Robust Reduced Order Modeling for Complex Multi-scale Problems

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Multilevel Autoencoder networks

J Xu, K Duraisamy  
Multi-level convolutional autoencoder networks for parametric prediction of spatio-temporal dynamics  
Computer Methods in Applied Mechanics and Engineering 372, 2019
Math + physics + structure for Learning

\[ \frac{1}{M} \sum_{i=1}^{M} \| \Psi(\Phi(x_i)) - x_i \|^2 \]

\[ \Phi(x) = \Phi_{dmd}(x) + \Phi_{nn}(x), \]
\[ \Psi(\Phi) = \Psi_{dmd}(\Phi(x)) + \Psi_{nn}(\Phi(x)) \]

Power of linear embedding

\[ \hat{x}_{j+1} = W_0 x_j + W_1 x_{j-1} + \ldots + W_L x_{j-L}, \]

On the Structure of Time-delay Embedding in Linear Models of Non-linear Dynamical Systems
Pan & Duraisamy, Chaos 2020
Metrics for Reduced order models

• Accuracy
• Robustness
• Realizability
• ‘True’ Predictivity*
• Efficiency*
• Time & complexity of development*
• Portability*
• Data requirements
  ➔ Type of data
  ➔ Amount of data

* Non-intrusive ROMs clearly win here

* Adaptive intrusive ROMs
A few things to take home

Stabilization

Limitations of static bases

Adaptivity

Multi-component ROMs

Non-intrusive ROMs

Introduction
- SP-LSVT ROMs
  - Formulation
  - Results
- Adaptive Basis
  - Formulation
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- ROM Networks
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- Non-Intrusive ROMs
  - Formulation
  - Results
- Summary
Let's define a test basis $\mathbf{W}$ and project the equation onto the test subspace,

$$\mathbf{q} = \mathbf{V}q_r + \mathbf{V}^\perp q_p.$$ 

Let's define a test basis $\mathbf{W}$ and project the equation onto the test subspace,

$$\mathbf{W}^T \mathbf{q}_r(0) = \mathbf{W}^T \mathbf{q}_0.$$ 

$$\frac{d\mathbf{q}_r(t)}{dt} = \left[\mathbf{W}^T \mathbf{V}\right]^{-1}\mathbf{W}^T \mathbf{f}(\mathbf{V}q_r(t), t), \quad \mathbf{q}_r(0) = \left[\mathbf{W}^T \mathbf{V}\right]^{-1}\mathbf{W}^T \mathbf{q}_0.$$ 

$$\frac{d\tilde{\mathbf{q}}(t)}{dt} = \mathbf{V}[\mathbf{W}^T \mathbf{V}]^{-1}\mathbf{W}^T \mathbf{f}(\tilde{\mathbf{q}}(t), t), \quad \tilde{\mathbf{q}}(0) = \mathbf{V}[\mathbf{W}^T \mathbf{V}]^{-1}\mathbf{W}^T \mathbf{q}_0.$$
Galerkin ROMs

Full Order Model
\[
\frac{d\mathbf{q}}{dt} = \mathbf{f}(\mathbf{q}, t), \quad \mathbf{q}(0) = \mathbf{q}_0, \quad \mathbf{q} : [0, T] \rightarrow \mathbb{R}^N
\]

define a trial basis \( \mathbf{V} \in \mathbb{R}^{n \times k} \) that spans a subspace \( \mathcal{V} \subset \mathbb{R}^n \).

\[
\mathbf{q} = \mathbf{Vq}_r + \mathbf{V}^\perp \mathbf{q}_p.
\]

Approximate
\[
\tilde{\mathbf{q}} = \mathbf{Vq}_r
\]

Substitute
\[
\frac{d\mathbf{Vq}_r(t)}{dt} = \mathbf{f}(\mathbf{Vq}_r(t), t), \quad \mathbf{Vq}_r(0) = \mathbf{q}_0
\]

Project
\[
\frac{d\mathbf{q}_r(t)}{dt} = \mathbf{V}^T \mathbf{f}(\mathbf{Vq}_r(t), t), \quad \mathbf{q}_r(0) = \mathbf{V}^T \mathbf{q}_0.
\]
Error Transport

\[ \epsilon(t) = q(t) - \bar{q}(t) \]
\[ = q(t) - Vq_r(t) \]
\[ = q(t) - \Pi q(t) + \Pi q(t) - Vq_r(t) \]
\[ = [(I - \Pi)q(t)] + [\Pi q(t) - Vq_r(t)] \]
\[ = \epsilon_{\Pi}(t) + \epsilon_{\|}(t). \]

\[ \frac{d\epsilon_{\|}}{dt} = \Pi [f(q(t), t) - f(\bar{q}(t), t)] \]
Stability

Let’s consider an autonomous linear system $f(q(t), t) = Aq(t)$, then

$$\frac{d\epsilon_\parallel}{dt} = \Pi A \epsilon_\parallel(t) + \Pi A \epsilon_\Pi(t).$$

$$\epsilon_\parallel^T \frac{d\epsilon_\parallel}{dt} = \epsilon_\parallel^T \Pi A \epsilon_\parallel + \epsilon_\parallel^T \Pi A \epsilon_\Pi$$

$$\frac{1}{2} \frac{d\epsilon_\parallel}{dt} = \frac{1}{2} \epsilon_\parallel^T [\Pi A + [\Pi A]^T] \epsilon_\parallel + \epsilon_\parallel^T \Pi A \epsilon_\perp$$

we get the necessary condition $^2$, that $\Pi A + [\Pi A]^T$ should be negative definite. Additionally, the interaction between the parallel and orthogonal errors may also affect stability in a profound manner.

In Galerkin ROMs, we do not have a great degree of control over $\Pi$. Petrov Galerkin methods give us additional control knobs to improve both accuracy and stability.
Galerkin & LSPG

**FOM**

\[ q^n = q^{n-1} + \Delta t A q^n \]

**Galerkin ROM**

\[
\begin{bmatrix}
I - \Delta t V^T A V
\end{bmatrix}
\begin{bmatrix} q^n_r \end{bmatrix}
= \begin{bmatrix} I \end{bmatrix}
\begin{bmatrix} q^{n-1}_r \end{bmatrix}
\]

**Least squares projection**

\[
\min_{q^n_r} \| V q^n_r - V q^{n-1}_r - \Delta t A V q^n \|^2_2
\]

**LSPG ROM**

\[
\begin{bmatrix}
I - \Delta t V^T A V - \Delta t V^T A^T V + \Delta t^2 V^T A^T A V
\end{bmatrix}
\begin{bmatrix} q^n_r \end{bmatrix}
= \begin{bmatrix} I - \Delta t V^T A^T V \end{bmatrix}
\begin{bmatrix} q^{n-1}_r \end{bmatrix}
\]

Farhat and co-workers, circa 2010
Linear Manifold ROMs

Continuous FOM
\[ \frac{dq}{dt} = f(q, t), \quad q(0) = q_0, \quad q : [0, T] \rightarrow \mathbb{R}^N \]

Discrete FOM
\[ r(q^n) \triangleq q^n + \sum_{j=1}^{l} \alpha_j q^{n-j} - \Delta t \beta_0 f(q^n, t^n) - \Delta t \sum_{j=1}^{l} \beta_j f(q^{n-j}, t^{n-j}) \]

Reduced representation in Linear subspace
\[ \tilde{q} = q_{\text{ref}} + P^{-1}Vq_r \]

\[
\begin{align*}
N \times 1 & \quad N \times N & \quad N \times k & \quad k \times 1
\end{align*}
\]
### Linear Stability: 1/2

#### Continuous FOM
\[
\frac{dq}{dt} = Jq, \quad q(0) = q_0,
\]

#### Discrete FOM
\[
(I - \Delta tJ)q^n = q^{n-1}, \quad q^0 = q_0
\]

#### Decomposition
\[
\tilde{q}(t) \triangleq Vq_r(t), \text{ where } V \in \mathbb{R}^{N \times k} \text{ and } q_r \in \mathbb{R}^k
\]

**Theorem 1:** If the Discrete FOM above is asymptotically stable in the sense of \[\| (I - \Delta tJ)^{-1} \|_2 \leq 1\], then the Backward Euler Galerkin ROM is also asymptotically stable if \[\lambda_n (I - 0.5\Delta t(J + J^T)) \geq 1\]

---

**Theorem 2:** If the Discrete FOM above is asymptotically stable in the sense of \( \left\| (I - \Delta t J)^{-1} \right\|_2 \leq 1 \), then the associated LSPG ROM is also asymptotically stable with no further assumptions required.
Linear Manifold Projection-based ROMs

\[
\frac{dq}{dt} = f(q, t), \quad q(0) = q_0, \quad q : [0, T] \to \mathbb{R}^N
\]

\[
r(q^n) \triangleq q^n + \sum_{j=1}^{l} \alpha_j q^{n-j} - \Delta t \beta_0 f(q^n, t^n) - \Delta t \sum_{j=1}^{l} \beta_j f(q^{n-j}, t^{n-j})
\]

\[
\mathcal{V} \triangleq \text{Range}(P^{-1}V)
\]

\[
\frac{dq_r}{dt} = V^T P f(\tilde{q}, t)
\]

\[
\tilde{q}^n \triangleq \arg \min_{\tilde{q}^n \in \text{Range}(V)} \|Pr(\tilde{q}^n)\|_2^2
\]
Multi-scale, Multi-physics, Complexity: An Example

- Non-linear, Multi-scale multi-physics interactions: acoustics, flow & reaction
- Flow – Large coherent structures + small shear layer dynamics
- Reaction – Highly intensive, distributed & intermittent thin flame
- High sensitivity to parameter changes

\[
\begin{align*}
Q &= \begin{pmatrix}
\rho \\
\rho u_i \\
\rho h^0 - p \\
\rho Y_i
\end{pmatrix}, \\
F_i &= \begin{pmatrix}
\rho u_i \\
\rho u_i u_j \\
\rho u_i h^0 \\
\rho u_i Y_i
\end{pmatrix}, \\
F_{v,i} &= \begin{pmatrix}
0 \\
\tau_{ij} \\
0 \\
\rho v_{i,j} Y_i
\end{pmatrix}, \\
H &= \begin{pmatrix}
0 \\
0 \\
0 \\
\dot{\omega}_i
\end{pmatrix}
\end{align*}
\]

Highly nonlinear and stiff source term:
\[e.g., \dot{\omega}_i = \frac{\rho Y_i}{M_1} A T^b \exp \left( \frac{-E_a}{R_y T} \right) \left( \frac{\rho Y_i}{M_1} \right)^{0.2} \left( \frac{\rho Y_2}{M_2} \right)^{1.3}\]
3 Things to take home

Key Enabler: Adaptivity
Part 1

Robustness & Accuracy

Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation C Huang, C Wentland, K Duraisamy, JCP, 2021
Discretely-consistent Petrov-Galerkin ROMs with Variable Transformation (1/3)

Conservative Equations

\[ \frac{q^{n+1} - q^n}{\Delta t} = f(q^{n+1}) \]

Pseudo time stepping

\[ \Gamma^{p-1} \frac{s^p - s^{p-1}}{\Delta \tau} + \frac{q^p - q^n}{\Delta t} = f(q^p) \]

Fully Discrete Residual

\[ r_s(s^p) \triangleq \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) I - \Delta t J^{p-1} \right] \Gamma^{p-1} (s^p - s^{p-1}) + (q^{p-1} - q^n) - \Delta t f(q^{p-1}) \]
Discretely-consistent Petrov-Galerkin ROMs with Variable Transformation (2/3)

Discrete equations

\[ \mathbf{r}_s(s^p) \triangleq \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) \mathbf{I} - \Delta t \mathbf{J}^{p-1} \right] \Gamma^{p-1} (s^p - s^{p-1}) + (q^{p-1} - q^n) - \Delta t \mathbf{f}(q^{p-1}) \]

Decomposition

\[ \tilde{s} \triangleq \tilde{s} + \mathbf{S} \mathbf{V} s_r \]

Scaling matrix for \( s \) → Basis vectors

Basis coefficients

Discretely-consistent Least-Squares formulation

\[ s_r^p \triangleq \arg \min_{s_r} \left\| Q \mathbf{r}_s(\tilde{s}) \right\|_2^2 \]

Scaling matrix for \( q \)
Discretely-consistent Petrov-Galerkin ROMs with Variable Transformation (3/3)

Discretely-consistent Least-Squares formulation

\[ s_r^p \triangleq \arg \min_{s_r} \| Q r_s (\tilde{s}) \|_2^2 \]

Test basis

\[ W^{p-1} \triangleq Q \left[ \left( \frac{\Delta t}{\Delta \tau} + 1 \right) I - \Delta t J^{p-1} \right] \Gamma^{p-1} SV \]

ROM

\[ [W^{p-1}]^T W^{p-1} (s_r^p - s_r^{p-1}) = -[W^{p-1}]^T Q r_q^{p-1} \]

Discretely-consistent, symmetrized, (globally)stable, conservative
Hyper-reduction

Re-define discrete least square formulation based on $N_s$ samples

\[
[W^{p-1}]^T W^{p-1} (s_r^p - s_r^{p-1}) = -[W^{p-1}]^T [PU]^k PQ r_q^{p-1}
\]

Preserves discrete consistency, but reduces complexity from $O(N)$ to $O(N_s)$
Parallel Data Processor (PDP) for Large scale ROMs

ROM Software Infrastructure Development → Efficient Data Processor

**CFD Code**

![Diagram of data flow](image)

**Parallel Data Processor (PDP)**
- Parallel toolset for data decomposition (POD/DMD) – shared with Air Force
- Compatible with different data formats
- Efficient basis generation, sparse sampling pre-calculations especially for large scale problems (e.g. POD with 100M DoFs x 1000 snapshots in less than 30 min)

**POD Basis, Sampling Points, …**
ROM Interface

ROM Software Infrastructure Development → Portable Parallel Interface

CFD Code

Some aspects of Intrusive ROM Framework can be portable

Portable Parallel Interface

Some aspects of Intrusive ROM Framework can be portable

Nonlinear model evaluations at sampling points

Basis & Sampling Points Adaptation

Read In POD Basis & Load Balance based on Sampling Points

(Dense matrix) Linear Solve

Reduction Order Model (ROM) Construction

MPI

$\Omega_1$

$\Omega_2$

$\Omega_i$

$\Omega_n$

n (<<N) processors

PDP

POD Basis, Sampling Points, …

Code Dependent
Further details on sampling

- First $d$ points selected by QR pivots of data (QDEIM)
- **GappyPOD+$+$R**: randomized oversampling
  - Remaining $N_s - d$ points are selected randomly
  - Cheap, simple, serial
- **GappyPOD+$+$E**: eigenvector-based oversampling
  - Minimize sampling error at every iteration
    \[
    \left\| [S_{m}^T U]^+] \right\|_2 = \frac{1}{\sigma_{min}(S_{m}^T U)}
    \]
  - Sample row of $U$ which maximizes update to smallest eigenvalue
    \[
    \lambda_{d}^{m+1} - \lambda_{d}^{m}
    \]

*Investigation of Sampling Strategies for Reduced-Order Models of Rocket Combustors, CR Wentland, C Huang, K Duraisamy, Proc. AIAA Scitech 2021 Forum*
Scalable Projection-Based Reduced-Order Models for Large Multiscale Fluid Systems,
CR Wentland, C Huang, K Duraisamy, AIAAJ 2023

Further details on sampling

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Fig. 19 Conservative variables time-average projection error.

Fig. 20 CVRC unsampled PROM time-average error, various $\Delta t$. 
Further details on sampling

Investigation of Sampling Strategies for Reduced-Order Models of Rocket Combustors, CR Wentland, C Huang, K Duraisamy, Proc. AIAA Scitech 2021 Forum
3D Truncated CVRC Injector with Downstream Forcing

Flamelet progress variable model with GRI-1.2 kinetics (32 species, 177 reactions)

Oxidizer @ T = 660K
Fuel @ T = 300K

Coarse 3D mesh (~ 590K cells)

Characteristic BC
4kHz @ 5% amp

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Model Performance

Oxidizer @ T = 660K
Fuel @ T = 300K

Coarse 3D mesh
(~ 590K cells)

Characteristic BC
4kHz @ 5%
amp

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**Introduction**

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**FOM**

**ROM 20 modes**

**ROM 60 modes**

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**T, K**

- 300
- 520
- 740
- 960
- 1180
- 1400
- 1620
- 1840
- 2060
- 2280
- 2500

---

**Oxidizer @ T = 660K**

**Fuel @ T = 300K**

**Coarse 3D mesh (~ 590K cells)**

**Characteristic B**

4kHz @ 5% amp

---

**Projected FOM**
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• Results

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FOM

ROM
(20 modes)

ROM
(60 modes)

T, K

300 520 740 960 1180
1400 1620 1840 2060 2280 2500

Oxidizer @ T = 660K
Fuel @ T = 300K

Coarse 3D mesh
(~ 590K cells)

Characteristic BC
4kHz @ 5% amp

3-4 Orders of magnitude cost reduction
Impact of projection error and sampling

- 60-mode POD Projection Error
- 60-mode ROM (no hyper-reduction)
- 60-mode ROM (hyper-reduction on 1% sampled mesh)
Non-linear Manifold SP-LSVT

- Dual-time formulation w/r/t primitive state

\[ \Gamma(s) \frac{\partial s}{\partial \tau} + \frac{\partial q(s)}{\partial t} - f(q) = 0, \quad \Gamma = \frac{\partial q}{\partial s} \]

- Introduce similar affine representation of primitive state

\[ s \approx \tilde{s} = \bar{s} + S \Psi(s_r) \quad ; \quad \Psi : \mathbb{R}^K \rightarrow \mathbb{R}^N \]

- \[ s^n_r = \arg\min_{a \in \mathbb{R}^K} \| Q r_s(\bar{s} + S \Psi(a)) \|^2_2 \]

\[ (W^{p-1})^T W^{p-1} [s_r^p - s_r^{p-1}] = - (W^{p-1})^T r_s(\tilde{s}^{p-1}) \]

\[ W^{p-1} = Q \frac{\partial r_s(\tilde{s}^{p-1})}{\partial \tilde{s}} S \left[ \frac{\partial \Psi}{\partial s_r} \right]^{p-1} \]

- Symmetrized at sub-iteration level!

- Notice two levels of scaling: \( Q \) and \( S \)
Reducing computational complexity of extreme multi-scale problems while preserving mathematical and physical fidelity

- In-situ adaptive sampling and projections to low-dimensional manifolds
- 2 orders of magnitude acceleration while preserving mathematical & physical fidelity
- Future state and parametric prediction of extremely complex chaotic flows with negligible off-line training
Enabling reduced complexity modeling without having access to full system simulations

- Train component based models
- Integrate components together as a full system
- Execute adaptive ROMs

Rocket combustor example

component ROM was replicated 3, 5, 7 times. It predicts flow characteristics well, even capturing emergent phenomena

Transverse instability!