



Division of Computational Physics... ...DCOMP

Physics Computing News

Spring 2003

Election Issue

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North Carolina State University

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Air Force Research Laboratory, and
DoD High Performance Computing
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Oregon State University

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Message from the Chair

Dear DCOMP Members,

We have just finished a very successful Annual Meeting in Austin, Texas. Our meeting, which was held in conjunction with the APS March Meeting, attracted about 300 contributed abstracts in Sessions and Categories co-sponsored by DCOMP. In addition, we co-sponsored 56 invited talks, which spread over eight symposia and six Focused Sessions. A number of our Symposia were exceptionally well attended, testifying to the vitality of our field. During the meeting, the Rahman Prize was presented to Steven White from University of California, Irvine. White, along with nine newly elected fellows, were then celebrated in an evening reception. Overall, it was an exciting and productive meeting, despite some problems with an unfinished Convention Center complex.

In accordance with our bylaws, the terms of office for some of our Executive Committee (EC) members expired at the Annual Meeting. Specifically, Jim Gubernatis, our devoted Past Chair, Peter Feibelman, and Renata Wentzcovich are leaving the EC, and Steve White will be retiring as Councilor when a new one is elected. Bob Peterkin and Harvey Gould are becoming Past Chair and Past Treasurer, respectively, but will stay on the EC for another year. Last but not least, Rubin Landau, our Newsletter Editor, agreed to serve for another year. We are all grateful to our retiring (and current) members for their many hours of dedicated and thoughtful service. Elections for new members of the EC is now being held. Please see pp. 6-10 of this Newsletter and vote on line! Electronic voting makes the process virtually painless, so please make your opinions count!

Our next **annual meeting** will be in **Montreal, Canada, March 22-26, 2004**. Barry Schneider, our Chair-Elect, will chair the Program Committee. In 2005, it is DCOMP's turn to hold the International Conference on Computational Physics (CPC), co-sponsored by IUPAP. The EC, after some discussion, decided to hold this meeting in conjunction with our Annual Meeting and with the 2005 March Meeting in Los Angeles, but to start CPC early, on the preceding weekend. This would enable a significantly enhanced scope and a larger number of invited speakers.

Let me end this note with some personal observations. Over the past year, I have attended several strategic planning meetings that dealt with grand challenges and future opportunities. Although the topics, agencies, and scopes of the meetings varied significantly, the computational themes were clearly visible in each meeting and were often prominent in terms of future growth. It became clear that both the US and the world are making large new investments in computer hardware, at both the high and the low ends. Several alternative high-end technologies are being pursued which promise to enhance the vitality of the field. Also, large investments in computer hardware are being made in all areas of computational sciences, which should lead to both breakthrough opportunities and excellent job prospects. This is an exciting time for computational physics!

Jerry Bernholc, Chair

DCOMP 2003-2004 Committees

DCOMP Nominating Committee:

Chair: Dale Koelling, DoE
Dale.Koelling@science.doe.gov

Vice Chair: Elaine Oran, NRL
oran@lcp.nrl.navy.mil

Members: Hudong Chen, Exa Corp
Adriana Moreo, Florida State
Vacant

Deadline for nominations to the DCOMP Executive Committee is 1 December.

DCOMP Program Chair:

Chair: Barry Schneider, NSF,
bschneid@nsf.gov

Deadline for nominations as invited speaker at the March meeting is 30 August.

DCOMP Fellowship Committee:

Chair: Robert E. Peterkin, AFRL,
Robert.Peterkin@kirtland.af.mil

Members: Roberto Car, Princeton
James Feagin, Cal State Fullerton
Birgitta Whaley, UCB

Deadline for nominations for fellowship is 12 April.

Aneesur Rahman Prize Committee:

Chair: Junko Shigemitsu, Ohio State U.,
shige@mps.ohio-state.edu

Vice Chair: Sidney Yip, Vice-Chair, MIT,
syip@mit.edu

Members: David Arnett, U. Arizona
David Landau, U. Georgia
Robert E. Peterkin, AFRL

Deadline for nominations is 1 July.
Information concerning this prize is at
<http://www.aps.org/praw/rahman/>.

Metropolis Award Committee

Chair: Bruce Boghosian, Tufts,
bruce.boghosian@tufts.edu

Vice Chair: Francis Alexander, LANL

Members: David Ceperley, U. Illinois
Vacant
Advisor of 2003 award recipient

Deadline for nominations is 15 September.
Information concerning this award is at
<http://www.aps.org/praw/metropol/>.

DCOMP International Liaison Committee

Chair: Rubin H Landau,
rubin@physics.orst.edu

Vice Chair: David Landau

Information Committee (Newsletter and Web)

Newsletter Editor: Rubin H Landau, Oregon State U.,
rubin@physics.orst.edu

Webmasters:

Rubin H Landau, Oregon State U.,
rubin@physics.orst.edu
Estela Blaisten-Barojas, George Mason U.,
blaisten@gmu.edu

DCOMP Home Page

The **DCOMP** home page, <http://www.aps.org/DCOMP>, provides information about the division's leadership, policies, and activities. It also contains the division's archive, listings of domestic and international meetings, information on DCOMP fellows, prizes and awards, and publications.

Please send your corrections and improvements to the **DCOMP** Webmasters listed above.

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

JOURNALS & PUBLICATIONS

At the beginning of 1999, the AIP journal *Computers in Physics* was merged with the IEEE journal *Computational Science & Engineering*. This created the bimonthly journal *Computing in Science and Engineering* as a joint publication of the American Institute of Physics and the IEEE Computer Society. The Educational Software contest, formerly sponsored by *Computers in Physics*, is continuing under the auspices of *Computing in Science and Engineering*. This contest provides recognition and reward to both professional and student authors of outstanding pedagogical software. Visit the CiSE site at <http://computer.org/cise/contest.htm> for details.

**Message from the DCOMP Past Chair,
Bob Peterkin**

Dear DCOMP Members,

My term as DCOMP Chair ended at the conclusion of the 2003 APS March meeting in Austin. Until I was elected to the DCOMP Executive Committee in 2000, I seldom attended March meetings because I believed that there were other conferences more relevant to my areas of expertise, plasma physics and gravity. The best part of being DCOMP's Chair was the opportunity to meet so many new physicists from subfields different from my own, and to learn so much physics from these new friends. At my first March meeting, I felt out of place; at the 2003 Austin meeting, I felt right at home. I thank the membership for the opportunity to serve, and I thank my colleagues on the DCOMP Executive Committee for making my job as Chair enjoyable and educational.

Our Division is in good shape. The breadth and depth of activities in computational physics is impressive. We are financially healthy, with over \$110K in our Division's account at APS. The bottom line has been growing at an annual rate of over 15% for the past few years due to membership dues and successful conferences. Outgoing Secretary-Treasurer Harvey Gould has done a tremendous job; be sure to thank him next time you see him.

After struggling with what to do with the DCOMP annual meeting, the Executive Committee decided to tie it firmly to the APS March meeting. DCOMP held its second IUPAP-sponsored Conference on Computational Physics (CCP2002) last year in San Diego, and will apply to IUPAP to host the next one in the western hemisphere (at the 2005 APS March meeting in Los Angeles). In addition, DCOMP will continue to participate substantially in the annual APS April meeting—scheduled for May in Denver in 2004! I wish to thank Steve Gottlieb for continuing to represent DCOMP's interests at the April meeting. Our new Chair, Jerry Bernholc did a tremendous job as DCOMP's program chair last year, and organized a great technical program including 56 invited talks and over 300 contributed abstracts at the Austin meeting. Chair-elect Barry Schneider is in charge of DCOMP's activities at next year's March meeting in Montreal. I look forward to seeing you all there next year.

With best wishes,

Robert E. Peterkin, Jr.

**DCOMP Election Candidates:
DCOMP Election Candidates:**

Vote on line by 6 June 2003 at

<http://physics.clarku.edu/dcomp/ballot03>

Vice Chair

Lee Collins

Stephen Foiles

Secretary/Treasurer

Mei-Yin Chou

David J. Singh

Division Councilor

Alexei M. Khokhlov

Richard M. Martin

Members at Large

David Bacon

Alex Friedman

Susan McKay

Malcolm Stocks

[See page 6
for candidate
statements
and bios.](#)

**Rahman Prize and Metropolis Award Call for
Nominees**

Division members who wish to nominate deserving colleagues or students for the Rahman or Metropolis Prizes are encouraged to do so. Nominations are open to scientists of all nationalities regardless of the geographical site at which the work was done. The Rahman 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.

More information can be found at the respective Web pages:

<http://www.aps.org/praw/rahman/> and

<http://www.aps.org/praw/metropol/>.

**Thanks for all the hard work for the Division by the
following individuals whose terms on the
Executive Committee expired in 2003:**

James E. Gubernatis, Past Chair

T11 B262, LANL

PO Box 1663, Los Alamos, NM 87545

Email: jg@lanl.gov

Phone: (505) 667-6727

Fax: (505) 665-4063

Condensed Matter Physics

Peter J. Feibelman, Member-at-Large

MS 1413, Sandia National Laboratories,

P.O. Box 5800, Albuquerque, NM 87185-1413

Email: pjfeibe@sandia.gov

Phone: (505) 844-6706

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Condensed Matter Physics

Renata M. Wentzcovitch, Member-at-Large

Dept of Chem Engr & Mater Sci, University of Minnesota

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Email: wentzcov@cems.umn.edu

Phone: (612) 625-6345

Condensed Matter Physics, Materials Physics

FELLOWSHIP PROGRAM

In 2002 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

Gennady P. Berman, Los Alamos National Laboratory

Citation: For his internationally recognized expertise in the areas of classical and quantum dynamical systems, dynamical chaos, dynamics of quantum computation, and modeling of nano-devices.

Ronald Elliott Cohen, Carnegie Institution of Washington

Citation: For contributions to the understanding of the physics of ferroelectrics, and for developments of methods and understanding of high pressure and temperature materials properties.

Tomas Diaz de la Rubia, Lawrence Livermore National Laboratory

Citation: For his contributions to multi-scale modeling of materials and seminal research on defect processes in solids under irradiation or high strain-rate conditions.

Lee Samuel Finn, Penn State University

Citation: For innovative contributions to the computational infrastructure for gravitational wave detection, detector modeling, data analysis and source simulations.

Alexei M. Khokhlov, Naval Research Laboratory

Citation: For the development of innovative computational techniques and their successful application to critical problems in astrophysics and combustion science.

Efstathios Manousakis, Florida State University

Citation: For innovative and original computational studies in the many-body problem including development of novel algorithms to tackle the many-fermion problem with very important applications to condensed-matter physics.

Andrew K. McMahan, Lawrence Livermore National Laboratory

Citation: For pioneering work on the computation of effective Hamiltonian parameters for superconducting oxides and phase transitions of materials under high pressure, and the subsequent solution of the associated models.

Michael Theodor Alfred Weinert, University of Wisconsin-Milwaukee

Citation: For his seminal contributions to the understanding of the electronic and magnetic properties of surfaces and bulk materials through the application and the development of first-principles methods.

K. Birgitta Whaley, University of California, Berkeley

Citation: For her contributions to theoretical understanding of quantum nanoscale phenomena, especially in superfluid helium droplets, and to control of decoherence in quantum information processing.

2003 Aneesur Rahman Prize Winner

Steve White is the recipient of the 2003 Aneesur Rahman Prize for Computational Physics. The Citation reads: "For his development, application, and dissemination of the numerical density matrix renormalization group (DMRG) method."

Steve was born in 1959 in Lawton, Oklahoma. He received his undergraduate degree from the University of California, San Diego, with a triple major in Physics, Mathematics, and Economics. Tired of the San Diego weather, he ventured to Cornell University to do graduate work in Physics and received his Ph.D. under the direction of John W. Wilkins and Kenneth G. Wilson. (John Wilkins is presently Chair-elect of the APS Division of Condensed Matter Physics, and Ken Wilson received the 1982 Nobel Prize in Physics and was the first recipient of the Rahman Prize in 1993.) Steve's dissertation, completed in 1987, was entitled "New Methods for Electronic Structure Calculations."

After a post-doc at the University of California, Santa Barbara, Steve has been on the faculty of the University of California, Irvine since 1989. Shortly after going to UCI, he invented the density matrix renormalization group, a numerical approach which has become widely used and which has proven to be remarkably successful for studying low-dimensional strongly correlated systems. His principal application of DMRG has been to models of the cuprate high temperature superconductors, where he has made substantial progress in understanding the properties of the striped states observed in many of these systems. In recent years, Steve has extended the range of DMRG to include higher-dimensional systems and to perform *ab initio* calculations of electronic structure.

In 1999, Steve was named a Fellow of the APS. He has served DCOMP as Councilor to the APS since 2000.

THE MONTE CARLO METHOD IN THE PHYSICAL SCIENCES

50th Anniversary Celebration of the Metropolis Algorithm
June 9-11, 2003, Los Alamos National Laboratory.

June 2003 marks the 50th anniversary of the Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller publication of what is now called the *Metropolis algorithm*. The Los Alamos National Laboratory is sponsoring the conference to celebrate this anniversary and its important role in the physical sciences. The conference will review the use of the Metropolis algorithm and Monte Carlo methods, highlight recent developments, and note the spread of Monte Carlo methods to other fields. More information is at

<http://cnls.lanl.gov/Conferences/MonteCarloMethods>
or

Jim E. Gubernatis, jeg@viking.lanl.gov

Recent Research in Computational Physics

Bringing Tranquility to Rough Virtual Times

Mark A. Novotny
Dept. of Physics and Astronomy
Mississippi State University

When times get rough in life, one often turns to prayer, meditation or the support of family, friends, and colleagues to seek tranquility. This news article describes the work of a DCOMP member-at-large, Mark A. Novotny, and his collaborators, to bring tranquility to rough virtual times in parallel simulations. Some content is new, but most is based on a recent article in *Science* [1] and a *Physical Review Letter* [2]. This work is supported by the National Science Foundation award administered by DMR by a grant entitled “ITR/AP (MPS): Non-Equilibrium Surface Growth and the Scalability of Parallel Discrete-Event Simulations for Large Asynchronous Systems” with Prof. Gvörgy Korniss of the Rensselaer Polytechnic Institute, as PI and Novotny as co-PI. (The DoE and the Research Corp also fund Coworkers on this project). The goal of the research is to construct and implement fully scalable parallel simulations of systems with asynchronous dynamics and short-range interactions.

Because the use of massive parallel computers is the only route to obtain the required huge amounts of computer power, the central question for all large-scale computations scalability. In parallel, discrete-event simulations (PDES), parts of a system are allocated and simulated on different processing elements (PE's). Each PE has its own local simulated time τ , often referred to as a virtual time, and as the simulation progresses, the virtual time horizon $\{\tau_i(t)\}_{i=1}^{N_{PE}}$ of the simulation progresses. Here N_{PE} is the number of PE's performing the simulation and t is the discrete number of parallel steps executed by all PE's (which is proportional to the wall-clock time). The dynamics of a large class of interacting systems is described by local state variables that have a finite number of states, and, hence, are simulated using PDES algorithms. As the system evolves, the state variables change asynchronously, and one must use a synchronization scheme to ensure causality. The dynamic interacting systems that PDES can simulate include financial market models, epidemic models of the spread of diseases in animal or human populations, dynamics of highly anisotropic magnetic systems, battlefield simulations, allocation of emergency personnel and resources following a natural or human-caused disaster, deliveries to a manufacturing plant or construction site, and queuing networks for systems such as cell phones.

The two basic ingredients of a PDES are the set of local simulated times τ_i and a synchronization scheme to preserve causality in the simulation. For a PDES scheme to be scalable, two criteria must be met as $N_{PE} \rightarrow \infty$: (i) the virtual time horizon should progress on average at a nonzero rate, and (ii) the typical spread of the time horizon should be bounded.

In the conservative implementation of PDES schemes on which we focus, the synchronization rule is that a PE can update its virtual time only if its virtual time is less than that of its neighboring PE's. Otherwise the PE idles. This rule ensures causality and has been shown [2] to lead to a virtual time horizon governed by the Kardar-Parisi-Zhang (KPZ) equation. This well-known equation from nonequilibrium surface growth has two consequences for scalability of PDES. First, because KPZ-like surfaces have slopes that are only short-range correlated, the density of local minima of

the virtual time horizon remains finite as $N_{PE} \rightarrow \infty$.

Consequently, criterion (i) is satisfied. However, criterion (ii) is violated because the virtual time horizon becomes macroscopically rough as XXX.

Criterion (ii) can be satisfied by forcing a PE to idle if its virtual time is too far ahead of the minimum virtual time [4]. However, this requires both a global calculation and global communication. The recent article in *Science* [1] illustrates that it is possible to satisfy criterion (ii) in a way that allows each PE to communicate only with a fixed, small number of other PE's. This is done by connecting each PE with another PE chosen at random from all N_{PE} processors. This connection is in addition to connections dictated by the physical system being simulated. An additional rule for the update is imposed a fraction p of the time, that is, the PE must also idle until its virtual time is less than that of its randomly connected PE. This leads to a small-world network connection. The small-world connection leads to a mean-field type of KPZ equation, and this equation has a time surface that is macroscopically smooth. Thus, criterion (ii) is satisfied.

In this way, references [1,2] demonstrate that for all short-ranged PDES simulations, perfectly scalable implementations are possible; i.e. criteria (i) and (ii) are both satisfied. Furthermore, using knowledge about non-equilibrium surface growth, and its relation to PDES, allows statements about the expected scalability for a finite value of N_{PE} for particular implementations [5, 6].

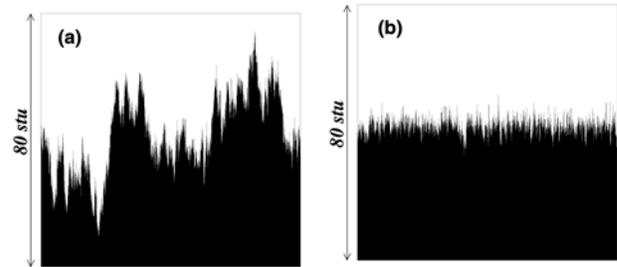


FIG. 1: The virtual times after 10^6 iterations are shown: rough virtual times in (a) with $p=0.0$ and tranquil virtual times in (b) for $p=0.1$.

*Electronic address: man40@ra.MsState.edu;

URL <http://www.msstate.edu/dept/physics/profs/novotny.html>

- [1] *Suppressing Roughness of Virtual Times in Parallel Discrete-Event Simulations*, G. Korniss, M.A. Novotny, H. Guclu, Z. Toroczka, and P.A. Rikvold, *Science* **299**: 677-679 (31 Jan 2003).
- [2] *From Massively Parallel Algorithms and Fluctuating Time Horizons to Non-equilibrium Surface Growth*, G. Korniss, Z. Toroczka, M.A. Novotny, and P.A. Rikvold, *Phys. Rev. Lett.* **84**, 1351-1354 (2000).
- [3] *Extremal-point Densities of Interface Fluctuations*, Z. Toroczka, G. Korniss, S. Das Sarma, and R.K.P. Zia, *Phys. Rev. E* **62**, 276-294 (2000).
- [4] *Algorithmic Scalability in Globally Constrained Conservative Parallel Discrete Event Simulations of Asynchronous Systems*, A. Kolakowska, M.A. Novotny, and G. Korniss, *Phys. Rev. E*, in press, preprint: <http://xxx.lanl.gov/abs/cs.DC/0211013>.
- [5] *Going Through Rough Times: from Non-Equilibrium Surface Growth to Algorithmic Scalability*, G. Korniss, M.A. Novotny, P.A. Rikvold, H. Guclu, and Z. Toroczka, *Materials Research Society Symposium Proceedings Series* Vol. 700, p. 297-308 (2002); invited paper.
- [6] *Parallelization of a Dynamic Monte Carlo Algorithm: a Partially Rejection-Free Conservative Approach*, G. Korniss, M.A. Novotny, and P.A. Rikvold, *J. Comp. Phys.* **153**, 488-508

Biographies and Statements for DCOMP Election Nominees

Vice Chair



Lee Collins biography

Lee Collins is a Laboratory Fellow at the Los Alamos National Laboratory, where he has been a staff scientist since 1977. He received a Ph.D. degree in Physics from Rice University in 1975. Editorial positions and honors include: Specialist Editor for Computer Physics Communications (1983-1991); Editorial Board Member (1991-1994) and Associate Editor (1994-present) of Physical Review A; APS Fellow (1995). He serves as Director of the Los Alamos Summer School (1992-present), a program aimed mainly at undergraduates with an emphasis on supercomputing, and as an Adjunct Professor at the University of New Mexico (1992-present). He has also been a member of the Executive, Fellowship, and Nominating Committees of the APS Topical Group on Few-Body Systems and Multiparticle Dynamics (GFB), the Executive Committee of the APS Forum for Physics and Society (FPS), and the Education Committee of the APS Division of Atomic, Molecular, and Optical Physics (DAMOP).

His research has spanned a diverse set of areas including astrophysics; heavy-particle collisions; scattering of electrons from atoms and molecules; molecular structure; interaction of matter with radiation - photoionization, intense field interactions, and quantum control; computational physics (large-scale 3D time-dependent quantum mechanical systems); and molecular dynamics simulations of dense liquids and plasmas as well as ultracold media.

Lee Collin's candidacy statement The Division should build on its considerable strengths as an interdisciplinary organization by continuing and expanding its collaborative efforts with other APS Divisions and Groups as well as international organizations and industry. Since computational methods permeate all areas of science and engineering, they form a natural bridge for linking seemingly unrelated research endeavors. We should further exploit these connections to interact with an even broader community through, for example, mutual sponsorship of conference sessions, topical meetings, and special projects.

Another area in which the Division can play an important role is education. Reports on the status of computational physics, for example from the NSF, stress the paucity of basic computational physics programs and courses for undergraduate and graduate students. While such students may exhibit competence with packaged mathematical programs as MATLAB and Mathematica, they many times lack a deeper understanding of the underlying numerical algorithms and formalism. We have also observed this deficiency for incoming students within the Los Alamos educational projects. The Division should aggressively address this issue along many fronts, for example, by sponsoring special student sessions at meetings, organizing its members to design special tutorial material, sponsoring specific forums to address these issues, and functioning as a hub for coordinating different institutions attacking this problem.

Stephen Foiles biography

Stephen Foiles received a B. S. with Distinction in Physics from Stanford University in 1978 and a M.S. and Ph.D. in Physics from



Cornell University in 1981 and 1983, respectively. His professional career has been with Sandia National Laboratories, first at the California site and currently at the New Mexico site. His work focuses on the atomic-level computation of the properties of metallic systems using methods ranging from empirical interatomic potentials to ab initio electronic structure methods. This includes work on the theory of liquids, the structure of surfaces and interfaces, defect properties, the effects of solutes, and the determination of thermodynamic properties. He was highly involved in the early development of the now widely used embedded atom method for the construction of interatomic interactions in metals.

The U.S. Department of Energy recognized Foiles for Sustained Outstanding Research in Metallurgy and Ceramics in 1987. He serves on the editorial board of the journal Modeling and Simulation in Materials Science and Engineering. He was elected a Fellow of the Institute of Physics in 1999 and was elected a Fellow of the American Physical Society in 2000.

Stephen Foiles's candidacy statement As we all know, computation and simulation have rapidly grown in importance in all sub-fields of physics as well as in science more generally. The synergism between the growth of computing resources and the advancement of computational algorithms enables this rapid growth in capabilities. The role of this division is to further this growth, educate the broader scientific community in the value of computations, and to encourage new students to enter this exciting discipline. While these goals are easily stated, they represent a daunting task. One of the underlying challenges and potential strengths of this division is its inherently interdisciplinary nature. Not only does it cross all of the sub-fields of physics, it also crosses strongly with related disciplines such as applied mathematics and computer science. One of the perennial challenges for the division, how to handle its annual meeting, is a manifestation of that challenge. The established meetings of the APS are focused around topical sub-fields. Although there are compelling logistical arguments for permanently aligning with one of these meetings, currently the March meeting, I feel this will ultimately disenfranchise a portion of the computational community and so defeat the purpose of this division. Therefore, I will push for periodic autonomous meetings sponsored by this division. The focus of the autonomous meeting will be on algorithmic advances that can be generalized to multiple sub-fields. To increase the value of these meetings, non-physicists should be invited to speak on generic algorithmic topics pertinent to physics.

Another role of the division is to enhance support for computational physics and to encourage students in this field. The collection and dissemination of success stories for computational physics will advance both of these goals. We all know ways that computation and simulation have aided our particular specialties. Few of us, though, can describe such successes outside our specialty. However, in order to inspire support and excite students, it is this broad view of the power of computations in science that is required.

Secretary/Treasurer

Mei-Yin Chou biography

Mei-Yin Chou received her Ph.D. in Condensed Matter Physics from the University of California, Berkeley in 1986. After working at Exxon Research and Engineering



Company as a postdoctoral research associate, she joined the Physics Department of Georgia Institute of Technology in 1989. She is currently a full professor of physics and holds the position of ADVANCE Professor of Science at Georgia Tech.

Her research field is computational materials physics, with an emphasis on first-principles studies of electronic, structural, and dynamical properties of solids, surfaces, and clusters. She has applied wavelet theory, density functional theory, and quantum Monte Carlo methods to large-scale electronic-structure calculations of materials. She is a recipient of the Alfred P. Sloan Research Fellowship (1990-1992), the David and Lucile Packard Fellowship (1990-1995), and the NSF Presidential Young Investigator Award (1991-1996). She is a Fellow of the American Physical Society.

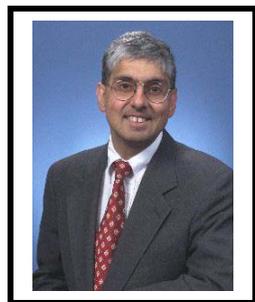
Chou has taken an active role in the community and has served in a variety of society functions. She was a co-organizer of the Focused Session, Theory of Materials: Surfaces, Interfaces, and Other Confined Systems, at the 1996 APS March Meeting, a member of the Executive Committee of the Physical Electronics Conference (1998-2000), the local Chair of the Twelfth Annual Workshop on Recent Developments in Electronic Structure Algorithms in Atlanta (2000), the elected U.S. Chair of the Gordon Research Conference on Hydrogen-Metal Systems (2001), and the co-Chair of the 62nd Physical Electronics Conference (2002).

Mei-Yin Chou's candidacy statement

The Division of Computational Physics draws members from every subfield of physics with a common interest in using computers to solve key scientific problems. The field has witnessed a phenomenal growth in the past two decades as simulations become increasingly capable of providing unique physical insights into complex problems that are invaluable to experiment and analytical theory. The Division must act aggressively to promote research and development in computational physics through meetings and workshops that bring together practitioners in mathematics, physics, chemistry, and biology to discuss common computational problems and to respond to emerging intellectual challenges. The Division should also facilitate the collection and dissemination of up-to-date information on software packages, algorithmic developments, and computer hardware technologies through publications, web pages, and special workshops. In addition, the Division should promote and participate in educational activities, and actively engage in policy issues regarding national computational facilities and federal research funding. Given the interdisciplinary nature of the Division and the diverse background of its members, it is important to maintain a dialogue between its officers and members so that the needs of the members can be properly addressed.

David J. Singh biography

David Singh was elected a Fellow of the Division of Computational Physics in 1997 for his contributions to the understanding of complex materials using first principles calculations and for development of the tools for such calculations. He received his Ph.D. in Physics from the University of Ottawa in 1985. He then held a postdoctoral fellowship with Henry Krakauer at



College of William and Mary from 1985, and joined the Naval Research Laboratory in 1988 as an NRC Associate with Warren Pickett. Since then, he has risen to his present position at NRL as Head, Theory of Functional Materials Section. He is the author or co-author of more than 200 scientific publications, mostly on methodology and applications of first principles approaches for properties of materials. He is a recognized expert on the linearized

augmented plane wave (LAPW) method and is the author of the book, *Planewaves, Pseudopotentials and the LAPW Method*, which was published in 1994. He served as co-chair and co-organizer of the International Conferences on Electronic Structure and Magnetism in Complex Materials (ESCM2000 and ESCM2002) and the Williamsburg Workshop, Fundamental Physics of Ferroelectrics (2003). Singh's current research interests include new electronic structure methods, magnetic oxides, piezoelectric materials, superconductors and thermoelectrics. Singh was awarded the NRL Sigma-Xi Pure Science Award for 2000 in recognition of his contributions in computational physics.

David Singh's candidacy statement

We in the DCOMP community live in exciting times. Computational physics is producing enormous scientific progress. The impact is broad and pervasive. We have, through computation, an engine for elucidating the detailed predictions of physical theories, a microscopic window into complex phenomena and a tool for exploring new horizons, where the technologies of tomorrow lie. At present, we witness an unprecedented explosion in computing and communications capabilities and availability. However, we also face severe funding pressures in many areas of computational physics. As a member at large, I will build on the core strengths and responsibilities of DCOMP, particularly promoting scientific communication, primarily through organization of the DCOMP meeting and participation in other meetings, and advocacy for federal and industrial support of computational physics. An important part of this is making the impact of computational work on science and technology more visible outside our community. In addition, I think that DCOMP can and should play a role in promoting discussion of broader issues affecting our community, e.g. the proper role of international collaboration and open access to high performance computing in our field. By its nature, DCOMP is interdisciplinary. Coordination with other APS units and participation in their meetings (for example through DCOMP sessions at the March and April meetings) is important. I will maintain and seek to strengthen the bridges to other APS units. My approach to service will emphasize consensus building and well thought out incremental change focusing on the core mission and strengths of DCOMP.

Councilor

Alexei M. Khokhlov biography

Alexei Khokhlov received his combined B.S./M.S. degree with honors in Astronomy from the Moscow State University in 1981, and his Ph.D. in Physics and Mathematics from the Institute of Space Research in Moscow in 1984. From 1984 to 1991 he worked at the Astronomical Council of the USSR Academy of Sciences. In 1991 he was a visiting scientist to the Max-



Planck-Institute for Astrophysics in Garching, and in 1992 he went to the Astronomy Department of the University of Texas at Austin. In 1995 he joined the staff of the Laboratory for Computational Physics and Fluid Dynamics at the Naval Research Laboratory in Washington DC.

His delayed-detonation model of Type Ia (SNIa) supernovae, proposed in 1991, led to a theoretical explanation of an empirical brightness-decline relation that is used to calibrate SNIa as cosmological standard candles. At the University of Texas, he carried out first three-dimensional simulations of SNIa explosions. His fully threaded tree adaptive mesh refinement algorithm made it possible to carry out reactive Navier-Stokes simulations of a deflagration-to-detonation transition (DDT) in premixed gaseous systems. This led to important insights into the nature of shock-

generated turbulence, the role of boundary layers in supersonic flame propagation, and mechanisms of DDT.

His current research includes physics of reactive flows, supernova explosions and experimental astrophysics, numerical general relativity, adaptive mesh refinement, and large-scale computer simulations. In 2003 he was elected a fellow of the APS, in the division of Computational Physics.

Alexei Khokhlov's candidacy statement

There is a common culture of computational physics that we all share. Similarities exist in how we approach our problems, use computers, build and validate codes, and how we gain understanding, intuition, and new ideas from simulations. This culture takes time and effort to communicate, learn, and appreciate. In attacking increasingly difficult, multi-scale, multi-process phenomena ranging from the microscale to the entire universe numerical modeling is critically important and often is the only possible approach to understanding of a highly non-linear behavior of a complex system. The role of computational physics is bound to increase rapidly with the opening of new and inter-disciplinary fields of research, the emergence of new computational principles and computer architectures, and invention of new and unexpected algorithms.

DCOMP is an important carrier and promoter of these new developments. Interaction with other divisions of the APS is crucial for extending computational methods to emerging fields of physics, and for bringing challenging new problems into the scope of computational physicists. One way of facilitating this is to hold DCOMP meetings together with meetings of other divisions of APS, organizing sessions focused on problems in new emerging fields, and sessions devoted to specific computational methods and approaches. Facilitating participation of students and young scientists in topical sessions of DCOMP may be very helpful. Another important goal of DCOMP and its interactions with the rest of the APS is to ensure that there are enough computational resources available to physicists, and that these resources are of the type and quality suitable for attacking new problems.

Richard M. Martin biography

Richard M. Martin received a B. S. in Engineering Physics from the University of Tennessee in Knoxville in 1964 and a Ph.D. in Physics from the University of Chicago in 1969. He was a post-doctoral member of the research staff at Bell Labs after which he joined the Xerox Palo Alto Research Center becoming Principal Scientist. In 1987 he joined the faculty of the Department of Physics



at the University of Illinois at Urbana-Champaign. He is a fellow of the American Physical Society and the American Association for the Advancement of Science and received the Alexander von Humboldt Foundation Senior Scientist Award.

His primary research area is the theory of electronic structure of solids, especially the development of practical methods to treat the many-body electron system in condensed matter and molecules. The methods include Quantum Monte Carlo simulations for the most exact calculations and density functional methods for prediction of broad ranges of material properties. Recent work has included computational algorithms for "Order-N" linear scaling methods and the theory and algorithms for calculations of polarization and localization in insulators. Examples of applications include prediction of the phase diagram of carbon at high pressure and temperature, simulations of large fullerenes, and prediction of the metal-insulator transition in hydrogen under

pressure. More information on research and courses is available at <http://www.physics.uiuc.edu/research/ElectronicStructure/>.

He has served the community as an elected member, Executive Committee, Division of Condensed Matter Physics, APS., 1994-97, and as Associate Editor of the Reviews of Modern Physics for Condensed Matter Theory. He is the co-founder of the ongoing annual workshop on New Methods for Electronic Structure Calculations and has long served on the organizing committee of the Workshop on Computational Physics: Total Energy and Force Methods at the ICTP in Trieste, Italy.

He is the author of a book, *Electronic Structure: Basic Theory and Methods* to be published in 2003, which typifies his approach - the confluence of theoretical ideas and computational algorithms to provide entirely new capabilities in science.

Richard Martin's candidacy statement

Computational physics is a vigorous, stimulating part of physics that brings unity to many subfields of physics and many other areas of science and technology. My goal is for the division to bring together scientists who identify intellectually challenging issues and advances that truly advance the frontiers. As one means of promoting the activities and synergism of the community, I believe the division should make a priority to organize symposia and sessions in the major physics meetings that bring out the cross-fertilization of different subfields. The symposia should combine aspects focused on specialized subfields and the strong relation to computations and algorithms utilized in other fields. A second priority should be education at the undergraduate and graduate levels to best prepare future scientists by encouraging integrated use of computation in all areas of science and engineering.

Members at Large

David Bacon biography

David Bacon received a S. B. in Physics and an S. B. in Mathematics from the Massachusetts Institute of Technology in 1977. He received a Ph.D. in Physics from Dartmouth College in 1982. Dr. Bacon started his career as an experimental plasma physicist working at the US Naval Research



Laboratory. He performed pulsed power experiments at NRL, the U.S. Army Harry Diamond Laboratories, and at Sandia National Laboratory. Dr. Bacon's doctoral research was in theoretical fluid dynamics, specifically the transition to turbulence.

Since 1982, Dr. Bacon has been a member of the staff of Science Applications International Corporation where he is currently the Director of the Center for Atmospheric Physics. In 1984, Dr. Bacon was introduced to the problem of numerical weather prediction and has spent much of the last 18 years trying to introduce modern computational fluid dynamic techniques to a community that was once the forefront of computational methods, but is now a backwater. The result is the Operational Multiscale Environment model with Grid Adaptivity (OMEGA), the first dynamically adapting, unstructured grid atmospheric simulation system.

Dr. Bacon's current interests span a wide range of applications of unstructured grid simulation including:

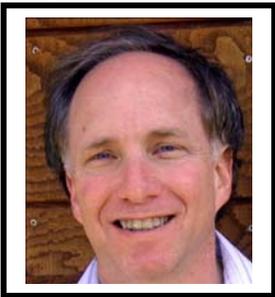
Atmospheric dispersion of aerosols and gases - especially boundary layer dispersion and dispersion in urban environments; Advanced numerical weather prediction - including remote sensing of surface properties (e.g., elevation, land/water fraction, land use, albedo, heat capacity, thermal conductivity, surface roughness, surface moisture, soil texture), remote sensing of the atmosphere (e.g., temperature, moisture, winds), data assimilation

techniques, numerical methods – including parallelization, and visualization and data dissemination; Multiscale atmospheric processes and simulation - including hurricane dynamics, thermodynamics, and microphysics; Air-surface processes and forecasting in Antarctica; and Simulation of the Martian atmosphere.

David Bacon's candidacy statement

Numerical weather prediction was once at the forefront of computational science – pushing computer architecture development, algorithm development, and basic mathematics – but its visionary period ended almost 40 years ago when the "computational" problem was deemed "solved" and the "physics" problem was still "unsolved." Unfortunately, as the physics problems were resolved, attention did not return to the numerical and computational issues. For the last 15+ years, I have tried to introduce modern computational methods to this problem that desperately needs a new paradigm to carry it into the future. This is the legacy I bring to the Division of Computational Physics.

Over the past decade, we have seen the sunset of large vector processors and the rise of massively parallel commodity processors. This changes the system paradigm in which our chosen scientific field is embedded. It raises new real and potential capabilities, but these must be communicated to the end users along with the reality of the new challenges that are faced by writing algorithms where communication and latency are as important as number of floating point operations and accuracy. The decline in computational science activity by the numerical weather prediction community occurred because it lost the interconnection between computational methods and the underlying physics. Other sub-disciplines are suffering from the same phenomena – the numerical issues were "solved" years ago. The problem is that those "solutions" do not make maximum use of the current architectures and capabilities. The Division of Computational Physics is uniquely positioned to serve as a champion for maintaining and expanding the interaction of numerical and computational scientists with their discipline colleagues.



Alex Friedman biography

Alex Friedman carried out his undergraduate and graduate studies from 1969 to 1978 at Cornell University, with support from a National Merit Scholarship and a Cornell Graduate Fellowship. His B.S. and Ph.D. degrees are in Engineering Physics and Applied Physics respectively; his thesis work consisted of the development and

application of a 3D particle-in-cell simulation code modeling the dynamics of "field reversed" rings of ions, a concept for fusion plasma confinement. During 1979 and 1980 he carried out research in computational plasma physics at the University of California at Berkeley. He then joined the scientific staff of Lawrence Livermore National Laboratory (LLNL), where he has carried out research in laser fusion, magnetic fusion, and heavy-ion fusion (HIF). The HIF concept uses intense beams of heavy ions (in contrast to lasers) to drive inertial-fusion target implosions, and is being pursued as an approach to electric power production. These beams are non-neutral plasmas and exhibit collective behaviors; their theoretical understanding is largely based on large-scale simulations.

Since 1998 Alex Friedman has served as the Beam Simulations and Theory Group Leader of the HIF Virtual National Laboratory, a joint enterprise of LLNL, Lawrence Berkeley National Laboratory (where he keeps his principal office), and the Princeton Plasma Physics Laboratory.

Alex Friedman is a Fellow of the American Physical Society, elected through DCOMP in 1997, and also a member of the APS Divisions of Plasma Physics and Physics of Beams. He is a member of Sigma Xi and Tau Beta Pi. He is a recipient of the LLNL Physics Department's Distinguished Achievement Award. He was elected to serve as a Fusion Program representative to the National Energy Research Scientific Computing Center Users Group's Executive Committee (NUGex). He recently became an Associate Editor of the Journal of Computational physics. His research interests include computational plasma physics and particle-beam (accelerator) physics, computational dynamics, four-dimensional (phase space) tomography, and numerical analysis.

Alex Friedman's candidacy statement

As a research scientist who believes that the proper status of computer simulation is that of a third path to physics understanding, complementing experiment and analytic theory, I will seek to promote that point of view more broadly throughout the APS. Specifically, I believe that computational physicists should be appointed to award and prize committees across the Divisions and Topical Groups (this is beginning to happen in DPP), so that excellent computational work may properly be recognized. In addition, I perceive an increasing compartmentalization of computational physicists, and note that the major application areas, such as plasma physics, accelerator physics, fluid dynamics, etc., tend to have their own separate meetings. I would seek to promote greater interchange among the areas, by encouraging periodic co-location of such topical meetings with the general DCOMP meetings; co-location with large general APS meetings has benefits but should not be allowed to exclude these other possibilities. Finally, I would encourage that conference program committees seek a greater emphasis on the presentation of improved computational methods, since that is where the true opportunity for cross-field benefit may be found. I would like to promote the notion that topical computational physics meetings should include a small number of invited talks "out of field" with an emphasis on methods.



Susan McKay biography

Susan McKay received her A.B. in Physics from Princeton University (1975), her M.S. in Physics from The University of Maine (1979), and her Ph.D. in Physics from M.I.T. (1987). In 1986, she joined the faculty of the Department of Physics and Astronomy at The University of Maine, where she is now

Professor and Chair of the Department. For the last two years, she has also served as the founding director of the University's Center for Science and Mathematics Education Research. Before joining the faculty at The University of Maine, she worked as an engineer in new product research and development at the Gillette Advanced Technology Laboratory (1975-1977), and held a research associate position in computational surface science at The University of Maine (1979-1981). She has served as a book department editor for Computers in Physics (1992-1998) and for Computing in Science and Engineering (1998-2002).

McKay has received several awards, including an IBM Predoctoral Fellowship in the Physical Sciences, an American Association of University Women Predoctoral Fellowship, Grants in Aid from Sigma Xi and Sigma Delta Epsilon, an American Vacuum Society Scholarship, a Josephine de Karman Fellowship, and two University of Maine Summer Faculty Research Awards. She was

also selected for an NSF POWRE Award, which supported her development of renormalization-group methods for driven non-equilibrium systems with quenched disorder.

McKay's research interests include a variety of problems and computational approaches within theoretical condensed matter physics. With her collaborators, she has studied phase transitions and critical phenomena in systems with quenched disorder, such as spin glasses and amorphous magnets, and in systems far from equilibrium. Part of this work has included the development of efficient computational strategies to retain the full distribution of interactions and fields under rescaling in renormalization-group treatments of spin glasses and the random-field Ising model. Another part of her research uses information theoretic quantities, such as the Shannon entropy and excess entropy, to characterize criticality and ordering in these systems. She and her collaborators have also investigated transitions to chaos and pattern formation in biological and physical systems, using both computational and analytical techniques.

Susan McKay's candidacy statement

The Division of Computational Physics holds a unique position as a group within the APS, in that computational physics is an important area for physicists working in many subfields. For this reason, the Division must represent a broad group of scientists and provide valuable, accessible information to them. Much of this information exchange happens through conference symposia and sessions, so the Division must make a strong effort to provide top-notch programs at major APS meetings and explore joint meetings with other groups of scientists, engineers, and applied mathematicians. These joint efforts are particularly important in order to foster multidisciplinary collaborations to advance computational strategies for problem solving.

The development of computational physics is best served if DCOMP includes opportunities and recognition for scientists working in this field at all levels of their careers. Travel awards for students to attend and present papers at conferences and invited speakers chosen from all professional stages enrich the computational physics community and encourage talented scientists to pursue this type of research. Short courses focused on computational topics at major meetings are also a high priority. A set of distinguished lecturers for departmental colloquia, publicized and partially supported by DCOMP, is another way to increase interest, knowledge, and rapid communication in the field. Essential, though, is to have the Division's activities reflect the breadth of its membership, in order to maintain value for all of its current members and attract new ones. This variety in programming is best accomplished by actively soliciting and using input from scientists practicing computational physics in many disciplines and in different types of workplaces.



Malcolm Stocks biography

Malcolm Stocks is Group Leader of the Theory Group of the Metals and Ceramics Division at Oak Ridge National Laboratory (ORNL). He obtained his education in the United Kingdom, obtaining an undergraduate degree in Applied Physics from the

University of Bradford in 1966 and a Ph.D. in Theoretical Physics from the University of Sheffield in 1969. After a postdoctoral position at ORNL from 1969-1972, he was on the Staff of the Physics Department at the University of Bristol from 1972-76 at which point he joined the research staff of the Theory Group at ORNL. In 1994, he was made Corporate Fellow, the highest distinction awarded an ORNL staff member. He became Group

Leader of the Theory Group in 2000. He has spent sabbaticals at the United Kingdom Science Research Council's Daresbury Laboratory (1981-82) and in the Department of Physics at the University of Bristol (1988-89). He has been an APS fellow since 1985. He has been awarded numerous honors including, on two separate occasions (1990,1998), the prestigious Gordon Bell Prize for innovative scientific application of parallel computing. He is a past chair of the Committee on Alloy phases of the TMS.

Stocks' major research activities are in development and application of first principles electronic structure techniques in materials science. His particular interest has been in multiple scattering Green's function methods, the theory of magnetism, alloy theory, semiconductor-oxide interfaces, and the application of parallel algorithms and computers to extend the size and complexity of systems amenable to ab initio study. He was a major contributor to the development of the Korringa-Kohn-Rostoker coherent-potential-approximation (KKR-CPA) method for calculating the electronic structure of disordered alloys as well a order-N scaling methods for treating large systems. He was a pioneer in the use of massively parallel computing in materials science. His current research is focused on the theory of the static and dynamic properties of inhomogeneous itinerant magnets, magnetic nano-structures, and the development of scalable parallel methods for performing calculations for realistic models of magnetic nanostructures. He has published more than 220 papers, has edited four books and has organized numerous international conferences and symposia including NATO Summers Schools, as well as APS, TMS and MRS symposia.

Malcolm Stocks' candidacy statement

According to the byelaws, one of the major objectives of DCOMP is to "promote research and development in computational physics; enhance prestige and professional standing of its members; encourage scholarly publication; and promote international cooperation in these activities." To my mind this provides an excellent guide for the efforts of DCOMP representatives at all levels. As computational physics continues to develop, it is important that DCOMP, through its representatives, exert significant influence on the national discussion regarding scientific research directions and the allocation of scarce research funds and resources. While at the level of the desktop, our community has benefited tremendously from the workstation revolution; it should also be recognized that, at the high end -- needed to address the most challenging computational problems --, our tools are expensive. Indeed, the demands of efficient leading edge computational physics facilities place funding demands that rival those of large experimental facilities. Furthermore, exploiting these facilities places considerable demands on the education of future physicists, requiring elements taken from many fields; including specific physics disciplines, computer science, and applied mathematics. In both of these areas, DCOMP should be proactive in order to ensure future high quality computational facilities and computational physicists. A second point of emphasis in the byelaws is to "provide to its members, and to all members of the Society, an opportunity for coordination and a forum for discussion and communication." Because DCOMP unites physicists by an approach rather than a particular topical area, it is important that individual representatives work to increase participation of their discipline specific colleagues in DCOMP. As one of the original co-organizers of the DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering (BES-DMSE) funded "Computational Materials Science Network," I hope that I am well placed to increase the participation of Computational Materials Physicists/Scientists in DCOMP. By doing this it is hoped that, as a whole, DCOMP increases the coordination across

computational physics and provides the broadest grass roots support for its activities and advocacy.

ROSTER OF EXECUTIVE COMMITTEE

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