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Book Review: *The Art of Molecular Dynamics Simulation*

The Art of Molecular Dynamics Simulation. D. C. Rapaport, Cambridge University Press, 2004, second edition.

This is an enlarged and improved second edition of a book on molecular dynamics (MD) simulations. The value of this book comes from both a clear presentation of the ideas and methods that are involved in understanding and performing modern MD simulations, and from the author's efforts to filter these ideas and to construct a representative set of concepts and case studies that can be easily used both for the education of newcomers and as a reference for the advanced practitioners.

MD simulations are being performed by a variety of scientists of different backgrounds. The ability to simulate a certain physical system in atomistic detail appeals to most modern researchers, as it offers a direct method for investigation and a better understanding of the processes that occur at atomic and molecular levels, where the boundaries between physics, chemistry, material science and molecular biology are blurred. In MD, concepts and application-motivated interests originating from different scientific disciplines coalesce and arguably create a powerful tool for new discoveries. Yet, this field is not without peril. There is always the danger that scientifically sound statistical methods and computational algorithms could be used in conjunction with imperfect force fields, nonrealistic simulation setups or, worse, in cases that are outside their intrinsic applicability limitations. Arising mainly from the complexity of the many-body systems that are the subjects of typical MD simulations, the various possible pitfalls confer an "artistic" aspect to the MD field. This perception is also supported by the recent development and availability of visually enhanced molecular visualization and animation programs. Nevertheless, this book reflects clearly the author's concerns regarding the above mentioned hazards, and thoroughly leads the reader through a series of fundamental MD concepts and computational algorithms.

As in the previous edition (first published in December 1995), the book starts with a short historical and theoretical introduction and with

a chapter on basic MD. The reader is given the opportunity from the very beginning to study and run a simple MD program. With its modular organization, the program provides the general framework that is used later in case studies throughout the book. Chapters 3 to 10 maintain the same structure as in the first edition, walking the reader through examples of gradually increasing complexity, from simple systems of Lennard–Jones spheres to simulations involving flexible molecules with various geometrical constraints. Along the way, a variety of routines are provided for typical MD setups such as integration schemes, neighbor lists and periodic boundary conditions, as well as for MD trajectory analysis, such as the calculation of transport coefficients, velocity autocorrelation functions or diffusion analysis. In this edition, new chapters (11, 12 and 16) have been added to the original content for the treatment of internal coordinates, many-body interactions, and granular dynamics. Methods for treating long-range interactions are now the subject of an entire chapter (13) presenting a detailed discussion and study cases for the Ewald sum, tree-code and fast-multipole methods. Finally, typical MD programming topics of a more technical nature (e.g. organizing the input data, configuration snapshot files, and managing extensive computations) are presented in a newly organized manner in Chapter 18. Overall, the book has an impressively comprehensive character regarding the number of MD-related methods and algorithms that are provided.

The electronic version of the software programs presented in the book can be downloaded from the following URL: http://www.ph.biu.ac.il/~rapaport/mdbook/getmdsw.php

All the codes are written in C, but the author uses a clear, "functional" style that facilitates the understanding of users of other programming languages such as Fortran. The programs presented in this new edition have been carefully rewritten and significantly extended to include new study cases. All the programs compiled successfully on a PC running Red Hat Linux 9.0 (gcc version 3.2.2). Thanks to their simple, conservative programming style they should require minimal changes for compiling correctly in most operating environments. While not emphasized in the book, the instructions presented in the "Using the software" section of the Appendix and in the *Readme* file provided with the electronic version of the software should be read by the users before compiling the first study cases. Notably, the *crun.sh* script would most probably fail to run on most default Linux installations since the current directory is not typically included in the user's path for security reasons. An easy fix is to replace "$b" with "./$b" in the last line of the *crun.sh* script. Another observation is that there is little or no description of the programs in their electronic version. Therefore, the user has to fully rely on the text from the

corresponding book chapter and on the list of variables from the Appendix. On the positive side, most chapters end with "Further study" sections, which could be very useful for the reader and often emphasize important concepts and ideas that could not be detailed in the current text. Just like the software, the list of references has been significantly extended and updated.

In his book, Rapaport shares with its readers his valuable experience in programming techniques that are involved in modern MD simulations. As stated by the author, this is intended to be a "recipe book". We note that, as any cookbook, it might miss some of the "family recipes" and "secret ingredients" that define the "state-of-the-art" of the MD cuisine. However, it provides in a clear manner the main concepts and tools that can improve both the understanding and the programming productivity of its readers, and it shows that while style is important, the scientific base of MD simulations is much more than just a matter of taste.

To sum up, this is a very useful and informative book that addresses the needs of a growing and diverse readership. Both students and researchers could benefit strongly from the coherent collection of theoretical and computational MD topics that are provided in this work.

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