The American Physical Society

Division of Computational Physics… …DCOMP

Physics Computing News

Summer 1999

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In This Issue

It is time for our Division to elect members of the *Executive Committee*. Ordinarily, the election for new officers is held prior to the divisional annual meeting at which time the new officers assume their positions. Due to the unusually early Divisional Meeting (which was part of the APS Centennial Meeting), unavoidable circumstances made it impossible to hold this election in a timely manner. Thus, at the end of the centennial meeting the Chair-Elect became Chair, and the Vice-chair became Chair-Elect.

Questions regarding the items in this newsletter or suggestions for future issues of *Physics Computing News* should be directed to Bob Peterkin, Newsletter Editor. His address is given at the end of the Roster of the Executive Committee.

APS and DCOMP Home Pages

The Division of Computational Physics has a home page that is available through the *APS Divisions, Topical Groups, Sections, and Forums* page attached to the APS home page at the **URL** http://www.aps.org. The latter can be reached by using Internet browsers such as Netscape and Microsoft Explorer.

The **DCOMP** home page, http://www.aps.org/DCOMP, provides up-to-date information about the Division's leadership, policies, and activities, including those regularly featured in this newsletter. It includes domestic and international meetings, fellowship in the APS, prizes and awards administered by DCOMP, journals and publications, and other issues that may arise from time to time.

Please send your suggestions for how to improve the DCOMP home page to the Newsletter Editor.

Note from the Past Chair

This past year has been both interesting and challenging. As a relatively new and very interesting vibrant division, DCOMP is constantly evolving. Add to this feature, the fact that this year we hosted our first IUPAP Conference on Computing in Physics (CCP99) in concert with the APS Centennial, and you can imagine how "interesting" the past year has been. Many people played quite significant roles and I would like to extend particular thanks to the Program Chair, Gary Doolen, and to Ralph Roskies who put together an exciting and very high visibility exhibit at the Centennial. In the future, CCP conferences will come to this country on a three-year cycle. Your Executive Committee has thus decided to hold next year's Divisional meeting together with the March APS meeting, to plan a "stand-alone" Divisional meeting in the San Francisco Bay area in 2001, and then CCP02 at an as yet undetermined location. The DCOMP Program Committee has also been directed to aggressively attempt to organize DCOMP sessions at all APS meetings! In addition, the Executive Committee has given their approval to a set of By-laws revisions. These will be presented to the Divisional membership for a vote according to the appropriate procedure. In closing, I would like to thank the many DCOMP members who assisted with various divisional duties and ask that you give the new Chair the same support.

With best wishes,
David P. Landau

APS CENTENTIAL MEETING

from the CHAIR-Gary D. Doolen

The Conference on Computational Physics, held jointly with the APS Centennial Meeting in Atlanta, was the largest meeting held by DCOMP. Over 11,000 registered for the Centennial Meeting and about 500 specifically registered for the concurrent Conference on Computational Physics, many more than expected. DCOMP had four days of sessions and the DCOMP Centennial Session on Friday morning was recorded and will be available on CDs (as will all the unit Centennial sessions). An outstanding exhibit show, organized by Ralph Roskies, included many computational demos from DCOMP.

Congratulations and thanks to the many organizers and volunteers including DCOMP Past Chair David Landau who helped make this meeting such a success. It is planned that this degree of success continues into the next century, when DCOMP will hold its annual meeting at the March APS meeting in Minneapolis.

This is a challenging and interesting time for Computational Physics, with computational capabilities continuing to grow exponentially and many fields demonstrating new computational capabilities. Beyond the individual research areas of our members, we must actively communicate the benefits of our fields to our elected representatives and to the public in general. DCOMP is your Division; help it remain vigorous and stimulating by helping to plan and participate in innovative programs at the upcoming meetings. Now is a good time to become active and fulfill your potential to contribute to DCOMP and to encourage others to do the same. All suggestions for improving DCOMP are encouraged; please send email to gdd@lanl.gov or call 505-667-8994.

ANEESUR RAHMAN PRIZE IN COMPUTATIONAL PHYSICS

The Aneesur Rahman Prize was established by the American Physical Society in 1992 to recognize and encourage outstanding achievement in computational physics research. The Prize is sponsored by the International Business Machines Corporation and Argonne National Laboratory, and consists of $5,000, an allowance for travel to the meeting of the Society at which the prize is awarded and where the recipient delivers the Rahman Lecture, and a certificate citing the contributions made by the recipient.

Past recipients of the Rahman Prize are: **Kenneth G. Wilson** (1993), **John M. Dawson** (1994), **Roberto Car**, **Michele Parrinello** (1995), **Steven Gwon Sheng Louie** (1996), **Donald H. Weingarten** (1997) and **David M. Ceperley** (1998).

1999 Aneesur Rahman Prize Winner: Michael L. Klein

The seventh Rahman Prize was awarded to **Michael L. Klein** of the University of Pennsylvania.
Background: Prof. Klein attended Bristol University where he received a B.Sc. in 1961 and a Ph.D. in 1964. He was a CIBA-GEIGY Fellow at the Instituto di Fisica, University of Genoa, Italy in 1964 - 1965 and an ICI Fellow in the Department of Theoretical Chemistry, at Bristol University, 1965 - 1967. In 1967 he moved to the United States to accept a position as a Research Associate in the Department of Physics at Rutgers University.

In 1968 he moved to the Chemistry Division of the NRCC in Ottawa, Canada, where he remained for 19 years, rising from Associate Research Officer to Principal Research Officer. During this period he was also Adjunct Professor at the University of Waterloo (1977 - 1983) and Professor of Chemistry (part-time), at McMaster University (1977-1988).

In 1987 he returned to the United States to accept his current position as Professor of Chemistry at the University of Pennsylvania, where he was appointed William Smith Professor of Chemistry from 1991-1993. Since 1993 he has been Hepburn Professor of Physical Science. In addition, Prof. Klein has been the Director of the Laboratory for Research on the Structure of Matter since 1993 and Director of the Penn Center for Molecular Modeling since 1994.

Prof. Klein is the author of over 400 scientific publications and editor of three books. His current research involves the structure and dynamics of disordered molecular systems using computer simulation techniques; systems of interest include molecular solids, conducting fluids, molecular overlayers, model membranes, micelles and membrane-bound proteins. His research has impacted broadly on topical problems ranging from condensed matter physics and materials science to chemistry, biochemistry and molecular biophysics.

2000 Aneesur Rahman Prize: Call for Nominees

Nominations for the eighth Rahman Prize are still open. Division members who wish to nominate deserving colleagues for the Rahman Prize are encouraged to do so before 1 July 1999. Announcements will appear periodically in *APS News* over the intervening months.

Nominations are open to scientists of all nationalities regardless of the geographical site at which the work was done. The prize shall ordinarily be awarded to one person, but a prize may be shared among recipients when all recipients have contributed to the same accomplishments.

Send the name of the proposed candidate and supporting information, including a *curriculum vitae* of the nominee, a description of the important contributions for which the nominee is being recognized, and a proposed citation, to: **Farid F. Abraham**, *Rahman Prize Committee Chair*, whose address is given in the Roster of the Executive Committee of this newsletter.

FELLOWSHIP PROGRAM

This year, the Division of Computational Physics had nine members elevated to Fellowship in the APS. We congratulate these colleagues on being so honored. The new Fellows are:

1. ***Bernard, Claude*****,** Washington University
   For his many contributions to the numerical study of quantum chromodynamics, particularly of the weak decays of strongly interacting particles.
2. ***Camp, William J.*****,** Sandia National Laboratories
   For contributions to computational methods in the theory of phase transition and in reactor safety physics, and for seminal efforts in high performance computing for science and engineering.
3. ***Cieplak, Marek*****,** Polish Academy of Sciences
   For his insightful contributions to the numerical studies of disordered systems.
4. ***Detar, Carleton Edward*****,** University of Utah
   For wide ranging contributions to hadronic and computational physics from the MIT bag model, to lattice studies of the spectrum, and especially for study of the quark-gluon plasma.
5. ***Kritz, Arnold H.,*** Lehigh University
   For the development of innovative simulation tools to study wave heating, current drive and transport in plasmas, and for inspired leadership in a teamed approach to large computations.
6. ***Ladd, Anthony*****,** University of Florida
   For a variety of contributions to numerical simulations of particle systems and especially for the development of lattice-gas and lattice-Boltzmann methods to particle suspension.
7. ***Landau, Rubin Harold*****,** Oregon State University
   For innovative developments and practical applications of computational quantum physics to the scattering and exotic bound states of elementary particles, and for original books in quantum mechanics and computational physics.
8. ***Matthaeus, William Henry*****,** University of Delaware
   For contributions to understanding of fluid and plasma relaxation processes, for pioneering work on novel lattice gas simulation methods, and for advances in understanding of turbulence and particle scattering in space plasmas
9. ***White, Steven R.*****,** University of Calif., Irvine
   For the development of the density matrix renormalization group method which provides a powerful numerical technique for investigating the properties of strongly correlated electron systems.

The annual deadline for nominations from DCOMP is 15 February.

JOURNALS & PUBLICATIONS

Computers in Physics: Educational Software Contest

The winners of the 1999 Educational Software contest were announced in the Nov/Dec issue of CIP. There have been 53 winners since the inception of the contest in 1990.

The Computers in Physics is no longer being published. At the beginning of 1999 CIP was merged with IEEE Computational Science & Engineering to create the bimonthly magazine *Computing in Science and Engineering*, which is a joint publication of the American Institute of Physics and IEEE Computer Society.

Peer-reviewed articles from the archival Journal Section of Computers in Physics for the years 1997 and 1998 only are available at *http://www.aip.org/cip/.* Additional materials including source code and a complete author and title index for the 12 volumes of Computers in Physics, extending from 1987 through 1998, are available on *CIP's legacy Web pages.*

The contest is continuing under the auspices of Computing in Science and Engineering.

DCOMP Annual Meeting

The next annual APS meeting will be held March 20th - 24th in Minneapolis, Minnesota.

The abstract deadline is 3 Dec '99. Information for electronic abstract submissions can be found at the URL
http://www.aps.org/meet/meet-abstract.html

For interesting physics news, including the latest on congressional actions, see ***"What's new"*** *by Bob Park at*
http://www.aps.org/WN/index.html

ROSTER OF EXECUTIVE COMMITTEE

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Term ends 2000; AMO Physics, Fluid Dynamics, Nuclear Physics, Plasma Physics

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Term ends 2001: Plasma Physics, Condensed Matter Physics

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Ex Officio; Statistical Physics, Condensed Matter Physics

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Term ends 2001; Fluid Dynamics

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Ex Officio; Plasma Physics, General Relativity

Thanks for all the hard work for the Division from the following individuals whose terms expired at the last Division meeting:

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Condensed Matter, Statistical Physics

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Condensed Matter

DCOMP ANNUAL ELECTION

In this year's election, we will elect a Vice-Chair, a Division Councilor, and two Members-at-Large for our Executive Committee. The candidates to be elected this year will serve on the Executive Committee of the Division for three years; their terms expire in the spring of 2002. The Vice-Chair becomes Chair-Elect next year, and the Chair of the Division in two years. The DCOMP Councilor serves a four-year term as the liaison between the APS Council and the DCOMP Executive Committee. Following each APS Council meeting, the DCOMP Councilor reports to the DCOMP Chair and the Secretary-Treasurer regarding APS Council actions that affect our Division. The Executive Committee of our Division has a total of six Members-at-Large.

For each of these positions we have two or more candidates. Their biographical information and policy statements are included to help inform you about them. Enclosed are a ballot sheet and a return envelope. Please vote for one candidate for the office of Vice-Chair, one candidate for Councilor and for two candidates among those running to be Members-at-Large.

Mail your ballot in the enclosed envelope to the Secretary-Treasurer of the Division. It must be received by September 20, 1999 for it to be counted.

INFORMATION ABOUT THE CANDIDATES

Vice-Chair

Jim Gubernatis
Los Alamos National Laboratory
Los Alamos, NM

In 1972 Jim Gubernatis received his Ph.D. in Physics from Case Western Reserve University. After one year as an assistant professor at Ohio Northern University and then two years as post-doctoral associate at Cornell University, he joined the staff of the Theoretical Division at the Los Alamos National Laboratory as a member of the Condensed Mater Theory and Statistical Physics group, serving as its Deputy Group leader from 1981 to 1984. At Los Alamos, he was a member of the committee charged with setting up the Center for Materials Science and for the past seven years served on the Executive Committee of Los Alamos's Center for Nonlinear Science. When the CM-2 computer first arrived at Los Alamos, he organized the CM-2 users group. From 1991-1993 he was a member of the National Academy of Science Panel on Mathematical Research for Materials Science and was the principal author of the chapter on mathematical and numerical methods in the panel's final report. He co-organized the spring of 1994 Institute for Theoretical Physics program on numerical methods for many-electron problems. In 1996 he was elected a Fellow of the American Society through the Division of Computational Physics. For the past 10 years he has been a member of the organizing committee for the annual workshop "Novel Methods for Electronic Structure Calculations" and has also help organize one conference and three cross-disciplinary international workshops devoted to Monte Carlo methods. Over his career he has authored 125 publications on such diverse topics as amorphous magnetism, effective medium theories for composites and polycrystals, non-destructive flaw detection and characterization using the scattering of elastic waves, quantum Monte Carlo simulations of strongly correlated electron systems, the uses of parallel computers in quantum simulations, Bayesian methods for statistical inference, and most recently, Monte Carlo approaches to problems with rough energy landscapes.

Candidate's Statement

About 15 years ago, when the first Cray computers become more readily accessible to the research community, I became fascinated with the possibility of applying this new computational power to difficult problems in quantum many-body theory and became a what now is being labeled a computational physicist. Rapidly I learned that the power of algorithm not the power the computer is often the limiting factor and my research has flipped back and forth between algorithmic development and applications of those algorithms. Until recently, this work focused intensely on quantum Monte Carlo methods for systems of interacting electrons. I also rapidly realized that research in other areas of physics often experiences similar algorithmic difficulties and these same difficulties are shared by our colleagues in chemistry, biology, and mathematics. While our applications may differ widely, our methods are similar, and our solutions to difficulties have wide impact provided that information is shared. The cross-disciplinary nature of computational physics has always excited me and is something I know from first-hand experience to be essential for the continued growth, development, and respectability of "numerical methods" in science and technology.

The Division of Computational Physics must continue to grow and to promote interest in computational science. To do this it needs to increase the co-ordination of its activities with the other Divisions in the American Physical Society and with its counterparts in other professional societies both nationally and internationally. The standard means to this end include jointly sponsored mini-symposiums, tutorials, workshops, and conferences. Many such activities are in place, we need to make them more widely known, more visible, and more integrated into the functions of the Division and the Society. What also needs attention is the educational function of the Division.

The Division should not simply be a "clearing house" of information but should be proactive in using and spreading that information. Besides keeping active researchers up-to-date, it needs to address the training of computational physicists. To do this, it should become a forum for teachers and developers of courses on the methods of computational physics. At many universities these courses are becoming as much a part of the required curriculum as traditional courses in methods of mathematical physics already are. While some of this educational role will be directed towards the undergraduate and graduate, some also needs to be directed towards professional researchers whether they work in universities,

industries or the government. Even if physicists do not use computational methods, they need to know what these methods do and do not do.

I also see opportunities for the Division to be more proactive in using the computer in its activities. While it is usually hard to beat face-to-face communication with a colleague for efficient exchange of information, the Web is an exceptionally exciting development for disseminating and gathering information and can be used to supplement face-to-face exchange in ways special to computational physics. What role should virtual conferences, workshops, and tutorials have in the Division's activities? Web-based courses are reshaping the way some courses are being taught at universities. Web publication is redefining the role of scientific journals. Should we be using the Web to reshape our scientific meetings? To redefine the conference proceeding?

Vice-Chair

Uzi Landman
School of Physics
Georgia Institute of Technology
Atlanta, GA

Uzi Landman received his B.S. (1965) and M.S. (1966) degrees in chemistry from the Hebrew University and the Weizmann Institute, respectively, and a D.Sc. (1969) degree in theoretical chemistry from the Israel Institute of Technology (Technion). Between 1970 and 1977 he worked at UC Santa Barbara, University of Illinois, Urbana-Champaign IL, University of Rochester, and the Xerox Research Center, Webster NY. In 1977 he joined the School of Physics at the Georgia Institute of Technology, where he is currently a Regents' and Institute professor, a Callaway Chair, and the director of the GA Tech Center for Computational Materials Science. In 1988 he served as an Associate Dean for Research at the college of Arts and Liberal Science at GA Tech. He is an elected fellow of the APS, an AVS Distinguished Lecturer, and the Editor-in-Chief of Computational Materials Science published monthly by Elsevier. His research interests are in the areas of condensed matter physics, surface science, clusters, nanoscale structures, nanotribology, and chemical dynamics, with an emphasis on the development and application of classical and quantum mechanical computational methodologies for modeling and simulations of physical and chemical phenomena.

Candidate's Statement:

Research endeavors using computer-based methodologies broaden our perspectives and deepen our insights in a wide spectrum of fields and disciplines, serving as tools for analysis of laboratory observations as well as for formulation and testing of unifying theoretical frameworks, and increasingly as a source of discovery of novel phenomena. Such computational modeling and simulation studies, which in practice often resemble experiments with a theoretical model serving as the interrogated system and the simulation itself employed as a computational microscopy or telescopy, are increasingly used in academia, government and industry in investigations of complex physical, chemical and biological systems characterized by varied interactions as well as involving a broad distribution of spatial and temporal scales. In the face of the diversity, interdisciplinarity and synergism characterizing modern computational science, and the new paradigm that it represents, it is the role of the DCOMP, and it will be my priority, to identify, foster and enhance links among members of our division and with our colleagues in other areas. I trust that such endeavors, which include the initiation and development of educational curricula and information exchange forums where computational and physical research issues are treated in an integrated manner, will open new opportunities, broaden and strengthen the impact of computational physics, and prepare us as researchers and students to face future challenges.

Councilor

James A. Warren
Nat'l Institute of Standard Technology
Gaithersburg, MD

James A. Warren was born in Cleveland in 1964 and spent an idyllic childhood there, until departing for Dartmouth College in 1983. After graduating from college near the top of his class he moved to the University of California, Santa Barbara. In 1992 he received his Ph.D. in Physics on the theory of solidification microstructure evolution. He has been with the Metallurgy Division of the Materials Science and Engineering Laboratory of the National Institute of Standards and Technology in Gaithersburg Maryland ever since. In 1994 he and several colleagues founded the Center for Theoretical and Computational Materials Science. In addition to his research responsibilities, Jim is now the Deputy Director of the CTCMS.

Candidate's Statement:

The Division of Computational Physics has a unique role in the structure of the APS; all of the remaining Divisions are focused on a particular discipline (Materials, Particles and Fields, etc.). As computers have emerged as a powerful tool for solving physics problems, a class of experts at using this tool has arisen, much as the experts in Electron Microscopy arose some years ago, whose ability to impact many areas of research is manifest. However, there is no Division of Electron Microscopy, why is there a Division of Computational Physics? I believe the answers to this question define my position as a candidate, as well as my vision for the future to DCOMP.

Certainly, computers as tools for solving problems in physics are ubiquitous. As physics is the discipline of applying quantitative methods to the study of nature, and computers are tools for solving quantitative problems, computation will continue its evolution into the central method of attack for problems of interest. It is this centrality that makes computaters a unique tool for analyzing the natural world.

Thus, the Division of Computational Physics should be a resource for scientists looking to enhance the applicability, speed, and usability of the computers they are able to access. DCOMP should also work to increase the accessibility of the best and most powerful computers. Often, DCOMP should collaborate with other Divisions in an effort to ensure the best

methods and resources are being applied to the pressing problems of the day.

Another way DCOMP can help the scientists it strives to serve is by promoting the development of computational tools (as opposed to methods). Often the major stumbling block to the implementation of a modeling technique is the demanding learning curve required of a researcher who has little time (and possibly interest) in computational methods. DCOMP can act as a bridge allowing those who develop the most advanced methods and techniques to reach those who desperately need these methods. By creating, for each problem, a network of scientists who can determine the relevant software design issues, develop the tools, and promote these tools to the physics community, DCOMP could dramatically increase its scientific impact. Finally, DCOMP needs to act as a policy forum for how the Nation spends its finite resources on computation. I believe we are in a position to influence policy, if we choose to make the effort.

Councilor

Steven R. White
Dept. of Physics and Astronomy
University of California
Irvine, CA

Steven White received a B.A. in Physics, Mathematics, and Economics from UC San Diego in 1982. As an undergraduate, he worked for three years with chemist Kent R. Wilson doing molecular dynamics simulations, co-authoring two papers. He obtained his Ph.D. in Physics from Cornell in 1988, where he worked with Kenneth G. Wilson and John Wilkins on applying renormalization group ideas to electronic structure calculations. From 1987 to 1989, he was a postdoc with D.J. Scalapino at UC Santa Barbara, where he developed and used quantum Monte Carlo methods for strongly correlated electron models. In 1989, he joined the faculty of UC Irvine, where he has remained since. His research interests are primarily in numerical studies of strongly correlated electron systems, particularly the high-temperature superconductors. In addition to using numerical techniques, he also works on developing new numerical approaches. In 1992 he developed the density matrix renormalization group, which is now widely used for numerical studies of low dimensional quantum systems. In the last several years he has worked to revise both the graduate and undergraduate physics curriculum at UCI to include more computational methods. In 1998 he was elected a fellow of APS, in the Computational Physics division.

Candidate's Statement

Most computational physicists identify themselves primarily with one of the traditional specialties, such as condensed matter physics or particle physics, rather than with computational physics. This is entirely appropriate--our primary goal is to understand the physics of our field. Nevertheless, we share a common set of tools, approaches, and practical problems with other computational physicists. One of the primary goals of the Division of Computational Physics should be to help foster communication between the various types of computational physicists, so that algorithms, tools, and experience can flow quickly between subfields. One way to do this is by promoting computationally oriented sessions at APS meetings. For example, sessions with pedagogically oriented overviews linked by a common numerical theme, but spanning various fields of physics could be proposed. Many of us can understand the numerical techniques of other fields quite quickly if jargon is kept to a minimum and if the physics aspects are kept at a colloquium level.

There are several current issues where we can profit greatly from the experiences of our fellow computational physicists. One is the incorporation of programming, numerical analysis, and computational physics into our undergraduate and graduate curricula. As numerical as well as general programming techniques become increasingly important in research and for many jobs that physics majors take, it becomes more and more important that our students be well grounded in these areas. What ways of incorporating them work best? How much should be handled by physics departments, as opposed to computer science and math departments? Another current issue is parallel programming.

Some of us are experts now on using parallel machines, while others are still able to solve our problems on good workstations. What pitfalls can be avoided when first going parallel? Which machines and parallelization techniques work best? Another issue is software in general: what advances in programming developed by computer scientists over the last few decades are useful for computational physics, and which are not? Can one write programs in an object-oriented language like C++ and still keep execution speed comparable to Fortran? Are there things one can do in a more modern language that are just not feasible in Fortran? Can we push the computer scientists to make future languages more numerically friendly? Again, the APS can help in these areas chiefly by fostering communication, both among computational physicists as well as between us and the rest of the world.

Member-at-Large

No Photo Available

David W. Arnett
Steward Observatory
University of Arizona
Tucson, AZ

Dr. Arnett received his Physics B.Sc. from the University of Kentucky, 1961 and his Ph.D. in Physics from Yale University 1965 (Ph.D. Advisor: A.G.W. Cameron). Professional Societies include, the American Astronomical Society (High Energy Astrophysics); the American Physical Society (Cosmic Physics \& Computational Physics); the International Astronomical Union, and the American Association for the Advancement of Science.

His past experience has been with NASA-NRC, postdoc, Goddard Institute for Space Studies, New York, 1965-6, Research Physicist, Lawrence Radiation Laboratory, Livermore, CA, 1966-7, postdoc, Kellogg Radiation Laboratory, Caltech, Pasadena, CA, 1967-9, Assistant Professor, Space Science, Rice University, Houston, TX, 1969-71, Associate Professor, Astronomy, University of Texas, Austin, 1971-74, Professor, Astrophysics, University of Illinois, Urbana, IL, 1974-

6, Professor, Astrophysics, Physics, Fermi Institute, University of Chicago, 1976-86, Program Leader (Supernova), Institute of Theoretical Physics, UCSB, 1980, *B. & E. Sunny,1986-89.* Distinguished Service Professor, University of Chicago, 1986-89.

Scholarships, Fellowships and Awards: Regents Professor, Steward Observatory, University of Arizona, 1989 - present. Member, Phi Beta Kappa, Visiting Fellow, Institute of Theoretical Astronomy, Cambridge, England, 1968-86, Alfred P. Sloan Fellow, 1970-1972, Visiting Fellow, Astrophysics, Oxford University, England, 1973, Visiting Distinguished Scientist, Philips Program, Haverford College, 1979, Visiting Scientist, Max-Planck-Institute for Astrophysik, Munich, 1979, Distinguished Graduate Award, Physical Sciences, Yale (with J. W. Truran), 1980, A. von Humboldt Prize (Senior Scientist), 1981, Distinguished Visiting Scientist, Stony Brook Astrophysics Program, S.U.N.Y., 1982, Fellow, American Physical Society, Member, National Academy of Sciences (1985-), and Member, American Academy of Arts and Sciences (1985-).

Dr. Arnett has written over 200 papers and is the author of several books.

Candidate's Statement

From designing a tic-tac-toe device as a boy to bringing up a Beowulf system this spring with my son, I have been interested in computers and their use. My collaborators and I have been fortunate enough to be involved in several pioneering efforts: the first use of radiation hydrodynamics for neutrino transport in core collapse supernovae and black hole formation, the development of what for many years was the method of choice for solution of nuclear reaction networks in astrophysics, detonations in type Ia supernovae, multidimensional hydrodynamics and hydrodynamic instabilities in SN1987A, and high energy density laser experiments which quantitatively scale to supernova conditions. I have created several computational science courses at the University of Arizona, in astronomy and in physics, at undergraduate and graduate levels. I have served on a number of national advisory committees, most recently the NRC studies on the readiness of the National Ignition Facility, and the Physics Survey Overview Committee (on which I represent computational physics). I believe that the millennium offers two strong challenges to those of us interested in computational physics. The first is to exploit the opportunity for communication, with the public, with the new generation from which we seek new scientists, with our colleagues in all areas of physics, and with scientists in other fields.

Computational physics is becoming a common language, cutting across old boundaries between disciplines. The internet and the PC are powerful attractions to potential new scientists and to interested adults. We can and should facilitate and coordinate efforts to communicate on all these levels. The second challenge is to connect the virtual reality of the simulation to the real world. As physicists, this challenge is our particular responsibility, both from our history and from the nature of our current practice of physics. We not only program computers, we invent and validate the rules the laws of physics upon which successful simulations must be based. Our traditions of vigorous interplay between theory and experiment are, I think, vital to successful development of computational science, and with our sister sciences, we should help lead in that direction.

Member-at-Large

David M. Ceperley
NCSA and Dept. of Physics
University of Illinois
Urbana-Champaign, IL

David Ceperley received his B.S. (1971) in physics at the University of Michigan and Ph.D. (1976) at Cornell University. After spending two years as a postdoc Orsay, France, New York University and Rutgers University, he joined the National Resource for Computational Chemistry at Lawrence Berkeley Laboratory. Following its closure, he became a staff scientist at Lawrence Livermore National Laboratory. He joined the University of Illinois physics department in 1987 with a position split with the National Center for Supercomputing Applications (NCSA).

With Richard Martin, he initiated an annual workshop series, "New Computational Methods for Electronic Structure", now in its eleventh year. He has also organized computational workshops at the Aspen Institute for Physics, the Institute for Physics at UC Santa Barbara and CECAM and two summer schools on computational approaches to materials. He is on the editorial board of *Computing in Science and Engineering, Journal of Physics, Condensed Matter* and *Computational Materials Science* and a Fellow of the American Physical Society and the American Academy of Arts and Sciences. He is the local team leader for the national NCSA group on nanomaterials and a member of the NCSA executive committee.

David Ceperley's research interests are in the area of computational statistical mechanics, in particular the simulation of quantum system using Monte Carlo methods. He has developed the diffusion Monte Carlo and Path Integral Monte Carlo algorithms and applied them to such systems as the electron gas, superfluid helium and high-pressure hydrogen. For this work he has received the Feenburg Metal (1996) and the Rahman Prize for Computational Physics of the American Physical Society (1998). He has been associated with high performance computing for 25 years.

Candidate's Statement

In my view, the primary role of this division is to foster research and education in computational physics. We are now entering the golden age of computational physics and opportunities abound. I think it is quite important to find more effective ways to communicate across disciplines, recognizing that the physical and social problems in computational physics are very much related to those in chemistry, biology, materials science, etc. Clearly better ways are needed to accomplish scientific interaction, possibly involving new technology.

Scientific progress has occurred to a large extent because scientists have been willing to document and share their data and methods. We want to encourage this in computational science by allowing permanent, documented links to open source code, and input and output data. Another aspect of scientific progress has been the institutionalizing of standards.

We owe much to those who a century ago succeeded in establishing the metric system, mathematical notation, chemical symbols, etc. Our division could play a role in promoting data and code standards. With widely used standards, the "seamless" integration of codes and interdisciplinary, multi-scale applications is made much easier and accessible to individual investigators.

Member-at-Large

Bulbul Chakraborty
Dept. of Physics
Brandeis University
Waltham, MA

Bulbul Chakraborty obtained her Ph.D. in Physics from SUNY at Stony Brook in 1979. She was a postdoctoral fellow at Argonne National Laboratory from 1979-1982. She spent the years between 1982 and 1986 in India and decided to come back to the United States in 1987. She joined the Brandeis University Physics Department as a faculty member in 1989 and is currently an Associate Professor there. Her research focuses on statistical mechanics and its applications to materials problems.

Candidate's Statement

I consider myself more as a condensed matter theorist rather than a computational physicist in spite of the fact that computer simulations have become an essential part of my research. As a member of the executive committee of DCOMP, I would like to work towards better dissemination of information amongst the community of physicists. The development of a database of computational physicists and their research interests would be of tremendous help to a newcomer in the field or someone looking for existing software. I would also like to see some resources devoted towards the coordination of educational software. A database of educational software that has been tested and recommended by members of the DCOMP would be an extremely valuable resource to Physics teachers everywhere.

Member-at-Large

John Kieffer
Dept. of Mat'ls Sci. & Eng.
University of Illinois
Urbana, IL

John Kieffer received his M.S. in Metallurgy and his Ph.D. in Applied Physical Chemistry from Clausthal Technical University in Germany. After appointments as a postdoctoral research associate at the Center for Solid State Science at Arizona State University, and the Department of Chemistry at Purdue University, he joined the faculty of the Department of Materials Science and Engineering at the University of Illinois in 1989. His research interests include the amorphous state of matter, liquids, structural phase transformations, fracture mechanics, and the application of chaos theory to characterize the behavior of molecular systems under non-equilibrium conditions. As research tools he develops and uses atomic- and meso-scale computer simulations, but he also has experience with various experimental techniques, and maintains close collaborations with experimenters that complement his computational efforts.

Candidate's statement:

Computational science and engineering is a rapidly growing area of expertise. Advancements in numerical algorithms and increased performance of computer hardware, facilitate computational approaches for increasingly complex problems, with more diverse applications, and produce more realistic results and reliable predictions. While the advancement of the field in these regards is driven by the talent of a growing number of researchers, the community as a whole will have to be concerned with the following issues: (i) in light of these developments, what are the requirements in terms of education and training of future scientists and engineers? (ii) given the diversity that already exists in the field of computational science, what can be done to avoid duplication of effort and promote cross-fertilization of ideas? (iii) In a community that grows at such a rapid pace, how can one identify and disseminate the most promising developments early on? Stewardship in such matters is an important responsibility of professional societies. Provided the opportunity to assist in the governance of APS/DCOMP, I will draw from my practice as an educator, my experience as an organizer of numerous conferences and symposia on computational materials science, as well as my familiarity with both the American and European educational and research systems.

1999 DCOMP BALLOT

Vice-Chair: Vote for one candidate

Jim Gubernatis

Uzi Landman

Councilor: Vote for one candidate

James A. Warren

Steven R. White

Members-at-Large: Vote for two candidates

David W. Arnett

David M. Ceperley

Bulbul Chakraborty

John Kieffer

Mail the completed ballot in the enclosed envelope to:

Bruce M. Boghosian
Secretary-Treasurer DCOMP
Center for Computational Science
Boston University
3 Cummington Street
Boston, MA 02215

The ballot must be received by September 20, 1999 for it to be counted.