

Robert E. Peterkin, current newsletter editor will be taking his new position as Vice Chair. Renata Wentzcovitch is the new DCOMP newsletter editor.

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IBM Almaden Research Center

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Message from the Chair

Dear DCOMP Membership,

For the DCOMP Executive Committee, I welcome DCOMP's newly elected officers. We look forward to working with you in creating an exciting program for 2000-2001. To the retiring officers, we express our sincere thank you for your many contributions that are making our Division successful.

We are planning to hold our DCOMP 2001 Meeting on the MIT campus during June 25 - 28. Professor Sidney Yip, Department of Nuclear Engineering, has accepted the responsibility of being Conference Organizer and has secured the help of several faculty members from MIT and the surrounding universities. We hope that Boston in June is an ideal location for attracting a large DCOMP attendance.

It is my hope that we can create a program that reflects the diversity of disciplines in computational physics. Maybe more important, we hope to stimulate cross-fertilization of novel computational techniques through special symposia with the intent of education and demonstration. Doing this successfully is challenging, but I feel that this is a primary & unique responsibility of DCOMP in contrast to the other Divisions of the APS.

Jim Gubernatis, DCOMP Chair-Elect, is the Program Chair of the 2001 Meeting and will be the driving force for a successful program.

In Jim's message, he will outline preliminary information about the program. Jim works at the Los Alamos National Laboratory and shared with our Executive Committee his recent experiences associated with the devastating fire. It was a very sensitive perspective of this unfortunate situation. I have asked Jim to write a similar message for our membership which is included in this newsletter.

Farid Abraham, farid@almaden.ibm.com
Chair

DCOMP Election Results

Vice chair: Robert Peterkin
Sec/Treas: Harvey Gould
Members at Large: Peter Feibelman
Renata Wentzcovitch

DCOMP welcomes you to the Executive Committee

The vote was extremely close, and we thank all the candidates for their participation. Farid

DCOMP 2001 Committees

The DCOMP Nominating committee:

The committee will be composed of the following individuals:

Chair: D. Papaconstantopoulos,
papacon@dave.nrl.navy.mil

Vice Chair: D. Truhlar

Members: J. Banavar
D. Rothman
D. Weingarten

The APS Executive Committee will appoint one additional member. The Nominating Committee prepares a slate of candidates for the positions Vice-Chair, Secretary-Treasurer, and Members-at-Large of the Executive Committee and advise the Chair on suitable candidates for Society committees. For more information, see

<http://www.aps.org/DCOMP/bylaws.html>

DCOMP Annual Meeting in 2001

Chair: Jim Gubernatis

Local Organizer: Sid Yip, syip@mit.edu
(617) 253-3809

Fellowship Committee:

Chair: James E. Gubernatis

Members: David Arnett
Daniel C. Barnes
Richard M. Martin
Claudio Rebbi

The deadline was April 14, 2000.

DCOMP Rahman Prize Committee:

Chair: Robert Sugar, sugar@vulcan.physics.ucsb.edu

Vice Chair: Tomas de la Rubia

Members: Daniel Meiron
Michael Klein ('99 recipient)
Shiyi Chen

Information concerning this award is in the following web address:

<http://www.aps.org/praw/rahman/descrip.html>

The nomination deadline was July 3rd.

Metropolis Award Committee

Chair: Sharon C. Glotzer

Members: Claudio Rebbi
Bruce Cohen
Michael Falk (2000 recipient)

Information concerning this award is discussed later in this Newsletter. The deadline is January 15, 2001.

DCOMP International Liaison Committee

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

Vice Chair: David Landau

The International Liaison Committee will develop and maintain relationships with other national and international physics societies. Because of the growing number of international organizations in computational physics, this responsibility is very important to DCOMP.

DCOMP Webmaster

Amy Bug, bug1@llnl.gov, has agreed to continue her role as Webmaster for DCOMP's APS Web site. Thank you Amy.

ANNUAL MEETING PROGRAM

We are just beginning to assemble the program and the invited speakers for the 2001 annual meeting. We are planning a number of general interest sessions of invited speakers, and we ask the membership to pass onto Jim Gubernatis (jg@lanl.gov) suggestions for topics and speakers. The topics should be of broad nature like turbulence, quantum information and computing, commodity computing, etc. The breath of disciplines under DCOMP's umbrella is difficult to embrace on the program committee. Outside help is welcome. Your input will be valuable. There will also be a poster session and sessions for contributed paper. More information will be given when the formal announcement of the meeting is made.

MARCH AND APRIL MEETING PROGRAMS

In 2001, DCOMP will still be a participating unit at the March and April meetings. Because our annual meeting will be stand alone that year, we are presently allocated only a small number of invited sessions at the March meeting. These sessions still represent an opportunity that the membership should not overlook. In recent years, the lack of response to the call for proposals for invited sessions has forced the program committee to generate these sessions. Your proposal for a DCOMP session, even with only few sessions allocated, is more likely to be successful than a proposal made to some other division. Keep your eye open for the formal call for invited proposals or contact Jim Gubernatis (jg@lanl.gov).

COOL APS LINKS:

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>

JOURNALS & PUBLICATIONS

Computing in Science and Engineering

At the beginning of 1999 the AIP journal *Computers in Physics* was merged with the IEEE journal *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. The URL for this new journal is <http://ojs.aip.org/cise/>.

Educational Software Contest

The Educational Software contest formerly sponsored by *Computers in Physics* is continuing under the auspices of *Computing in Science and Engineering* which wishes to recognize and reward both professional and student authors of outstanding pedagogical software. Visit the information site at <http://computer.org/cise/contest.htm> for details.

PC CLUSTERS

One of the best-attended sessions at DCOMP 2000 in Minneapolis was the session on PC Clusters organized by Prof. Steven Gottlieb (Indiana). Prof. Gottlieb and the speakers have graciously arranged it so the vignettes of these sessions are on the Web at <http://physics.indiana.edu/~sg/pccluster.html>.

APS and DCOMP Home Pages

The DCOMP home page, <http://www.aps.org/DCOMP>, provides 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. In the future, use of the web for divisional business including posting up-to-date news and running annual elections will increase.

Please send your suggestions for how to improve the DCOMP home page to the DCOMP Webmaster Amy Bug, bug1@lnl.gov

THE FIRE IN LOS ALAMOS

Because of the ties many in the computational community have to Los Alamos, Farid Abraham asked me to share my experiences and perspectives about the Cerro Grande fire.

My house did not suffer any fire or smoke damage. In the middle of the night, my family and I were ordered to evacuate and we spent four days in the first vacant motel room we could find in Santa Fe. We were among the first permitted to move back to town, moving back Mother's day evening, which was a nice present for my wife. My group

was one of the first permitted to return to work, surely not because we are essential to Laboratory operations (although most of the time we act like we are) but because our building suffered almost no smoke and fire damage. I have been a very fortunate person.

The fire devastated a fairly large part of the town and destroyed much of the natural beauty of the area. Because of the large number of homes destroyed in a relatively small town, everyone knows multiple families who lost their home or suffered significant damage. My post-doc's rental was completely burned to the ground, and he lost almost everything. He is uninsured. Local businesses, clubs, and churches and national businesses and relief organizations have been very supportive of the fire victims, as have the Department of Energy, the University of California, and the Laboratory. At this writing (Memorial Day), most of the livable homes are now re-occupied, and most of them have both their electricity and gas back on. For those who lost their home, they have a major problem in finding places to stay. Housing in Los Alamos has never been abundant or inexpensive. The nearest towns are 20 and 35 miles away. Federal assistance is promised.

The Lab's buildings suffered remarkably little fire damage. There are several scorched trees nearby our building. For some buildings, smoke damage is a problem. In particular, the smoke played havoc with the sophisticated ventilation systems in some buildings. This type of problem delayed my wife's returning to work for two days after me. My son, who will work as a summer student, still has not been called to work. He has been "on hold" for 3 weeks.

The fire is now well to the north of town, although flare-ups in the nearby hills occurred most of the past week. Officials were predicting that today the fire would be finally contained. Then it will allow itself to burn out, a process that will probably take 2 to 4 weeks.

Some of the nearby hills and canyons are badly blackened, and because the slopes of these hills are now ash-covered; the forest floor is now a poor absorber of moisture. The town is on a flash flood alert. A hard rain could generate another disaster. Our monsoon season is about 6 weeks away so there is time to prepare and reduce the danger.

New Mexico is one of the poorest and most sparsely populated states in the Nation. Many of its residents live in poverty. Los Alamos is one of the smallest and wealthiest counties in the Nation. Few of its residents live in poverty. What was truly remarkable was the amount of food, clothing, and money collected for the fire victims from others throughout the state, from towns in the state as far as 350 miles away. Some people were donating things that they themselves needed. This genuine generosity and caring is overwhelming many people, even those like me who do not need any aid. Out of all this, I believe Los Alamos will become a better community. I have yet to talk with anyone who is not looking forward to tomorrow.

Jim Gubernatis
Chair-Elect

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), **David M. Ceperley** (1998) and **Michael L. Klein** (1999).

2000 Aneesur Rahman Prize Winner: Michael John Creutz

The eighth Rahman Prize was awarded to **Michael John Creutz** of the Brookhaven National Laboratory.

Background: Dr. Michael J. Creutz received his BS degree in physics from Caltech in 1966 and his Ph.D. in physics from Stanford University in 1970. He worked as a Fellow of the Center for Theoretical Physics at the University of Maryland in 1970 and joined the staff at Brookhaven National Laboratory in 1972 where he is currently employed. His present field of research includes theoretical particle physics, numerical simulations of quantum field theory, and computational physics.

Dr. Creutz serves on the editorial board of several technical publications including *Computing in Science and Engineering*, *International Journal of High Speed Computing*, and the *International Journal of Modern Physics C*. He has served on the Executive Board of the Division of Computation Physics, including Chair of the Division in 1994 - 1995. He also was member of the APS Division of Particles and Fields Executive Committee from 1986 - 1988. He is a Fellow of the APS and has received the Brookhaven Research and Development Award as well as the Andrew Sobczyk Memorial lectureship from Clemson University in 1997.

Aneesur Rahman Prize: Call for Nominees

Division members who wish to nominate deserving colleagues for the Rahman Prize are encouraged to do so. Announcements for this prize appear periodically in *APS News*.

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: **Robert L. Sugar**, *Rahman Prize Committee Chair*, Phys Dept, University of California, Santa Barbara, Santa Barbara, CA 93106.

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. **Hudong Chen**, Exa Corporation
For contributions to fundamental fluid and magnetohydrodynamic turbulence theory, pioneering work in discrete many-body systems and Lattice Boltzmann representations, and industrial applications and practical numerical methods based upon these ideas.
2. **Carlo Jacoboni**, Modena University
For outstanding research and leadership in computational analysis of transport phenomena in solids.
3. **Michael John Mehl**, Naval Research Laboratory
For outstanding contributions to the development of density functional theory and to its applications using the LAPW method, tight-binding Hamiltonians and methods based on localized charge densities.
4. **Mark R. Pederson**, Naval Research Laboratory
For significantly enhancing the density-functional-based predictive capabilities in molecular and cluster physics by unique developments, implementations and applications of novel computational algorithms.
5. **L. Ramdas Ram-Mohan**, Worcester Polytechnic Institute
For his development of powerful analytic and computational methods for the investigation of the properties of novel semiconductor heterostructures.
6. **Mark Owen Robbins**, Johns Hopkins University
For his contributions to our understanding of the molecular origins of friction, lubrication, spreading and adhesion.
7. **Fausto Succi Sauro**, IAC-CNR
For development and application of lattice Boltzmann and other computational methods that successfully marry continuum and statistical mechanical approaches to complex physics problems.
8. **Priya Vashishta**, Louisiana State University
For contributions in computational quantum, classical and statistical mechanical physics.
9. **Su-Huai Wei**, National Renewal Energy Laboratory
For contributions to the understanding of electronic structures and stabilities of compounds, alloys, interfaces, super lattices and impurities using first-principles calculations and for development of the methods for such calculations.

The annual deadline for nominations from DCOMP is 1 April.

2000 MARIA GOEPPERT-MAYER AWARD

to
Sharon C. Glotzer *N.I.S.T*

Citation:

"For her ingenious use of computational physics to probe a wide range of novel materials under different conditions, and for demonstrating the existence and nature of spatially-correlated dynamic heterogeneities in glass-forming liquids."

Background:

[Dr. Sharon C. Glotzer](#) is a physicist in the [Polymers Division](#) of the [Materials Science and Engineering Laboratory](#) at [NIST](#), and the co-founder and director of the [NIST Center for Theoretical and Computational Materials Science](#). She received a B.S. in Physics from UCLA in 1987, and a Ph.D. in Physics from Boston University in 1993 with Professor H. Eugene Stanley. Dr. Glotzer joined NIST in 1993 as a National Research Council postdoctoral fellow in the Polymers Division.

Dr. Glotzer's research focuses on the theoretical and computational study of the structure and dynamics of soft materials, including polymers, dense liquids, glasses, colloids, liquid crystals and granular materials. Current interests include characterization of emergent spatial patterns in slow dynamics of disordered structures; filled polymers and nanocomposites; controlling fabrication and processing of mesoscale structure in blends; deformation and flow of amorphous structures and bulk metallic glasses; emergence of nanoscale structure and self-assembly in soft materials; multiscale modeling, acceleration algorithms, and massively parallel simulation of soft materials; molecular dynamics, Monte Carlo, and time-dependent Ginzburg-Landau methods; computational materials science techniques, tools and applications to soft materials.

Dr. Glotzer is a recipient of the 1998 Presidential Early Career Award for Scientists and Engineers, the 1997 Department of Commerce Bronze Medal, a 1996 Senior Visiting Fellowship Award at the Centre for Chemical Physics, University of Western Ontario, an NRC Postdoctoral Fellowship Award from 1993-1995, a TRW Graduate Fellowship Award from 1987-1992, and the 1986 Sigma Delta Epsilon Society of Graduate Women in Science Scholarship Award for Exceptional Promise in Science. Her first paper, written while an undergraduate in 1987, was in 1991 voted "One of the 50 Most Memorable Papers," published in the American Journal of Physics. Dr. Glotzer has served the APS Division of Computational Physics as a member of the Nomination Committee and in vice-chairing the Metropolis Award committee. She is also a member of MRS, ACS, AIChE, and AAAS.

Nicholas Metropolis Award

The purpose of this award is to recognize doctoral thesis research of outstanding quality and achievement in computational physics and to encourage effective written and oral presentation of research results.

The award consists of \$1,500 and a certificate to be presented at an awards ceremony at the DCOMP's annual meeting and an additional allowance of up to \$500 to travel to the meeting. The recipient will be invited to present his or her work in an appropriate session of the meeting. The award is sponsored by the Journal of Computational Physics. Further information can be found at <http://www.aps.org/praw/metropol/descrip.html>

Please note that because of the late annual meeting in 2001, the deadline for nominations has been changed from July 3, 2000 to January 15, 2001.

2000 NICHOLAS METROPOLIS AWARD

to

Michael Lawrence Falk

University of California at Santa Barbara

Citation:

"For developing novel computational diagnostics to visualize the microscopic processes controlling deformation and fracture in simulated amorphous solids, and for using the insights obtained from the simulations to develop a dynamical theory of low-temperature shear deformation in those materials."

Background:

Dr. Falk received his B.A. in physics (1990) and M.S.E. in computer science (1991) at the Johns Hopkins University where he engaged in computational physics research regarding screening in colloidal system with Prof. M.O. Robbins. In 1991 he was awarded the Luce Scholarship for travel to East Asia, and spent a year in Taejeon, South Korea at the Systems Engineering Research Institute of the Korean Institute of Science and Technology. While in Korea Dr. Falk collaborated with Dr. G. Ihm of the Korean Research Institute of Standards and Science investigating localization in quantum-wells and wires.

Upon returning to the United States in 1992 Dr. Falk began his graduate studies in physics at the University of California at Santa Barbara. His Ph.D. research, under the guidance of Prof. J.S. Langer, investigated the deformation and fracture of amorphous solids. From 1995-98 he was a recipient of the Department of Energy Computational Sciences Graduate Fellowship. He completed his Ph.D. research in 1998, and was chosen to serve as the graduate commencement speaker. After completing his doctorate he accepted a postdoctoral position at Harvard University in the Division of Engineering and Applied Sciences working with Prof. J.R. Rice and Prof. D.S. Fisher on problems of crack branching and crack front waves. He was also a visiting scholar at the Center for Theoretical and Computational Materials Science at the National Institute of Standards and Technology in the summer of 1999. Dr. Falk is a member of the American Physical Society, the Materials Research Society and Amnesty International USA. His research currently focuses on microscopic theories of plasticity, nonequilibrium phenomena in materials and the dynamics of fracture.

ROSTER OF EXECUTIVE COMMITTEE

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Term ends 2002

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Plasma Physics, General Relativity
Term ends 2003

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Term ends 2003

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Term ends 2002

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Condensed Matter Physics and Materials Physics
Term ends 2003

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Plasma Physics, Condensed Matter Physics

Thanks for all the hard work for the Division by the following individuals whose terms on the Executive Committee expired in 2000:

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Condensed Matter, Statistical Physics

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Condensed Matter Physics, Chemical Physics

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