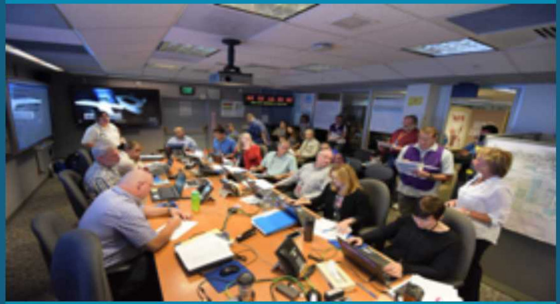
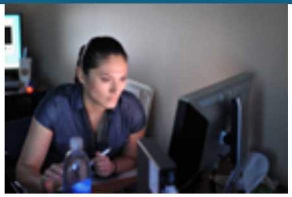
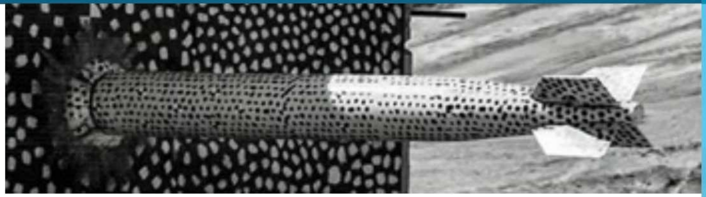
SAND2020-8784PE



Projection-based ROMs at SNL: How? (Methods)

PRESENTED BY

Eric Parish

Limitations of projection-based reduced-order models
(pre-Sandia contributions)

- **Linear time-invariant systems**: **mature**
  - ✓ ***Accurate, certified***: sharp *a priori* error bounds
  - ✓ ***Property preservation***: guaranteed stability
  - ✓ ***Inexpensive***: pre-assemble operators

- **Elliptic/parabolic PDEs**: **mature**
  - ✓ ***Accurate, certified***: sharp *a priori* error bounds
  - ✓ ***Property preservation***: preserve operator properties
  - ✓ ***Inexpensive***: pre-assemble operators

- **Nonlinear dynamical systems**: **ineffective**
  - ✗ ***Unstable and inaccurate:*** pROM solution can "blow up"
  - ✗ ***Structure not preserved***: physical properties ignored
  - ✗ ***Not generalizable***: Can perform poorly for extrapolation
  - ✗ ***Not certified***: error bounds can grow exponentially in time
  - ✗ ***Expensive***: projection insufficient for speedup

- **Many of Sandia's applications are defined by nonlinear dynamical systems**
  - Hypersonic reentry
  - Magnetohydrodynamics
  - Geophysical fluid dynamics
  - Electromagnetics

Existing pROM technologies are not well suited for Sandia's applications

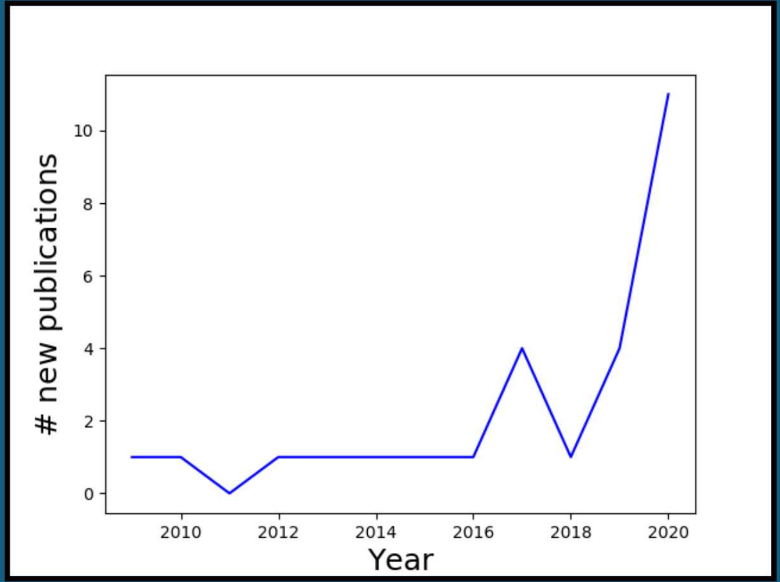
Our research is focused on developing pROMs for nonlinear dynamical systems relevant to Sandia's applications

Research investment areas

- ***Stabilized pROMs***
  - How can we keep pROMs stable and accurate?
- ***Structure preservation***
  - How can we make pROMs satisfy important physical properties
    - Conservation of mass, momentum, and energy
    - Lagrangian structure
- ***Generalization***
  - Can we make pROMs that extrapolate?
- ***Qualification & Certification of pROMs***
  - Can we rely on the pROM solution?

Sandia pROM research highlights (2009-present)

- 26 peer reviewed publications
- 705 citations
- 16 different Sandia authors
- JCP top cited since 2017 list [Carlberg & Barone]
- JCP most downloaded 2020 list [Lee & Carlberg]

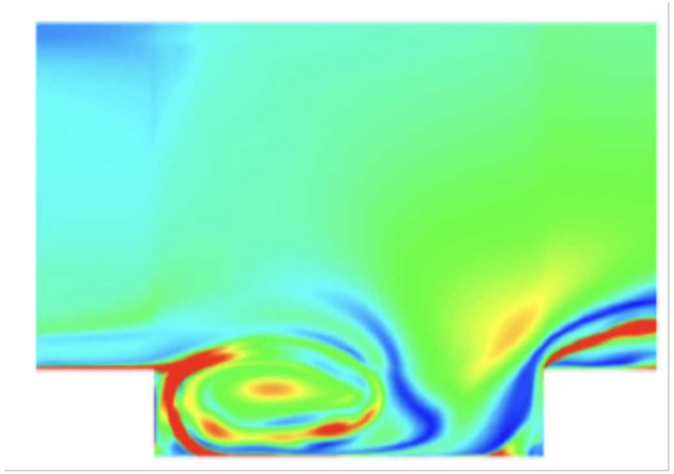


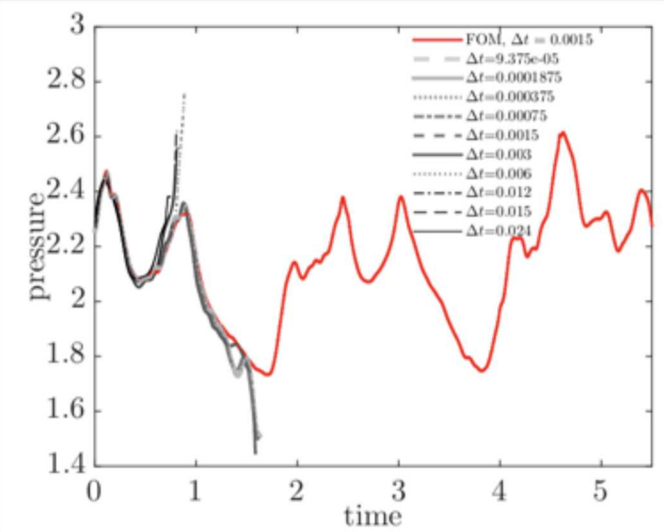
Stabilized pROMs

- **Question:** How can we make stable and accurate pROMs?
- **Challenge:** Standard pROMs be unstable for nonlinear and nonsymmetric systems

When applied to our engineering problems:

- Standard pROM is often unstable
- Exhibits exponentially growing error bounds





K. Carlberg, M. Barone, and H. Antil, Galerkin v. least-squares Petrov-Galerkin projection in nonlinear model reduction, Journal of Computational Physics, 330 (2017), pp. 693–734.

Standard pROMs are unsuitable for Sandia's application use cases

Stabilized pROMs – minimum residual pROMs

- **Question:** **How can we make stable and accurate pROMs?**
- **Challenge:** **Standard pROMs be unstable for nonlinear and nonsymmetric systems**

How are we addressing this?

- Standard Galerkin pROM is constructed via residual orthogonality
  - Fails for nonsymmetric systems

- **We compute solutions that minimize the FOM residual**

$$\tilde{\boldsymbol{x}}(t, \boldsymbol{\mu}) = \arg\min_{\boldsymbol{y} \in \mathcal{V}} \|\dot{\boldsymbol{y}} - \boldsymbol{f}(\boldsymbol{y}, \boldsymbol{\mu}, t)\|_{\mathbf{A}}^2$$

  - Yields **stable, accurate,** and **robust** approximations

- Sandia has been a pioneer in **minimum-residual pROMs**

We compute solutions that best satisfy the governing equations given our data

Sandia min-res literature:
- K. Carlberg, M. Barone, and H. Antil [2017]
- Y. Choi and K. Carlberg [2019]
- E. Parish and K. Carlberg [2020]

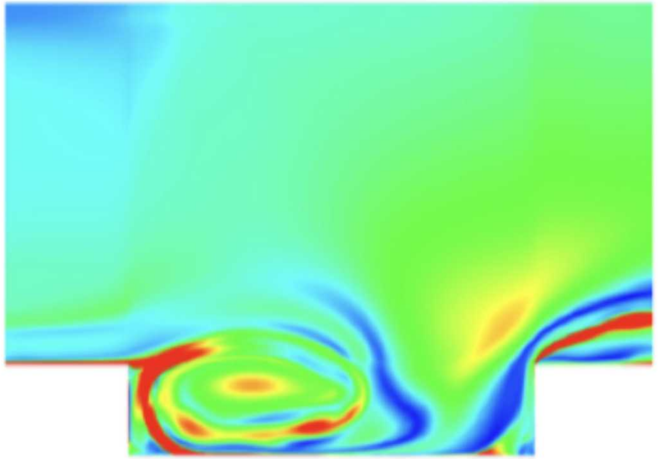
Other Sandia literature on stabilized pROMs
- Barone, I. Tezaur, et al [09,10]
- I. Tezaur. et al [16]
- I. Tezaur, B. van Bloemen Waanders, S. Arunajatesan, M. Barone [14]
- Parish et al. [20]

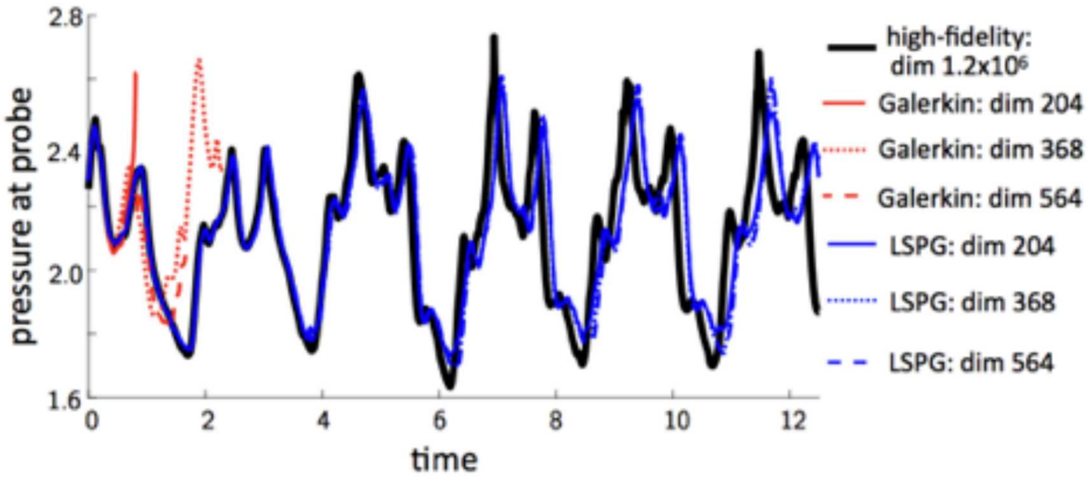
Stabilized pROMs – minimum residual pROMs

- **Question:** How can we make stable and accurate pROMs?
- **Challenge:** Standard pROMs be unstable for nonlinear and nonsymmetric systems

When applied to our engineering problems:

- Minimum-residual pROMs yield stable and accurate solutions





K. Carlberg, M. Barone, and H. Antil, Galerkin v. least-squares Petrov-Galerkin projection in nonlinear model reduction, Journal of Computational Physics, 330 (2017), pp. 693–734.

Sandia's research on minimum residual projections enables pROMs for Sandia's applications

Structure preservation

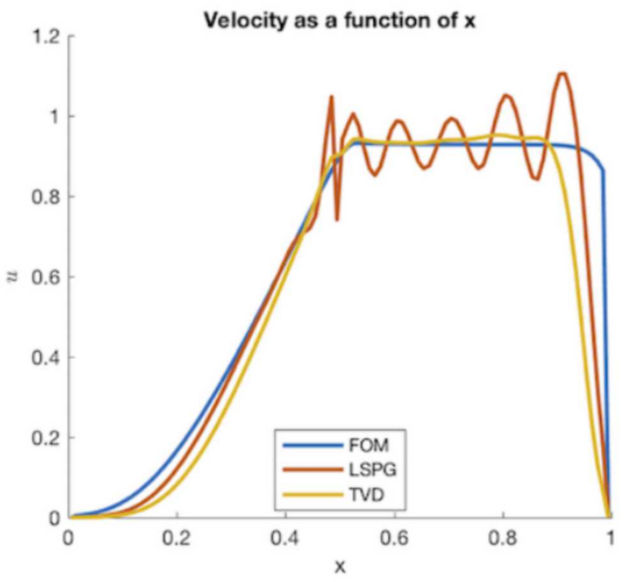
Tezaur, Fike, Carlberg, Barone, Maddox, Mussoni, Balajewicz, *Advanced Fluid Reduced Order Models for Compressible Flow.* [17]

- Many systems underlying Sandia's applications have important **structure**
  - Conservation of mass, momentum, and energy in fluid dynamics
  - Solenoidal fields in magnetohydrodynamics
  - Lagrangian structure in solid mechanics

- Minimum residual formulation naturally allows for **constraints**

$$\text{minimize} \|\dot{\boldsymbol{y}} - \boldsymbol{f}(\boldsymbol{y}, \boldsymbol{\mu}, t)\|_{\mathbf{A}}^2$$

$$\text{subject to } \ldots$$



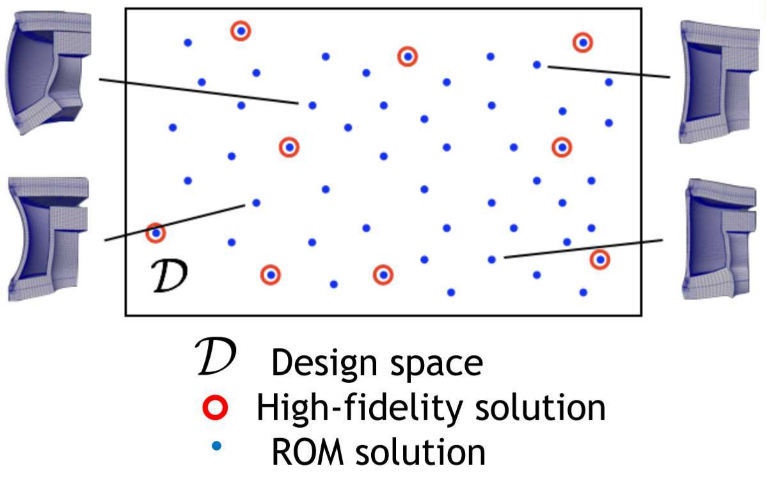
Total variation diminishing constrained ROM

Sandia structure preservation literature:
- Carlberg, Tuminaro, and Boggs [15]
- Pen, Carlberg [15]
- Carlberg, Choi, Sargsyan [17]
- Lee, Carlberg [20]

Constrained minimum-residual pROMs enable formulations that preserve structure

Generalization

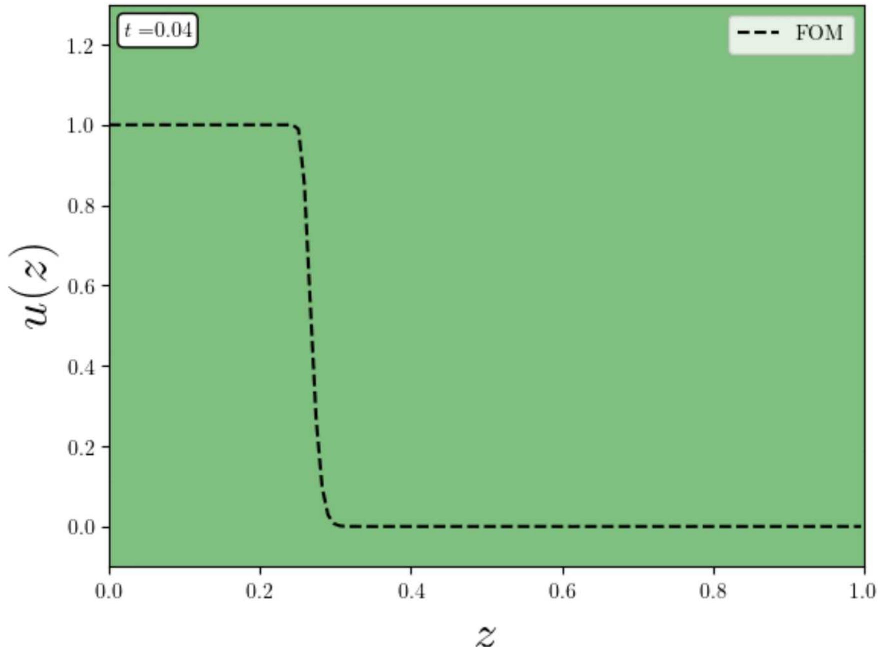
- **Question:** How can we obtain accurate solutions when we apply our pROMs in new regimes?
- **Challenge:** standard approaches fail for certain problems



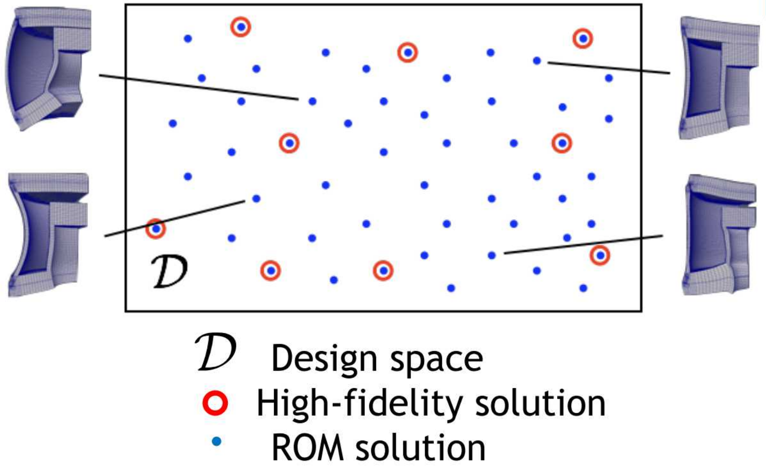
- Example: building a pROM of the linear convection equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial z} = 0$$

  - Solution is a wave propagating left to right
  - Build a pROM using data for $t \in [0, 0.5]$
  - Use the pROM to predict for $t \in [0, 1]$



Generalization

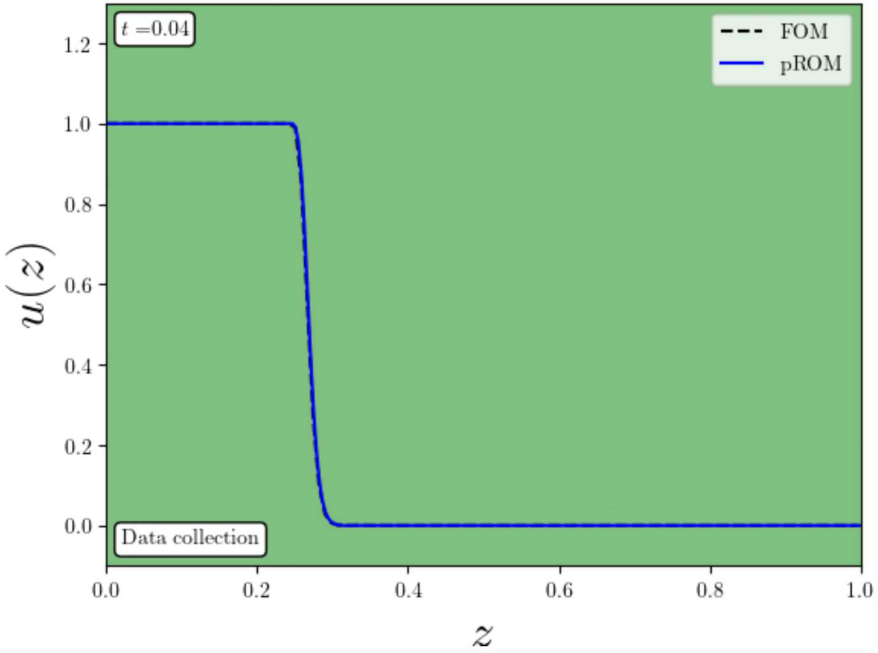


- **Question:** How can we obtain accurate solutions when we apply our pROMs in new regimes?
- **Challenge:** standard approaches fail for certain problems

- Example: building a pROM of the linear convection equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial z} = 0$$

  - Solution is a wave propagating left to right
  - Build a pROM using data for $t \in [0, 0.5]$
  - Use the pROM to predict for $t \in [0, 1]$



PCA fails to identify low-dimensional structure!

Generalization: can we leverage advancements in ML?

Sandia ML-ROM literature
- **Lee & Carlberg [2020]**
- **Tencer & Potter [2020]**

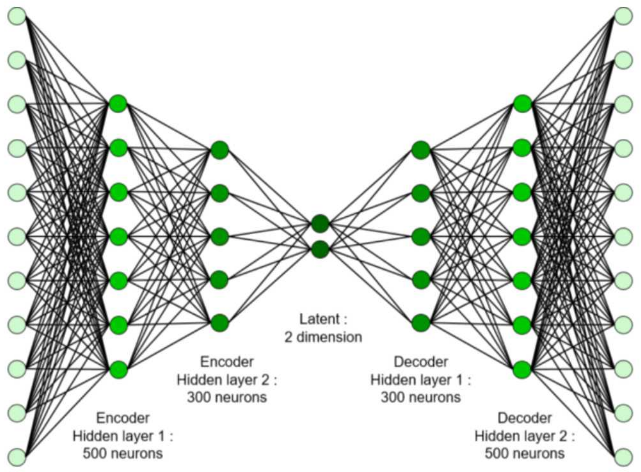
- **PCA fails to identify low-dimensional structure**
  - Precludes the use of pROMs for many important problems!

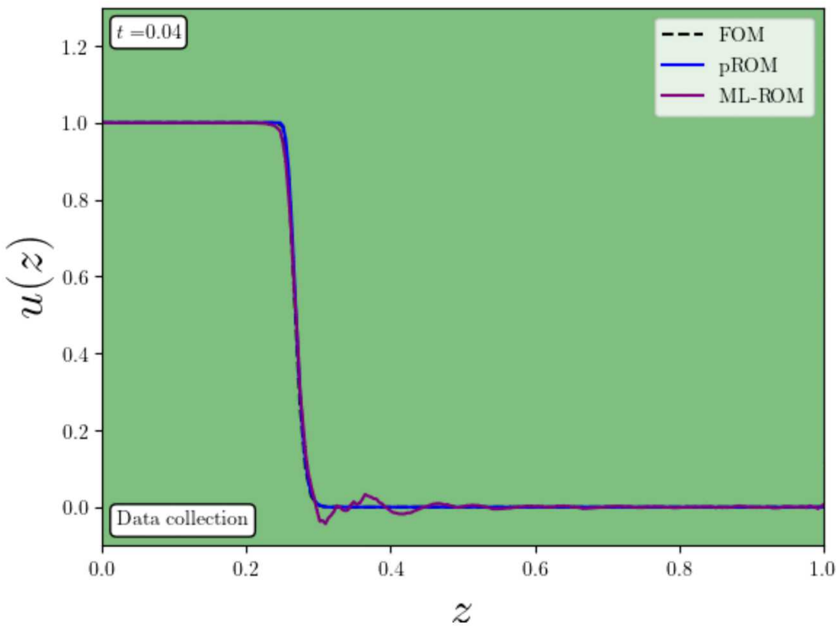
- **How are we addressing this?**
  - PCA identifies **linear** subspaces
  - We use machine learning to **identify nonlinear manifolds**
    - Use neural networks to identify low-dimensional structure
    - Minimize the residual on the resulting low-dimensional nonlinear manifold

Linear: $\tilde{\boldsymbol{x}}(t, \boldsymbol{\mu}) \equiv \boldsymbol{\Phi} \boldsymbol{x}(t, \boldsymbol{\mu})$

Nonlinear: $\tilde{\boldsymbol{x}}(t, \boldsymbol{\mu}) \equiv \boldsymbol{g}\left(\hat{\boldsymbol{x}}(t, \boldsymbol{\mu})\right)$

ML-pROMs improve generalization!

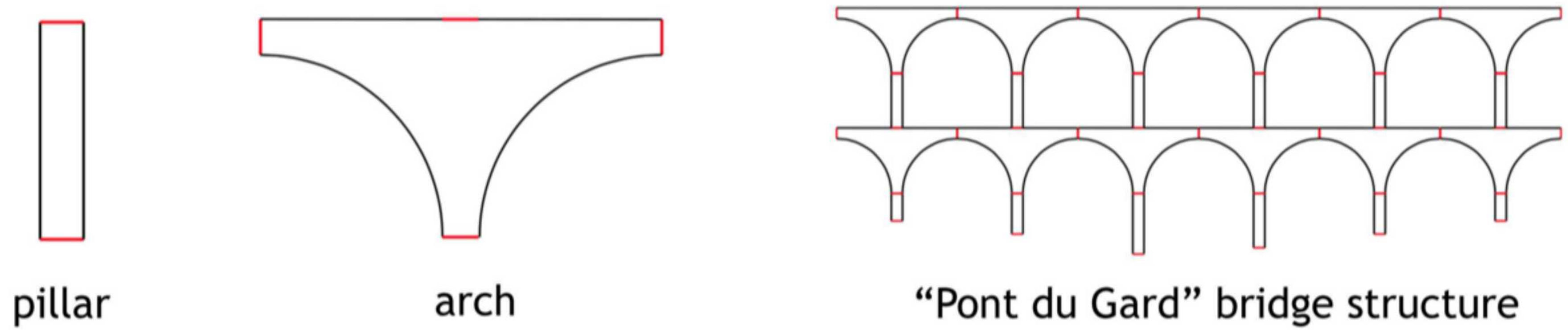




Generalization: additional work

Sandia ML-ROM literature
- Lee & Carlberg [2020]
- Tencer & Potter [2020]

- **Domain decomposition pROMs** [Hoang, Choi, Carlberg 20]
  - Decomposes pROM problem into subdomains



(Courtesy from Huynh et al., 2013)

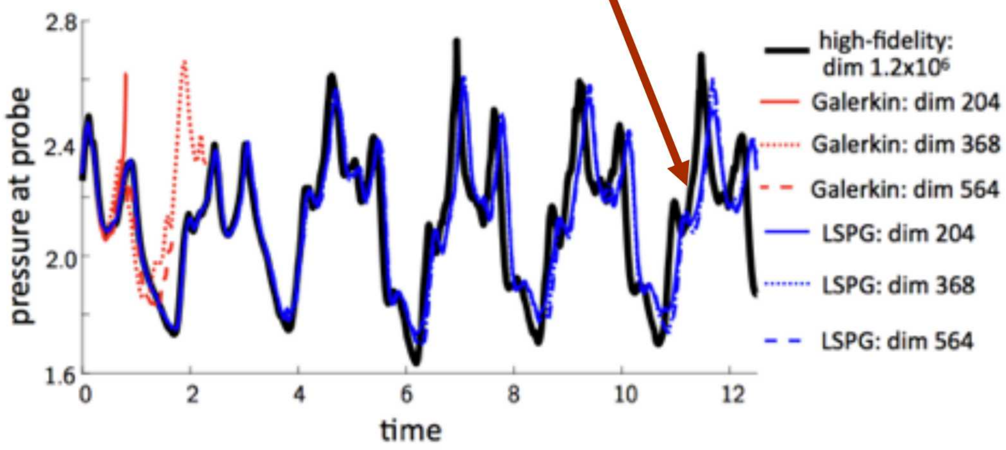
- **h-adaptivity** [Etter, Carlberg 20, 14]
  - Adapts pROM basis on the fly for improved generalization

Qualification & Certification of pROMs

- **Question:** How can we quantify the accuracy of pROM solutions?

- Traditional approaches for error quantification
  - *A posteriori* error bounds
  - Dual weighted residuals
- Traditional approaches can lack sharpness/accuracy and can be difficult to compute

pROMs incur errors!



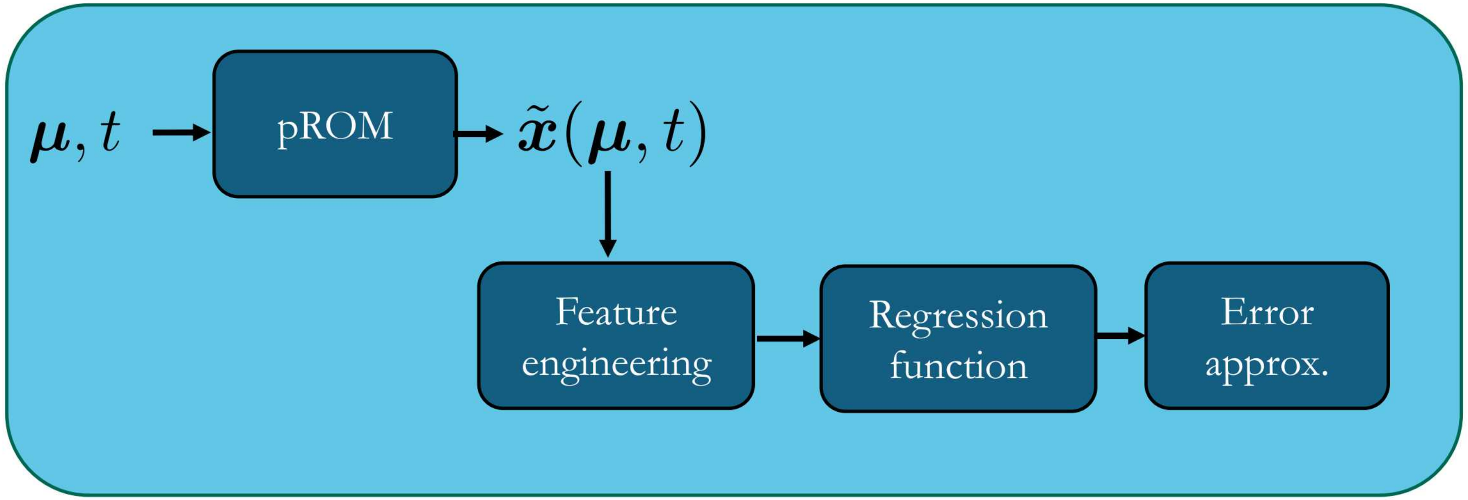
- **Traditional approaches for error quantification are not practical for pROMs applied to Sandia's applications!**

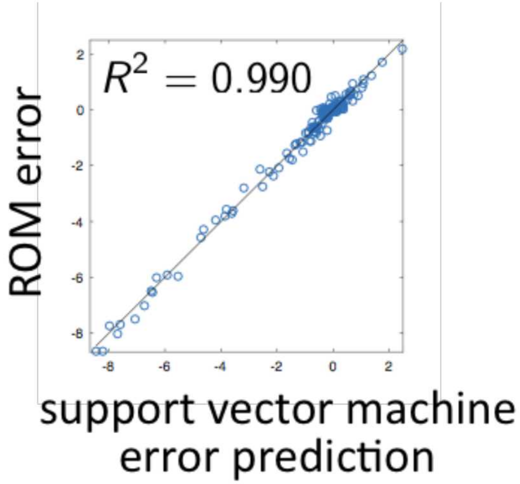
Qualification & Certification of pROMs

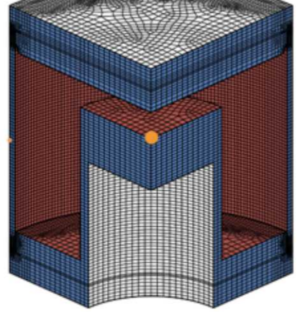
Example: Component Structural Model

- **Question:** How can we quantify the accuracy of pROM solutions?

- **How are we addressing this?**
  - We take a data-driven approach**: machine learning error models**
  - Main idea: build a **feature-error** mapping via a regression function







B. Freno and K. Carlberg, "*Machine-learning error models for approximate solutions to parameterized systems of nonlinear equations*", CMAME, 19.

Enables statistically certified ROMs!

Sandia error modeling literature:
- Drohman & Carlberg [2015]
- Trehan, Carlberg, Durlofsky, [2017]
- Freno & Carlberg [2019]
- Parish & Carlberg [2020]

Research summary

Standard pROM technologies for nonlinear dynamical systems

✗ ***Unstable and inaccurate:*** ROM solution can "blow up"

❑ **We are developing stabilized pROM formulations**

✗ ***Structure not preserved***: physical properties ignored

❑ **We are developing constraint-based pROMs**

✗ ***Not generalizable:*** Can perform poorly for extrapolation

❑ **We are developing ML-pROMs, DD-pROMs, and h-adaptive pROMs**

✗ ***Not certified***: error bounds can grow exponentially in time

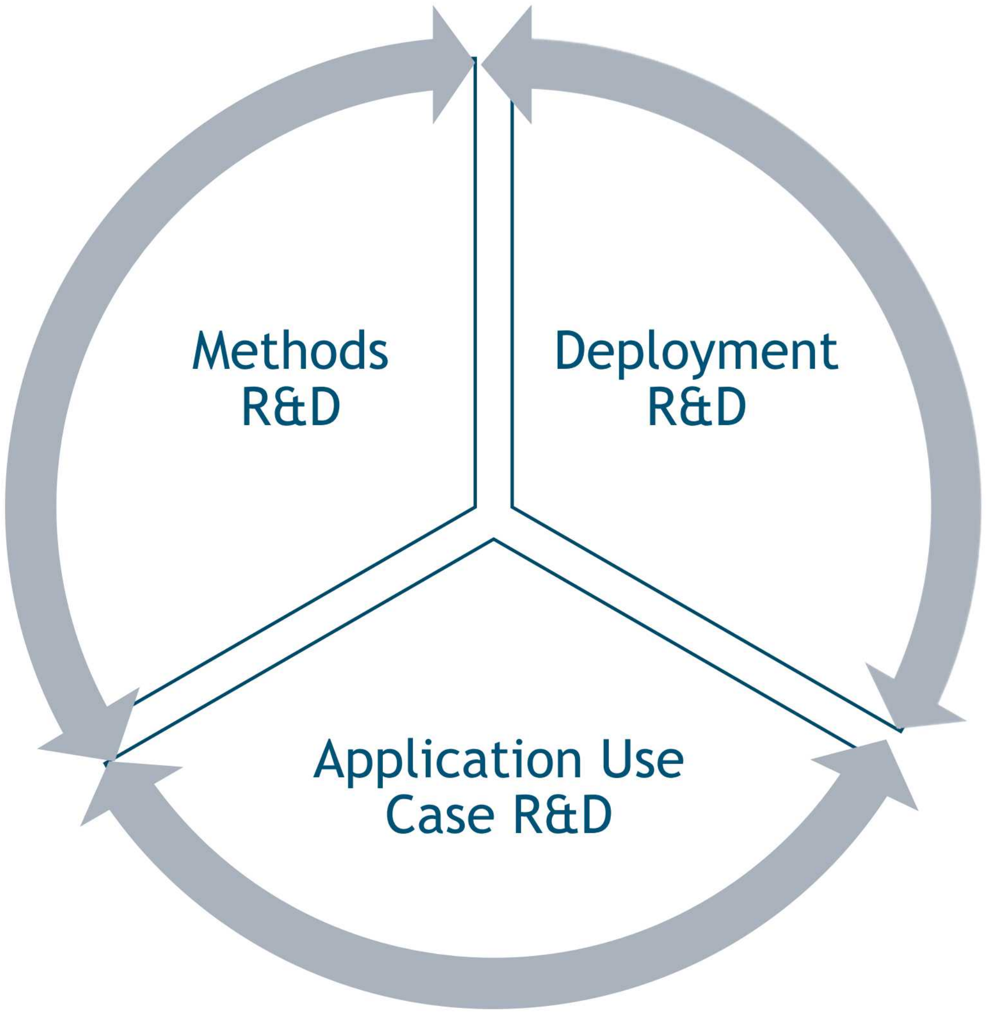
❑ **We are developing machine learning error models**

We are continuing to

- **Advance these technologies and integrate them in Pressio**
- **Pursue research to address challenges encountered by the application team**

Conclusions

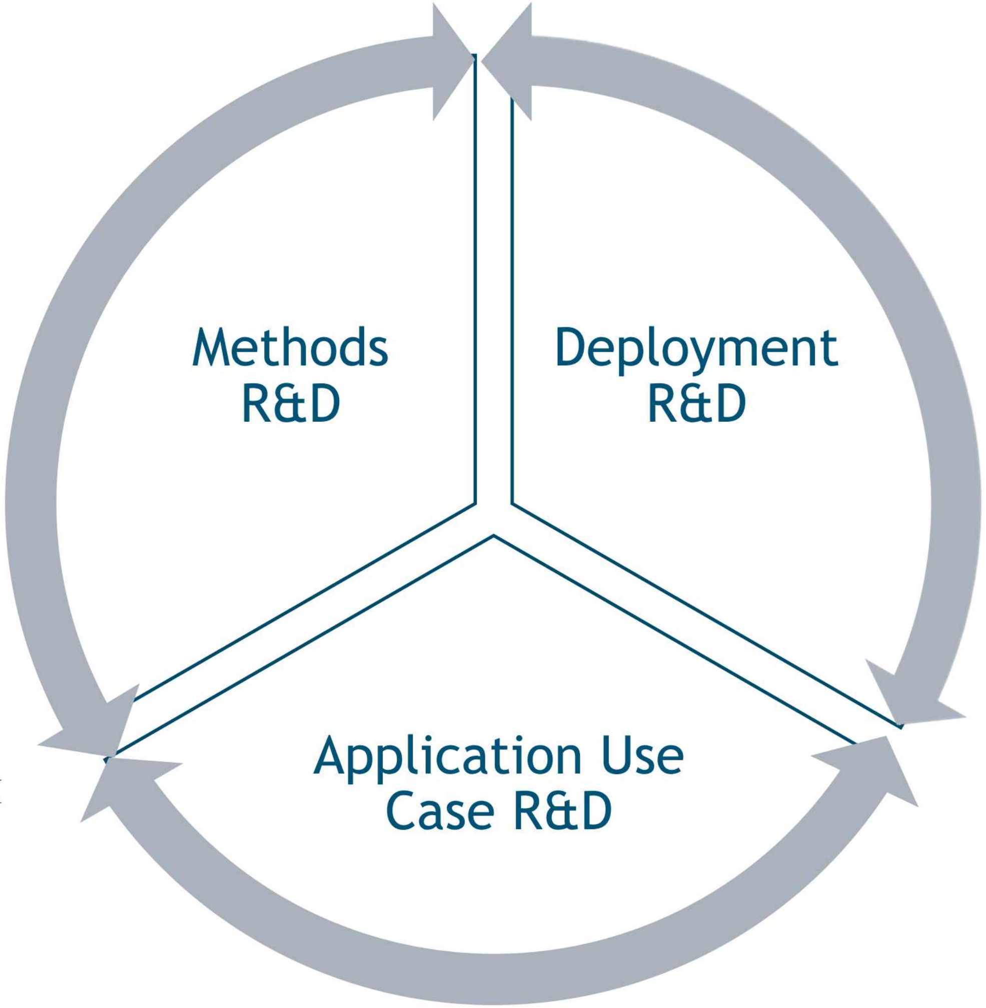
- pROMs are powerful tools for surrogate modeling
- Sandia's investments in pROM technology has been growing
- pROMs have been integrated into Aria and SPARC
  - Yield <1% errors with >100x speed-up in wall-time
- Integration is achieved via Pressio
  - Computational framework aimed at enabling pROMs in application codes
- For project management, pROM work has been subdivided:
  - Application Use Case R&D
  - Deployment R&D
  - Methods R&D



Conclusions

- We are looking for your feedback!

1. How could pROM R&D contribute to your (team's/department's) activities?
2. What gaps within the current pROM R&D projects need to be addressed to make pROMs useful?
3. Which staff are interested in engaging pROM R&D? What areas of R&D are they interested in (i.e., methods, deployment, and/or application use case)?
4. Which mechanics areas are interested in engaging in pROM R&D?
   - Who are the right SMEs for those areas?
   - Would current funding streams support engagement or would joint funding need to be pursued?
5. What are barriers and pathways to deploying pROM on mission problems?
   1. What kind of accuracy/performance would an application need to be usable?
   2. What metrics are important and how would you measure accuracy?
6. What reduced-physics and/or data-driven surrogate modeling efforts at Sandia should the pROM team engage?
7. What technical, funding, personnel, and teaming constructs are required to support eventual productization of the pROM capability?



Thank you for your time!

Backup slides

We achieve large improvements in the generalization criteria with manifold model reduction

2D Chemically reacting flow

$$\frac{\partial \mathbf{w}(\vec{x}, t; \boldsymbol{\mu})}{\partial t} = \nabla \cdot (\kappa \nabla \mathbf{w}(\vec{x}, t; \boldsymbol{\mu})) - \mathbf{v} \cdot \nabla \mathbf{w}(\vec{x}, t; \boldsymbol{\mu}) + \mathbf{q}(\mathbf{w}(\vec{x}, t; \boldsymbol{\mu}); \boldsymbol{\mu})$$

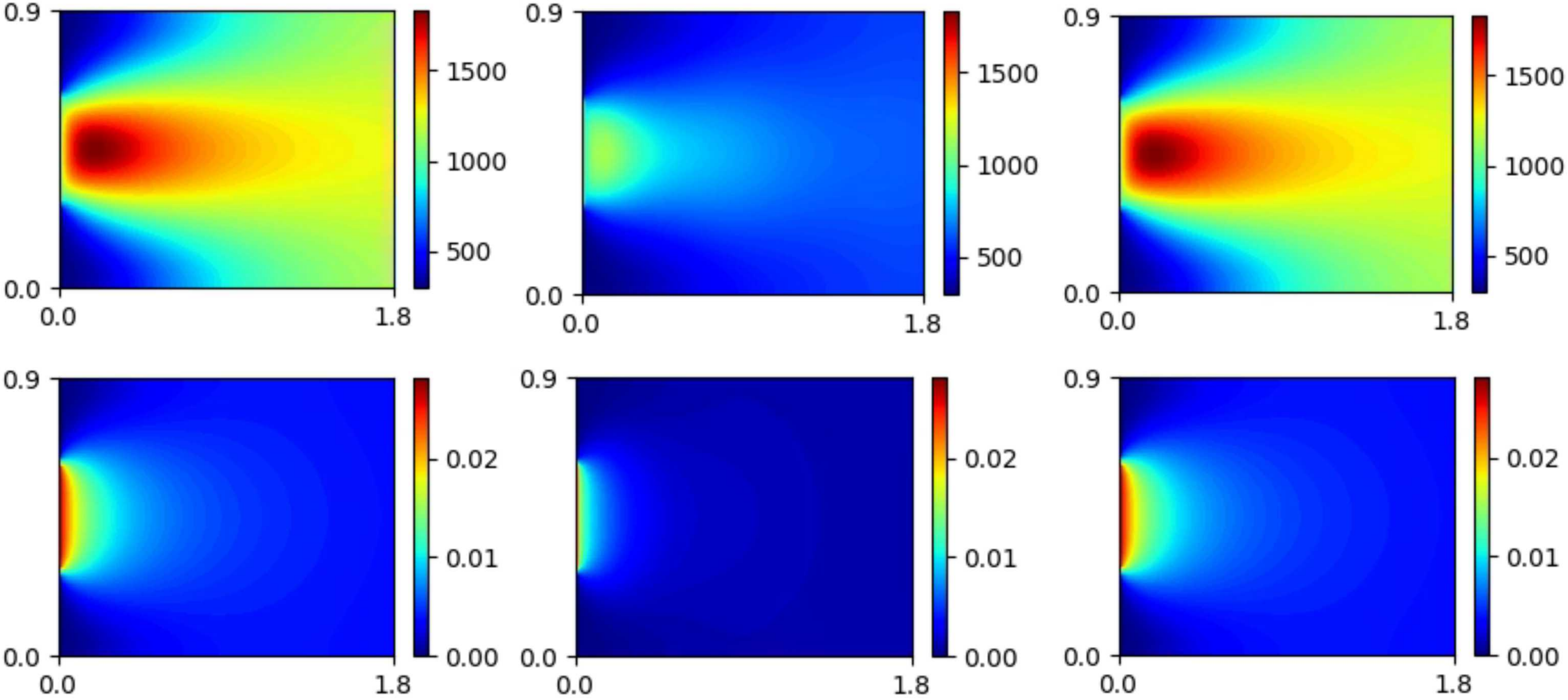
high-fidelity model

LSPG w/ PCA
ROM dimension=5

Manifold LSPG w/ autoencoder
ROM dimension=5

temperature

H2 fraction



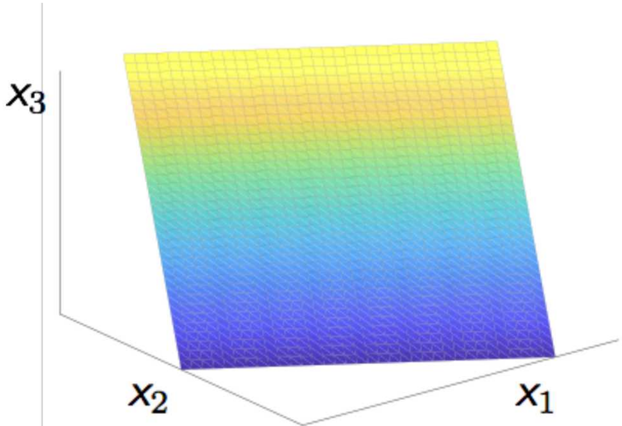
[Lee & Carlberg, 2020]

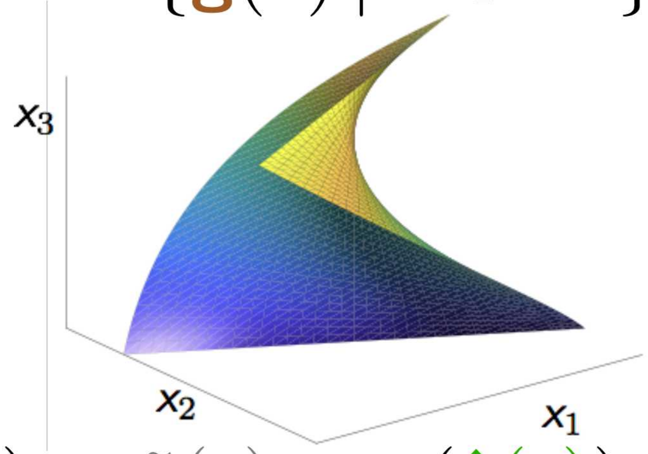
Manifold LSPG projection uses a nonlinear function instead of a linear basis, resulting in more capacity [Lee & Carlberg, 2019]

$$\text{range}(\boldsymbol{\Phi}) := \{\boldsymbol{\Phi}\hat{\mathbf{x}} \,|\, \hat{\mathbf{x}} \in \mathbb{R}^p\}$$

$$\mathcal{S} := \{\mathbf{g}(\hat{\mathbf{x}}) \,|\, \hat{\mathbf{x}} \in \mathbb{R}^p\}$$

Example:
N=3
P=2





$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t) \in \text{range}(\boldsymbol{\Phi})$$

$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \mathbf{g}(\hat{\mathbf{x}}(t)) \in \mathcal{S}$$

Decoder:
One choice of
nonlinear
function