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Editors

Machine Learning and Its Application to Reacting Flows

ML and Combustion

Springer

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Preface

Machine learning (ML) has been around for many decades and has been explored in the past for many practical applications. Currently, ML is interpreted in a broader context and finding its way into a number of sectors such as Engineering, Health Care, Transport including Traffic Prediction and Control, driverless car, Information Technology, Big Data Analysis and Processing, Agriculture, Agronomy, etc. It has found its way also into our daily life, for example, temperature and lighting controls and information searches on the internet. In a nutshell, ML is nothing but statistical interference using data collected or knowledge gained through past targeted studies or real-life experiences. The sophistication level of ML depends on the intended application and the advanced nature of the algorithms used for statistical learning and inference. This area has attracted huge interest recently because of the advent of the computational power, technology and algorithms required for data training, verification and validation, and the readiness and availability of these algorithms for application to a wide range of fields and practical systems. Hence, it is very timely to overview the various ML techniques or algorithms for big data analyses with a specific application to combustion science and technology.

This particular topic is chosen because of the important role of combustion systems and technologies covering more than 90% of the world's total primary energy supply (TPES). Although alternative renewable energy technologies are coming up, their shares for the TPES are less than 5% currently and one needs a complete paradigm shift to replace combustion sources. Whether this is practical or not is entirely a different question and an answer to this question is likely to depend on the respondent. However, a pragmatic analysis suggests that the combustion share to TPES is likely to be more than 70% even by 2070 as discussed in the chapter "Introduction" of this book. Hence, it will be prudent to take advantage of ML techniques to improve combustion sciences and technologies to better combustion system design and development so that the emission of greenhouse gases can be curtailed along with improving overall efficiencies. The level of interest in applying ML to combustion is clearly evident from the recent surge in research activities on this topic. Hence, the aim of this volume is to bring this knowledge together and make it readily accessible for researchers and graduate students interested in this multi- and cross-disciplinary topic. We attempted to keep the discussion accessible to students and researchers interested in turbulent combustion, ML techniques, and its application to turbulence and combustion on a simple physical basis while highlighting the need for ML.

Chapter "Introduction" gives an introduction to the role of combustion technologies in the future purely based on the current practical and scientific evidence. This chapter also identifies the opportunities to use ML algorithms (MLA) while investigating turbulent combustion. The chapter "Machine Learning Techniques in Reactive Atomistic Simulations" surveys various ML techniques and discusses their application for estimating atomic potential energies, required for chemical kinetics, through molecular dynamics simulation as an example. The chapter "A Novel In Situ Machine Learning Framework for Intelligent Data Capture and Event Detection" introduces in situ training for MLA which is a useful idea as it can save considerable efforts required in the training phase while using MLA. The chapter "Machine-Learning for Stress Tensor Modelling in Large Eddy Simulation" discusses the use of ML to estimate subgrid scale stresses and fluxes needed for large eddy simulation of turbulent combustion. The application of ML for combustion chemistry is discussed in the chapter "Machine Learning for Combustion Chemistry". The turbulence-chemistry interaction is a highly nonlinear stochastic problem ideally suited for ML and chapters "Deep Convolutional Neural Networks for Subgrid-Scale Flame Wrinkling Modeling–AI Super-Resolution: Application to Turbulence and Combustion" give different perspectives on the use of ML for estimating filtered reaction rate. Data-driven approaches can also be leveraged for reduced-order modeling of turbulent combustion and this is discussed in the chapter "Reduced-Order Modeling of Reacting Flows Using Data-Driven Approaches". The use of ML for thermoacoustics is described in chapter "Machine Learning for Thermoacoustics". Some of these chapters are written in a tutorial fashion and also provide hyperlinks to access the associated computer codes. The concluding remarks and future directions are summarised in the final chapter. Each of the chapters provides ample references for further reading by curious readers.

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