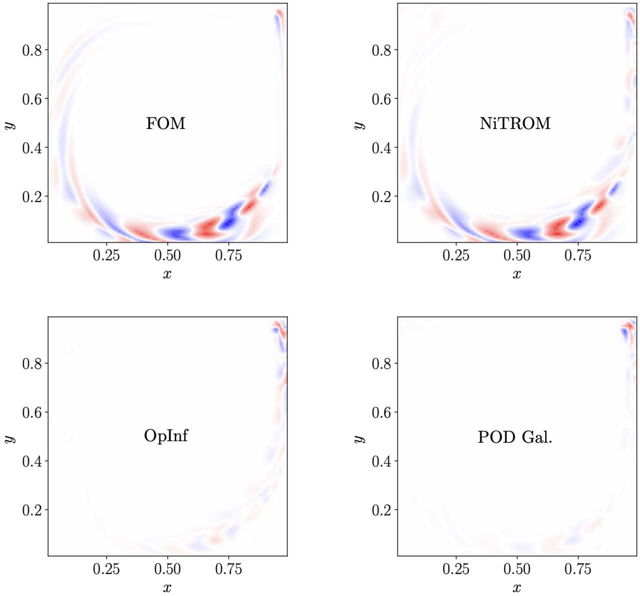
Data-driven model reduction via non-intrusive optimization of projection operators and reduced-order dynamics

Alberto Padovan*, Blaine Vollmer*, and Daniel J. Bodony*

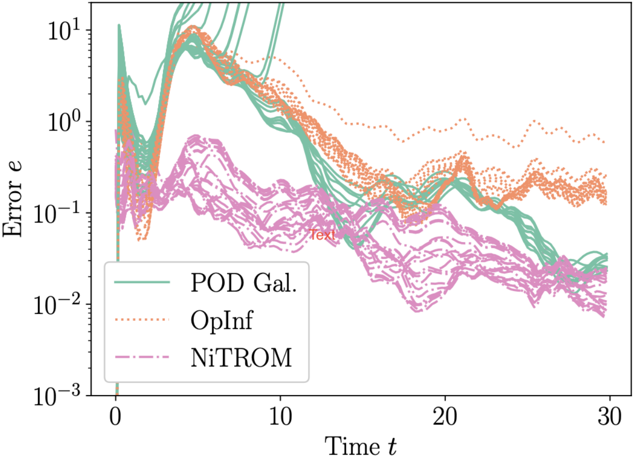
Abstract. Computing reduced-order models using non-intrusive methods is particularly attractive for systems that are simulated using black-box solvers. However, obtaining accurate data-driven models can be challenging, especially if the underlying systems exhibit large-amplitude transient growth. Although these systems may evolve near a low-dimensional subspace that can be easily identified using standard techniques such as Proper Orthogonal Decomposition (POD), computing accurate models often requires projecting the state onto this subspace via a non-orthogonal projection. While appropriate oblique projection operators can be computed using intrusive techniques that leverage the form of the underlying governing equations, purely data-driven methods currently tend to achieve dimensionality reduction via orthogonal projections, and this can lead to models with poor predictive accuracy. In this paper, we address this issue by introducing a non-intrusive framework designed to simultaneously identify oblique projection operators and reduced-order dynamics. In

- Idea:
  - Guess subspaces for projection
  - Determine an approximate model using operator inference
  - Use the adjoint of the inferred model to compute gradients needed for gradient descent
  - Update subspaces and iterate

Example: lid-driven cavity flow



Training error for lid-driven cavity flow



Takeaways

- PCA often does not give the best subspaces for reduced-order models
- Can generalize balanced truncation to nonlinear systems by balancing state covariance and gradient covariance
- Gradient covariance matrices computed efficiently from adjoint simulations
- Iterative method for further refining these subspaces, using loss function based on trajectories
- These methods are intrusive (require knowledge of the full dynamics)
- However, they play very nicely with non-intrusive methods (Operator Inference)

Acknowledgements and papers

- Alberto Padovan (Postdoc, UIUC)
- Sam Otto (Asst. Prof, Cornell)
- Funding from Air Force Office of Scientific Research

- Papers
  - Covariance balancing: SE Otto, A Padovan, and CW Rowley, SIAM J Scientific Computing, 45(5):A2325–A2355, 2023
  - Trajectory-based optimization: SE Otto, A Padovan and CW Rowley, SIAM J Scientific Computing 44(3):A1681–A1702, 2022.