APS AMERICAN PHYSICAL SOCIETY

Division of Computational Physics… …DCOMP

Physics Computing News

Winter 2004

Election Issue

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Rubin H. Landau
Oregon State University

Message from the Chair

Dear DCOMP Members,

It has been a good year for computational science and computational physics. We are witnessing big investments in computational hardware by everyone: governments, academic institutions and industry. Expectations are high, and it appears that the, by-now well-known, paradigm shift of computation as the third pillar of science and as an (almost?) equal partner to experiment and theory, is finally being taken seriously in most scientific disciplines. While for some areas of study, such as global warming and of thermonuclear explosions, computation is the only practical option, major advances in other programs, such as controlled fusion and even nanotechnology, may also hinge on progress in computational modeling. In the many cases, successful modeling not only supplants technically challenging experiments, but also leads to novel designs and directions.

In contrast to the recent past, we are again seeing substantial diversity in hardware, from large clusters of personal computers, to computational grids, and even to "ultra scale" massively parallel vector processors. Clearly, the powers-that-be are realizing that what really matters it is not just the cost per delivered flop, but mostly the cost to benefit ratio, with timeliness playing a major role. While some problems and models parallelize trivially, others require specific architectures as well as major algorithmic and programming efforts. Although the progress in hardware has been the most visible, the progress in computational methods has been equally robust and no less important. Achieving optimum impact will require substantial investments in computational methodology, including algorithms and program design. The diversity in architectures is, in my mind, an advantage, since one can use the optimal, or most cost-effective architecture, for a problem at hand. But it also increases the need for theorists and software experts. Should we expect this to result in major job opportunities? I certainly hope so! I believe that rapid progress in key areas will require substantial multidisciplinary teams, including computational and computer scientists, as well as experimentalists. I am optimistic about the potential for future breakthroughs, but they will all require investments in both people and hardware.

Let me now turn to divisional issues. It is again time for the elections, which were accelerated somewhat by the switch of our Annual Meeting to the March Meeting. At that meeting, Robert Peterkin, our past Chair and Harvey Gould, our past Secretary/Treasurer will be stepping down from the Executive Committee. We are all grateful for their many years of dedicated service. Estela Blaisten-Barojas and Steven Louie are

DCOMP Annual Meeting
Montreal, March 20-26, 2004

Message from the Chair-Elect

Dear DCOMP Members,

We are just finishing the process of finalizing the program for the March Meeting in Montreal, March 22-26, 2004. The meeting received approximately 6100 abstracts, the largest ever, in spite of the concerns of many of us about visa issues for foreign scientists. DCOMP is sponsoring or co-sponsoring ten focused sessions and seven invited symposia. In addition, at the meeting we will honor our respected prize winners: Farid Abraham (Raman Prize), Frans Pretorius (Metropolis Prize in 2003), and Joerg Rottler (Metropolis Prize in 2004). Details of the program can be found at the DCOMP Web site:

http://www.aps.org/units/dcomp

I would like to draw your attention to the Special Symposium on Wednesday, March 24 at 5 PM entitled, "The Impact of High Performance Computing on Physics Research". Ralph Roskies (Scientific Director, Pittsburgh Supercomputer Center), Ray Orbach (Office of Science, Department of Energy), and Peter Freeman (Assistant Director, CISE, National Science Foundation) are the speakers, with a panel discussion to follow. For those interested in the future of high performance computing in the US, that's the place to be on Wednesday evening. We will co-sponsor an evening reception on Tuesday with DMP in which we celebrate the prize winners and announce the recently elected Fellows. Our **business meeting** will be held on Thursday at 5:30PM in the Peribonka room of the Fairmont Queen Elizabeth hotel, followed by the Executive Committee dinner in Richelieu room.

The 2005 DCOMP meeting will be held in conjunction with the 2005 APS March Meeting in Los Angeles, California, March 21-25. In addition, it is DCOMP's turn to host the 2005 International Conference on Computational Physics. This is an IUPAP sponsored conference, and I am in the process of obtaining the necessary approval from IUPAP. I should note that IUPAP has become very sensitive to the manner in which the US government has been treating some foreign nationals wishing to come to scientific conferences in the US. Specifically, they are talking about withdrawing IUPAP support for US meetings if there is no change in policy. The APS and others are working on the problem. After discussing the question with the DCOMP Executive Council, it was decided to proceed with the application and wait for IUPAP to approve or disapprove. If approval is given, and the CCP meeting occurs, DCOMP activities will begin on the previous weekend in order to accommodate the additional needs of CCP. This should lead to a significantly enhanced scope to the 2005 DCOMP meeting, as well as to a larger number of invited speakers.

also stepping down as members of the Executive Committee. They have done their parts well and deserve our heartfelt thanks for their efforts. Barry Schneider will become the Chair of the Division, and we will elect a new Vice-Chair and two Members-at-Large. The vote is electronic and thus extremely fast and easy. A few clicks are all it takes to make your voice heard. Please read the candidate statements in this Newsletter and please vote!

Finally, I am looking forward to seeing many of you at our Annual Meeting in Montreal. Despite the concerns with the visas, the Montreal meeting has a record number of submitted abstracts and promises to be an exciting meeting in a very attractive location. Barry Schneider, our Program Chair, has worked very hard and assembled a very strong program (please see his article on this page). Please come and please do not forget about the reception on Tuesday evening, which will honor our prize winners and new Fellows!

Jerry Bernholc, Chair

I will be taking over as Chair of DCOMP at the March Meeting. I would like to express my thanks to Jerry Bernholc for his constant support as I "learned the ropes" and to other DCOMP members who helped with the organization of the program for this years meeting in Montreal.

Barry I Schneider, Chair-Elect

Future DCOMP Meetings

2004 APS March Meeting
March 22-26, 2004
Montreal, Canada

2004 APS April Meeting
May 1-4, 2004
Denver, CO

2005 APS March Meeting
March 21-25, 2005
Los Angeles, CA

2005 APS April Meeting
April 16-19, 2005
Tampa, FL

DCOMP 2003-2004 Committees

DCOMP 2003-2004 Committees

Information Committee

- **Rubin Landau,** ***Newsletter Editor & Chair*** - rubin@physics.orst.edu
Estela Blaisten-Barojas, ***Web Editor*** - blaisten@gmu.edu
Peter Reynolds, ***Membership Coordinator*** - pjr@ohm.nrl.navy.mil

Nominating Committee

- **Dale Koelling (DoE),** ***Chair (2001-2003)*** - Dale.Koelling@science.doe.gov
Members: Hudong Chen (Exa Corp.) *2001-03*, Adriana Moreo (Florida State U) *2003-05*, Rubin Landau (Oregon State) *2003-05*, Samuel Trickey (U. Florida) *2003-05*, Donald Hamann (Lucent Tech) *APS representative (1 year term)*.

Deadline for nominations to the DCOMP Executive Committee is October 14, 2003.

Program Committee

- **Barry Schneider (NSF),** ***Chair*** - bschneid@nsf.gov
Members: Jerry Bernholc (bernholc@ncsu.edu); Mei-Yin Chou (meiyin.chou@physics.gatech.edu); Lee Collins, lac@lanl.gov; Rubin Landau (rubin@physics.orst.edu); Steven Gottlieb (sg@fuji.physics.indiana.edu); Hong Guo (guo@physics.mcgill.ca); Steven White (srwhite@uci.edu); Warren B. Mori (mori@physics.ucla.edu); Luis Lehner (lehner@lsu.edu)

The deadline for nominations of invited speakers at DCOMP 2004/ March meeting was August 30, 2003.

International Liaison Committee

- **Rubin R. Landau (Oregon State U),** ***Chair*** - rubin@physics.orst.edu
Members: David Landau (U. Georgia), Estela Blaisten-Barojas (George Mason U).

2004 Metropolis Award

Joerg Rottler for his thesis "Deformation and Failure of Glassy Materials", and its innovative research on the simulation and analysis of craze and fracture in glassy materials.

Computational Nanotechnology Schools in US and Europe.

2004 Summer School on Computational Materials Science:
Introduction to Computational Nanotechnology

June 7-18, 2004
University of Illinois at Urbana-Champaign

Organized by the Materials Computation Center sponsored by the NSF

http://www.mcc.uiuc.edu/SummerSchool04/

Spring College on Science at the Nanoscale

24 May - 11 June 2004
Abdus Salam International Centre for Theoretical Physics (ICTP)
Miramare - Trieste, Italy

Some travel support, for qualified US participants is offered by the NSF through the Materials Computational Center, Univ. Illinois of Urbana-Champaign
Please apply directly at:
http://www.mcc.uiuc.edu/travel/index.htm

International Conference on Computational Science ICCS 2004

June 7-9, 2004
Krakow, Poland
http://www.cyfronet.kra

See page 6 for candidate statements and bios.

Computational Physics in Physical Review

Are you aware that Physical Review E has a computational physics section? In 1993, the computational physics section E-16 was added in response to a request from the community. PRE publishes computational physics papers that describe substantial improvement in the general computational methods that address significant physics problems. These papers are intended to reach a wider audience of physicists than that reached by specialized journals. All the Physical Review journals are available online at <http://publish.aps.org/>, and abstracts of articles and letters published in the past three years are freely available to all. The journal now offers free color online only for authors supplying color PostScript files. See the announcement at <http://publish.aps.org/color03.html>.

There is considerable advantage to publishing in PRE. Since the journal covers a wide range of topics in statistical, nonlinear and soft matter physics, including many-body physics, a broader, international audience is reached.

We would like to take this opportunity to thank Gerald Hedstrom, Associate Editor for the Computational Physics section, who will retire from that position February 2004. Gerald started as Associate Editor for Physical Review A in 1992 and was one of the founding editors of PRE when it was started the following year. Following Gerald's retirement, Burkhard Dünweg from the Max Planck Institute for Polymer Research, Mainz, Gerrmany and Gary Grest will take over editing the Computational Physics section.

The current editorial board member for computational physics is Harvey Gould. We try to be considerate of the referees and not overburden them with review requests, so it is helpful when current referees and authors recommend new potential referees. So that our review requests are on target, we encourage referees to log onto our referee server <http://referees.aps.org/> in order to update their expertise and contact information.

Gary Grest, Editor, Physical Review E
Margaret Malloy, Associate Editor

FELLOWSHIP PROGRAM

In 2003 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 ??

Doolen, Gary Dean
Los Alamos National Laboratory

Citation: For frontier computational research in fluid dynamics modeling, one-component plasmas, complex-rotation methods for atomic resonances, and laser-plasma interactions.

Galli, Giulia
Lawrence Livermore National Laboratory

Citation: For important contributions to the field of ab initio molecular dynamics and to the understanding of amorphous and liquid semiconductors and quantum systems.

Johnson, Duane Douglas
University of Illinois

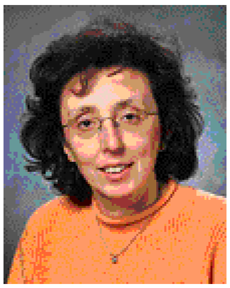
Citation: For theoretical and computational contributions to our understanding of physical properties of disordered alloys which have uncovered the microscopic underpinnings of the thermodynamics and phase transformations of alloys.

Lin, Hai Qing
Chinese University of Hong Kong

Citation: For his contributions in developing and applying computational methods to quantum many body systems.

DCOMP
2004 ELECTION CANDIDATES

Candidates for Vice-chair:



Giulia Galli is the Quantum Simulations Group Leader in the Physics and Advanced Technologies Directorate at the Lawrence Livermore National Laboratory (LLNL). She received a Ph.D. degree in Physics from the International School for Advanced Studies in Trieste, Italy in 1986. After postdoctoral positions at the University of Illinois at Urbana Champaign and the IBM Research Division in Zurich, Switzerland, she joined the Swiss Institute for Numerical Research at the Swiss Poly-technical School in Lausanne, where she was Senior Researcher and then Senior Scientist. In 1998 she moved to LLNL as a Staff Scientist. In 2000, she received a Department of Energy/Defense Program award of excellence for " Technical Excellence in Advanced Simulations" and in 2001 she was awarded two LLNL Awards of Excellence, by the Defense and Nuclear Technology and the Computation Directorates, respectively. She was elected a Fellow of the American Physical Society in 2003. Her current research activity is focused on computational investigations of systems and processes relevant to condensed matter physics, physical chemistry, materials and nano-science, using quantum simulations, in particular ab-initio Molecular Dynamics and Quantum Monte Carlo techniques. Topics of current interest include nanostructures and complex surfaces, as well as modeling bio-molecules in solution and fluids and solids under pressure.

Candidacy statement. In the last decade, scientific computing has been playing an increasingly important role in solving key problems in different disciplines encompassing Physics, Chemistry and Biology. Computer simulations are now reaching the point where they are on a par with laboratory experiment and mathematical theory as predictive tools for innovative research in science and engineering. Building on its strength as an interdisciplinary organization, the Division of Computation Physics should facilitate the exchange of information about algorithmic advances, new computational techniques and codes among the traditional Physics disciplines represented in the APS, as well as establish connections to the divisions of other Societies devoted to the promotion of scientific computing (e.g. Computational Chemistry of the ACS, SIAM and the MRS). This may be accomplished by joint special workshops, joint tutorial activities at National Meetings and web sites with up to date information about new computational techniques and related applications. The Division should also be involved in promoting educational activities in Computational Physics and Scientific Computing, in particular help promoting new curricula including a robust formation in numerical algorithms and modern programming techniques.

Robert Swendsen is a Professor of physics at Carnegie Mellon University. He received his PhD from the University of Pennsylvania in 1971. He spent the next two years as a post-doc at the University of Cologne, followed by three years at the Institut für Festkörperforschung at the KFA Jülich. In 1976, he went to Brookhaven National Laboratory, where he stayed until 1979, when he joined the IBM Zurich Research Laboratory. He has been at Carnegie Mellon since 1984, where he was Associate Dean of the Mellon College of Science in 1993-94 and Head of the Department of Physics from 1994 through 1999. Swenson' s research has been primarily in the area of Monte Carlo simulations. He has participated in the development of the Monte Carlo renormalization group, the Swendsen-Wang algorithm, the Replica Monte Carlo simulations, the Multiple-Histogram method (also known as the Weighted Histogram Analysis Method), Dynamically Optimized Monte Carlo, Transition Matrix Monte Carlo, inverse Monte Carlo renormalization group transformations, and recently the Adaptive Integration Method. He participated in early computer simulations demonstrating the effect of particle segregation by shaking (with A. Rosato, F. Prinz, and K.J. Strandburg), and the existence of an equilibrium quasi-crystalline state (with M. Widom and K.J. Strandburg).

He is a Fellow of both the APS and the AAAS. In 1993, he was chair of DCOMP. He is currently a member of the Advisory Board for the RealityGrid project in Great Britain. In 1982, he received an IBM Outstanding Achievement Award. In 1991, he received the Forefronts of Large-Scale Computational Problems Award for " Molecular Dynamics Studies of DNA Structure" with S. Kumar, J. M. Rosenberg, and P. A. Kollman.

Candidacy statement. Although computational physics has grown enormously in recent years in both intellectual sophistication and scientific impact on a wide variety of fields, it is far from settling into the mold of a standard discipline. Novel computational approaches to both new and old problems continue to be generated. Interdisciplinary teamwork has come to be taken for granted, as the benefits of such collaborations have become increasingly recognized. A major goal of DCOMP is the promotion of research and the development of computational physics. This is an exciting task because of the dramatic growth in the field and the important consequences of our work. But it is also a major challenge, since we must continue to expand and develop our contacts with scientists from virtually every field of endeavor. The international aspect of all scientific efforts today is yet another dimension of the breadth that DCOMP must cover. Running interesting interdisciplinary meetings, workshops, short courses and tutorials is extremely important in supporting computational science. DCOMP is doing an excellent job, and current activities should be maintained at the high level that has been established. DCOMP can also serve an important role by connecting computational physicists with scientists in other relevant fields, for roles ranging from speakers to potential research collaborators. These interdisciplinary connections can create new research possibilities as well as communicating them.

Although computational physics is already a major part of the scientific endeavor, there is still a great deal of work to do to introduce computational methods into educational programs. The advantages are enormous. Computer graphics provides an immediate and compelling feedback for students that a red mark on a homework assignment can never achieve. Perhaps more importantly, computational approaches can bypass the non-physical approximations that were used by old courses to make problems tractable for students. A great deal of important work is being done in this direction, which should be supported strongly by DCOMP.

Candidates for Member-at-large:

Elbio Dagotto received his Ph.D. in Physics from the Instituto Balseiro, Bariloche, Argentina (1985). After

postdoctoral appointments at the University of Illinois and the Institute for Theoretical Physics (ITP) at Santa Barbara, he joined the Department of Physics and National High Magnetic Field Lab at Florida State University (FSU) (1992). He recently was hired as Distinguished Scientist by the University of Tennessee and Oak Ridge National Lab (starting June 2004). Dagotto has been associated with high performance computing for close to 20 years, first working in lattice gauge theory while at Illinois, and then in superconductivity and magnetism since his appointments at the ITP and FSU.

Elbio Dagotto's research interests are currently in the area of condensed matter theory, in particular computational studies of models for correlated electrons. This includes transition-metal oxides, such as cuprates and manganites, as well as nanostructures, like quantum dots and molecular conductors, where correlations lead to interesting effects. Dagotto has written close to 200 papers, including several reviews, and also a book for Springer Verlag (2002) on Colossal Magnetoresistance. At the APS level, he co-organized the 2004 Focus Session on Magnetoresistive Oxides, he was divisional associate editor of the Physical Review Letters for four years, and also a member of the board of editors of Solid State Communications. He has been or currently is principal investigator of several grants by NSF, ONR, and other agencies. Dagotto is a Fellow of the American Physical Society.

Candidacy statement. I will focus on promoting research in computational physics. We are entering a golden age in this area of investigations and many opportunities abound. Although difficult initially, the community has finally accepted that computational research is an excellent unbiased way to clarify the true behavior of many theoretical systems. Well-known cases include strongly correlated electrons, as in the Hubbard model. However, in spite of this progress, much remains to be done. The role of computational research as a `third way' to do physics must be cemented in the community, and for this goal to materialize a concerted effort must be carried out. We must make sure that computational physics is well represented in conferences, and efforts using this type of tools receive the recognition they deserve. As the younger generations acquire more responsibilities the task will become easier, but certainly we still must continue the education of some of our colleagues that resist accepting the key role of computer-oriented research.

It is also very important to find effective ways to communicate across disciplines, since the problems in computational physics are much related to those in materials science, chemistry, biology, and others. Progress in algorithms in one area of investigations should rapidly become known to others. To achieve this goal it is imperative that frequent workshops/conferences with multidisciplinary participation and emphasis on computational aspects be regularly organized. Even within physics, studies in the area of particle physics, nuclear physics, condensed matter, and biophysics, to name a few, share a common set of tools and practical problems, and as a consequence strong communication among the many areas should be pursued. Computationally oriented sessions at all APS meetings should be promoted, particularly involving pedagogical focus sessions.

Mark Jarrell received a B.S. in physics from Drexel University in 1983, and a PhD in physics from the University of California at Santa Barbara in 1987, working with D.J. Scalapino. From 1987-1990 he was a postdoc with Daniel Cox at The Ohio State University, and since 1990 he is a professor at the University of Cincinnati, Department of Physics. His research is focused on the study of correlated electronic systems and the development of related computational techniques. Together with collaborators, he developed algorithms to address the problem of analytic continuation of Quantum Monte Carlo data. He was one of the developers of the Dynamical Mean Field Theory, and is presently involved in its cluster extensions. He has applied these methods to study a variety of correlated systems, from the cuprates and heavy

Fermion systems, to more recent studies of lower dimensional systems. He is also active in the development and distribution of open-source physics courseware.

Candidacy statement. The computational sciences are a rich and emerging area with tremendous opportunities for fundamental research, education and funding. In part, this is driven by new experiments involving complex systems, such as lower-dimensional nanoscale systems and systems of biological importance. These experiments involve complex systems, which are very difficult to treat analytically. Thus, simulations are an essential counterpart to experiment. Some of the most interesting new results fall outside of conventional physics and overlap with chemistry, biology, and electrical and materials engineering, etc. The applicability of computational physics techniques to these systems has lead to the emergence of interdisciplinary computational sciences research. I believe that the division should continue to foster the growth of interdisciplinary computational physics research and education.

John Kogut is a professor of physics at the University of Illinois at Urbana-Champaign. He received his Ph. D. from Stanford University in 1971 and was a research associate at Princeton's Institute for Advanced Study from 1971 to 1973. He has held a Sloan Foundation Fellowship (1976-1978), a Guggenheim Fellowship (1987-1988) and was elected a Fellow in the American Physical Society in 1983. He has spent considerable time and effort in developing computational methods for high energy physics as well as improving the computational infrastructure of the field. He pioneered and advocated the use of supercomputers in the context of high energy physics and co-invented the lattice gauge theory algorithms, which incorporate quarks into computer simulations. Since quarks are fermions which satisfy the Pauli exclusion principle and cannot be represented by ordinary numbers, this represented an important development in the field. These fermion algorithms are now the backbone of the simulation methods used by a large fraction of the practitioners of lattice gauge theory to turn Quantum Chromodynamics into a predictive and quantitative theory, relevant to both Nuclear/High Energy and Condensed Matter physics. He pioneered the use of lattice gauge theory and computer simulations to understand Quantum Chromodynamics in hot, dense environments for application to the evolution of the early universe, the interiors of dense neutron stars, the RHIC experiments etc. He is an active proponent of the use of lattice gauge theory in novel applications relevant to the development of new technologies, such as high temperature superconductivity, Quantum Computing and Quantum Information Theory. In the early 1980's he helped initiate the program of National Supercomputer Centers for the NSF and was a Principal Investigator on the first successful center proposal, the National Center for Supercomputing Applications (NCSA) at Illinois. His experience in industry with Floating Point Systems and Cray Research, where he consulted in the development of multi-processor operating systems and compilers, were important components in making the national program a reality.

Candidacy statement. There are several reasons why I would like to serve as Member at Large of the Division of Computational Physics of the APS. First, I would like to see computational physics, especially in the arena of high energy physics, become a more influential and central part of the field. High energy physics is a discipline which has been dominated by ideas in symmetries and perturbation theory and a typical theorist in the field is not aware of the possibilities of computational methods. This is a pity because computational methods can lead to progress surmounting the bottlenecks of theoretical particle physics, moving it beyond traditional perturbative calculations. Many seemingly esoteric problems in cosmology, the early universe, new and exotic states of matter require the application of numerical methods for their formulation as well as their solution. Second, I would like to see computational methods become a more respected tool in the hands of inventive, broadly talented physicists. Much of computational physics deals with getting numbers out of well-understood, mature fields, as is certainly appropriate. However, there is the creative side of the field where new algorithms and applications are invented. I believe that this segment of the field should be actively promoted. A broad knowledge of physics is needed to achieve this goal. For example, in lattice gauge theory one must understand critical phenomena, field theory, statistical physics, algorithms and parallel processing. This basis then allows one to contribute to many disciplines and constantly reinvigorate and reinvent them all. In order to promote computational methods in theoretical physics I have written a textbook on lattice gauge theory entitled "The Phases of Quantum Chromodynamics:From Confinement to Extreme Environments" with M.A. Stephanov of the University of Illinois at Chicago, have compiled a three volume reprint series entitled "Milestones in Lattice Gauge Theory" and have organized a one semester workshop, scheduled for early 2005, at the Kavli Institute for Theoretical Physics entitled "Modern Challenges for Lattice Gauge Theory" with M. Creutz, H. Neuberger and T. Wettig.

Michael Mehl received his B. A. in Physics from the University of Kansas in 1973. He received his M.S. in physics from Indiana University, Bloomington, in 1995,

and his Ph.D. in Physics IU in 1980. In 1979 he became a postdoctoral fellow at Rutgers University in New Brunswick, New Jersey, working with Prof. David Langreth on the Density Functional Theory of electrons. This work culminated in the development of the ``Langreth-Mehl'' generalized gradient approximation to Density Functional Theory. Following another postdoctoral position at the University of Maryland, he began work at the Naval Research Laboratory as a contractor for Sachs-Freeman Associates in 1983, working with the then Theory Section of the Condensed Matter Branch of the Condensed Matter and Radiation Sciences Division. In 1986 he became a government employee, working for what is now the Center for Computational Materials Science at NRL. He is currently Head of the Surfaces and Interfaces Section of the Center. He has published over 100 scientific papers, focusing on the computational understanding of the electronic and mechanical behavior of materials. He was elected a Fellow of the Division of Computational Physics in 2000 for his contributions to density functional theory and its applications.

Candidacy statement. Computational physics is at an interesting time. Increasing power at decreasing cost allows a desktop computer to outperform the supercomputer of a decade ago. Clustering these cheap CPUs allows us to build machines with capabilities not even imagined a few years ago. In parallel, sophisticated software packages have been developed and made available to scientists who do not write code. For example, the U.S. Department of Defense's CHSSI program makes a large number of scalable parallel computational packages available to researchers. In my own field of research there are also well-documented commercial (e.g. Wien LAPW and Vienna pseudopotential) and open source (AbInit) packages for determining the electronic structure and energetics of a solid.

These developments came about because of readily available, easily modified software, and a large number of physical and computer scientists who developed or optimized these codes for use in computational physics. In the future we will need even more of these scientists to take develop and take advantage of new computational algorithms. One of the goals of DCOMP should therefore be the recruiting and training of new physicists who can perform these tasks. Of course, the new techniques developed by these researchers must be communicated to the community, and this is another place where DCOMP should be heavily involved, by supporting workshops, focus sessions at major meetings, and sponsored lectures at Colleges, Universities, and National Laboratories. These steps will ensure that we keep expanding our capabilities.

ROSTER OF EXECUTIVE COMMITTEE

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