PREFACE

The Office of Health and Environmental Research (OHER) has supported and continues to support development of computational approaches in biology and medicine. OHER's Radiological and Chemical Physics Program initiated development of computational approaches to determine the effects produced by radiation of different quality (such as high energy electrons, protons, helium and other heavy ions, etc.) in a variety of materials of biological interest—such as water, polymers and DNA; these include molecular excitations and sub-excitations and the production of ionization and their spatial and temporal distribution. In the past several years, significant advances have been made in computational methods for this purpose. In particular, codes based on Monte Carlo techniques have been developed that provide a realistic description of track-structure produced by charged particles. In addition, the codes have become sufficiently sophisticated so that it is now possible to calculate the spatial and temporal distribution of energy deposition patterns in small volumes of subnanometer and nanometer dimensions. These dimensions or resolution levels are relevant for our understanding of mechanisms at the molecular level by which radiations affect biological systems.

Since the Monte Carlo track structure codes for use in radiation chemistry and radiation biology are still in the developmental stage, a number of investigators have been exploring different strategies for improving these codes. Nevertheless, the scientific community here in the United States and the European communities felt that all the international experts working in this field ought to be brought together to discuss the computational advances, evaluate the state of the art, and to provide directions for future research in this field. In addition, the scientific community and OHER recognized that discussions of the ongoing computational approaches in radiological and chemical physics should also consider other major advances in the field of computational biology, evaluate the impact of the increased technology and computational methods that have taken place in the last few years, and suggest new approaches to enhance this unique capability for further advancing the goals of track structure methods.

Considering the importance of this research and the unprecedented opportunities that are available, OHER organized and sponsored a workshop on computational approach Monte Carlo methods in molecular radiation biology at the National Academy of Sciences facilities in Irvine, California. In order to have sufficient information and input from outside experts, the organizers made special efforts to bring internationally recognized experts in other fields, such as structural biology, computational biology, statistics and mathematics to the workshop. By all accounts, interaction and exchange of information and ideas between the participants was outstanding. Eighteen invited scientific papers were presented and ample time was provided for discussions. These proceedings provide a complete record of

the reports and discussions at the workshop, documents the progress in this field and points to future research directions. We are extremely thankful to Lawrence Berkeley Laboratory and the staff of the Life Sciences Division for untiring help in the local arrangements of the workshop, and for editing and proofreading the proceedings. Special thanks are due Ms. Cathy Sage and Ms. Martha Franklin for coordinating the prepublication of these proceedings.

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