Data-driven Reduced-order Models via Regularized Operator Inference for a Single-injector Combustion Process

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Key Outcomes

- Variable transformations expose a polynomial structure in a system of nonlinear partial differential equations, enabling efficient non-intrusive learning of accurate polynomial reduced-order models (ROMs) from data via Operator Inference (OpInf).
- The minimization problem requires careful regularization. We establish a principled approach for regularization selection that balances training error and long-term integration behavior.
- A two-dimensional single-injector combustion process presents a challenging application for traditional model reduction techniques, but properly regularized OpInf ROMs compare favorably with a state-of-the-art intrusive approach.

Regularized Operator Inference

- Operator Inference forms a polynomial ROM with the structure defined by transformed PDEs by learning operators $\hat{\mathbf{c}}, \hat{\mathbf{A}}, \hat{\mathbf{H}}, \hat{\mathbf{B}}$ from data:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{q}}(t) = \hat{\mathbf{c}} + \hat{\mathbf{A}}\hat{\mathbf{q}}(t) + \hat{\mathbf{H}}(\hat{\mathbf{q}}(t) \otimes \hat{\mathbf{q}}(t)) + \hat{\mathbf{B}}\mathbf{u}(t), \qquad t \in [t_0, t_f].$$

- To obtain training data,
  1. Simulate the high-fidelity model, generating raw snapshots.
  2. Transform the raw snapshots to the learning variables.
  3. Compute a rank-r POD basis from the transformed snapshots.
  4. Use the basis to project the transformed snapshots.
  5. Estimate projected time derivatives from projected snapshots.

- The projected snapshots $\{\hat{\mathbf{q}}_j\}_{j=0}^{k-1}$ and estimated time derivatives $\{\dot{\hat{\mathbf{q}}}_j\}_{j=0}^{k-1}$ drive the minimal-residual OpInf learning problem:

$$\min_{\hat{\mathbf{c}}, \hat{\mathbf{A}}, \hat{\mathbf{H}}, \hat{\mathbf{B}}} \sum_{j=0}^{k-1} \left\| \hat{\mathbf{c}} + \hat{\mathbf{A}}\hat{\mathbf{q}}_j + \hat{\mathbf{H}}(\hat{\mathbf{q}}_j \otimes \hat{\mathbf{q}}_j) + \hat{\mathbf{B}}\mathbf{u}_j - \dot{\hat{\mathbf{q}}}_j \right\|_2^2.$$

- The OpInf minimization problem can be written in standard least-squares form, decoupled into r individual problems, and augmented with a Tikhonov regularization:

$$\min_{\mathbf{o}} \|\mathbf{D}\mathbf{o}_i - \mathbf{r}_i\|_2^2 + \|\lambda \mathbf{o}_i\|_2^2, \qquad \mathbf{o}_i = i^{\text{th}} \text{ row of } \mathbf{O} = [\hat{\mathbf{c}}\ \hat{\mathbf{A}}\ \hat{\mathbf{H}}\ \hat{\mathbf{B}}].$$

- The regularization parameter $\lambda > 0$ is chosen to minimize training error while maintaining a bound on the integrated coefficients $\hat{\mathbf{q}}(t)$ over the time domain of interest $[t_0, t_f]$.

Combustion Process

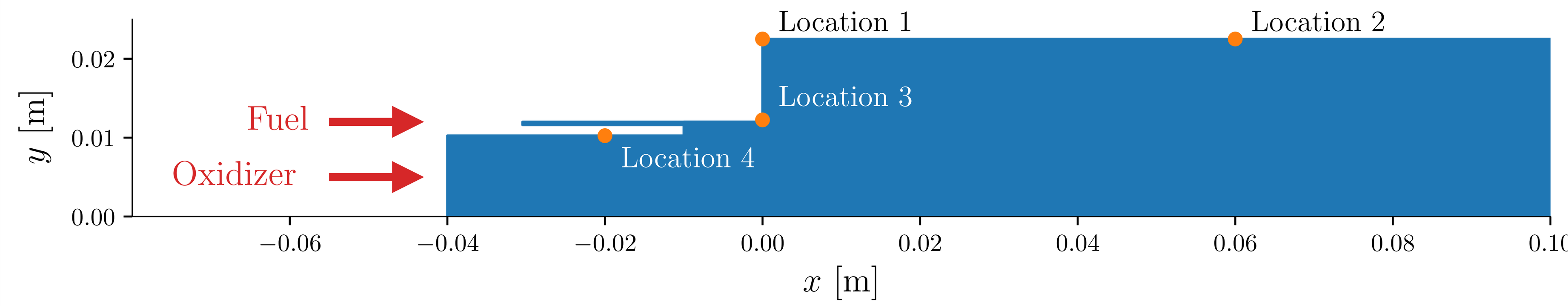


Figure 1: Computational domain with point trace monitoring locations.

- Governing equations describe conservation of mass, momentum, energy, and chemical species,

$$\frac{\partial \vec{q}_c}{\partial t} + \nabla \cdot (\vec{K} - \vec{K}_v) = \vec{S},$$

where $\vec{q}_c = [\rho \quad \rho v_x \quad \rho v_y \quad \rho e \quad \rho Y_{CH_4} \quad \rho Y_{O_2} \quad \rho Y_{H_2O} \quad \rho Y_{CO_2}]^T$ are the conservative variables. Chemical species are modeled with a one-step combustion process,

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O.$$

- Conservation equations are solved at high fidelity with the finite-volume based General Equations and Mesh Solver (GEMS).
- Variable transformations expose a nearly quadratic polynomial structure in the learning variables $\vec{q} = [p \quad v_x \quad v_y \quad T \quad 1/\rho \quad c_{CH_4} \quad c_{O_2} \quad c_{H_2O} \quad c_{CO_2}]^T$.

Results: Sensitivity to Training Data

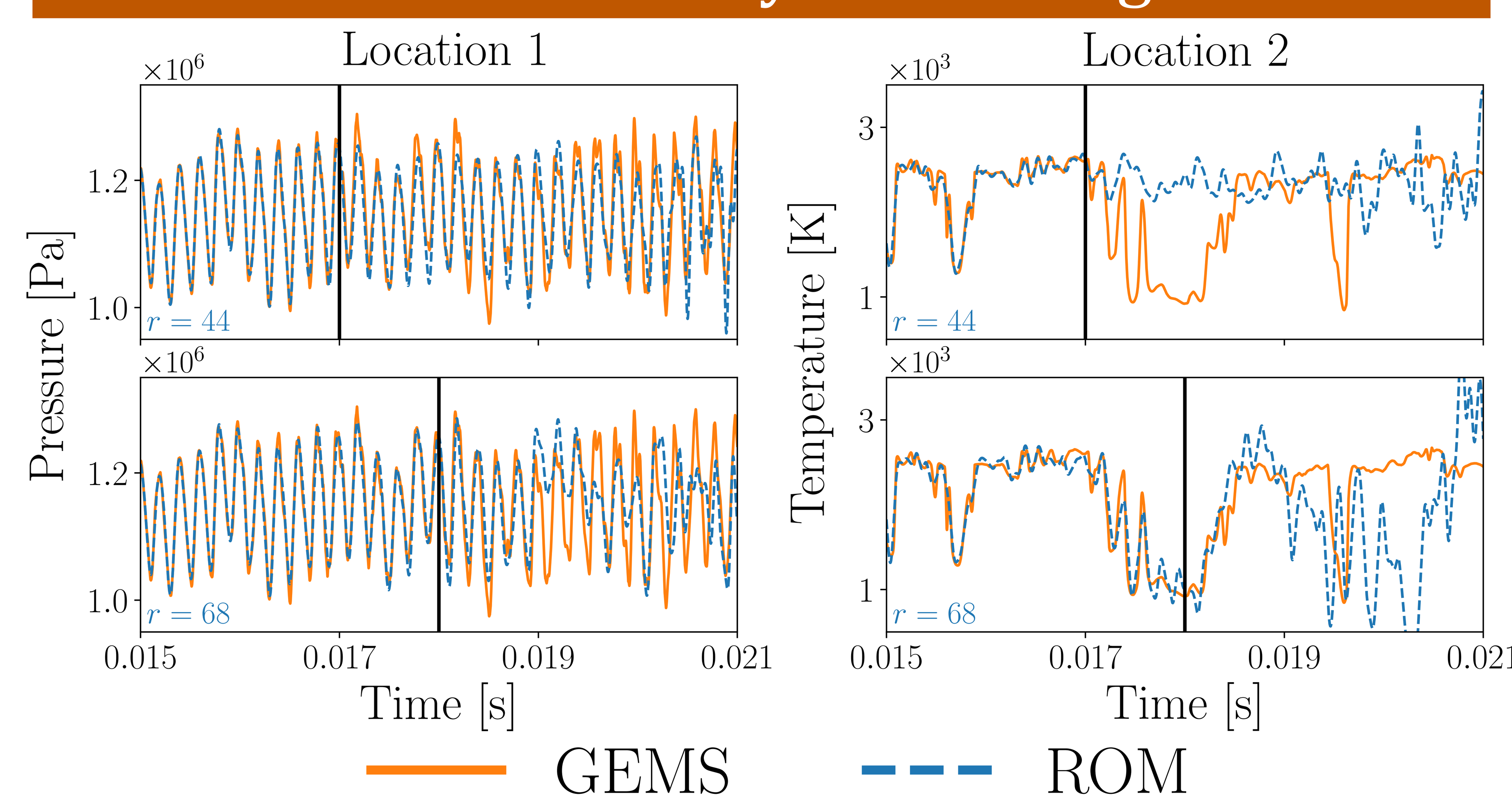


Figure 2: Point traces of GEMS training data and predictions from two OpInf ROMs. Each ROM exhibits high accuracy in re-predicting the training regime and acceptable accuracy in predicting future dynamics, while achieving close to a million times speedup in computational cost compared to GEMS.

Results: Comparison to POD-DEIM

We compare regularized Operator Inference to a state-of-the-art intrusive method that uses a least-squares Petrov-Galerkin POD projection coupled with the discrete empirical interpolation method (DEIM). The OpInf ROMs provide the same or better accuracy at approximately one thousandth of the computational cost.

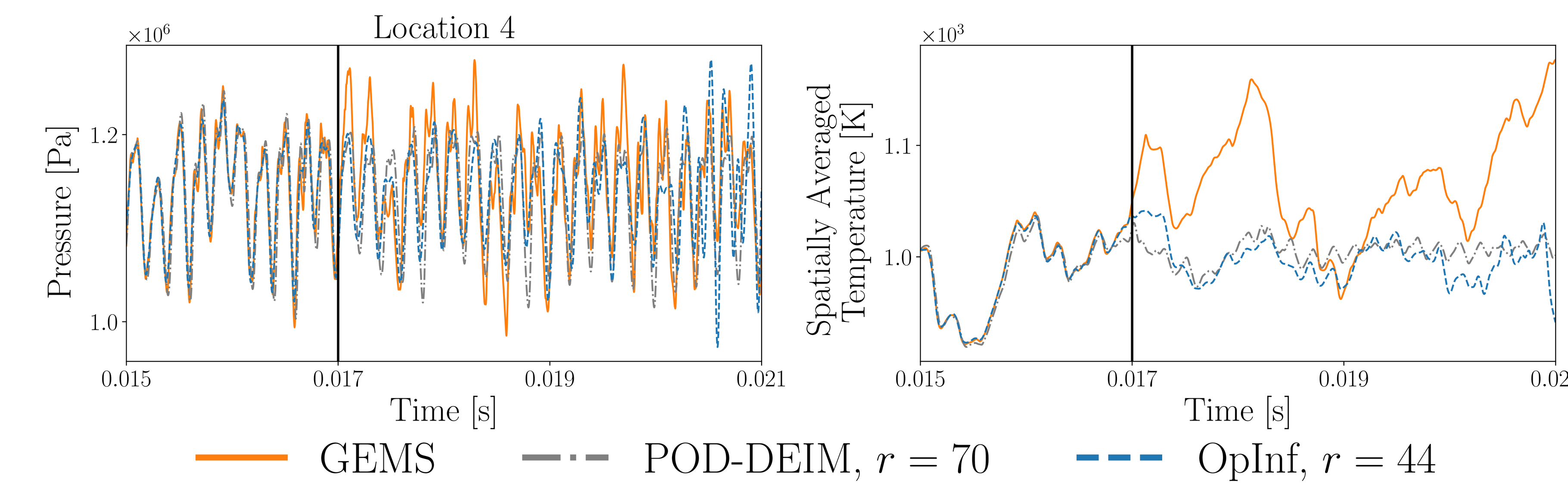
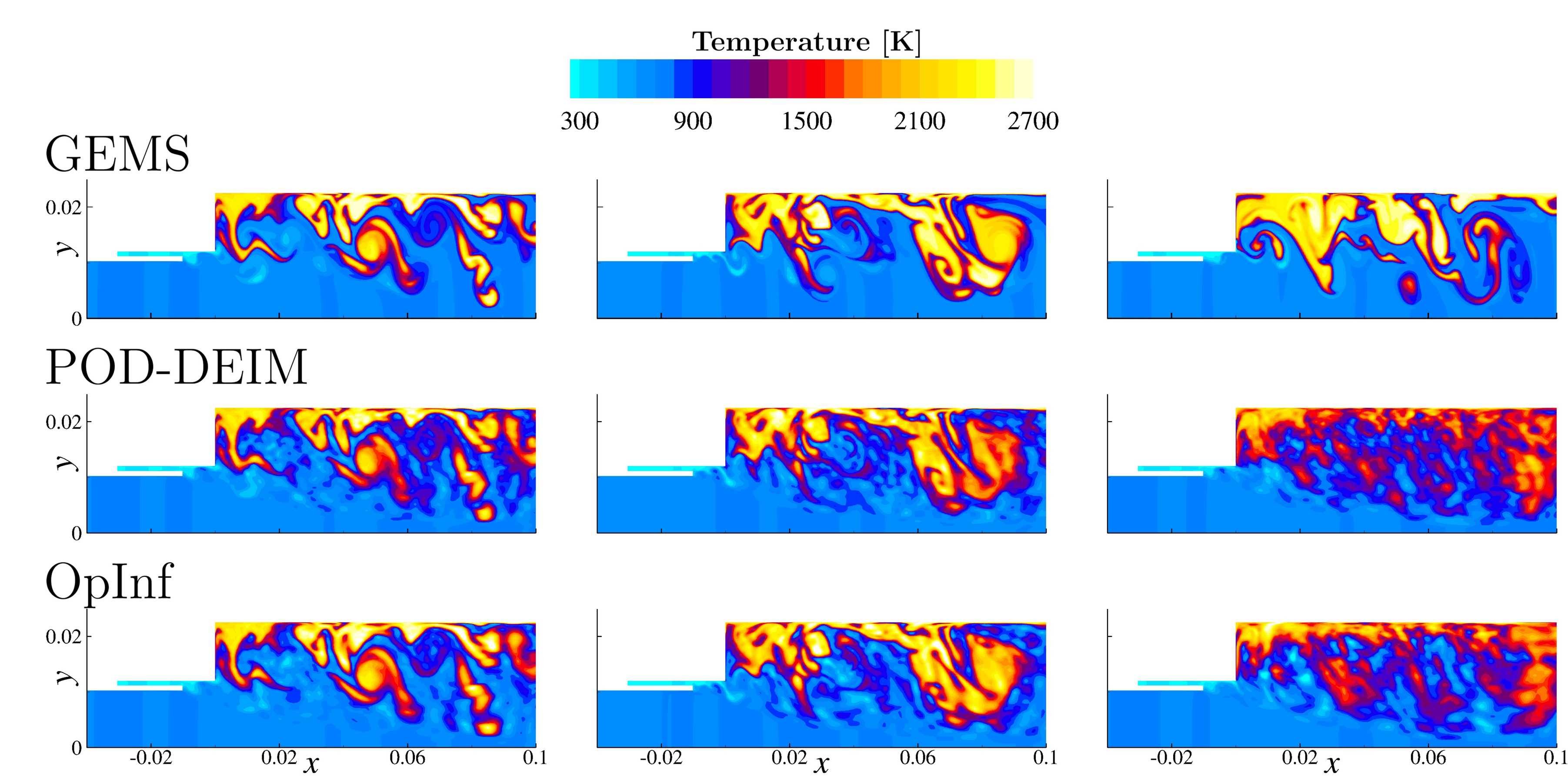


Figure 3: Comparison of an OpInf ROM to a POD-DEIM ROM, trained with the same amount of data. Both approaches reconstruct the training data well and maintain appropriate pressure oscillation frequencies, but they struggle to predict the erratic temperature dynamics beyond the training horizon.



(a) training regime (b) end of training (c) prediction regime

Figure 4: Full-domain temperature reconstructions in the training regime, at the end of the training, and into the prediction regime.

Resources

- McQuarrie SA, Huang C, Willcox K. 2020. Data-driven reduced-order models via regularized operator inference for a single-injector combustion process. arXiv:2008.02862.
- https://github.com/Willcox-Research-Group/ROM-OpInf-Combustion-2D