Computer Simulations in Molecular and Protein Conformations

Preface

In recent years, more and more researchers in Computer Science and Global Optimization have found Computational Biology, Computational Chemistry, Protein Folding and other related "real sciences" to be wonderful sources of test problems for global minimization algorithms. At the same time, researchers in those real sciences have come to recognize Computer Science and Global Optimization as a powerful tool in solving their problems. As the sciences blend, together with the advent of massively parallel high performance computers, we have all witnessed the advances in Computational Biology, Computational Chemistry and Protein Folding: better solutions have been found; larger problems have been solved! In 1994, we edited the first special issue of JOGO on Advances in Computational Biology and Protein Folding, which proved to be a great success. In 1995, the editors coorganized an international workshop on this topic (at the DIMACS Center) bringing together well known active researchers. Many new results have been obtained since the last special issue. We thought that it is time to publish a second high quality special issue on this topic.

We are pleased to present to you this special issue of JOGO featuring Computer Simulations in Molecular and Protein Conformations. All papers published in this issue are refereed. We take this opportunity to thank all the authors and the referees without whose time and effort this special issue wouldn't have been possible. The research of the two editors were supported in part by the National Science Foundation under grants BIR-95-05919 and ASC-94-09285.

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