



Preface

Quantum Monte Carlo is a field experiencing considerable growth as advances in computer technology and algorithms are making possible the simulation of a variety of phenomena that would be extremely difficult to investigate by other means. When approached by several of my Los Alamos colleagues about helping to organize a conference on the field, I was quite excited about the idea. I thought that such a conference was timely scientifically, and as a relative newcomer to these types of simulations, I also thought it would be a marvelous opportunity for me to learn more and to meet other researchers interested in the field.

What is “quantum” about quantum Monte Carlo, of course, is the statistics the particles and fields obey. These seemingly simple requirements, however, make the quantum simulations difficult to perform, and often orders of magnitude more computing time are needed than for comparably sized classical systems. Perhaps somewhat mind-boggling are the simulations being attempted in lattice gauge theory that have already pushed today’s supercomputers to their limits, even though relatively small systems are being used.

A variety of quantum Monte Carlo methods exist, so making general statements about the field is difficult, if not misleading, but I think it is fair to say that the variety is largely a consequence of the absence of a clear algorithmic choice for the various problems, and in some cases the results of the simulations are as much a demonstration of the algorithm used as they are a demonstration of new physical results obtained. Interesting science is being done; it is just that one would like to do more and to do it better. Unsurprisingly, in today’s age of supercomputers, new method development is often linked to computer architecture and special computer designs for maximum efficiency. This linkage is likely to be the opportunity of the times, for even when more efficient and effective algorithms are in place, scaling up the system size and exploring the richer physics of more complex systems will be the order of the day.

In this issue of the *Journal of Statistical Physics*, we present the proceedings of our conference, *Frontiers of Quantum Monte Carlo*, held September 3–6, 1985, in Los Alamos, New Mexico. The conference was successful in capturing the excitement of recent developments in addition to creating an opportunity for exchange between practitioners and potential

newcomers. We planned the conference around sessions of extended talks, presenting detailed descriptions of different aspects of quantum Monte Carlo, and used a poster session to generate additional discussion and exchange. By publishing the proceedings, we hope to share its results with a larger community.

The papers in these proceedings were contributed by the speakers and the poster session participants, with some poster session participants preferring to be represented by extended abstracts. In organizing the proceedings, I grouped the papers by "discipline." Many papers are, however, multidisciplinary, so scanning the Table of Contents should prove valuable. Two papers, the ones by Professors Kogut and Scalapino, were designed to be of a more introductory nature and have been grouped separately.

The conference also had a festive intent. We at Los Alamos are proud of the role that our colleague, Nick Metropolis, played in developing importance sampling for use in computer simulations. The Metropolis algorithm remains one of the most powerful algorithms yet developed for numerical simulations of statistical mechanical problems. In the year of Nick's seventieth birthday, we dedicated the conference to him, hoping it would be a fitting tribute, and in recognition of his broader interests and his extensive contributions to the use of computers, we held a special session on Computers in Science. Two papers from that session are reproduced here: Professor Anderson's historical account of the earliest uses of computers, detailing the important role Nick played, and Professor Lax's talk on the important advances that occur when the physical sciences, mathematics, and computers interplay. These papers are highly recommended. For me they provide a provocative perspective on theoretical sciences.

In planning the conference I was fortunate to have David Campbell, Jim Doll, Gerry Guralnik, Jim Louck, Paul Stein, and Chuck Zemach helping to recruit speakers and participants. I am particularly grateful to David Campbell for his advice and encouragement. We all are thankful to the Centers for Materials Science and Nonlinear Studies and the Theoretical Division at Los Alamos for the financial support to conduct the conference and to Mary Frances Gomez, Laurie Lauer, and Valerie Ortiz for making sure that everything ran smoothly. The person I would like to thank most is Nick. I bought away from the conference not just the hoped for new information and colleagues, but also a better appreciation of the man and his achievements. I feel richer because of this.

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