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COMPUTER SOFTWARE REVIEWS

MOBY. Version 1.41

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MOBY[1] is a program for molecular modeling. It can be run on IBM compatibles (with 640K of RAM, 80 × 87 arithmetic coprocessor, hard disk, VGA, EGA, or HERCULES graphics adapters). The use of a mouse is optional. Both English and German versions are available. The program is shipped on two 5.25-in. or 3.5-in. diskettes that are not copy-protected.

The program can be run in demo mode allowing the user to get acquainted with some of its capabilities. In protocol mode the whole session is captured to a disk file, which may be edited and shown in demo mode. A manual for the program contains a thorough description with an extensive tutorial.

MOBY allows the user to draw structures (up to 2000 centers and bonds) with a 3D editor, read it from disk (a number of formats including MNDO, Brookhaven Protein Database, MACCS II, SHAKAL, and freely definable format are supported), display the structure and its van der Waals or solvent surfaces, define a fragment (up to 150 centers), carry out force-field calculations (extended AMBER force field) with exact calculation of their interaction with all centers (molecular dynamics simulation, conformational analysis for up to six torsion angles, calculations under geometry constraints and with periodic boundaries are supported), and conduct semiempirical quantum chemical calculations with MNDO and AM1 methods for systems up to the size of glucose. Matching of structures and interactive docking are also provided.

It is worthwhile mentioning the flexibility of the force-field calculations. Hydrogen atoms bound directly to carbon atoms can be considered explicitly or implicitly ("united atom" approximation). Either all terms or only the valence terms of the force field can be used for the energy calculations. Geometry optimization can be run with constraints specified by the user for interatomic distances, bond lengths, valence, and torsion angles. For special cases periodic boundaries can also be specified. The conjugate gradient and the steepest descent optimizer can be selected, and various options and criteria for geometry optimization can be defined. Easy switching between force-field and quantum chemical calculations provides the ability to use charges calculated by the AM1 method for molecular mechanics calculations and to use the geometry optimized by the force-field method for quantum chemical calculations.

The main feature distinguishing MOBY from many other molecular modeling programs on PCs is its orientation toward biochemistry. The program uses the AMBER force field,[2] known to be well-suited for proteins and other biological molecules. Protein structures can be read directly from the Brookhaven Database. The program displays the protein and any of its parts in many different ways (all atoms and bonds, backbone, sequence of amino acid residues, etc.). The user can define a fragment in the protein and investigate its conformational behavior. Examples in the tutorial illustrate the modeled denaturation of a polyalanine helix in cytochrome C and substrate binding to the enzyme adenylate kinase. The coloring ability is a very interesting feature of the program. All centers can be colored in accordance with their properties (charge, energy, etc.). This makes the process of geometry optimization quite unusual in appearance.

MOBY can be used in various fields such as biochemistry, enzyme catalysis, and drug design, but it cannot be recommended for the use in conformational analysis in areas outside biochemistry because of the relatively "poor" parameterization of AMBER force field. In such cases programs like PCMODEL are preferable. We have tried to compare these two programs by calculating the conformational energy of a methyl group. PCMODEL (extended MM2 force field) gave 1.78 kcal/mol while MOBY gave 1.10 kcal/mol. The experimental value in aprotic solvent is 1.70 kcal/mol.

Also, it must be pointed out that it is not easy to use this program without having studied the manual or tutorial, since pleasant features of user-friendly programs such as pop-up helps or use of the ESC key for exiting are absent.

Overall, the program is recommended, especially for biochemistry and drug design.

REFERENCES AND NOTES

(1) MOBY is available from Springer-Verlag, New York, Inc., P.O. Box

2485, Secaucus, NJ 07096-2491. Telephone (212)460-1622. A single copy costs $498 for academic users, $998 for others. For 5–9 copies, the prices are $200 and $598 per copy and for 10 or more copies, $150 and $400, respectively.

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BOOK REVIEWS

New Trends in Animation and Visualization. Edited by Nadia Maganenat Thalmaan and Daniel Thalmaan. Wiley Professional Computing. John Wiley & Sons: New York. 1991. 285 pp. $49.95 (cloth). ISBN 0-471-93020-2.

New Trends in Animation and Visualization is a compilation of contributions from several authors on recent advances in animation and visualization techniques. The book is divided into four parts. The first part, which covers almost half of the book, gives an overview of the principles, issues, and techniques of object-oriented design and scientific visualization. It also addresses specific issues such as filling, clipping, and interrogation of shapes. Other topics covered include hypermedia, 3D hierarchies, and virtual environments.

Part 2 deals with specific problems and applications of visualization. Theoretical aspects of visualization in scientific experiments and in building/landscape design are discussed here. Part 3 is about the rendering of natural phenomena like fur, water, and hair, and Part 4 is about visualization and animation of human bodies.

This book is aimed at people who already have a background in computer visualization and animation techniques and who are involved in the development of such products. This is not meant to be a review, though, interested people could use the ample references listed at the end of each chapter for that purpose. *New Trends in Animation and Visualization* has a pleasant typeface in spite of its multi-author origins and has several color illustrations. The price listed (cloth version) seems reasonable. This book is recommended for Engineering and Computer Science Libraries.

Jayashri Nagaraja, *Princeton University*

Chemometrics: Applications of Mathematics and Statistics to Laboratory Systems. By Richard G. Brereton. Ellis Horwood Series in Chemical Computation, Statistics and Information. Ellis Horwood: New York. 1990. 307 pp. ISBN 0-13-131350-9.

This book is aimed at the user of chemometric methods rather than at the chemometrics researcher. It begins with an introduction that includes a history of chemometrics and a survey of the possible applications in laboratory chemistry. The author emphasizes that the text does not require extensive knowledge of mathematics and statistics, a fact supported by the generous use of graphics and the sparse use of equations. For the more curious reader, references to appropriate articles in the literature are included for every topic discussed in the book. The introduction even has a general survey of the chemometrics literature that will prove valuable for scientists who are new to chemometrics.

Chapter 2 is concerned with the appropriate design of multivariate laboratory experiments, with emphasis on the simplex optimization method and factorial design. Chapter 3 addresses the problems of sampling sequential, time-based data. Only a limited number of topics are discussed in the third chapter (it is the shortest of the book), a mere 25 pages, and it does not describe in sufficient detail even the chosen procedures. The chapter includes some discussion of the statistics of time-based data distributions, autocorrelation and averaging methods, and the Nyquist criteria for sampling frequency.

Chapter 4 introduces principal components analysis, information theory, ANOVA, and Fourier and Hadamard spectroscopies under the heading "Choosing and optimizing analytical conditions". Portions of the book, and this chapter especially, suffer from an attempt to provide a comprehensive introduction in a small number of pages, which inevitably leads to a somewhat arbitrary clustering of topics.

Chapter 5 considers the processing of univariate signals. Fourier transform methods are discussed here as separate procedures from their applications in optical spectroscopy. Averaging, deconvolution techniques, and filtering for signal processing are given one of the better treatments in this chapter.

Chapter 6 considers the processing of multivariate signals. This is usually the heart of chemometrics texts, but it is given short treatment in this book. Perhaps this is just as well since the subject is thoroughly covered in other general books and articles. Factor analysis, principal components regression, and partial least squares for quantitative calibration are introduced with a modest discussion of their application. Pattern recognition is the subject of Chapter 7, and the text introduces all of the now-classic methods, such as SIMCA and KNN. Supervised and unsupervised pattern recognition are discussed in general terms, with an even treatment given to each method.

The major drawback of this book is that it is too short for a comprehensive introduction to such a disparate subject as chemometrics. A longer book or a more thorough introduction to fewer methods might have minimized the disorganized feel of the text. Additionally, some subjects are introduced in what might seem inappropriate chapters. Fourier trnasform analysis, for example, is introduced with principal components analysis in a chapter on optimization of analytical conditions.

A small annoyance that will have varying effects on different readers in the appearance of the typesetting. The type suffers from the "camera-ready" look, and readability has been sacrificed by condensing the text and equations. In this regard it is no different than many other books published in this way, but the text deserves better.

The book works best as an introduction to chemometric methods for laboratory scientists—its stated intention—but it also would be valuable as a textbook for a graduate-level course in chemometrics. The extensive references would make coupling a supplement of research articles a minor task. Although the book is rather short, the author has produced one of the best introductions to the subject of chemometrics that exists today.

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