Preface

The original driver for this book is the author's research on electrochemical energy applications such as the development of reliable and systematic descriptions of batteries and fuel cells. Very quickly it became apparent that taking into account multiple scientific aspects using the language of physics and mathematics requires a broad but combined view of fundamental established scientific fields to systematically and reliably capture highly complex and interlinked physical, chemical, thermodynamic, mathematical, and practical engineering systems. Moreover, a clear understanding of involved processes such as chemical reactions is limited, since it is very difficult to obtain the preferred measurements/data from operational electrochemical devices, for instance. This difficulty of gaining operational data and measurements of real-time systems, without disturbing or modifying their inner workings, is a general challenge present in many applications such as chemistry (danger of modifying processes), biological multicell processes and signalling (e. g., broken communication), data-link networks (e. g., ghosts in sensor-fusion-control-actuator systems or degradation in quality of information such as the participants' locations) and social dynamics (e. g., invasive sensors preventing natural interaction). At the same time, many new technologies are increasingly a result of combining existing scientific developments and engineering products often by connecting them to smart networks. Examples are reaction networks (Catalysis), the Internet of Things (IoT), Command and Control (C2) Systems and their associated sensor and communication networks, and machine learning (ML) as well as artificial intelligence (AI) with their combination, extension, training, and development of novel neural networks and their corresponding training methods.

As a consequence, future technology represents itself often as interacting, network-like structures, which we systematically identify as CHeSs in this book. This broad and application-driven view is a result of various impressions, experiences, and efforts daily gained at international research places and different scientific and engineering departments, which had a crucial impact on the final scope and form of this book as motivated in the following subsequent paragraphs.

The scientific journey of this book starts at the Eidgenössische Technische Hochschule Zürich (ETH), the author's Alma Mater. The historically grown understanding and view, in part due to the Einstein's impact, that both Physics and Mathematics are not opposing fields, but rather synergetic scientific building blocks reaching their ultimate, optimal understanding by taking the different views from both fields into account. As a result, studying mathematics at ETH meant taking the same lectures in physics and mathematics as the physicists do and vice versa. At the turn of the millennium, the community of students and professors also induced and spread a general, ideal view on science, its fundaments, and its role in society. This certainly provided a motivating and healthy view to develop a scientific career. Moreover, the immediate transition from middle school classes (K-12) with at most 30 students to lectures at university with over hundreds of students can, depending on one's character, lead to a strong development

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of independence in learning and understanding new and complex theories by working out the necessary concepts and solutions by oneself.

Originally, I started my dissertation under the supervision of Andreas Prohl at ETH on *Modeling, Analysis, and Numerics in Electrohydrodynamics*[4] late 2005. In 2007, A. Prohl kindly offered me the chance to continue my work in a different research environment. This means that I got the opportunity to complete and defend my dissertation on the rigorous development of reliable and convergent finite element schemes of the models, previously developed and analyzed at ETH, at the Universität Tübingen. My interdisciplinary PhD topic combines applications with rigorous mathematics supported by physical and chemical sciences and therefore immediately caught my interest and the necessary focus. Hence, it naturally builds a solid ground for my subsequent years of research leading to this book. In this context, I am grateful to A. Prohl for the initial shaping of my scientific thinking and for giving me the freedom to develop my independence by focusing on physically consistent and quantitative aspects of real-world problems. My arrival at the Numerical Analysis Group (NAG) in Tübingen was exactly at the time when Christian Lubich was finishing his book on numerical schemes for Schrödinger equations,[5] which served to me as an excellent and motivating entry into Quantum Mechanics. The computational view on Quantum Mechanics gained hereby together with the continuous advances in the development of Quantum Computers (QCs) over the last decade provided a motivating and solid basis for discussing the usefulness of QCs in the context of this book. In fact, the complexity of QC itself provides already a formidable example of a Complex Heterogeneous System (CHeS), deserving its own dedicated book.

Thanks to a prospective researcher grant awarded by the Swiss National Science Foundation (SNSF) and to my host, Martin Z. Bazant, who supported my planned research work, I could benefit from two intensive research years at the Massachusetts Institute of Technology (MIT), Cambridge. The research environment I had experienced so far was primarily driven by the goal of gaining a complete understanding by taking all possible aspects and details of a process of interest into account. Hence, it was enlightening to observe a primarily application-driven view for gaining useful physical and scientific insight by rewriting dimensional equations into their corresponding nondimensional form. This means that the naturally arising dimensionless parameters in such reformulations allow us to systematically discuss the physical and mathematical justification for neglecting certain terms (physical processes) depending on the scenario of interest.[6] This is what I have taken as the scientific basis of and the motivation

4 M. Schmuck, *Modeling, Analysis, and Numerics in Electrohydrodynamics*, Universität Tübingen, 2008.

5 M. Lubich, *From quantum to classical molecular dynamics: reduced models and numerical analysis*, European Math. Soc., 2008.

6 Related discussions I enjoyed with Roman Stocker (Professor at MIT at that time, now at ETH Zürich), whom I want to thank for his time and insights into his modeling approaches.

for the following general phrase building a fundamental cornerstone of MIT's research culture, i. e., "*Keep It Simple*".[7] Also during my time at MIT, I met Peter Berg (University of Alberta and Brock University) when he visited Cambridge, MA. Our discussions during that time extended my focus in electrochemistry to look into working principles of fuel cells. Thanks to Peter Berg's previous efforts in fuel cell research, we identified a fundamental prototype catalyst layer formulation allowing us to reliably and systematically derive effective catalyst layer equations for Proton-Exchange Membrane (PEM) fuel cells. Moreover, we rigorously derived how *microscopic, incompressible fluid systems* can become *compressible on the macroscale*.

Toward the end of my SNSF-funded research project at MIT in 2011, I came across a highly interesting research theme offered in a joint Research Associate position at Imperial College, London, by Serafim Kalliadasis (Chemical Engineering) and Grigorios A. Pavliotis (Mathematics). My research efforts led me to acquire and to extend a *Renormalization Group* technique and to combine it with a *Maximum Entropy Principle* toward a novel *Stochastic Mode Reduction* strategy in the context of the *Kuramoto–Sivashinksy equation*.[8] Finally, London's size with its Universities and Colleges as well as its history provide a truly international, scientific, and cultural melting pot. The stimulating and supporting environment in both research departments offered peaceful and inspiring working conditions. This finally allowed me to secure my first permanent academic position as Lecturer/Assistant Professor in Edinburgh in 2013.

Motivated and driven by historical developments such as the redesign of the steam engine by James Watt and its subsequent driver for the theory of Thermodynamics as well as the microscopic and probabilistic view on mechanics by James Clerk Maxwell and his contributions to Electrodynamics, I slowly acquired step by step fundamental aspects about the nature of heat in complex systems. In this context, I feel also fortunate for getting the opportunity to talk to Oliver Penrose[9] about the rigorous application of concepts from Thermodynamics and Statistical Mechanics. Hence, the research environment at the Maxwell Institute for Mathematical Sciences and the Heriot-Watt University provided an inspiring and calm enough environment for young aspiring researchers to pursue their ambitious scientific goals. Triggered by discussions on Li_xFePO_4-batteries in M. Z. Bazant's research group in 2009, I finally got the time to elaborate and develop a basic understanding of the important thermodynamic concept referred to as *Phase Transitions*. In fact, the highly heterogeneous character of $FePO_4$-electrodes represents

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7 "Keep It Simple" means here that we should not work with unnecessarily complex model equations if the application of interest implies that certain physical forces/terms are negligible. Indeed, the requirement of simplicity is much older and often referred to as Occam's razor, in honor of the late 13th- to early 14th-century English philosopher William of Ockham (= Oak Hamlet).

8 M. Schmuck et al., *New Stochastic Mode Reduction Strategy for Dissipative Systems*, PRL 110:244101 (2013).

9 O. Penrose, *Foundations of Statistical Mechanics – A Deductive Treatment*, Pergamon Press, 1970.

a formidable prototype problem where systematically derived effective macroscopic descriptions by techniques such as upscaling and homogenization are of great practical interest. These efforts turned into the derivation of the effective macroscopic Cahn–Hilliard phase field formulation and its rigorous verification by error estimates. These error estimates additionally provide *convergence rates* quantifying how quickly the full microscopic description approaches the upscaled Cahn–Hilliard equation while increasing the heterogeneity (that is, $\epsilon \to 0$). Starting with investigations on modeling and analysis in electrohydrodynamics during my PhD, fundamental thermodynamic building blocks such as free energies appeared naturally as useful analytical quantities, e. g., an *entropy law* obtained in the process of deriving *a priori estimates* for establishing the solvability (i. e., the existence of solutions). The deeper study and understanding of free energies, in particular, their main usage in equilibrium thermodynamics, during my time in Edinburgh suddenly raised the following central and crucial question: *What are the systematic principles governing the consistent nonequilibrium thermodynamic (i. e., dynamic) description of systems relying on both reversible and irreversible processes?* At first, I believed the answer is to define the dynamics as a gradient descent of the system's free energy in the appropriate function space.[10] However, despite the fact that this still leaves us with a choice between different possible gradient descent schemes, the answer to the original question is still not convincing enough. After coming across the General Equations for Non-Equilibrium Reversible–Irreversible Coupling (GENERIC) developed by Hans Christian Öttinger and Miroslav Grmela, it is currently the most systematic framework available (to the best of my knowledge) for the physical derivation of reliable dynamic descriptions of time-dependent physical processes. On this occasion, I would like to express my gratitude to Hans Christian Öttinger (ETH Zürich) for his hospitality and the discussions on GENERIC for electrohydrodynamic and phase field formulations, which are elaborated and presented in this book, respectively.

In 2018, triggered by an E-Mail invitation from the ETH Alumni network about a rare opportunity to work on a uniquely designed radar environment taking the geographic features of the Swiss Alps into account, I took this chance to work as a governmental scientific analyst and researcher[11] in a highly interdisciplinary environment of a Command and Control (C2) system. The sensor-oriented nature of radar systems naturally depend on essential aspects such as Measurement Theory, Noise Filtering, and Uncertainty Quantification. These practical concepts strongly motivated me to account for the observer/measurement system in the formulation of Complex Heterogeneous Systems

10 The (continuous) gradient flow formulation is the vanishing limit of a time discretization parameter associated with the descent scheme. Indeed, gradient flows are frequently exploited in mathematical analysis, e. g., G. Perelman, *The entropy formula for the Ricci flow and its geometric applications*, arXiv:math/0211159v1, (2002), or R. S. Hamilton, *Three manifolds with positive Ricci curvature*, J. Diff. Geom. 17:255–306 (1982).

11 Official role reads Scientific Research & Development Engineer.

(CHeSs), which is the main driver and focus of this book. The highly interdisciplinary nature of the underlying C2 system, with different sensor and control applications requiring data and information fusion realized on dedicated computational resources such as Data Centers (DCs), represents a truly interesting and stimulating working environment, to which the author is grateful for being able to contribute.

Obviously, the highly interdisciplinary character of CHeSs and the goal of the book is to foster a general interest in establishing a concise theory and framework for capturing universal principles naturally emerging from the underlying structure of CHeSs. This motivates that interdisciplinary scientists, scientific engineers, and graduate and postgraduate students with an affinity in mathematical concepts are the most likely target audience for this book. The reader will benefit by having a basic knowledge in functional analysis and calculus of variations, both with a focus on partial differential equations, as well as in quantum mechanics. Certain sections of the book can well serve as introductory courses in “Homogenization”, “Smart Interacting Systems”, and “Quantum Computing”, for instance.

Finally, this review of essential impressions and experiences, leading to the present form of the book, does not intend to be complete, and hence, the author would like to thank any person not explicitly mentioned in this preface or the previous acknowledgement for the hospitality, inspirations, and stimulating discussions that might have influenced in some form the content of this book. Hopefully, this text stimulates future research on CHeSs and related topics and leads to novel promising and practically useful findings and publications. Naturally, the author appreciates readers giving reference to such stimuli.

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