

# Data Driven Fluid Mechanics

Combining First Principles and  
Machine Learning

MIGUEL A. MENDEZ

*von Karman Institute for Fluid Dynamics, Belgium*

ANDREA IANIRO

*Universidad Carlos III de Madrid, Spain*

BERND R. NOACK

*Harbin Institute of Technology, China  
Technische Universität Berlin, Germany*

STEVEN L. BRUNTON

*University of Washington, USA*

# Contents

<i>Preface</i>	<i>page xi</i>
<i>List of Contributors</i>	<i>xviii</i>
<b>Part I Motivation</b>	<b>1</b>
<b>1 Analysis, Modeling and Control of the Cylinder Wake</b>	<b>3</b>
1.1 Introduction	3
1.2 The cylinder wake	4
1.2.1 Configuration	5
1.2.2 Unforced transients	6
1.2.3 Wake dynamics	7
1.3 Features	8
1.3.1 Multi-dimensional scaling	9
1.3.2 Local linear embedding	10
1.3.3 Other features	11
1.4 Low-dimensional representations	11
1.4.1 Proper orthogonal decomposition	11
1.4.2 Clustering	12
1.4.3 Comparison and discussion	12
1.5 Dynamic models	14
1.5.1 POD Galerkin method	14
1.5.2 Mean-field model	14
1.5.3 Manifold model	15
1.6 Control	16
1.6.1 Model-based control	16
1.6.2 Model-free machine learning control	18
1.7 Conclusions	19
<b>2 Coherent structures in turbulence: a data science perspective</b>	<b>20</b>
2.1 Introduction	20
2.2 Coherent structures	24
2.2.1 Free-shear flows	26
2.2.2 Wall-bounded flows	27
2.2.3 Conceptual experiments	32

2.3	Discussion	32
<b>3</b>	<b>Machine Learning in Fluids: Pairing Methods with Problems</b>	<b>34</b>
3.1	Overview	34
3.1.1	Kinematic and dynamics modeling of fluid flows	37
3.2	Machine Learning Basics	39
3.2.1	Machine learning categorizations	41
3.2.2	Neural networks	44
3.2.3	Cross validation	46
3.3	Flow feature extraction	46
3.3.1	Dimensionality reduction	46
3.3.2	Clustering and classification	48
3.3.3	Sparse and randomized methods	49
3.3.4	Super resolution and flow cleansing	50
3.4	Modeling flow dynamics	51
3.4.1	Linear models: DMD and Koopman analysis	51
3.4.2	Neural network modeling	52
3.4.3	Parsimonious nonlinear models	53
3.4.4	Closure models with machine learning	54
3.5	Control and optimization	56
3.6	Challenges for machine learning in fluid dynamics	58
<b>Part II</b>	<b>Methods from Signal Processing</b>	<b>61</b>
<b>4</b>	<b>Continuous and Discrete LTI Systems</b>	<b>63</b>
4.1	On Signals, Systems, Data and Modeling of Fluid Flows	63
4.2	A note about notation and style	66
4.3	Signal and Orthogonal Bases	67
4.3.1	Discrete Signals	67
4.3.2	Continuous Signals	69
4.4	Convolutions and Eigenfunctions	71
4.5	Causal and Stable Systems	73
4.6	LTI Systems in their Eigenspace	74
4.6.1	Laplace and Z Transforms	75
4.6.2	Discrete and Continuous Frequencies	76
4.6.3	The Convolution Theorem	77
4.6.4	Differential and Difference Equations	78
4.7	Application I: Harmonic Analysis and Filters	80
4.7.1	From Laplace to Fourier	80
4.7.2	Multiresolution Analysis and Digital Filters	82
4.8	Application II: Time Series Analysis and Forecasting	87
4.8.1	Stochastic LTI Systems	87

---

4.8.2	Time Series Forecasting via LTI Systems	88
4.9	What's next?	90
<b>5</b>	<b>Time-Frequency Analysis and Wavelets</b>	<b>91</b>
5.1	Introduction	91
5.2	Windowed Fourier Transform	93
5.2.1	Windowed FT and Gabor Transform	93
5.2.2	Discrete Gabor Transform	94
5.3	Wavelet Transform	97
5.3.1	Fundamentals	97
5.3.2	The Continuous Wavelet Transforms	99
5.3.3	Wavelet series: the path to Discrete Wavelet Transform	101
5.3.4	Multi-resolution analysis	102
5.3.5	The DWT and filter banks	105
5.4	Tutorials and examples	110
5.4.1	Time Frequency Analysis of Hot-Wire Data: CWT vs WTF	110
5.4.2	Filtering and compression	113
5.5	Conclusions	116
<b>Part III</b>	<b>Data-Driven Decompositions</b>	<b>117</b>
<b>6</b>	<b>The Proper Orthogonal Decomposition</b>	<b>119</b>
6.1	Introduction	119
6.2	The singular value decomposition	120
6.2.1	The singular value decomposition: definition	120
6.2.2	The singular value decomposition: properties	121
6.3	The POD of discrete data	124
6.4	The POD of continuous systems	126
6.5	The POD for projection-based modeling	128
6.6	Extensions of the POD	129
6.7	Examples	129
<b>7</b>	<b>The Dynamic Mode Decomposition</b>	<b>135</b>
7.1	Introduction	135
7.2	The Koopman idea	137
7.3	The dynamic mode decomposition	141
7.4	Sparsity promotion for finding amplitudes	143
7.5	Applications	146
7.6	Extensions and generalizations	152
7.7	Summary and conclusions	154
<b>8</b>	<b>Generalized and Multiscale Modal Analysis</b>	<b>155</b>
8.1	The Main Theme	155

8.1.1	The scope of modal decompositions	156
8.1.2	How many decompositions?	156
8.2	The General Architecture	158
8.2.1	A note on notation and style	158
8.2.2	Projections in Space <i>or</i> Time	159
8.2.3	Projections in Space <i>and</i> Time	161
8.2.4	The Fundamental Factorization	162
8.2.5	Amplitudes and Energies	164
8.3	Common Decompositions	166
8.3.1	The Delta Decomposition	166
8.3.2	The Discrete Fourier Transform (DFT)	166
8.3.3	The Proper Orthogonal Decomposition (POD)	168
8.3.4	The Dynamic Mode Decomposition (DMD)	170
8.4	The Multiscale POD (mPOD)	173
8.4.1	Frequency Constrained POD	173
8.4.2	From Frequency Constraints to MRA	177
8.4.3	The mPOD Algorithm	179
8.5	Tutorial Test Cases	181
8.5.1	Test Case 1	181
8.5.2	Test Case 2	182
8.6	What's next?	184
<b>9</b>	<b>Good Practice and Applications of Data-Driven Modal Analysis</b>	<b>185</b>
9.1	Introduction	185
9.1.1	A brief recall of the snapshot POD procedure	187
9.2	Dataset Size and Richness	188
9.2.1	Effect of the number of samples on the convergence of the statistics	188
9.2.2	The effect of noise	190
9.2.3	An example: Noisy measurements in a turbulent channel	192
9.3	Extracting Phase Information	192
9.3.1	An example: The wake of two cylinders in ground effect	195
9.4	Extended POD	196
9.4.1	An application: Time-resolved flow sensing with the EPOD	198
9.4.2	An exercise: The turbulent Heat Transfer in a Pipe Flow	200
<b>Part IV</b>	<b>Dynamical Systems</b>	<b>205</b>
<b>10</b>	<b>Linear Dynamical Systems and Control</b>	<b>207</b>
10.1	Linear Systems	207
10.2	PID feedback control	210
10.3	The root locus plot	214
10.4	Controllability and observability	215
10.5	Full-state feedback	216

---

10.5.1	Pole placement	216
10.5.2	Optimal control	217
10.6	Additional control techniques and considerations	218
10.6.1	State estimation	219
10.6.2	Robust control	219
10.6.3	Nonlinear control	219
10.6.4	Application of feedback control in fluids	220
<b>11</b>	<b>Nonlinear Dynamical Systems</b>	<b>221</b>
11.1	Introduction	221
11.2	Dynamical systems	222
11.2.1	Continuous-time systems	222
11.2.2	Discrete-time systems	223
11.2.3	Linear dynamics and spectral decomposition	224
11.2.4	Bifurcations	225
11.3	Goals and challenges in modern dynamical systems	226
11.4	Koopman theory	229
11.4.1	Mathematical formulation	229
11.4.2	Koopman mode decomposition	232
11.4.3	Examples of Koopman embeddings	234
11.4.4	History and recent developments	236
<b>12</b>	<b>Methods for System Identification</b>	<b>238</b>
12.1	Model reduction and system identification	238
12.2	Balanced model reduction	239
12.2.1	The goal of model reduction	240
12.2.2	Change of variables in control systems	241
12.2.3	Balancing transformations	243
12.2.4	Balanced truncation	245
12.2.5	Computing balanced realizations	247
12.3	System identification	251
12.3.1	Eigensystem realization algorithm	251
12.3.2	Observer Kalman filter identification	254
12.4	Sparse identification of nonlinear dynamics (SINDy)	256
<b>13</b>	<b>Modern Tools for the Stability Analysis of Fluid Flows</b>	<b>261</b>
13.1	Introduction	261
13.2	Definitions of stability	265
13.3	General formulation	268
13.4	Reduced formulation for special cases	274
13.5	Practical issues and implementation details	279
13.6	Tonal noise analysis: quantifying a complex feedback mechanism	286
13.7	Further extensions	290

13.8	Summary and conclusions	290
<b>Part V</b>	<b>Applications</b>	<b>291</b>
<b>14</b>	<b>Machine Learning for Reduced-Order Modeling</b>	<b>293</b>
14.1	Introduction	293
14.2	POD Galerkin model	294
14.2.1	Flow configuration	294
14.2.2	Proper Orthogonal Decomposition	295
14.2.3	Galerkin method	297
14.2.4	Closures and stabilizers	297
14.2.5	Model identification	298
14.2.6	Applications	299
14.3	Cluster-based reduced-order modeling	300
14.3.1	Clustering	300
14.3.2	Cluster-based Markov models	301
14.3.3	Cluster-based network models	301
14.3.4	Generalizations	302
14.4	General principles	302
14.5	Tutorial: xROM	304
14.5.1	Numerical Setup	304
14.5.2	General characteristics of xROM	304
14.5.3	Exercises	307
<b>15</b>	<b>Advancing Reacting Flow Simulations with Data-Driven Models</b>	<b>310</b>
15.1	Introduction	311
15.2	Combustion data sets	312
15.2.1	Data preprocessing	315
15.3	Feature extraction using dimensionality reduction techniques	315
15.3.1	Description of the analyzed data set	316
15.3.2	Extracting features with data reduction techniques	316
15.4	Transport of Principal Components	326
15.4.1	Nonlinear regression models	327
15.4.2	Validation of the PC-transport approach in LES simulations	327
15.5	Chemistry acceleration via adaptive-chemistry	331
15.5.1	Description of the approach	331
15.5.2	Application of the approach	332
15.6	Available software	334
15.7	Summary	334
<b>16</b>	<b>ROMs for Aerodynamic Applications and MDO</b>	<b>336</b>
16.1	Introduction and Motivation	336
16.2	Reduced-Order Modeling	338
16.2.1	POD-based ROMs	338

---

16.2.2	ROMs based on Isomap	340
16.3	Implementation	340
16.4	Applications	341
16.4.1	Parametric ROM based on POD and Isomap for LANN wing	342
16.4.2	Parametric ROM based on POD and Isomap for XRF-1	344
16.4.3	Reduced-order Modeling for Static Aeroelastic Problems	346
16.4.4	ROMs in the Context of Multidisciplinary Design Optimization	349
16.4.5	Aeroelastic ROM based on Synthetic Modes and Gappy POD	350
16.4.6	Nonlinear Dimensionality Reduction by Autoencoder Networks	351
16.4.7	Unsteady Physics-based Nonlinear Reduced-order Modeling	355
16.5	Conclusions	355
<b>17</b>	<b>Machine Learning for Turbulence Control</b>	<b>356</b>
17.1	Introduction	356
17.2	Goals, tools and principles	357
17.2.1	Goals	357
17.2.2	Tools	358
17.2.3	Principles	359
17.3	Model-based control	360
17.3.1	Linear dynamics	361
17.3.2	Weakly nonlinear dynamics	362
17.3.3	Moderately nonlinear dynamics	364
17.4	Model-free machine learning control	366
17.4.1	Cluster-based control	366
17.4.2	Linear genetic programming control	367
17.5	MLC Tutorial	367
17.5.1	Generalized mean-field model	368
17.5.2	Installation	369
17.5.3	Execution	370
17.5.4	My MLC problem	373
<b>18</b>	<b>Deep Reinforcement Learning applied to Active Flow Control</b>	<b>374</b>
18.1	The promise of deep reinforcement learning in fluid mechanics	374
18.2	A brief introduction to deep reinforcement learning	376
18.2.1	Learning through trial and error	376
18.2.2	Q-learning	378
18.2.3	Policy gradient methods	380
18.2.4	Current research directions in deep reinforcement learning	382
18.3	Recent applications of deep reinforcement learning to fluid mechanics problems	384



18.3.1	Swimming and locomotion	384
18.3.2	Feedback active flow control	385
18.4	A guide to deploying DRL in fluid mechanics	389
18.4.1	Problem identification and coupling to DRL framework	389
18.4.2	Problem modeling: invariances, reward shaping, and parallelization	391
18.4.3	Other techniques: normalization, actuation frequency, and transfer learning	392
18.5	Perspectives and remaining questions	395
<b>Part VI</b>	<b>Perspectives</b>	<b>397</b>
<b>19</b>	<b>The Computer as Scientist</b>	<b>399</b>
19.1	Introduction	399
19.2	2-D turbulence: a case study	401
19.2.1	Data generation and analysis	401
19.2.2	Verification and validation	406
19.3	Vortices and dipoles	409
19.4	Discussion and conclusions	410

# Preface

This book is for scientists and engineers interested in data-driven and machine learning methods for fluid mechanics. Big data and machine learning are driving profound technological progress across nearly every industry, and they are rapidly shaping fluid mechanics' research. This revolution is driven by the ever-increasing amount of high-quality data, provided by rapidly improving experimental and numerical capabilities. Machine learning extracts knowledge from data without the need for first principles and introduces a new paradigm: use data to discover, rather than validate, new hypotheses and models. This revolution brings challenges and opportunities.

Data driven methods are an essential part of the methodological portfolio of fluid dynamicists, motivating students and practitioners to gathering practical knowledge from a diverse range of disciplines. These fields include computer science, statistics, optimization, signal processing, pattern recognition, nonlinear dynamics, and control. Fluid mechanics is historically a *big data* field and offers a fertile ground to develop and apply data-driven methods, while also providing valuable shortcuts, constraints, and interpretations based on its powerful connections to first principles physics. Thus, hybrid approaches that leverage both data-driven methods and first principles approaches, are the focus of active and exciting research. This book presents an overview and a pedagogical treatment of some of the data-driven and machine learning tools that are leading research advancements in model-order reduction, system identification, flow control, and data-driven turbulence closures.

## About the Book and the VKI Lecture Series

This book originated from a one-week course from the von Karman Institute (VKI) for fluid dynamics (<https://www.vki.ac.be/>). The course was hosted by the Université libre de Bruxelles (ULB) from 24 to 28 February 2020, in the classic VKI lecture series format. These are one-week courses on specialized topics, selected by the VKI faculty and typically organized 8-12 times per year. These courses have gained a worldwide recognition and are among the most influential and distinguished European teaching forums, where pioneers in fluid mechanics have been training young talents for many decades.

The lecture series was co-organized by Miguel A. Mendez from the von Karman Institute (Belgium), Alessandro Parente from the Université libre de Bruxelles (Bel-

gium), Andrea Ianiro from Universidad Carlos III de Madrid (Spain), Bernd R. Noack from Harbin Institute of Technology, Shenzhen (China) and TU Berlin (Germany) and Steven L. Brunton from University of Washington (US).

## Online Material

The book is supported by supplementary material, including codes, experimental and numerical data, exercises, and the video lectures recorded from the course. All material is hosted on the course website:

<https://www.datadrivenfluidmechanics.com/>

The supplementary material covers more exercises, tutorials, and practicalities than could be included in this book while preserving its conciseness. Readers interested in gaining a working knowledge on the subject are encouraged and expected to download this material, study it along with the book, and test it on their own data. The large repertoire of computing tools implemented, together with the relevant datasets provided, offer a unique opportunity to learn by practicing with real experimental and numerical data.

## The Audience

The book is intended for anyone interested in the use of data-driven methods for fluid mechanics. We believe that the book provides a unique balance between introductory material, practical hands-on tutorials, and state-of-the-art research. While keeping the approach pedagogical, the reader is exposed to topics at the frontiers of fluid mechanics research. Therefore, the book could be used to complement or support classes on data-driven science, applied mathematics, scientific computing, and fluid mechanics, as well as to serve as a reference for engineers and scientists working in these fields. Basic knowledge of data processing, numerical methods, and fluid mechanics is assumed.

## The Book's Roadmap

Like the course from which it originates, this book results from the contribution of many authors. The use of machine learning methods in fluid mechanics is in its early days, and a large team of lecturers allowed the course attendees to learn from the expertise and perspectives of leading scientists in different fields.

Here we provide a roadmap of the book to guide the reader through its structure and link all the chapters into a coherent narrative. The book chapters can be clustered into six interconnected parts, slightly adapted from the VKI lecture series.

**Part I: Motivation.** This part includes the first three chapters, which introduce the motivation for data-driven techniques from three perspectives.

**Chapter 1**, by B.R. Noack and coauthors, opens with a tour de force on machine learning tools for dimensionality reduction and flow control. These techniques are introduced to analyze, model, and control the well-known cylinder wake problem, building confidence and intuition about the challenges and opportunities for machine learning in fluid mechanics. **Chapter 2**, by J. Jiménez, takes a step back and gives both a historical and a data-science perspective. Most of the dimensionality reduction techniques presented in this book have been developed to identify patterns in the data, known as *coherent structures* in turbulent flows. But what are coherent structures? This question is addressed by discussing the relationship between data analysis and conceptual modelling and the extent to which artificial intelligence can contribute to these two aspects of the scientific method. **Chapter 3**, by S. Brunton, gives an overview of how machine learning tools are entering fluid mechanics. The chapter provides a short introduction to machine learning, its categories (e.g. supervised versus unsupervised learning), its subfields (regression and classification, dimensionality reduction and clustering) and the problems in fluid mechanics that can be addressed by these methods (e.g. feature extraction, turbulence modelling and flow control). This chapter contains a broad literature review, highlights the key challenges of the field, and gives perspectives for the future.

**Part II: Methods from Signal Processing.** This part brings the reader back to classic tools from signal processing, usually covered in curricula crossed by experimental fluid dynamicists, although with a large variety of depth. This part of the book is motivated by two reasons. First, tools from signal processing are, and will likely remain, the first ‘off-the shelf’ solutions for many practical problems. Examples include filtering, time-frequency analysis, and data compression using filter banks or wavelets, or the use of linear system identification and time series analysis via autoregressive methods. The second reason – and this is a central theme of the book – is that much can be gained by combining machine learning tools with methods from classic signal processing, as later discussed in Chapter 8. Therefore, **Chapter 4**, by M. A. Mendez, reviews the theory of linear time-invariant (LTI) systems along with their properties and the fundamental transforms used in their analysis: the Laplace, Fourier, and Z transforms. This chapter draws several parallels with more advanced techniques. For example, the use of the Laplace transform to reduce ordinary differential equations (ODEs) to algebraic equations parallels the use of Galerkin methods to reduce the Navier Stokes equation to a system of ODEs. Similarly, there is a link between the classical Z-transform and the modern dynamic mode decomposition (DMD). **Chapter 5**, by S. Discetti, complements the previous chapter by focusing on time-frequency analysis. The fundamental Gabor and continuous/discrete Wavelet transforms are introduced along with the related Heisenberg uncertainty principle and multiresolution analysis. The methods are illustrated on a time-series obtained from hot-wire anemometry in a turbulent boundary layer and from flow fields obtained via numerical simulations.

**Part III: Data-Driven Decompositions.** This part of the book consists of four

chapters dedicated to a cornerstone (and rapidly growing sub-field) of fluid mechanics: modal analysis. This part is mostly concerned with methods for linear dimensionality reduction, originally introduced to identify, and “objectively” define, coherent structures in turbulent flows.

**Chapter 6**, by S. Dawson, is dedicated to the proper orthogonal decomposition (POD), the first and most popular tool introduced in the fluid mechanics community in the 1970s. The chapter reviews the link between POD with the singular value decomposition (SVD), its essential properties (e.g. optimality, relation to eigenvalue decomposition, and generalization to weighted inner products), its practical computation on discrete datasets, and its extension to continuous systems. This chapter closes with illustrative exercises that guide the reader to practical computation. **Chapter 7**, by P. Schmid, is dedicated to the dynamic mode decomposition (DMD), a powerful alternative to POD introduced by P. Schmid a decade ago. This chapter reviews the derivation of DMD and its roots in dynamical systems and Koopman operator theory. The main DMD algorithm is presented along with its “sparsity promoting” variant, and the chapter is enriched by three applications to experimental and numerical data, as well as a brief outlook at new extensions and generalizations.

**Chapter 8**, by M. A. Mendez, presents a generalized framework for deriving, computing, and interpreting *any* linear decomposition. Modal decompositions are analyzed in terms of matrix factorization and viewed as a special case of 2D discrete transforms. This framework is used to combine multiresolution analysis via filter banks with the classic POD, and derive the multiscale POD (mPOD). The mPOD is a recent decomposition that generalized the energy-based (POD-like) and the frequency-based (DMD-like) formalism. The chapter includes several exercises and tutorials, allowing the reader to test these decompositions on experimental data. Finally, this part on modal analysis closes with **Chapter 9**, by A. Ianiro, with an overview of good practices and applications of modal analysis. This chapter addresses essential questions on the statistical convergence of POD, the impact of random noise, and the possibility to extract phase information about the modes even if the data is not time-resolved. Moreover, the chapter presents interesting applications of the extended POD – in which decompositions of different datasets are correlated – to experimental and numerical data.

**Part IV: Dynamical Systems.** This part of the book consists of four chapters dedicated to various aspects of dynamical systems. **Chapter 10**, by S. Dawson, gives a brief overview of linear dynamical systems and linear control. This is one of the most developed disciplines in engineering, with applications across robotics, automation, aeronautics, and mechanical systems in general. Linear techniques provide a standard approach for closed-loop control and have been successfully used in fluid flows. This chapter illustrates the main concepts (state-space representation, controllability and observability, and optimal control) and tools (root locus, pole placement, PID controllers) focusing on a specific example from fluid mechanics, namely the stabilization of a wake flow. An overview of additional control techniques and a brief literature review for flow control are also provided.

**Chapter 11**, by S. Brunton, provides an overview of nonlinear dynamical systems.

The chapter introduces fundamental concepts such as flow maps, attracting sets and bifurcations, and gives a modern perspective on the field, with its current goals and open challenges. These include recent advances in the operator-theoretic views that seek to identify a linear representation of nonlinear systems and identify dynamical systems from data, further discussed in the following chapter. **Chapter 12**, also by S. Brunton, builds on the previous chapter and Part III of the book to introduce several advanced topics in model reduction and system identification. The chapter opens with a review of balanced model reduction goals for linear systems and builds the required mathematical background and the fundamentals of balanced POD (BPOD). Linear and nonlinear identification tools are introduced. Among the linear identification tools, the chapter presents the eigensystem realization algorithm (ERA) and the observer Kalman filter identification (OKID). Among the nonlinear identification tools, the chapter presents the sparse identification of nonlinear dynamics (SINDy) algorithm, which leverages the LASSO regression from statistics to identify nonlinear systems from data.

This part closes with **Chapter 13**, by P. Schmid, providing a modern account of stability analysis of fluid flows. The chapter begins with a brief review of the classic definition of stability (e.g., Lyapunov, asymptotic, and exponential stability) and moves towards a modern formulation of stability as an optimization problem: unstable modes are those along which the growth of disturbances is maximized. The chapter introduces a powerful, adjoint-based, iterative method to solve such an optimization and shows how to recover common stability and receptivity results from the general framework. Finally, an illustrative application to the problem of tonal noise is given.

**Part V: Applications.** This part of the book is dedicated to the application of data-driven and machine learning methods to fluid mechanics.

**Chapter 14**, by B.R. Noack and co-workers, is dedicated to reduced-order modeling. The chapter gives an overview of the classic POD-Galerkin approach, reviewing the main challenges in closure and stabilization as well as classic applications. It then moves to emerging cluster-based Markov models and their possible generalization. A detailed tutorial is also provided to offer the reader hands-on experience with reduced-order modeling.

**Chapter 15**, by K. Zdybal and co-workers, focuses on the use of data-driven models for studying reacting flows. The numerical simulation of these flows is extremely challenging because of the vast range of scales involved. This chapter gives a broad overview of how machine learning techniques can help reduce the computational burden. The key challenges of high dimensionality are discussed along with an overview of dimensionality reduction methods, ranging from classic principal component analysis (PCA) to local PCA, non-negative matrix factorization (NMF), and artificial neural network (ANN) autoencoders. The application of these tools to reduce dimensionality in the modelling of transport and chemical reactions is illustrated in a challenging test case.

**Chapter 16**, by S. Görtz and co-workers, is dedicated to the application of reduced-order modelling for multidisciplinary design optimization in aerodynamics. The design of an aircraft involves thousands of extremely expensive numerical simulations.

This chapter shows how linear and nonlinear dimensionality reduction tools can help speed up the process. POD, cluster POD, and Isomaps, combined with nonlinear regression, are discussed and demonstrated in industrially relevant cases such as the aero/structure optimization of an entire aircraft.

**Chapter 17**, by B.R. Noack and co-workers, is dedicated to flow control and how machine learning might revolutionize the field. The chapter gives first an overview of flow control, its purposes, goals, tools, and strategies. Then, two paradigms for flow control are introduced and compared. On the one hand, there are model-based approaches, rooted in first principles and our ability to derive models that predict how a system responds to inputs. On the other hand, there are model-free approaches rooted in powerful optimization strategies that can “learn” the best control laws from data, by simply interacting with the system. Cluster-based control and linear genetic programming are illustrated, and the chapter closes with a tutorial on an illustrative nonlinear benchmark problem.

**Chapter 18**, by J. Rabault and A. Kuhnle complements the previous chapter with an overview of deep reinforcement learning (DRL) for active flow control. Reinforcement learning is one of the three paradigms of machine learning. Contrary to the other two (supervised and unsupervised learning), a reinforcement learning algorithm starts with no data and learns through experience, i.e., via trial and error. This framework is meant to tackle decision-making processes, such as teaching a computer to play chess or drive a car or, as the authors show, to control a fluid flow. This chapter introduces the main approaches of reinforcement learning (e.g. Q-learning versus policy gradient methods), the current research directions, and the recent applications to fluid mechanics problems. Guidelines to practically deploy DRL are given, along with a perspective for the future of the field.

**Part VI: Perspectives.** The book closes with **Chapter 19**, by J. Jiménez, with a fascinating perspective and important questions for the field. Combined with Chapter 2, this chapter explores how much the progressive synergy between machine learning and fluid dynamics, fostered by ever increasing computational capabilities, could promote the ‘automation’ of science and ultimately turn machines into colleagues. This, as masterfully illustrated with a simple case study, ultimately depends on whether ‘blind’ randomized trials can be integrated in the process of formulating hypothesis, eventually giving computers the ability to ask questions rather than just providing answers.

## A note on the Notation

The reader will quickly realize that different chapters have (slightly) different notation. Among these, the same symbol is sometimes used for different purposes, and different symbols are sometimes used for the same quantities. This choice is deliberate. First, the book covers a wide range of disciplines, each with well-established notations. For example, the symbol  $u$  usually denotes the actuation in control theory and the velocity field in fluid mechanics. In reinforcement learning, the actuation is denoted

by  $a_t$  and called the ‘action’ while the sensor measurement is denoted by  $s_t$  and called ‘state’ (while it is usually denoted by  $\mathbf{y}$  in control theory). Resolving these ambiguities would make it difficult for readers to link the material in this book with the literature of the various intersected disciplines. Thus, each chapter represents the starting point towards more advanced and specialized literature, in which a standard notation has not yet been settled. Keeping the notation as close as possible to the cited literature helps the reader make essential connections. We hope that the reader will approach each chapter with the required flexibility, and we welcome comments, corrections and suggestions to benefit students for the next reprint.



# List of Contributors

**Abu-Zurayk, Mohammad**

Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR),  
Germany

**Aversano, Gianmarco**

Université Libre de Bruxelles and Vrije Universiteit Brussels, Belgium  
Université Paris Saclay, France

**Bekemeyer, Philipp**

Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR),  
Germany

**Brunton, Steven**

University of Washington, USA

**Coussement, Axel**

Université Libre de Bruxelles and Vrije Universiteit Brussels, Belgium  
Université Paris Saclay, France

**D'Alessio, Giuseppe**

Université Libre de Bruxelles and Vrije Universiteit Brussels, Belgium  
Université Paris Saclay, France

**Dawson, Scott**

Illinois Institute of Technology, USA

**Discetti, Stefano**

Universidad Carlos III de Madrid, Spain

**Ehlert, Arthur**

Technische Universität, Berlin, Germany  
Industrial Analytics, Berlin, Germany

**Fernex, Daniel**

Technische Universität Braunschweig, Germany

**Franz, Thomas**

Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR),  
Germany

**Görtz, Stefan**

Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR),  
Germany

**Ianiro, Andrea**

Universidad Carlos III de Madrid, Spain

**Jiménez, Javier**

Universidad Politécnica Madrid, Spain

**Kuhnle, Alex**

University of Cambridge, United Kingdom

**Lusseyran, François**

Université Paris-Saclay, France

**Maceda, Guy C.**

Université Paris-Saclay, France

**Malik, Mohammad, R.**

Université Libre de Bruxelles and Vrije Universiteit Brussels, Belgium

**Mendez, Miguel A.**

von Karman Institute for Fluid Dynamics, Belgium

**Morzynski, Marek**

Poznań University of Technology, Poland

**Nayeri, Christian N.**

Technische Universität Berlin, Germany

**Noack, Bernd R**

Harbin Institute of Technology, Republic of China  
Technische Universität Berlin, Germany

**Parente, Alessandro**

Université Libre de Bruxelles and Vrije Universiteit Brussels, Belgium

**Rabault, Jean**

Norwegian Meteorological Institute, Norway

University of Oslo, Norway

**Ripepi, Matteo**

Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR),  
Germany

**Schmid, Peter**

Imperial College London, United Kingdom

**Semaan, Richard**

Technische Universität Braunschweig, Germany

**Sutherland, James C.**

University of Utah, USA

**Zdybal, Kamila**

Université Libre de Bruxelles and Vrije Universiteit Brussels, Belgium