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Invariant Manifolds for Physical and Chemical Kinetics

Springer

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Invariant Manifolds in Chemical Kinetics

To our parents

Preface

This book is about model reduction in kinetics. Is this physics or mathematics? There are at least four reasonable answers to this question:

- It is physics, it is not mathematics;
- It is mathematics, it is not physics;
- It is both physics *and* mathematics;
- It is neither physics, nor mathematics, it is something else (but what could that be?).

Of course, it is physics. Model reduction in kinetics requires physical concepts and structures; it is impossible to make an expedient reduction of a kinetic model without thermodynamics, for example. The entropy, the Legendre transformation generated by the entropy, and the Riemann structure defined by the second differential of the entropy provide the elementary geometrical basis for the first approximation. The physical sense of the models gives many hints for their further processing. So, it is not mathematics; we care about the physical sense more than about rigorous proofs. We should deal with equations even in the absence of theorems about existence and uniqueness of solutions. Mathematics assimilates the physical notions with a considerable delay in time, but any such an assimilation leads to further insights.[1]

But, without doubt, it is mathematics. The story about invariant manifolds for differential equations began inside mathematics. The first significant steps were taken by two great mathematicians, A.M. Lyapunov and H. Poincaré, at the end of the XIXth century. Then N.M. Krylov and N.N. Bogolyubov, A.N. Kolmogorov, V.I. Arnold and J. Moser, J.E. Marsden, M.I. Vishik, R. Temam, and many other mathematicians developed this field of science, and many elegant theorems and useful methods were created. This is not only pure mathematics, the wide field of applications was developed too, from hydrodynamics to process engineering and control theory and methods. This is *pure and applied dynamics.* The language of model reduction, the basic notions that we use, the theorems and methods, all this either came from

[1] The closest example: after mathematicians discovered how the entropy functional may be important for the theory of the Boltzmann equation, then they proved the existence theorem (P.L. Lions and R. DiPerna, this work was awarded the Fields medal in 1994).

pure and applied dynamics directly, or bears the visible imprint of its ideas and methods. Maybe the book presents a specific chapter on this subject?

But, of course, the problems came from physics, from engineering. Maybe it is both physics *and* mathematics? Or perhaps it is something different, but what can it be? It is not so easy to answer the question, what is the subject of our book, even for the authors. But we can say what we want it to be. We want it to be a special "meeting point" of pure and applied dynamics, of physics, and of engineering sciences. This meeting point has a sufficient number of specific problems, methods and results to deserve a special name. We propose the name *Model Engineering*. As long as it is engineering, it is synthetic subject: if it is possible to prove something exactly, this is great, and we should follow this possibility, but if the physical sense gives us a seminal hint, well, we should use it even if the rigorous foundations are far from complete. *The result is the model that works.* In this enormous field of intellectual activity our book tends to be in the theoretical corner; we focus our study on constructive *methods*, and the examples that fill up more than three-quarters of the book are used for motivation, demonstration and development of the methods.

Which scientific disciplines should meet at the meeting point we build in our book? The last century demonstrated the emergence of two disciplines, of the theory of dynamical systems in mathematics, and of statistical physics. Nonequilibrium statistical physics, in short, is a science about slow-fast motion decomposition. Dynamic theory is about general features of long-time typical behaviour. Our book is about what dynamic theory has to say about nonequilibrium systems. The very brief answer is – it makes the theory of nonequilibrium systems the theory of slow invariant manifolds. But the reverse impact of physics on methods is also significant. Applied mathematics and computational physics create a "second (computational) reality". This is a beautiful intellectual building, but in each element of this building, at each step of the work, we should take into account the basic physics; the violation of a physical law at one place can destroy an important part of the whole construction.

The presented methods to construct slow invariant manifolds certainly reflect the authors' preference and their own work. Much effort was spent to coordinate the developed methods with the basic physics at each step.

The book can be used for various purposes:

– As a collection of tools for model reduction in kinetics;
– As a source of mathematical problems;
– As a guide to physical concepts useful for model reduction;
– As a collection of successful examples of model reduction;
– As a source of recent literature on model reduction, invariant manifolds and related topics.

We wrote the book for our colleagues and for our students in order to avoid in the future the usual excessive explanation: to explain the basic notions and physical sense, to answer the common questions about invariant manifolds and model reduction, about our point of view, about the balance between physics, mathematics (dynamics) and engineering in our work. Now we can simply hand over this book and suggest reading approaches. There are many possible approaches for different purposes. Some of them are presented in the introduction.

As useful background for reading the book, three graduate courses should be mentioned: differential equations and dynamical systems, kinetics and thermodynamics, and elementary functional analysis.

Once upon a time Lev Landau gave the following advice: If the Contents of a book is interesting to you, close the book and try to write it. If it is too difficult a task, then look through the first chapter and try to write it. If it is still too hard, go ahead and try to write a section, a subsection, a paragraph, a formula. We completely agree with this advice with just one addition: please send us your results, because your book will contain another point of view, and will be highly interesting.

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