

Physics-informed machine learning for reactive mixing

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Abstract

Reduced-order models (ROMs) for reactive mixing in a vortex-based velocity field are developed using machine learning algorithms. Datasets based on high-fidelity simulations of anisotropic reaction-dispersion are used for training the algorithms. A recently developed non-negative finite element formulation is used for the high-fidelity simulations. We show that the developed ROMs are accurate compared to high-fidelity simulations with a R^2 -score is greater than 0.9 while the computational time of ROMs are five orders of magnitude faster than high-fidelity simulations.

Introduction

Subsurface models are computationally intensive due to the complexities of coupling various processes (such as flow, heat and mass transfer, chemical reactions, damage/fracturing, and mechanical deformation), size of the domains, and length of time of interest. Typically, high-fidelity numerical simulations of these models take hours to days on several thousands of processors, and may not be feasible for real-time calculations and uncertainty quantification where one needs to run thousands of such simulations. Hence, there is a pressing need to develop simpler, more computationally efficient models (which take seconds to run on a laptop) while still accurately predicting the desired quantities of interest for real-time applications. An attractive way to construct computationally efficient models is through reduced-order modeling that are fast. Herein, we present a physics-informed machine learning (ML) framework to construct reduced-order models (ML-ROMs) for reactive mixing quantities of interest (QoIs) based on high-fidelity numerical simulations. QoIs include species decay, product yield, and degree of mixing.

Methodology

High-resolution datasets for constructing ML-ROMs are generated by solving anisotropic reaction-dispersion equations using a non-negative finite element formulation [1, 2] for different input parameters for perturbed vortex-based velocity fields. A fast reaction $A + B \rightarrow C$ is used and more than 2000 realizations with a spatial-temporal resolution of $81 \times 81 \times 1000$ are used for generating the datasets. The non-negative finite element formulation ensures that species concentration is non-negative on coarse computational grids even under high degree of anisotropy. The input parameters are a time-scale associated with flipping of velocity, a spatial-scale controlling small/large vortex structures of velocity, a perturbation parameter of the vortex-based velocity, anisotropic dispersion strength/contrast, and molecular diffusion. Methods such random forests, F-test, and mutual information criterion are then used to evaluate the importance of model inputs/features with respect to QoIs. Support Vector Machines (SVM) and Support Vector Regression (SVR) are then used to construct ROMs based on the model inputs. Then, SVR-ROMs are used to predict scaling QoIs, and compared against the high-fidelity predictions.

Results

We observed that anisotropic dispersion strength/contrast is the most important feature and time-scale associated with flipping of velocity is the least important feature. Qualitatively, SVR-ROMs were able describe the trends observed in the scaling laws associated with QoIs. Moreover, it is observed that SVR-ROMs accuracy measured in terms of R^2 -score is greater than 0.9. Meaning that, we have a good quantitative prediction using SVR-ROMs. Figure 1 shows the concentration profile of product C for two realizations and the predictions of the concentrations of the reactants and product using the SVR-ROMs. The scaling law exponent dependence on model inputs/features were also evaluated using k -means clustering. Based on clustering analysis, we infer that incomplete mixing occurs at high anisotropic contrast and the system is well-mixed for low anisotropic contrast. In terms of computational time, the proposed SVM-ROMs and SVR-ROMs are $\mathcal{O}(10^5)$ times faster than high-fidelity numerical simulations. Overall, the developed ML-ROMs are fast and provide reasonably good predictions. This makes them applicable for real-world reactive-transport problems such as model predictions of contaminant fate and transport as well as for real-time analyses and interpretation of monitoring data.

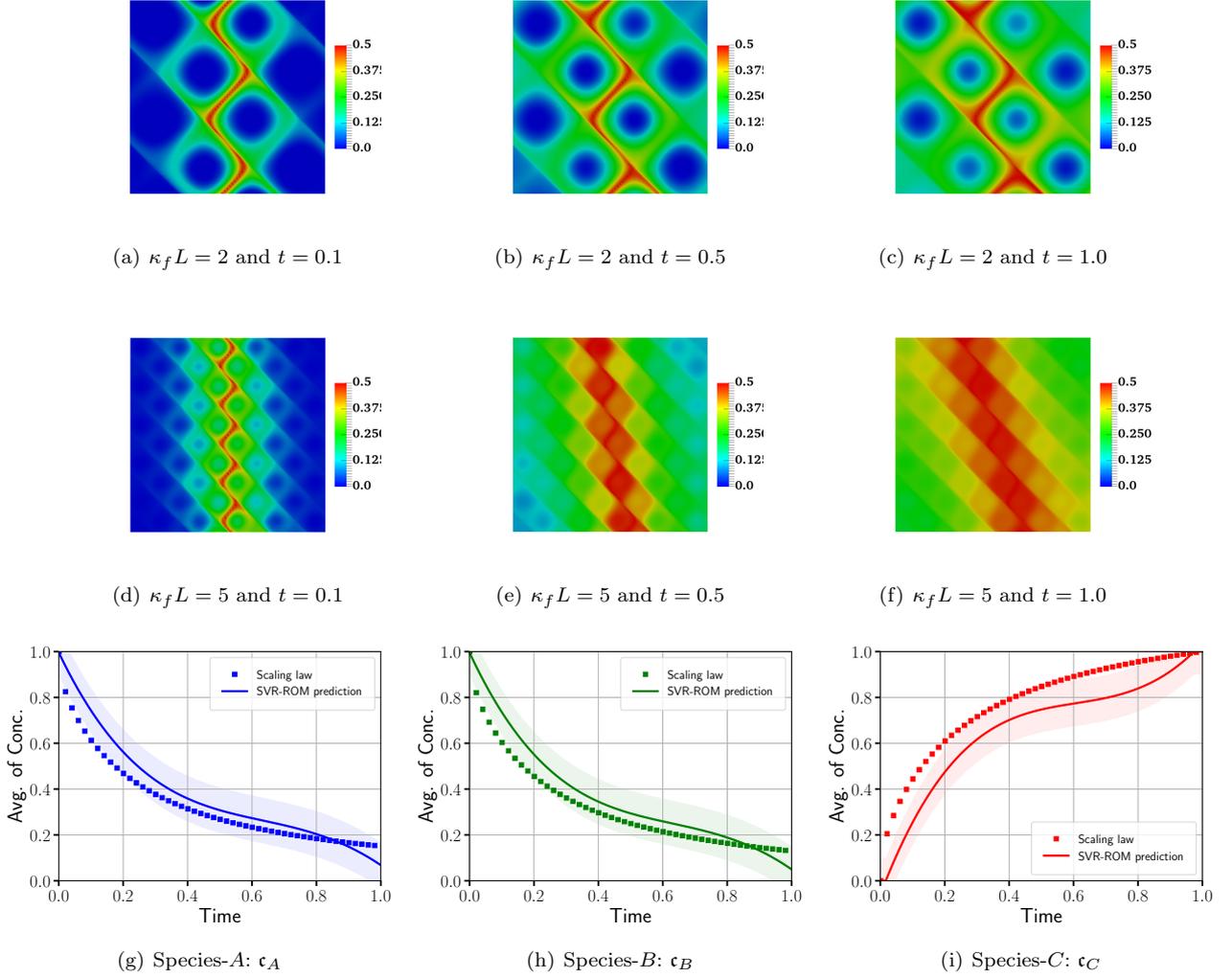


Figure 1: Concentration of product C at time $t = 0.1, 0.5, 1.0$ for two realizations are shown in (a)-(f). κ_f controls the spatial scales of the vortices. From (a)-(f) figures it is clear that for smaller values of $\kappa_f L$, product C concentration is zero in certain regions. As $\kappa_f L$ increases, we can see that number of regions with zero product C concentration decrease. This is because the velocity field contains a lot of small-scale vortices that are spread across the domain. Prediction of average of concentrations of reactants A , B and product C using Support Vector Machines based reduced-order models are shown in (g)-(i) [3]. High-fidelity predictions are also shown for comparison.

References

- [1] K. B. Nakshatrala, M. K. Mudunuru, and A. J. Valocchi. *A numerical framework for diffusion-controlled bimolecular-reactive systems to enforce maximum principles and non-negative constraint*, Vol.253, 278-307, (2013).
- [2] M. K. Mudunuru and K. B. Nakshatrala. *On enforcing maximum principles and achieving element-wise species balance for advection-diffusion-reaction equations under the finite element method*, Vol.305, 448-493, (2016).
- [3] M. K. Mudunuru, S. Karra, and V. V. Vesselinov. *On physics-informed machine learning models for reactive-transport applications*, LA-UR-17-27784, (2017).