

Nedunchezian Swaminathan · Alessandro Parente  
Editors

# Machine Learning and Its Application to Reacting Flows

ML and Combustion

 Springer

### *Editors*

Nedunchezian Swaminathan  
Department of Engineering  
University of Cambridge  
Cambridge, UK

Alessandro Parente  
Aero-Thermo-Mechanics Laboratory  
École polytechnique de Bruxelles  
Université Libre de Bruxelles  
Brussels, Belgium

Brussels Institute for Thermal-fluid  
Systems, Brussels (BRITE)  
Université Libre de Bruxelles and Vrije  
Universiteit Brussel  
Brussels, Belgium



ISSN 2195-1284

ISSN 2195-1292 (electronic)

Lecture Notes in Energy

ISBN 978-3-031-16247-3

ISBN 978-3-031-16248-0 (eBook)

<https://doi.org/10.1007/978-3-031-16248-0>

© The Editor(s) (if applicable) and The Author(s) 2023. This book is an open access publication.

**Open Access** This book is licensed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>), which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license and indicate if changes were made.

The images or other third party material in this book are included in the book's Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the book's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG  
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

# 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.

The idea for this book came during a collaborative project, ALCHEMY (mAchine Learning for ComplEx MultiphYsics problems), between Cambridge University and ULB funded by Fondation Wiener-Anspach, ULB, Brussels. The funding from this foundation is gratefully acknowledged. We cannot understate the dedication of the contributors to this volume and we thank them for their contributions.

Cambridge, UK  
Brussels, Belgium  
May 2022

Nedunchezhian Swaminathan  
Alessandro Parente