Learning non-intrusive data-driven reduced models: application to large-scale systems

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Workshop on Data-driven & Reduced Order Modeling for Multi-Scale Problems

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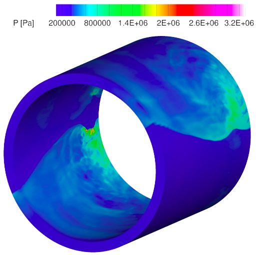
August 31, 2023

Learning predictive data-driven reduced models of rotating-detonation rocket engine combustion chambers via Operator Inference



Goals

- construct physics-based data-driven reduced models of large-scale RDRE simulations with sufficient engineering accuracy
- use these ROMs for downstream tasks such as design optimization

Computational challenges

- the high-fidelity LES simulations are large-scale and computationally very expensive (a single simulation typically requires $\mathcal{O}(10^6)$ core-hours on supercomputers)
- the resulting training data sets are often sparse
- they comprise down-sampled time instants from the high-fidelity simulation
- only few parametric instances can realistically be simulated to generate training data

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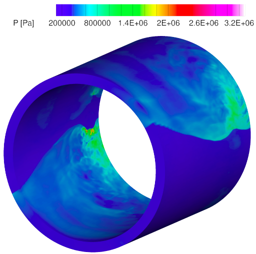

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Part I: constructing ROMs for large-scale simulations for predictions beyond the training time horizon

Discrete operator inference: general idea

- starting point: a physics-based model, typically described by PDEs or ODEs
- variable transformations that expose polynomial structure in the model
- lens of projection to define the form of a structure-preserving low-dimensional model

} define the structure of the reduced model

Operator inference learning problem

- non-intrusive learning by inferring reduced model operators from data

$$\underset{\hat{\mathbf{O}}}{\operatorname{argmin}} \|\hat{\mathbf{D}}\hat{\mathbf{O}} - \hat{\mathbf{R}}\|_F^2 + \text{regularization}$$

  - $\hat{\mathbf{O}}$: low-dimensional operators define the reduced model as a discrete system
  - $\hat{\mathbf{D}}, \hat{\mathbf{R}}$: data matrix/forcing from simulation and/or experimental data
  - minimum residual formulation leads to linear least-squares minimization
  - regularization is key to reduce overfitting, account for model misspecification etc.

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Steps to perform discrete operator inference

I. Start: full-order model. Suppose the process of interest is described through (possibly after applying a lifting transformation) the high-dimensional quadratic discrete model

$$\mathbf{w}[k+1] = \mathbf{A}\mathbf{w}[k] + \mathbf{H}(\mathbf{w}[k] \otimes \mathbf{w}[k])$$

II. Discrete operator inference:

1. training data: compute a set of n_t full-order model solutions (snapshots)
2. training data manipulation (lifting, centering, scaling) to get the snapshot matrix of the transformed variables $\mathbf{Q} \in \mathbb{R}^{n \times n_t}$
3. subspace identification: determine rank-r reduced basis $\mathbf{V}_r \in \mathbb{R}^{n \times r}$ via the (thin) singular value decomposition of $\mathbf{Q}$
4. projection: project each transformed snapshot: $\hat{\mathbf{Q}}[k] = \mathbf{V}_r^\top \mathbf{Q}[k] \in \mathbb{R}^{r \times n_t}$
5. learn reduced operators $\hat{\mathbf{A}} \in \mathbb{R}^{r \times r}$, $\hat{\mathbf{H}} \in \mathbb{R}^{r \times r^2}$, and $\hat{\mathbf{c}} \in \mathbb{R}^r$ via operator inference with regularization

III. Finish: reduced-order model. The learned reduced operators define the ROM

$$\hat{\mathbf{q}}[k+1] = \hat{\mathbf{A}}\hat{\mathbf{q}}[k] + \hat{\mathbf{H}}\left(\hat{\mathbf{q}}[k] \otimes \hat{\mathbf{q}}[k]\right) + \hat{\mathbf{c}}$$

We then use the reduced model to issue predictions beyond the training time horizon

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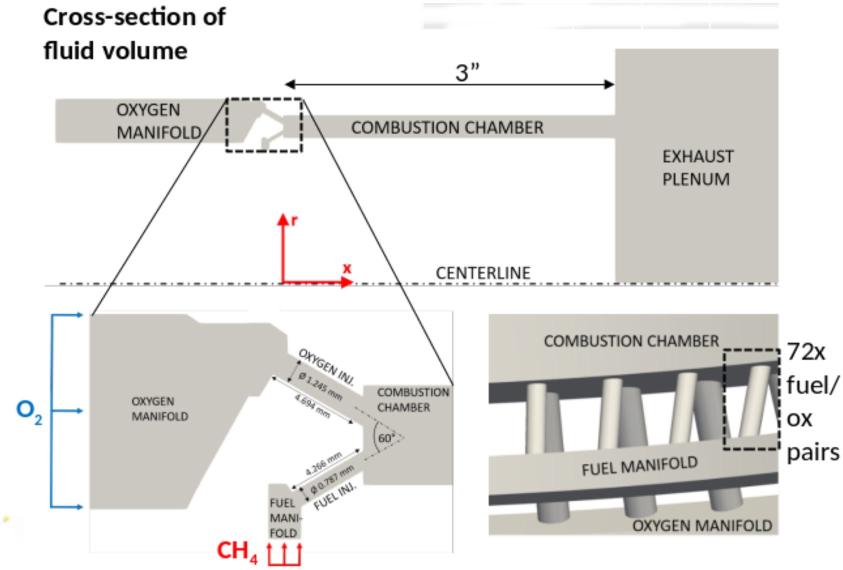
Numerical demonstration

Modeling the combustion chamber of a rotating detonation rocket engine



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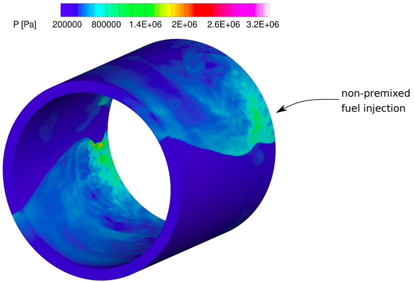

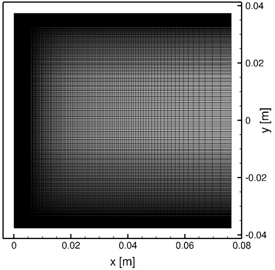

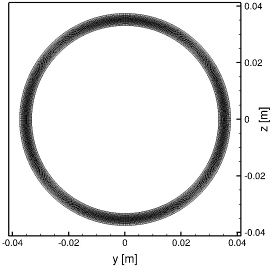

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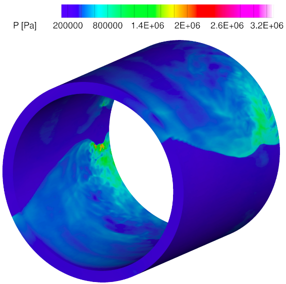
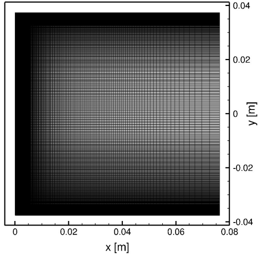
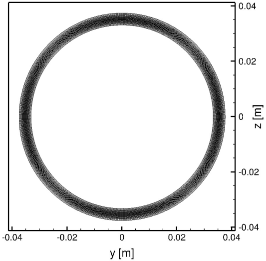
- injector design with 72 discrete injector pairs



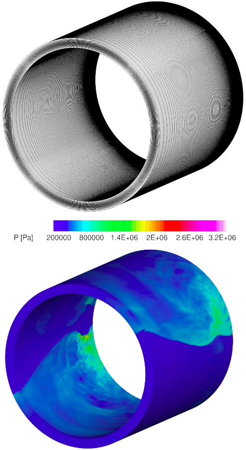




Modeling the combustion chamber of a rotating detonation rocket engine

1. Generate training data + data manipulation

- $\dot{m} = 0.267\ \mathrm{kg} \cdot \mathrm{s}^{-1}$ and $\Phi = 1.16$
- 2 ms of full-state solutions generated ~6M CPU hours on $>$ 16K cores
- the original simulation data has been interpolated on a structured mesh comprising $n_x = 4,204,200$ spatial DoF
- time step size $\Delta t \sim 10^{-9}$ s
- available data: 501 down-sampled snapshots over $[2.50, 3.75]$ ms (~4 periods of two-wave system)
- 18 transformed state variables: specific volume, pressure, 3D velocity, temperature, 12 species mass fractions (full chemistry data)
- training data: snapshot matrix $\mathbf{Q} \in \mathbb{R}^{76M \times 375}$

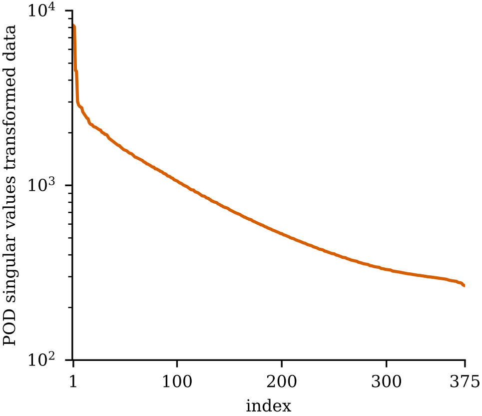


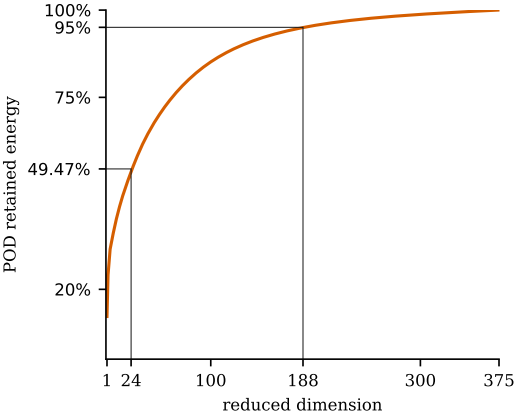
Two dominant co-rotating waves in the quasi-limit-cycle behavior of the flow

Modeling the combustion chamber of a rotating detonation rocket engine

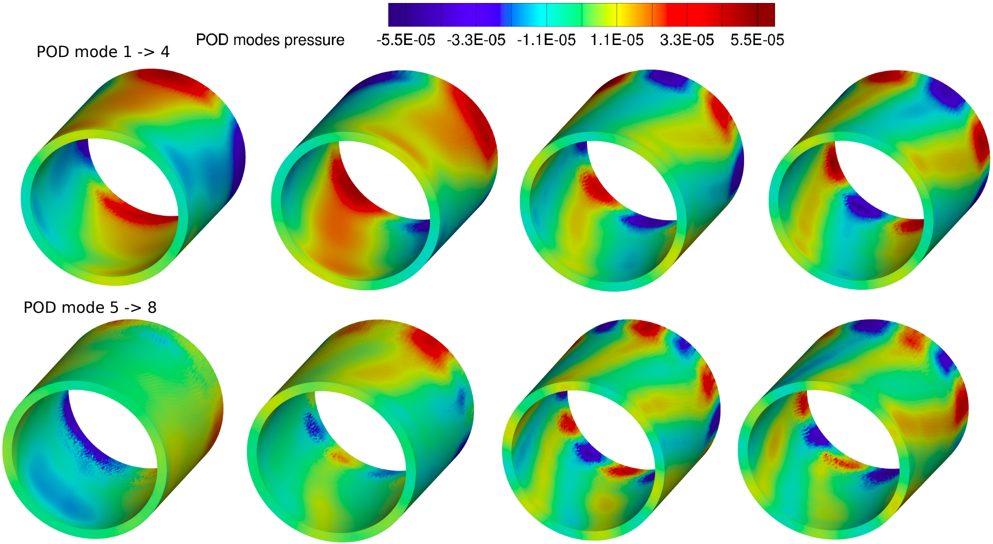
2. Compute POD basis

- snapshot matrix of transformed variables
- scale and center snapshot data
- compute POD basis $\mathbf{V}_r \in \mathbb{R}^{76M \times r}$
- low-data regime limits size of the non-intrusive ROM



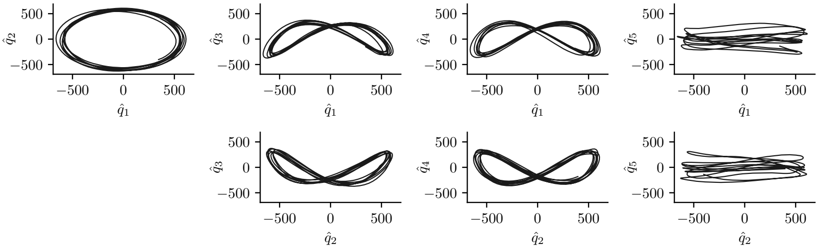


Modeling the combustion chamber of a rotating detonation rocket engine

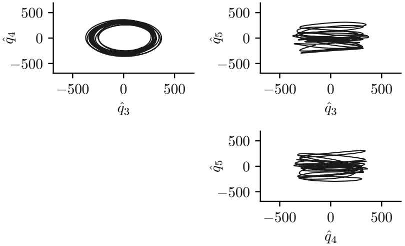


Modeling the combustion chamber of a rotating detonation rocket engine

Two-dimensional phase portraits of POD amplitudes



note that these amplitudes represent the data used in the OpInf inference problem

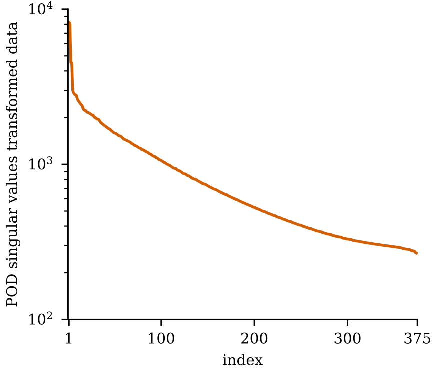


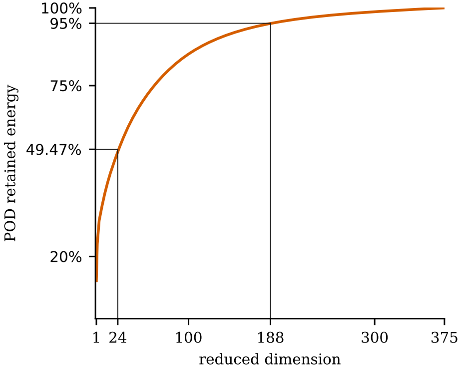
Modeling the combustion chamber of a rotating detonation rocket engine

3. Infer reduced operators

- compute reduced snapshot matrix $\hat{\mathbf{Q}} = \mathbf{V}_r^\top \mathbf{Q} \in \mathbb{R}^{r \times 375}$

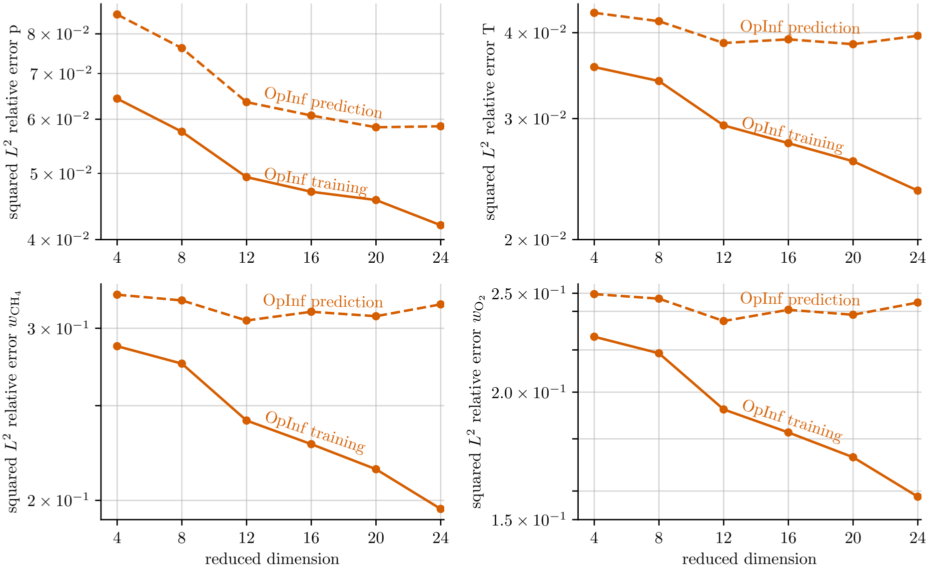
- learn a fully discrete quadratic ROM
- solve linear least squares to infer reduced operators



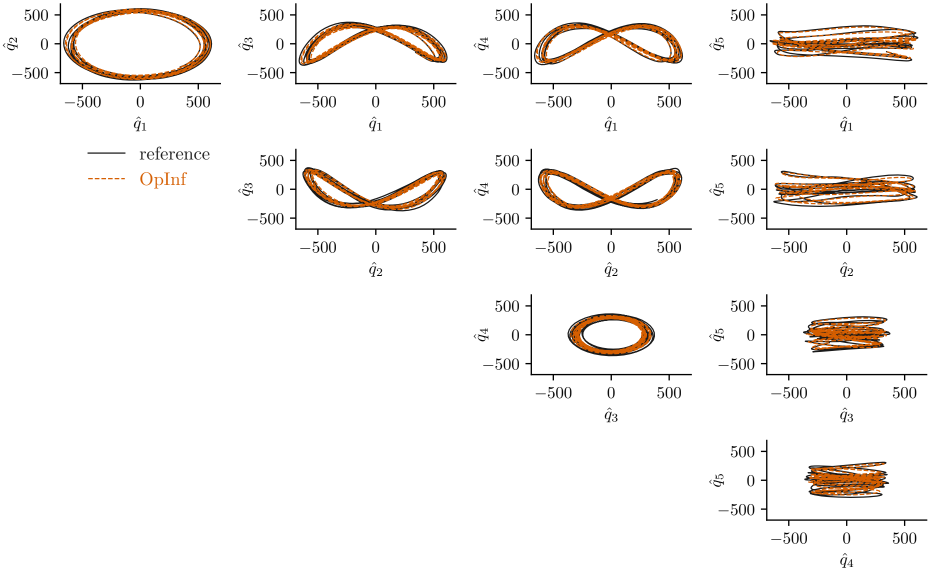


resulting reduced model is completely decoupled from the original CFD code

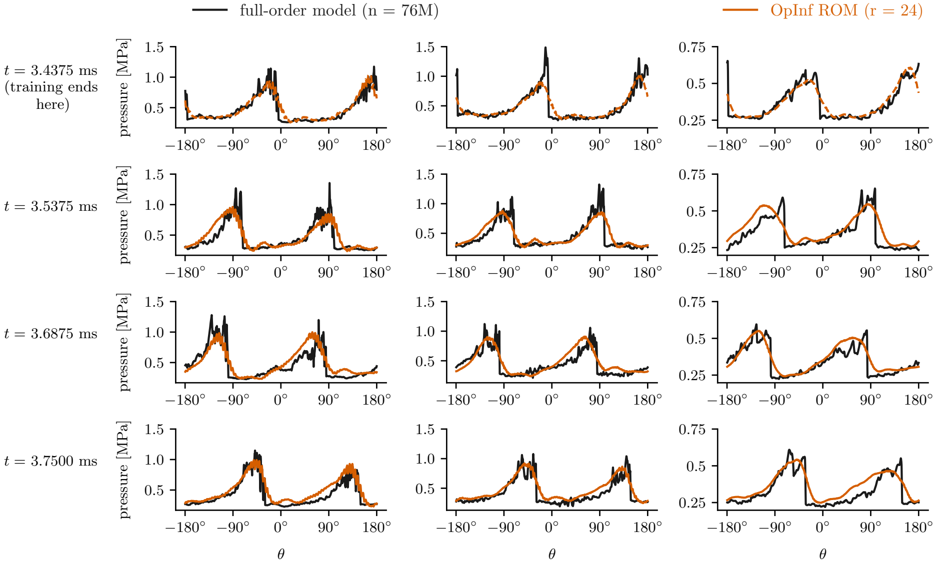
OpInf reduced model relative error



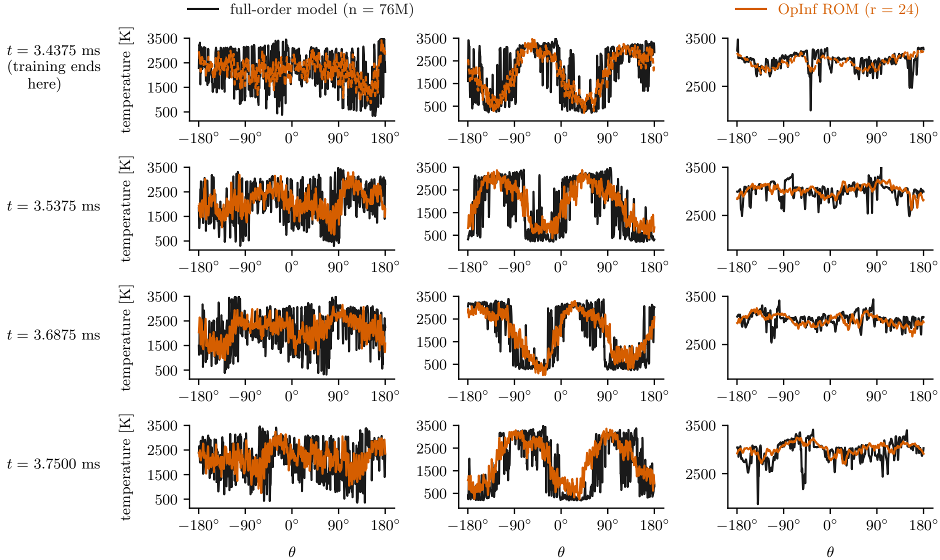
OpInf predictions for two-dimensional phase portraits



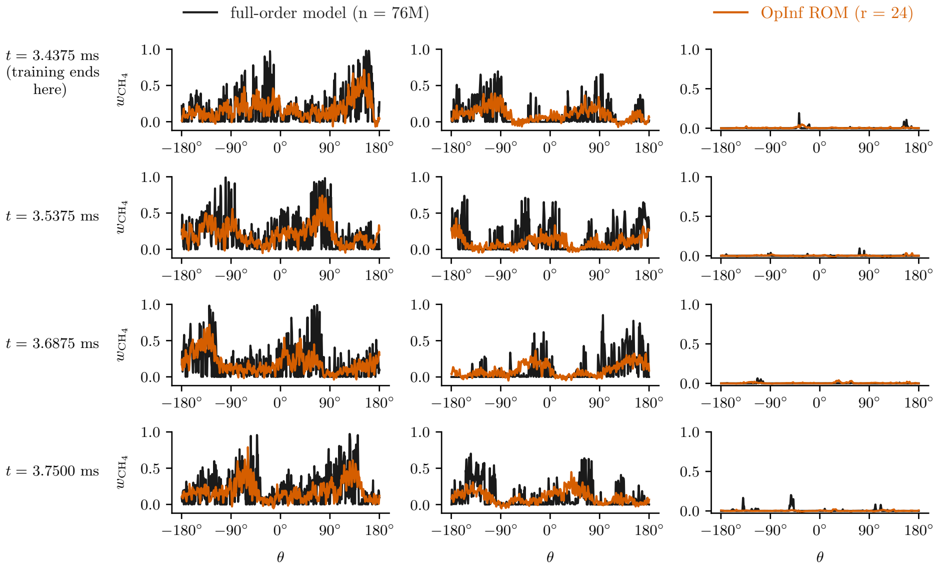
One-dimensional circumferential pressure profiles



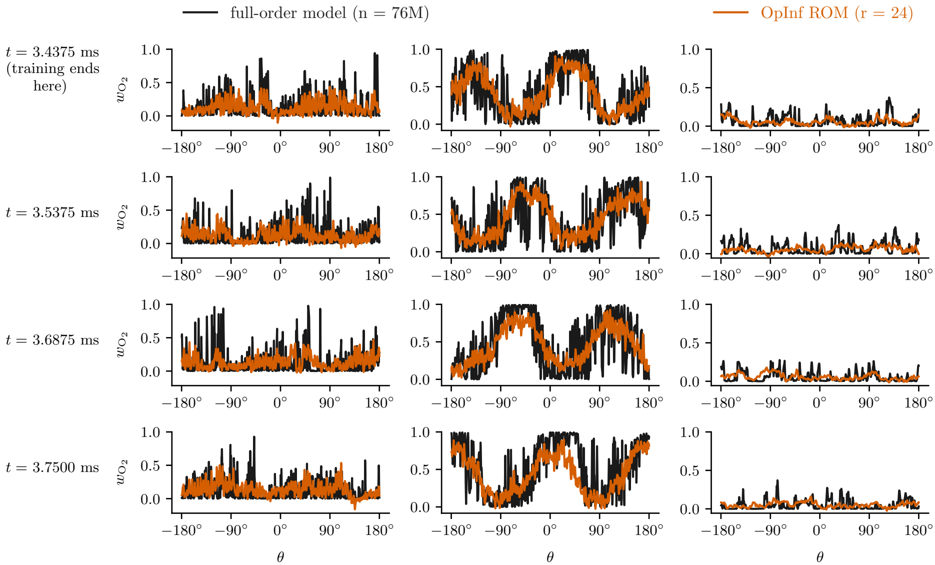
One-dimensional circumferential temperature profiles



One-dimensional circumferential fuel mass fraction profiles



One-dimensional circumferential oxidizer mass fraction profiles



Part II: towards predictive parametric ROMs of large-scale RDRE combustion chamber simulations

Parametric discrete operator inference: general idea

- a parametric physics-based model, typically described by PDEs or ODEs
- variable transformations that expose polynomial structure in the model
- lens of projection to define the form of a structure-preserving low-dimensional parametric model

} define the structure of the parametric reduced model

Discrete parametric operator inference learning problem

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Steps to perform parametric discrete operator inference

I. Start: full-order model that depends on a d-dimensional parameter $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^d$. Suppose that the process of interest can be described (possibly after a lifting transformation) through the high-dimensional parametric quadratic discrete model

$$\mathbf{w}[k+1] = \mathbf{A}(\boldsymbol{\mu})\mathbf{w}[k] + \mathbf{H}(\boldsymbol{\mu})\left(\mathbf{w}[k] \otimes \mathbf{w}[k]\right)$$

We seek a to construct a parametric reduced model via OpInf with reduced dimension $r \ll n$.

To this end, we consider a quadratic-bilinear model form for the parametric model:

$$\mathbf{w}[k+1] = \underbrace{\mathbf{A}_0\mathbf{w}[k]}_{\text{linear}} + \underbrace{\sum_{i=1}^{d} \mu_i \mathbf{A}_i \mathbf{w}[k]}_{\text{bilinear}} + \underbrace{\mathbf{H}_0\left(\mathbf{w}[k] \otimes \mathbf{w}[k]\right)}_{\text{quadratic}} + \underbrace{\sum_{i=1}^{d} \mu_i \mathbf{H}_i\left(\mathbf{w}[k] \otimes \mathbf{w}[k]\right)}_{\text{quadratic-linear}},$$

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Steps to perform parametric discrete operator inference

II. Parametric OpInf for the quadratic-bilinear ROM:

1. training data: compute n_t full-order model snapshots for each training parameter instance $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_m \in \mathbb{R}^d$
2. training data manipulation (lifting, centering, scaling) to obtain the snapshot matrix of transformed data $\mathbf{Q} \in \mathbb{R}^{n \times m n_t}$
3. subspace identification: rank-r global POD basis $\mathbf{V}_r \in \mathbb{R}^{n \times r}$ using the thin SVD of $\mathbf{Q}$
4. projection: project each snapshot to obtain $\hat{\mathbf{Q}} = \mathbf{V}_r^\top \mathbf{Q} \in \mathbb{R}^{r \times m n_t}$
5. learn reduced operators $\hat{\mathbf{A}}_i$, $\hat{\mathbf{H}}_i$ and $\hat{\mathbf{c}}_i$ for $i = 0, 1, \dots, d$ via operator inference with regularization

Steps to perform parametric discrete operator inference

III. Finish: parametric reduced-order model.
The learned reduced operators define the parametric quadratic-bilinear reduced model

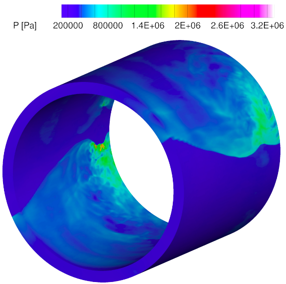
$$\hat{\mathbf{q}}[k+1] = \hat{\mathbf{A}}_0\hat{\mathbf{q}}[k] + \sum_{i=1}^{d} \mu_i \hat{\mathbf{A}}_i \hat{\mathbf{s}}[k] + \hat{\mathbf{H}}_0 \left(\hat{\mathbf{q}}[k] \otimes \hat{\mathbf{q}}[k]\right) + \sum_{i=1}^{d} \mu_i \hat{\mathbf{H}}_i \left(\hat{\mathbf{q}}[k] \otimes \hat{\mathbf{q}}[k]\right) + \hat{\mathbf{c}}_0 + \sum_{i=1}^{d} \mu_i \hat{\mathbf{c}}_i$$

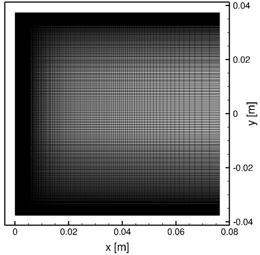
Given $\boldsymbol{\mu} \in \mathbb{R}^d$, we use the parametric ROM to issue parametric predictions beyond the training set

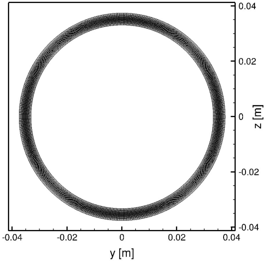
Numerical demonstration

Parametric modeling of an RDRE combustion chamber

- LES simulations of the reactive, viscous 3D Navier-Stokes equations
- skeletal chemistry mechanism based on the Foundational Fuel Chemistry Model (FFCMy-30)
- non-premixed fuel injection (gaseous methane and oxygen)
- injector design with 72 discrete injector pairs
- parametric variations in the flow conditions







Parametric modeling of an RDRE combustion chamber

Parametric description

- parametric variations in flow conditions (mass flow-rate, $\dot{m}$ $[\mathrm{kg} \cdot \mathrm{s}^{-1}]$, and equivalence ratio, Φ)
- these variations are characterized in our model using a scalar parameter $\mu \in \mathbb{R}$

$$\mu = \frac{\dot{m}}{\dot{m}_0} + \frac{\Phi}{\Phi_0},$$

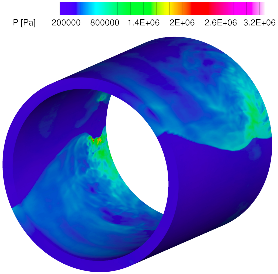
  where $\dot{m}_0$ and Φ_0 are the respective maximum mass flow-rate and equivalence ratio
- we have simulation data for three parameter instances

μ	Flow Condition	$\dot{m}$ $[\mathrm{kg} \cdot \mathrm{s}^{-1}]$	Φ	Time Interval	Periods	Dominant Waves	Secondary Waves
$\mu_1 = 1.41$	nominal	0.267	1.16	$[3.7525, 4.0000]$ ms	1.97	5	0
$\mu_2 = 1.73$	high Φ	0.266	1.71	$[1.8425, 2.0900]$ ms	1.64	6	8
$\mu_3 = 1.55$	high $\dot{m}$	0.333	1.09	$[3.7525, 4.0000]$ ms	1.97	5	0

Parametric modeling of an RDRE combustion chamber

1. Generate training data + data manipulation

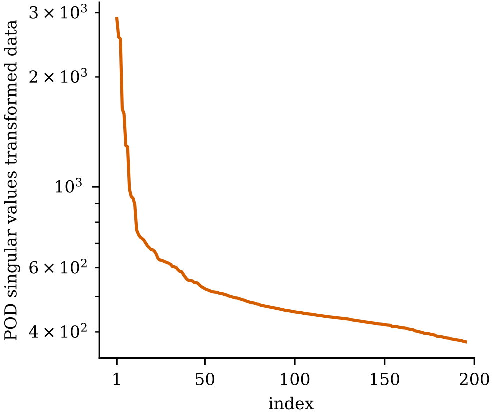
- 2 ms of full-state solutions for all three parameter instances generated ~6M CPU hours on > 16K cores
- the original simulation data has been interpolated on a structured mesh comprising $n_x = 4,204,200$ spatial DoF
- time step size $\Delta t \sim 10^{-9}$ s
- available data: 100 down-sampled snapshots for each parameter instance (about 0.25 ms of physical time)
- 8 transformed state variables: specific volume, pressure, 3D velocity, temperature, 2 species mass fractions (fuel and oxidizer)
- train ROM using data corresponding to μ_1 and μ_2, make ROM predictions for μ_3
- training data: snapshot matrix $\mathbf{Q} \in \mathbb{R}^{34M \times 200}$

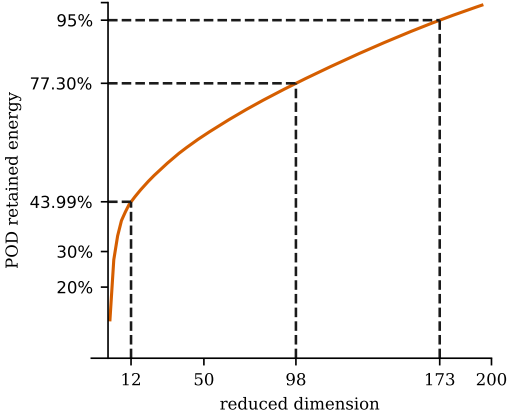


Parametric modeling of an RDRE combustion chamber

2. Compute (global) POD basis

- snapshot matrix of transformed variables
- scale and center snapshot data
- compute POD basis $\mathbf{V}_r \in \mathbb{R}^{34M \times r}$
- low-data regime limits size of the non-intrusive ROM

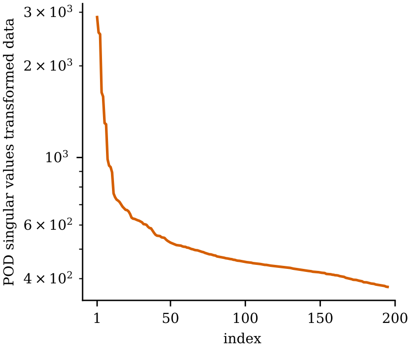


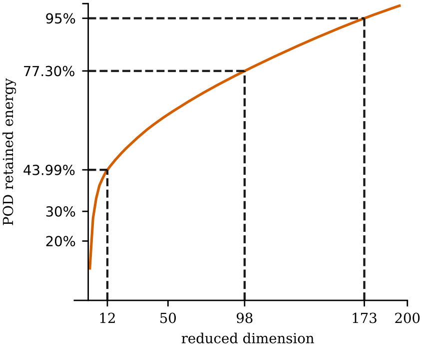


Parametric modeling of an RDRE combustion chamber

3. Inference reduced operators

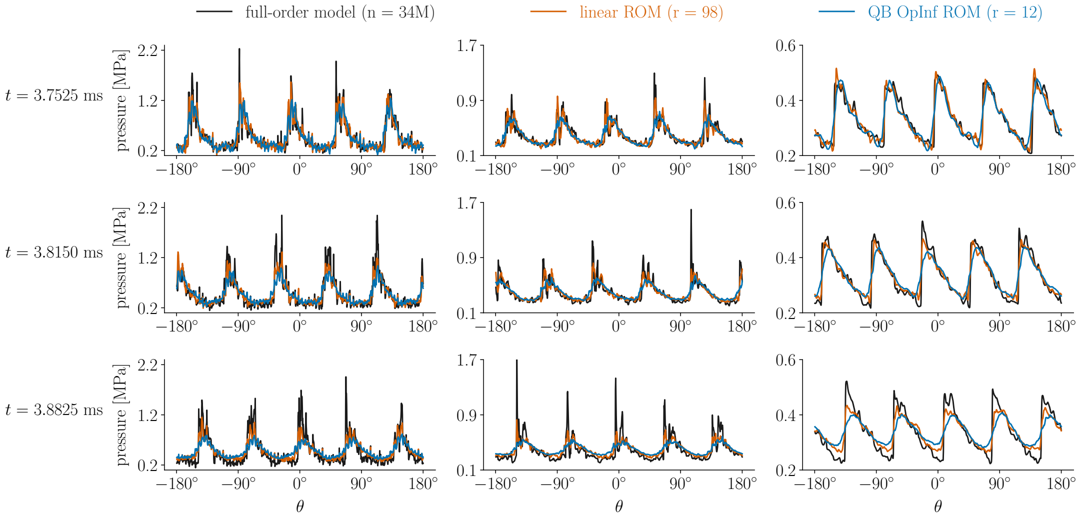
- compute reduced snapshot matrix $\hat{\mathbf{Q}} = \mathbf{V}_r^\top \mathbf{Q} \in \mathbb{R}^{r \times 200}$
- learn a fully discrete parametric ROM
- solve linear least squares to infer reduced operators



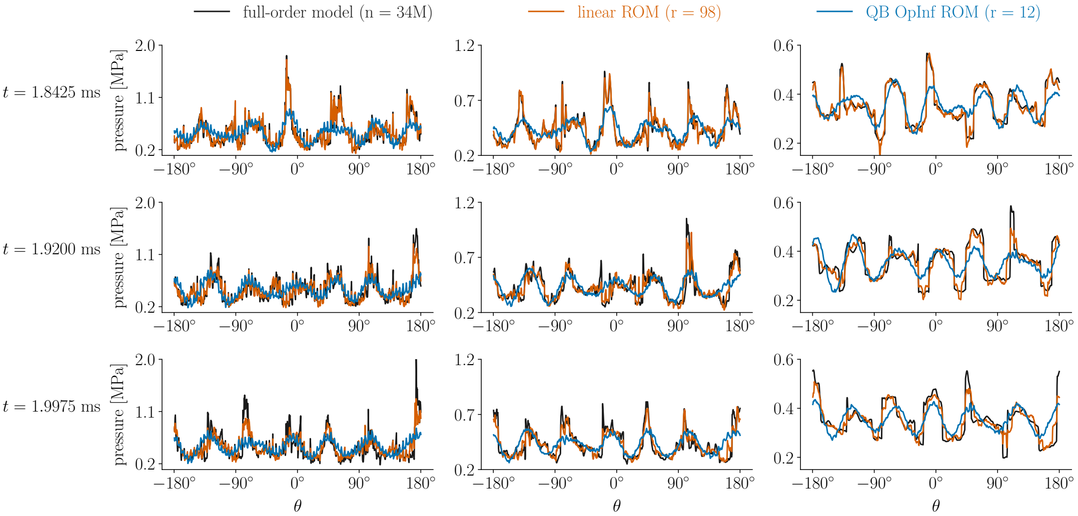


Due to the scarcity of the available data, we also consider linear parametric reduced models

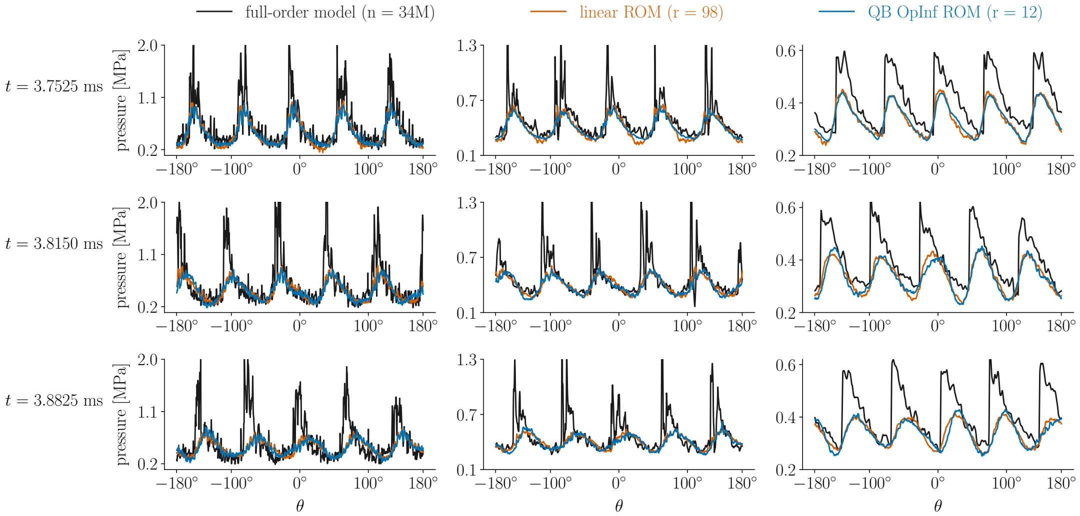
One-dimensional circumferential pressure profiles: 1st training parameter (nominal flow condition)



One-dimensional circumferential pressure profiles: 2nd training parameter (high equivalence ratio)



One-dimensional circumferential pressure profile prediction outside of the training set (3rd parameter, high mass flow-rate case)



Outlook

Domain-decomposed data-driven reduced models

- basis localization can lead to faster singular value decay $\rightarrow$ smaller r_i, although now have ROM of dimension r_i for each subdomain $i = 1, 2, \ldots, k$
- the decomposition also mitigates computational complexity of offline snapshot processing

Preprocess the training data set via filtering

- filter the snapshots in the training data set – variable by variable – prior to training the ROM
- filtering can reduce overfitting, improve the prediction accuracy of the ROM, and improve the condition of the Operator Inference learning problem

Summary - Non-intrusive ROMs

- non-intrusive formulation enables rapid deployment, ROM derivation without access to source code, and variable transformations to promote structure
- it moreover enables ROM development across multiple sites without the need to transfer large-scale data sets (e.g., training data generation, data manipulation, and POD basis computation at ARFL, and OpInf ROM construction and postprocessing at UT Austin)
- Operator Inference ROMs are completely decoupled from CFD code and very fast to simulate
- our ROMs evaluate within milliseconds on a laptop computer
- Operator Inference can be used to construct both ROMs for predictions beyond the training time horizon and parametric ROMs
- slow singular value decay is a challenge for linear-subspace approximations
- generation of training data is a major expense; for realistic combustion problems we generally lack sufficient training data to fully resolve the dynamics
- domain decomposition and filtering are promising approaches to address these challenges

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