Book Review

P. M. Pardalos, D. Shalloway, and G. Xue (eds.), *Global Minimization of Nonconvex Energy Functions: Molecular Conformation and Protein Folding.* DIMACS Series in Discrete Mathematics and Theoretical Computer Science, Vol. 23, American Mathematical Society, 1995, ISBN 0-8218-0471-5.

This book contains seventeen refereed papers presented at an interdisciplinary scientific conference attended by leading biochemists, computer scientists, engineers and mathematicians working in global optimization held at DIMACS in March 1995. It describes the recent development of a variety of new methods which have been developed for solving one of the most significant and challenging problems in molecular biophysics and biochemistry which consists of computing the native 3-dimensional conformation (folded state) of a globular protein given its amino acid sequence, possibly in the presence of additional agents as well as related problems. Numerical methods require on one hand determination of suitable energy functions that can reliably model protein behavior, and on the other hand optimization methods that can find or approximate global minima of these functions. Given the many degrees of freedom available to protein structures this task can hardly be achieved by standard nonliner programming techniques. Therefore, ingenious new methods have to be developed combining experimental knowledge-based methods to provide good initial guesses with a variety of approaches including heuristics, stochastic methods, various approximation techniques, dynamic systems, parametrized global optimization techniques, smoothing and decomposition. The book reflects very much of the state–of the-art in all these directions which is exhibited by the following table of contents:

- PATRICIA AMARA, JIANPENG MA, AND JOHN E. STRAUB: Global Minimization on rugged energy landscapes

- ROBERT E. BRUCCOLERI: Energy directed conformational search of protein loops and segments

- RICHARD H. BYRD, ELIZABETH ESKOW, ANDRÉ VAN DER HOEK, ROBERT B. SCHNABEL, CHUNG-SHANG SHAO, AND ZHIHONG ZOU: Global optimization methods for protein folding problems

- BRUCE W. CHURCH, MATEJ OREŠIČ, AND DAVID SHALLOWAY: Tracking metastable states to free-energy global minima

- JUN GU AND BIN DU: A multispace search algorithm for molecular energy minimization

- HERBERT A. HAUPTMAN: A minimal principle in the phase problem of X-ray crystallography

- XICHE HU, DONG.KU, KENNETH HAMER, KLAUS SCHULTEN, JUERGEN KOEPKE, AND HARTMUT MICHEL: Knowledge based structure prediction of the light-harvesting complex II of *Rhodospirillum molishianum*

- J. KOSTROWICKI AND H.A. SCHERAGA: Some approaches to the multiple-minima problem in protein folding

- C.D. MARANAS, I P. ANDROULAKIS, AND C.A. FLOUDAS: A deterministic global optimization approach for the protein folding problem

- JORGE J. MORÉ AND ZHIJUN WU: ε -optimal solutions to distance geometry problems via global continuation

- RUTH PACHTER, ZHIQIANG WANG, JAMES A. LUPO, STEVEN B. FAIRCHILD, AND BRIAN SENNET: The design of chromphore containing biomolecules

- A.T. PHILLIPS, J.B. ROSEN, AND V.H. WALKE: Molecular structure determination by convex global underestimation of local energy minima

- ANDREJ ŠALI, EUGENE SHAKHNOVICH, AND MARTIN KARPLUS: Thermodynamics and kinetics of protein folding

- GOMATHI RAMACHANDRAN AND TAMAR SCHLICK: Beyond optimization: Simulating the dynamics of supercoiled DNA by a macroscopic model

- MICHAEL VIETH, ANDRZEJ KOLINSKI, C.L. BROOKS, III, AND JEFFREY SKOLNICK: A hierarchial approach to the prediction of the quaternary structure af GCN4 and its mutants

- G.L. XUE, A.J. ZALL, AND P. M. PARDALOS: Rapid evaluation of potential energy functions in molecular and protein conformations

- MARKUS M. ZACHARIAS AND DIOSISIOS G. VLACHOS: Simulated annealing calculations for optimization of nanoclusters: The roles of quenching, nucleation, and isomerization in cluster morpholoy

This book is highly recommended to graduate students and researchers in mathematical programming, molecular biology, biochemistry, computer science, engineering and operations research.

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