SAND2019-8800C

Data-informed Reduced-order Models with Memory Effects

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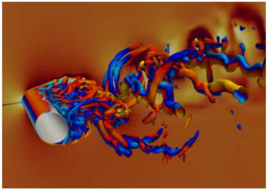
Motivation

- Many query problems of dynamical systems
  - Shape optimization
  - Parameter estimation



- Direct solutions to dynamical systems can be computationally intractable
  - 10k CPU hours
- **Forward model is a computational bottleneck**

Motivation

- Model reduction makes many query problems tractable
  - POD-Galerkin ROM
  - Cost savings of over $100\times$
- Challenges in model reduction
  - Reduced-order models generate approximate solutions
    - Can be **inaccurate** and **unstable**
- Leads to epistemic uncertainty
- Desirable **quantify** and **reduce** this uncertainty

Approaches for error reduction and quantification in ROMs

- *A posteriori* error bounds
  - Rigorous bounds on the error
  - Quantifies, but doesn't *reduce* errors
  - Bounds are often loose
- *A posteriori* error models
  - Can be used to reduce state or QoI errors
  - Quantifies *and* reduces errors
  - Can be challenging to create and validate
- Subgrid-scale Modeling
  - Models impact of truncated dynamics in ROM
  - Reduces state errors
  - Intrusive

Overview

- Propose a data-informed subgrid-scale modeling framework
  - Quantifies *and* reduces errors
  - Only requires the data that was used to generate the ROM
- Framework combines ideas from subgrid-scale modeling, error modeling, and machine learning
  - Framework is based on Mori-Zwanzig subgrid-scale models
  - Models unresolved effects as a deterministic function + noise
  - Parameters in the proposed models are learned from snapshot data used to construct the ROM trial space
- Demonstrate applicability on the advection-diffusion and shallow water equations

Problem Description

Full-Order Model

- Focus on the parametric full-order model (FOM)

$$\frac{d}{dt}\mathbf{u}(\boldsymbol{\eta}, t) = \mathbf{R}(\mathbf{u}, \boldsymbol{\eta})$$

  - State vector: $\mathbf{u} \in \mathbb{R}^N$
  - Spatial discretization scheme: $\mathbf{R} : \mathbb{R}^N \times \mathbb{R}^{N_\eta} \to \mathbb{R}^N$
  - System parameters: $\eta \in \mathbb{R}^{N_\eta}$

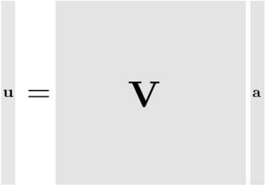
- **Principle Challenge:** Full-order model is high dimensional
  - Computationally expensive
- Require computationally efficient methods of approximating the FOM

Reduced-Order Models: Coordinate Transformation

- State variable can be expressed in an orthonormal, hierarchical coordinate system,

$$\mathbf{u}(\boldsymbol{\eta}, t) = \mathbf{V}\mathbf{a}(\boldsymbol{\eta}, t)$$

  - Full-order trial basis: $\mathbf{V} \in \mathbb{R}^{N \times N}$
  - Generalized coordinates: $\mathbf{a}(\boldsymbol{\eta}, t) \in \mathbb{R}^{N}$



- FOM can be written in this coordinate system as

$$\frac{d}{dt}\mathbf{a}(\boldsymbol{\eta}, t) = \mathbf{V}^T\mathbf{R}(\mathbf{V}\mathbf{a}(\boldsymbol{\eta}, t), \boldsymbol{\eta})$$

POD Reduced-Order Model: Basis Generation

- POD is a popular approach to construct the basis
- **Requires offline training:**
  - Solve full-order model for high fidelity data

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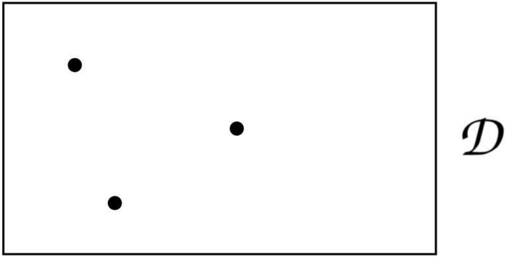

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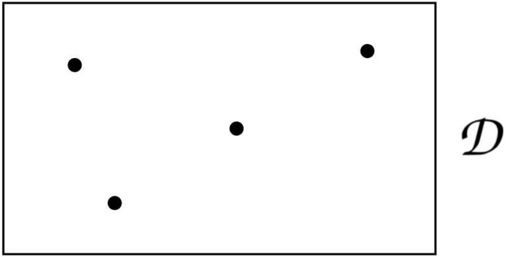

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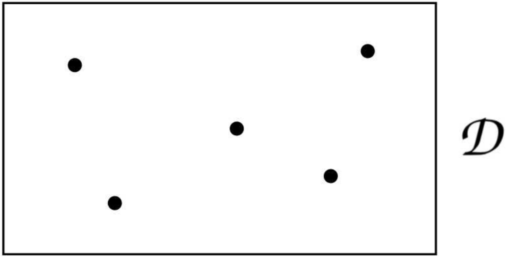


- Use data to generate K dimensional basis $\tilde{\mathbf{V}}$ ($K \ll N$)

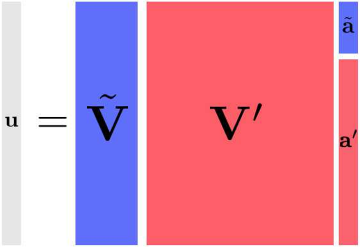
Reduced-Order Models: Basis decomposition

- Trial basis decomposition

$$\mathbf{V} = \left[\tilde{\mathbf{V}}; \mathbf{V}'\right], \qquad \mathbf{a} = [\tilde{\mathbf{a}}, \hat{\mathbf{a}}],$$

  - POD trial space: $\tilde{\mathbf{V}} \in \mathbb{R}^{N \times K}$
  - Resolved generalized coordinates: $\tilde{\mathbf{a}} \in \mathbb{R}^{K}$
  - Unresolved trial space: $\mathbf{V}' \in \mathbb{R}^{N \times (N-K)}$
  - Unresolved generalized coordinates: $\hat{\mathbf{a}} \in \mathbb{R}^{N-K}$

- State decomposition:



Reduced-Order Models: Basis decomposition

- FOM can be decomposed into two equations,
  - Coarse-scale ROM equation:

$$\frac{d}{dt}\tilde{\mathbf{a}} = \tilde{\mathbf{V}}^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \eta)$$

  - Fine-scale equation:

$$\frac{d\hat{\mathbf{a}}}{dt} = \mathbf{V}'^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \eta)$$

- **Objective of ROMs is to solve the coarse-scale equation**

Reduced-Order Models: Closure Problem

- Coarse-scale ROM depends on the unresolved scales

$$\frac{d\tilde{\mathbf{a}}}{dt} = \tilde{\mathbf{V}}^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \boldsymbol{\eta})$$

- Need to approximate fine-scales for closed system

$$\mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \boldsymbol{\eta}) = \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}}, \boldsymbol{\eta}) + \mathcal{M}(\tilde{\mathbf{a}})$$

- Approximation for the fine-scales is referred to as a "subgrid-scale" model

Modeling Challenge

- Unclosed coarse-scale equation:

$$\frac{d\tilde{\mathbf{a}}}{dt} = \tilde{\mathbf{V}}^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \boldsymbol{\eta})$$

- Model for unresolved physics:

$$\downarrow$$

$$\mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \boldsymbol{\eta}) = \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}}, \boldsymbol{\eta}) + \mathcal{M}(\tilde{\mathbf{V}}\tilde{\mathbf{a}}, \boldsymbol{\eta})$$

- Closed coarse-scale equation:

$$\downarrow$$

$$\frac{d\tilde{\mathbf{a}}}{dt} = \tilde{\mathbf{V}}^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}}, \boldsymbol{\eta}) + \mathcal{M}(\tilde{\mathbf{V}}\tilde{\mathbf{a}}, \boldsymbol{\eta})$$

- How to construct $\mathcal{M}$?

Subgrid-scale Modeling

- ROM Subgrid-scale modeling techniques:
  - Eddy viscosity models (Iliescu et al.)
  - Variational multiscale models (Codina et al., Iliescu et al.)
  - Data-driven models (Iliescu et al., Carlberg et al.)
  - Mori-Zwanzig models (Chorin et al., Stinis et al., Venturi et al.)

Subgrid-scale Modeling

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  - **Data-driven models** (Iliescu et al., Carlberg et al.)
  - **Mori-Zwanzig models** (Chorin et al., Stinis et al., Venturi et al.)

Mori-Zwanzig Formalism

- Exact ROM equation:

$$\frac{d\tilde{\mathbf{a}}}{dt} = \tilde{\mathbf{V}}^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}} + \mathbf{V}'\hat{\mathbf{a}}, \boldsymbol{\eta})$$

- Mori-Zwanzig formalism allows for

$$\frac{d\tilde{\mathbf{a}}}{dt} = \tilde{\mathbf{V}}^T \mathbf{R}(\tilde{\mathbf{V}}\tilde{\mathbf{a}}, \boldsymbol{\eta}) + \int_0^t \mathbf{K}(\tilde{\mathbf{a}}(t-s), s, \boldsymbol{\eta}) ds$$

- Advantages:
  - Exact equation for the resolved POD modes
  - Only depends on the resolved variables
- Challenges:
  - Computing the memory integral is not practical
- Appealing starting point for developing accurate ROMs

Mori-Zwanzig Models

- MZ framework serves as the basis of many models:
  1. Renormalized *t*-model
  2. Bachelor series expansion models
  3. Finite memory models
  4. τ-model
  5. Faber series models
- **Challenges:**
  - Challenging to determine the best model *a priori*
  - Many models contain parameters which must be selected

Subgrid-scale Modeling

- We propose a data-driven subgrid-scale modeling framework for ROMs
  - Use (MZ-based) subgrid-scale models to approximate unresolved effects
  - Leverage data used for construction of ROM trial space to calibrate model parameters
  - Perform model selection based on desired performance metrics

Data-Calibrated Subgrid-Scale Modeling Framework

Modeling Framework

- Propose approximations to the memory of the form,

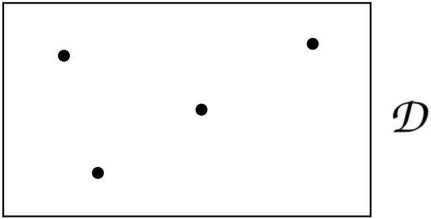
$$\int_0^t \mathbf{K}(\tilde{\mathbf{u}}(t-s), s, \boldsymbol{\eta})ds \approx \mathcal{N}\left(\mathbf{f}(\mathbf{w}(\boldsymbol{\eta}), \tilde{\mathbf{u}}, \boldsymbol{\eta}), \sigma^2(\boldsymbol{\eta})\right)$$

  - $\mathcal{N}$: Normal distribution
  - $\mathbf{f}$: Deterministic subgrid-scale model
  - $\mathbf{w}$: Model paramaters
  - σ^2: Noise variance

- Offline framework steps:
  1. Form the primitive ROM
  2. Select candidate subgrid-scale models, $\mathbf{f}$
  3. Learn model parameters, $\mathbf{w}$
  4. Learn the noise variance, σ^2
  5. Select optimal ROM

Data-Calibrated POD Reduced-Order Model

- Constructing data-calibrated POD ROM consists of:
  1. **Offline training:** Solve full-order model for high fidelity data



  2. **Offline ROM construction**:
     - Identify low dimensional subspace, $\tilde{\mathbf{V}}$

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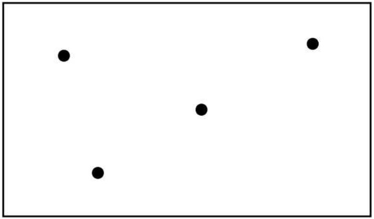

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  2. **Offline ROM construction**:
     - Identify K dimensional linear subspace, $\tilde{\mathcal{V}}$, with $K << N$
     - **Close coarse-scale ROM with candidate subgrid-scale models**

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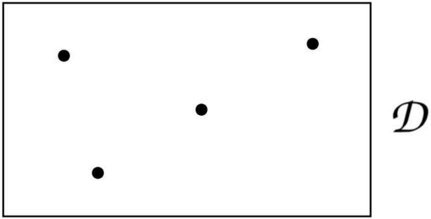


  2. **Offline ROM construction**:
     - Identify K dimensional linear subspace, $\tilde{\mathcal{V}}$, with $K << N$
     - **Close coarse-scale ROM with candidate subgrid-scale models**
     - **Use ROM training data to perform subgrid-scale model calibration and selection**

Selection of the Subgrid-Scale Models

- First step involves selection of candidate SGS models
- Consider here four methods
  1. Galerkin truncation:

$$\mathbf{f}(\mathbf{w}, \tilde{\mathbf{u}}, \boldsymbol{\eta}) = 0$$

  2. Renormalized t model:

$$\mathbf{f}(\mathbf{w}, \tilde{\mathbf{u}}, \boldsymbol{\eta}) = c(\boldsymbol{\eta}) t \mathbf{K}(\tilde{\mathbf{u}}(t), 0, \boldsymbol{\eta})$$

  3. τ model:

$$\mathbf{f}(\mathbf{w}, \tilde{\mathbf{u}}, \boldsymbol{\eta}) = \tau(\boldsymbol{\eta}) \mathbf{K}(\tilde{\mathbf{u}}(t), 0, \boldsymbol{\eta})$$

  4. Exponential kernel model:

$$\mathbf{f}(\mathbf{w}, \tilde{\mathbf{u}}, \boldsymbol{\eta}) = \int_0^t c(\boldsymbol{\eta}) e^{\frac{1}{\tau(\boldsymbol{\eta})}(t-s)} \mathbf{K}(\tilde{\mathbf{u}}(t), 0, \boldsymbol{\eta}) ds$$

Supervised Learning for the Model Parameters

- Models contain unknown model parameters
  - eg. Markovian τ model: $\mathbf{w} = \tau(\boldsymbol{\eta})$
- Learn model parameters with a supervised learning method

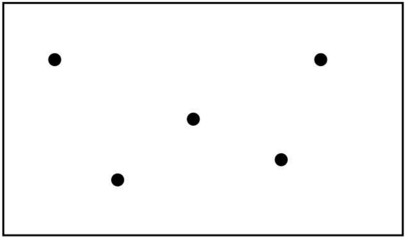
$$\mathbf{w}(\boldsymbol{\eta}) \approx \hat{\mathbf{w}}(\theta, \boldsymbol{\eta})$$

  - $\hat{\mathbf{w}}$: regression function from supervised learning (e.g. neural network)
  - θ: regression model weights

- **Takeaway: Use supervised learning methods to learn the parameterization of the model constants**

Supervised Learning for the Model Parameters

- Leverage data used in ROM training process to learn weights
- Evaluate ROM at same training points



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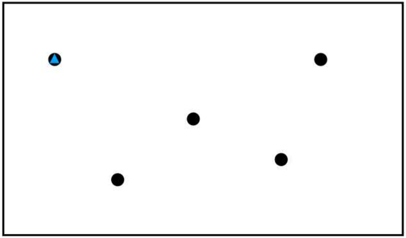

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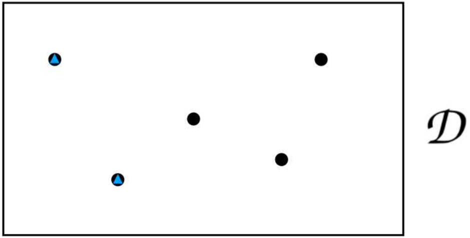

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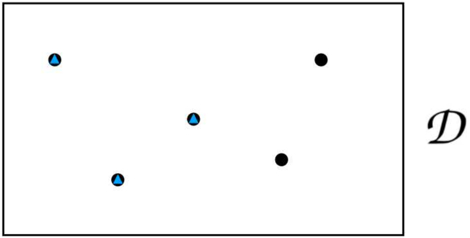


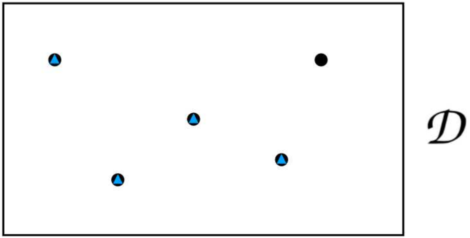
Problem Description

Data-Calibrated Subgrid-Scale Modeling Framework

Numerical Experiments

Supervised Learning for the Model Parameters

- Leverage data used in ROM training process
- Evaluate ROM at same training points



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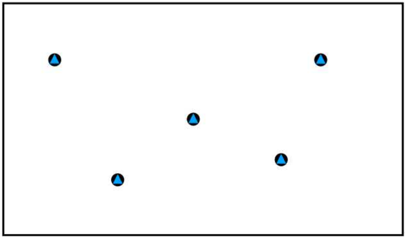

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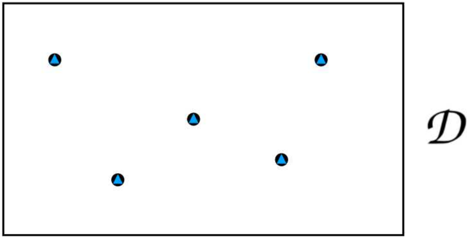

- Train each SGS model by minimizing the misfit between the ROM and FOM
- Calibrate the noise variance based on validation frequencies

Supervised Learning for the Model Parameters

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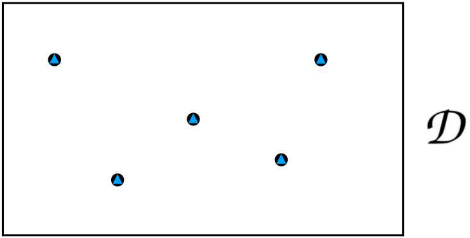


- Train each SGS model by minimizing the misfit between the ROM and FOM
- Calibrate the noise variance based on validation frequencies

Model Selection

- Previous step gives a set of calibrated ROMs
- Perform model selection by:
  1. Evaluate each calibrated ROM on the training set
  2. Compute performance metrics
     - e.g. mean squared error (MSE) or MSE / CPU time
  3. Select ROM with best metric

- **Leads to an optimal "calibrated" ROM**
  - Maintained the same trial space
  - Did not require any additional data

Data-Driven ROM Framework: Summary

1. Sample the parameter domain and solve FOM
2. Compute optimal basis of rank K (POD)
3. Form primitive ROM through Galerkin projection
4. Select subgrid-scale model(s)
5. Optimize for model parameters for parameter instance
6. Learn model parameters as a function of input features
7. Optimize for noise variance based on validation frequencies
8. Learn noise variance as a function of input features
9. Perform model selection

Numerical Experiments

Numerical Example: Advection Diffusion ROM

- Examine the parameterized advection-diffusion equation

$$u_t = u_x + \frac{1}{Re} u_{xx}$$

$$u(0,t) = u(2,t) = 0$$

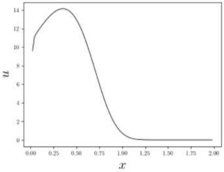
$$u(x,0) = x(2-x)\exp(2x)$$

- Parameters:
  - $Re \in [50, 500]$: Reynolds number

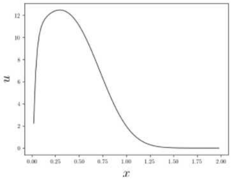
- Truth model is a finite difference scheme

$$\frac{du_k}{dt} = p_0 \frac{u_{k+1} - u_k}{\Delta x} + p_1 \frac{u_{k+1} - 2u_k + u_{k-1}}{\Delta x^2},$$

  - $N = 100$



Re = 237



Re = 50

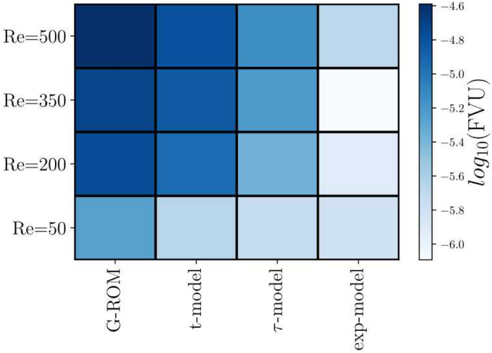
Generation of Data-Informed Reduced Model

1. Solve truth model for $\mathrm{Re} = [50, 200, 350, 500]$
2. POD of solution snapshots to generate trial basis
   - Select basis size from 99% energy criteria
3. Form baseline ROM through Galerkin projection
4. Calibrate SGS models on $\mathrm{Re} = [50, 200, 350, 500]$ cases
   - Gaussian process regression is used to calibrate parameters
5. Calibrate noise model based on 95% validation frequency

Training Results

- Evaluate trained models based on FVU metric:

$$FVU = 1 - r^2$$



- **exp-model performs the best across all parameter instances**

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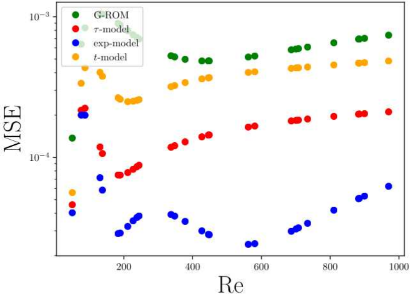
Test Set Results

- All ROMs are evaluated on 30 samples for $Re \in [20, 500]$
- Accuracy assessed from mean-squared error

	MSE	% Reduction
G-ROM	2.11e-3	0%
t-model	3.65e-4	43.4%
τ-model	1.47e-4	77.1%
exp-model	**4.94e-5**	**93.9%**

MSE and percent reduction in error



MSE as a function of Reynolds number

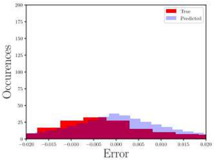
- **exp-model performs the best across all parameter instances**

Uncertainty Propagation

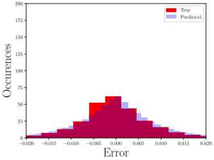
- Propagate uncertainty through the noise model
- Predicted versus true confidence intervals:

	G-ROM	τ-model	exp-model
68%	82.2%	83.4%	82.1%
95%	**94.4%**	**94.9%**	**94.9%**
99%	96.7%	97.0%	97.3%

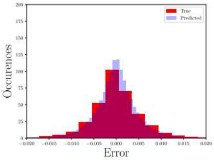
- Distributions predicted by noise models are *not* statistically accurate
  - Temporal correlations are ignored
  - Gaussian distribution is inaccurate
  - etc.
- **Validation frequencies used in training are accurate**



G-ROM



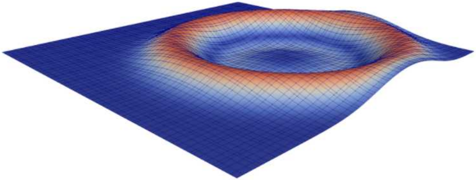
τ-model



exp-model

Numerical Example: ROM of Shallow Water Equations

- Solve the shallow water equations parameterized by
  - Gravity: $g = [2, 9]$.
  - Water height: $h_0 = [0.05, 0.2]$.



- Truth model is a 4th order discontinuous Galerkin scheme
  - Contains 12k degrees of freedom

Construction of Reduced Order Model

- Full-order model is solved for a grid $g = [3, 6, 9]$, $h = [0.05, 0.125, 0.2]$
- POD of solution snapshots to generate trial basis
  - Select basis size from 99.9% energy criterion (226 modes)
- Form primitive ROM through Galerkin projection
- Calibrate SGS models on FOM runs used for trial basis generation
  - Multivariate linear regression is used to calibrate parameters

- *Note: No hyper-reduction is used to accelerate the non-linear residual evaluation*

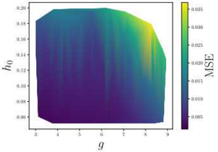
Results

- ROMs are solved for 100 random samples of the parameters
- Error is assessed through MSE

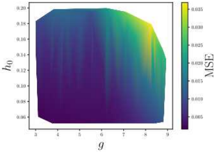
	MSE	% Reduction
G-ROM	0.0112	0%
τ-model	0.0106	5.4%
exp-model	0.0052	53.3%

MSE and percent reduction in error

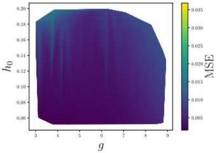
- Non-local subgrid-scale model leads to significant error reduction



G-ROM



τ-model



exp-model

Summary

- Quantifying and reducing errors in reduced-order models is of critical importance
- Outlined a data-driven framework for subgrid-scale model calibration and selection
  - Use MZ-based method to model unresolved effects in ROMs
  - Utilized ROM training data to perform model calibration
    - Supervised learning methods are used to learn model parameters
  - Utilized ROM training data to perform model selection
- Demonstrated method on advection diffusion and shallow water equations
  - Framework led to significant error reductions in all cases
  - exponential MZ model performed the best in all cases

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Problem Description

Data-Calibrated Subgrid-Scale Modeling Framework

Numerical Experiments

Thank you for your time!

- Funding sources:
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