

Preface

The dynamics of molecular systems is an essential tool of systems biology. It helps figuring out what is the effect of the perturbation of a system, or what is the best dose for a drug or what could be an effective combined therapy. Simulation is the essence of *what-if* experiments that help us make informed decisions for the next lab experiments by saving time and resources.

We felt the lack of a comprehensive textbook collecting the most relevant and state-of-the-art simulation algorithms that can be a reference for students and the researchers entering the field. In particular, the book is intended for practitioners of the systems biology field with mathematical/computing backgrounds, who want to understand simulation algorithms and algorithmic systems biology. The book can also be used in advanced undergraduate courses on modeling and simulation of biological systems. It also contains many examples used as benchmarks that can help students gain a practical grasp on the main concepts throughout the book. Some knowledge of basic molecular biology and basic computer science can help, but the aim of the book is to be a self-contained approach to the field. All chapters propose further reading about the topics introduced, to drive the reader to deeper treatments of the topics in the book. All of these references are collected in the bibliography reported at the end of the book. The appendices briefly recall relevant knowledge needed to completely appreciate the book.

The book approaches three different classes of simulation algorithms: stochastic, deterministic and hybrid. As a final remark, we stress that we were forced to choose among many different algorithms and methods to constrain the book to a reasonable size. The choice was driven by our experience both as researchers and teachers working in the field. We are aware that there are many other excellent solutions to the problems addressed in the book that we were not able to include. The references are intended to manage this issue at least partially.

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