Vidhyayana - ISSN 2454-8596
An International Multidisciplinary Peer-Reviewed E-Journal
www.vidhyayanaejournal.org
Indexed in: Crossref, ROAD & Google Scholar

66

Machine Learning in Engineering: A Necessity for Viksit Bharat

Arijit Ganguli

School of Engineering and Applied Sciences, Ahmedabad University, Ahmedabad, 380009

Abstract

In the present era of Artificial Intelligence (AI) and Machine Learning (ML), it is very evident for everyone to think of Natural Language Processing (NLP) or Robotics as the innovations of AI/ML that has revolutionized the world. Machine Learning can play a vital role in predicting important parameters in new and existing Engineering Applications if trained well by data. ML models can save time and computational power upto 10 times the conventional models. The data can be generated via experiments or via Computational fluid Dynamics (CFD) simulation-based analysis. The present article presents the opportunities that lie in building machine learning models in industries including Chemical processes, Mechanical Equipments, Nuclear Reactors etc. The procedure is substantiated with a case study to show the power of a Machine Learning Model to reduce time and computational power. A transient CFD simulation for a rectangular tank heated with water filled in it is performed and the data generated is used to train a Machine Learning model. The predictions match the actual data to 98% accuracy.

Introduction

Engineering applications need a lot of predicted capabilities from their genesis till their lifetime. For example, chemical industries have batch reactors operating in smaller volumes. It might take a few number of days to deliver a single product. The design of such reactors from lab to commercial scale, CFD simulations are carried out to optimize the design which may take months for one successful simulation. The performance in such reactors depends on the flow inside the reactor which depends on time and spatial resolution of the reactor. It also depends on operating parameters like the speed of the agitator. If data of CFD simulations with space and time are stored and used for training a Machine learning model the same results can be obtained in one tenth the time needed for optimization using CFD. Similarly in Nuclear Applications an innovative safety design for a 400 MW power plant might need a few crores of investment and space to build a pilot scale experimental setup. A CFD simulation might need a 16 core computer to run for three months continuously which means cost of computation and air conditioning for all the time period mentioned. However, a trained ML model would need nearly 15 days to provide good predictions from the trained data.

In the current work, we take the example of a safety operation of a Nuclear Reactor. To understand the same, a small lab experiment is undertaken which takes 6 to 7 hours for attaining steady state. Two dimensional CFD simulation for mimicking this phenomena would take 15 days with a 4 core machine. The objective is to build an ML model with the CFD data and make efforts to predict results and compare with the results of the CFD data.

Literature survey

Few researchers have conducted CFD(Computational Fluid Dynamics) simulations of flows in such cavities . The enclosure flows most widely studied are differentially heated (heated from one vertical side and cooled from the other opposite vertical side), which might have different geometrical shapes (rectangular, square, rhombic, curved), different orientations (for example inclined, tilted), having obstacles inside the geometries (baffles, corrugations) and having different boundary conditions (one side maintained at constant temperature or top surface at constant temperature while bottom surface being adiabatic) (. These are transient flows with a wide range of spatio-temporal variation during the development of the flow. These flows are computationally intensive, with a single simulation in the magnitude of weeks. Approaches to Reduced Order Modeling (ROM) include Proper Orthogonal Decomposition (POD); Galerkin projection (GP) methods or GP-POD where GP is combined with POD. These are also referred to as intrusive techniques. POD decomposes the flow field into a set of basis functions that optimally describe the original system in the form of the highest energies, referred to as modes . Another approach is the hybrid approach of both intrusive and nonintrusive techniques (POD-GP), which is computationally intensive and involves high costs (Pathak et al., 2018; Rahman et al., 2018; Wan et al., 2018; Xie et al., 2018). Another alternative approach that is being used by fluid mechanics researchers to solve spatiotemporal problems is a hybrid approach by combining Artificial Neural Networks (ANNs) with nonintrusive ROM frameworks (like POD) (Gamboa, 2017; Kutz, 2017; Brunton et al., 2020). These approaches make time-series predictions using Long short-term memory (LSTM), an ANN. In contrast, the flow physics is captured using a lower number of POD modes. One of the advantages of LSTM architecture is its ability to predict even noisy sequential time series into stable predictions closer to actual solutions using its internal dynamics. Development of ROM using POD and LSTM has been carried out by only a few works (Wang et al., 2018; Rahman et al., 2019).

Methodology

The CFD study is carried out using Ansys Fluent commercial software. The methodology involves using appropriate grid and solving discretized Navier-Stokes Equations using appropriate numerical schemes. The exact transient solver throughout this work is the pressure-implicit with the splitting of operators (PISO) algorithm . Each simulation is run for 15000 s, while training and testing uses the flow field from 1 s to 1000 s.

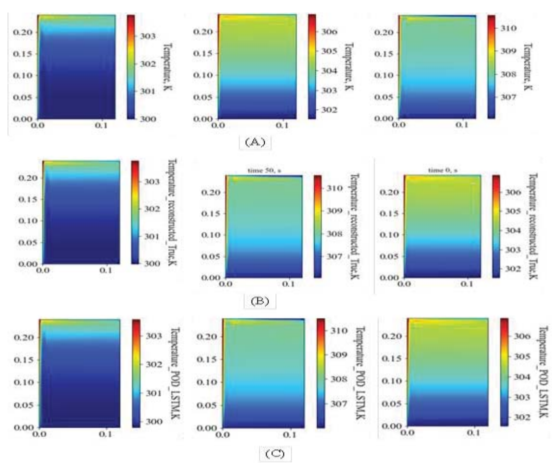
This section describes the Nonintrusive Reduced Order Modeling (NIROM) methodology referred to as POD-LSTM framework for predicting the flow fields at different times. A solely data-driven neural network approach is used to predict the time coefficients. The snapshot data obtained from the CFD simulations undergoes a POD transform and provides us with the time-dependent modal coefficients essentially a sequence of temperature or velocity data for time. As is generally the case with ROMs, this methodology comprises a computationally heavy offline training phase to build the POD-LSTM framework and an

Vidhyayana - ISSN 2454-8596
An International Multidisciplinary Peer-Reviewed E-Journal
www.vidhyayanaejournal.org
Indexed in: Crossref, ROAD & Google Scholar

efficient online phase for reconstructing flow fields for valid particularization of the parameters.

Results and Discussion

Figures A to C show the actual CFD results, ones by POD and reconstructed POD-LSTM framework for three different time instants, 100, 1000, and 5000 seconds. It should be noted that the first two instants are the ones used for training while the last instant is the one that is a new dataset. It can be observed that the POD-LSTM methodology can capture both the qualitative and quantitative trends for the times reported than those for which it has been trained, viz., the dynamics of both the hydrodynamic and thermal boundary layers and stratification are similar to that observed in the physical CFD models.



Statistical analysis was performed to evaluate the performance of the POD-LSTM framework. Root Mean Square Error (RMSE) was computed to determine the statistical deviation between POD- LSTM-based predictions and CFD-based results. The following expression gives RMSE:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n_\lambda}\left(\Delta\rho_{i,\lambda}\right)^2}{n_\lambda}}$$

where n_λ is the total number of node points in the computational domain λ, i takes values from 1 to the total number of node points, $\rho_{i,\lambda}$ is the variable (either velocity or temperature) at each node point for a particular time instant t since RMSE is found at a particular time instant t and $\Delta\rho_{i,\lambda}$ is the difference between the predicted values of the POD-LSTM framework and the values of CFD-based results at a particular time instant.

The structural similarity index (SSIM) and correlation coefficient (r) are used to assess the accuracy of the qualitative features of the velocity and temperature contours predicted by the POD-LSTM framework. SSIM uses the colour, texture, intensity, and structural information and matches the structure, luminescence, and contrast of the predicted velocity or temperature contour pixels by the POD-LSTM framework at a particular instant to the reference velocity or temperature contour. The correlation coefficient measures the linear relationship between the pixel values of velocity or temperature contours predicted by the POD-LSTM Framework with the reference contours to assess their similarity. It indicates the spatial consistency of the proposed method across the predicted contour image. the training and validation loss trends are the same, and the deviation is less than 5%, which shows that LSTM performance is good. All the energy is contained in mode 1 for temperature basis mode. In contrast, in the case of velocity basis modes, the first 4 modes consist of 97.5 to 99% of the energy, after which the energy is 100%.

Conclusions

1. The ML model qualitatively and quantitatively predicts the velocity and temperature patterns accurately when compared with the CFD model with an accuracy of ~97-99% based on RSME, correlation coefficient and SSIM for any time instant.
2. The ML model for the problem considered is estimated to reduce the computational time and power requirement by 10 times compared to that required for CFD methodology.
3. This study provides a good platform for building generalized ML models for equipments performance for Engineering Applications

References

Aubry, N, R Guyonnet, and R Lima. "Spatio-Temporal Symmetries and Bifurcations Via Bi-Orthogonal Decompositions." *Journal of Nonlinear Science* 2 (1992): 183-215.

Basak, Tanmay, S Roy, and AR Balakrishnan. "Effects of Thermal Boundary Conditions on Natural Convection Flows within a Square Cavity." *International Journal of Heat and Mass Transfer* 49, no. 23-24 (2006): 4525-35.

Berkooz, Gal, Philip Holmes, and John L Lumley. "The Proper Orthogonal Decomposition in the Analysis of Turbulent Flows." *Annual review of fluid mechanics* 25, no. 1 (1993): 539-75.

Das, Debayan, Monisha Roy, and Tanmay Basak. "Studies on Natural Convection within Enclosures of Various (Non-Square) Shapes–a Review." *International Journal of Heat and Mass Transfer* 106 (2017): 356-406.

Gupta, Akhilesh, V Eswaran, Prabhat Munshi, NK Maheshwari, and PK Vijayan. "Thermal Stratification Studies in a Side Heated Water Pool for Advanced Heavy Water Reactor Applications." *Heat and mass transfer* 45 (2009): 275-85.

Issa, Raad I. "Solution of the Implicitly Discretised Fluid Flow Equations by Operator-Splitting." *Journal of computational physics* 62, no. 1 (1986): 40-65.

Pathak, Jaideep, Alexander Wikner, Rebeckah Fussell, Sarthak Chandra, Brian R Hunt, Michelle Girvan, and Edward Ott. "Hybrid Forecasting of Chaotic Processes: Using Machine Learning in Conjunction with a Knowledge-Based Model." *Chaos: An Interdisciplinary Journal of Nonlinear Science* 28, no. 4 (2018).

Rahman, Sk M, Suraj Pawar, Omer San, Adil Rasheed, and Traian Iliescu. "Nonintrusive Reduced Order Modeling Framework for Quasigeostrophic Turbulence." *Physical Review E* 100, no. 5 (2019): 053306.

Rahman, Sk Mashfiqur, Omer San, and Adil Rasheed. "A Hybrid Approach for Model Order Reduction of Barotropic Quasi-Geostrophic Turbulence." *Fluids* 3, no. 4 (2018): 86.

Rowley, Clarence W, Tim Colonius, and Richard M Murray. "Model Reduction for Compressible Flows Using Pod and Galerkin Projection." *Physica D: Nonlinear Phenomena* 189, no. 1-2 (2004): 115-29.

Sadeghi, Mohamad Sadegh, Naghmeh Anadalibkhah, Ramin Ghasemiasl, Taher Armaghani, Abdul Sattar Dogonchi, Ali J Chamkha, Hafiz Ali, and Amin Asadi. "On the Natural Convection of Nanofluids in Diverse Shapes of Enclosures: An Exhaustive Review." *Journal of Thermal Analysis and Calorimetry* (2020): 1-22.

Sieber, Moritz, C Oliver Paschereit, and Kilian Oberleithner. "Spectral Proper Orthogonal Decomposition." *Journal of Fluid Mechanics* 792 (2016): 798-828.

Wan, Zhong Yi, Pantelis Vlachas, Petros Koumoutsakos, and Themistoklis Sapsis. "Data-Assisted Reduced-Order Modeling of Extreme Events in Complex Dynamical Systems." *PloS one* 13, no. 5 (2018): e0197704.

Xie, Xuping, Muhammad Mohebujjaman, Leo G Rebholz, and Traian Iliescu. "Data-Driven Filtered Reduced Order Modeling of Fluid Flows." *SIAM Journal on Scientific Computing* 40, no. 3 (2018): B834-B57.