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This book provides a complete and comprehensive reference/guide to Pyomo (Python Optimization Modeling Objects) for both beginning and advanced modelers, including students at the undergraduate and graduate levels, academic researchers, and practitioners. The text illustrates the breadth of the modeling and analysis capabilities that are supported by the software and support of complex real-world applications. Pyomo is an open source software package for formulating and solving large-scale optimization and operations research problems. The text begins with a tutorial on simple linear and integer programming models. A detailed reference of Pyomo's modeling components is illustrated with extensive examples, including a discussion of how to load data from data sources like spreadsheets and
databases. Chapters describing advanced modeling capabilities for nonlinear and stochastic optimization are also included. The Pyomo software provides familiar modeling features within Python, a powerful dynamic programming language that has a very clear, readable syntax and intuitive object orientation. Pyomo includes Python classes for defining sparse sets, parameters, and variables, which can be used to formulate algebraic expressions that define objectives and constraints. Moreover, Pyomo can be used from a command-line interface and within Python's interactive command environment, which makes it easy to create Pyomo models, apply a variety of optimizers, and examine solutions. The software supports a different modeling approach than commercial AML (Algebraic Modeling Languages) tools, and is designed for flexibility, extensibility, portability, and maintainability but also maintains the central ideas in modern AMLs.

The aim of this book volume is to explain the importance of Markov state models to molecular simulation, how they work, and how they can be applied to a range of problems. The Markov state model (MSM) approach aims to address two key challenges of molecular simulation: 1) How to reach long timescales using short simulations of detailed molecular models. 2) How to systematically gain insight from the resulting sea of data. MSMs do this by providing a compact representation of the vast conformational space available to biomolecules by decomposing it into states sets of rapidly interconverting conformations and the rates of transitioning between states. This kinetic definition allows one to easily vary the temporal and spatial resolution of an MSM from high-resolution models capable of quantitative agreement with (or prediction of) experiment to low-resolution models that facilitate understanding. Additionally, MSMS facilitate the calculation of quantities that are difficult to obtain from more direct MD analyses, such as the ensemble of transition pathways. This book introduces the mathematical foundations of Markov models, how they can be used to analyze simulations and drive efficient simulations, and some of the insights these models have yielded in a variety of applications of molecular simulation.

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