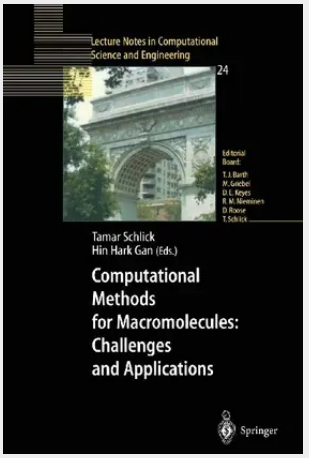
Schlick / Gan

Computational Methods for Macromolecules: Challenges and Applications

Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling, New York, October 12-14, 2000



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3 The workshop on Methods for Macromolecular Modeling (M), held at New York University on 12- 14 October 2000, attracted 187 participants from Eu rope, Asia, the Americas, and the Middle East. (see monod.biomath.nyu.eduj rvhganjconfOO.html for more information). The exciting program was made possible by the dedicated work of the international advisory committee whose members were P. Deuflhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, T. Schlick, and R. Skeel. We are indebted to the following agen cies and institutions for their generous support: the Burroughs Wellcome Fund, Department of Energy, National Science Foundation, National Insti tutes of Health, Computational Biomedicine Initiative at Mount Sinai School of Medicine, and NYU's Courant Institute of Mathematical Sciences, Depart ment of Chemistry, and Science Council. This volume is a collection of 19 review and original articles by the speak 3 ers and participants of the M workshop. The topics covered include molecu lar dynamics methods, Monte Carlo methods, other conformational sampling methods, free energy methods, long range interactions and fast electrostatics, and statistical approaches to protein structures. A perspective article intro duces the contributions in this volume and reflects on future prospects in macromolecular modeling.

Methods for Macromolecular Modeling (M3): Assessment of Progress and Future Perspectives.- I Biomolecular Dynamics Applications.- Mathematics and Molecular Neurobiology.- Structural and Dynamical Characterization of Nuclei Acid Water and Ion Binding Sites.- II Molecular Dynamics Methods.- A Test Set for Molecular Dynamics Algorithms.- Internal Coordinate Molecular Dynamics Based on the Spectroscopic B-Matrix.- The Sigma MD Program and a Generic Interface Applicable to Multi-Functional Programs with Complex, Hierarchical Command Structure.- Overcoming Instabilities in Verlet-I/r-RESPA with the Mollified Impulse Method.- III Monte Carlo Methods.- On the Potential of Monte Carlo Methods for Simulating Macromolecular Assemblies.- Structure Calculation of Protein Segments Connecting Domains with Defined Secondary Structure: A Simulated Annealing Monte Carlo Combined with Biased Scaled Collective Variables Technique.- IV Other Conformational Sampling Methods.- Hierarchical Uncoupling-Coupling of Metastable Conformations.- Automatic Identification of Metastable Conformations via Self-Organized Neural Networks.- V Free Energy Methods.- Equilibrium and Non-Equilibrium Foundations of Free Energy Computational Methods.- Free-Energy Calculations in Protein Folding by Generahzed-Ensemble Algorithms.- Ab Initio QM/MM and Free Energy Calculations of Enzyme Reactions.- VI Long Range Interactions and Fast Electrostatics Methods.- Treecode Algorithms for Computing Nonbonded Particle Interactions.- A New Reciprocal Space Based Method for Treating Long Range Interactions in Ab Initio and Force-Field Based Calculations for Surfaces, Wires, and Clusters.- Efficient Computational Algorithms for Fast Electrostatics and Molecular Docking.- VII Statistical Approaches to Protein Structures.- FoldRecognition Using the OPLS All-Atom Potential and the Surface Generalized Born Solvent Model.- Identification of Sequence-Specific Tertiary Packing Motifs in Protein Structures using Delaunay Tessellation.- Appendix: Color Plates.

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