



Division
of Computational
Physics...
...DCOMP

Physics
Computing
News

Fall 2001

CCP2002
San Diego
25-28 August 2002
Details Inside

Message from the Chair

Dear DCOMP Members,

This is the time of the year to welcome the newly elected members to the Executive Committee and thank its departing members for their contributions. Thanks also go to those who served on the Program, Fellowship, and Rahman and Metropolis Prize committees and to those who acted as Newsletter editor and Webmaster. There are too many to thank explicitly in this short note, but I do need to give particular thanks to the departing Chair, Farid Abraham. It has been a pleasure working with him, and we all should thank him for his positive contributions to the Division over the past several years.

A lot has happened since the last Newsletter. We held our annual meeting from June 25-28 in Cambridge, Massachusetts on the campus of MIT. It was a well-attended success. Bob Peterkin, now Chair-Elect and the 2002 Program Chair, has already started planning our next meeting. It will be in San Diego, August 25-28, and we are pleased that it will be jointly sponsored by the International Union of Pure and Applied Physics and will be internationally known as CCP2002. Please mark these dates on your calendar and try to attend. Bob is putting a lot of energy and skill into making this the best attended DCOMP meeting yet. Short articles on both meetings appear later in this Newsletter. Your comments and suggestions about these meetings are always welcomed.

During the past year we proposed some changes to our bylaws to reshape some of our appointed committees to make them more attuned with the present needs of the Division. We will all be voting on these changes when we hold our next election sometime this Winter. In the meantime, please look at http://www.aps.org/DCOMP/bylaws_web/index.htm for a discussion. This year, for the first time, we used Web balloting in our elections. The voting increased by 50%. We were pleased to see this increase. Hopefully, it is a trend.

Right now we are planning our invited sessions for the March and April meetings. If you attend those meetings, please look for DCOMP sessions.

I am looking forward to my coming year as Chair. Please do not hesitate to contact me (jg@lanl.gov) with suggestions and comments.

CHAIR

James Gubernatis
Los Alamos National Laboratory

PAST CHAIR

Farid F. Abraham
IBM Almaden Research Center

CHAIR-ELECT

Robert E. Peterkin, Jr.
Air Force Research Laboratory

VICE-CHAIR

Jerzy (Jerry) Bernholc
North Carolina State University

SECRETARY-TREASURER

Harvey A Gould
Clark University

MEMBERS-AT-LARGE

David Arnett
University of Arizona

Estela Blaisten-Barojas
George Mason University

David Ceperley
University of Illinois

Peter Feibelman
Sandia National Laboratories

Steven Louie
U. California, Berkeley

Renata M. Wentzcovitch
University of Minnesota

Jim Gubernatis, Chair
jg@lanl.gov

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DCOMP Election Results

Vice chair: **Jerzy (Jerry) Bernholc**
Members at Large: **Estela Blaisten-Barojas**
Steven Louie

We thank all the candidates for their participation.

DCOMP 2001-2002 Committees

The DCOMP Nominating committee:

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

Vice Chair: Donald Trular

Members: Hudong Chen
Dale Koelling
Elaine Oran

DCOMP Annual Meeting in 2002: CCP2002

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

Local Organizer: Robert E. Peterkin

Preliminary information about the 2002 meeting is discussed latter in this Newsletter. Specific questions can be sent to
CCP2002@merlin.plk.af.mil.

Fellowship Committee:

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

Members: Daniel C. Barnes
David Ceperley
Michael Creutz
Richard M. Martin

The 2002 nomination deadline is April 1, 2002.
The 2002 Chair will be Jerzy (Jerry) Bernholc,
bernholc@ncsu.edu.

DCOMP Rahman Prize Committee:

Chair: Tomas de la Rubia, delarubia@llnl.gov

Vice Chair: Priya Vashista

Members: Shiyi Chen
Michael Creutz
Richard M. Martin

Information concerning this award is at
<http://www.aps.org/praw/rahman/>. The nomination deadline for 2002 was July 2, 2001.

Metropolis Award Committee

Chair: Bruce Cohen, bcohen@llnl.gov

Members: Bruce Berne
David Ceperley
Steve Louie
Bob Rosner
Doug Toussaint

Information concerning this award is at
<http://www.aps.org/praw/metropol/>.

The DCOMP International Liaison Committee

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

Vice Chair: David Landau

Newsletter Editor

Robert E. Peterkin, Robert.Peterkin@kirtland.af.mil

DCOMP Webmasters

Rubin Landau, rubin@physics.orst.edu, and Estella Blaisten-Barojas, eblaiste@gmu.edu.

JOURNALS & PUBLICATIONS

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 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.

DCOMP Home Page

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 Webmasters Rubin Landau, rubin@physics.orst.edu, and Estella Blaisten-Barojas, eblaiste@gmu.edu.

Rubin and Estela are taking over for Amy Bug who in turn has become a department chair. We thank Amy for her contributions and service.

Help Wanted: Newsletter Editor Needed

DCOMP needs a new Newsletter editor. The current editor, Bob Peterkin, is stepping down to better address his responsibilities as Chair-Elect and Program Chair. The Newsletter is published at least once a year. The position of Editor carries an appointment to DCOMP's executive committee. Interested people should contact Jim Gubernatis, jg@lanl.gov.

DCOMP Annual Meeting Announcement

Conference on Computational Physics:

CCP2002

at the Hyatt Regency Islandia

25-28 August 2002

San Diego, CA, USA

The Division of Computational Physics is organizing and hosting the annual Conference on Computational Physics in 2002 (CCP2002). This international conference is sponsored jointly by the American Physical Society, the European Physical Society, and the International Union of Pure and Applied Physics. CCP2002 will serve as our Division's annual meeting in 2002, and will take place 25-28 August at the Hyatt Regency Islandia in San Diego, California, USA: http://www.hyatt.com/usa/san_diego/hotels/hotel_sanis.html.

CCP2002 will highlight basic and applied computational physics and its applications worldwide to the university, industrial and laboratory communities. San Diego (<http://www.sandiego.org/>) is located on the southern California coast and offers easy access for travelers from the U.S., Europe and Asia via the San Diego International Airport.

The Conference Chairman is our Division's Chair-elect: Robert E. Peterkin of the Air Force Research Laboratory. For Conference information, please check the DCOMP meetings web site <http://www.aps.org/DCOMP/meetings.html>.

Conference organizers can be contacted at CCP2002@merlin.plk.af.mil. We are planning for 300 attendees. There will be morning plenary session talks for the full assemblage of participants. The afternoons will have a variety of sessions on computational physics, each with an invited speaker to begin the session and contributed talks following. The invited speakers will be chosen by special invitation and by a selection from the submitted abstracts.

DCOMP01

The 2001 Regular Meeting

The 2001 Regular Meeting of Division was held in Cambridge, Massachusetts, June 25-28, on the campus of the Massachusetts Institute of Technology. The Program Chair was Jim Gubernatis (Los Alamos) and the Local Committee Chair was Sid Yip (MIT). While a number of students and faculty from nearby universities dropped in for select talks and sessions, 241 people did register for the meeting, and of these 25% were students. The attendance met our optimistic target.

The scientific program was organized around plenary, focus, and poster sessions. The plenary sessions were designed by the program committee around topics,

issues, and developments of general interest to the computational physicist. Session scientific themes ranged from looking at cutting edge uses of large-scale computation to solve significant scientific and engineering problems to gazing at the future as represented by quantum computing. In between were sessions exploring themes such as the latest in scientific visualization, the building of PC clusters, and the challenges, opportunities, and experiences of physicists working in the computer and financial industries.

The focus sessions targeted research in disciplinary areas. Each focus session had at least one invited speaker highlighting recent research. The remainder of the session consisted of contributed papers selected by the program committee. The committee was able to accommodate about 90% of those who preferred an oral presentation instead of a poster presentation. The disciplines represented by these sessions covered almost the entire range of disciplines under the umbrella of the Division. About 20% of the abstract contributors preferred a poster session. This session was held on Wednesday evening along with a reception and was well attended.

A special session, a Town Hall meeting, was held on "Advances Important to Computational Physics Education." On Sunday, on the Boston University campus, a tutorial on how to build a Beowulf Cluster was conducted by Steve Gottlieb (Indiana). 16 participants each built one node of a possible cluster while another 25 observed. We believe this hands-on tutorial was the first of its kind.

The lectures associated with the awards of the Rahman and Metropolis prizes were given in a special awards session. Alex Zunger of NREL received the Rahman prize and John Pask of UC-Davis, now at the NRL, received the Metropolis prize.

March and April 2002 Meeting Programs

In 2002, DCOMP will still be a participating unit at the March and April APS meetings. Because our annual meeting will be stand alone that year, we are presently allocated only a small number of invited sessions at each meeting. To increase our presence at the March meeting we will be jointly sponsoring several sessions with several other participating Divisions. We will have some DCOMP only sponsored sessions. These sessions 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 DCOMP's Vice-Chair, Jerry Bernholc at bernholc@ncsu.edu.

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.

Additional information can be found at <http://www.aps.org/praw/rahman>.

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), **Michael L. Klein** (1999) and **Michael John Creutz** (2000).

2001 ANEESUR RAHMAN PRIZE WINNER: ***Alex Zunger*** National renewable Energy Laboratory

The ninth Rahman Prize was awarded to **Alex Zunger** of the National Renewable Energy Laboratory. Dr. Zunger's research field is Condensed Matter Theory of Real Materials. He developed in 1977 the first-principles density functional pseudopotentials. In 1978, he co-developed the Momentum space total energy method. In 1981, he developed with John Perdew the now most widely used exchange and correlation energy functional and the Self-Interaction Correction. In 1983, he developed a novel theoretical method for simultaneous relaxation of atomic positions and charge densities in self-consistent LDA calculations. Recently, he developed methods for calculating the electronic properties of semiconductor quantum nanostructures. The Bardeen Award was given to A. Zunger on his "seminal contributions to the theoretical understanding and prediction of "spontaneous ordering" in alloys whereas the Rahman award was given "for his pioneering work on the computational basis for first-principles electronic structure theory of solids." He is the winner of the DOE/MRI 1980 and 1990 Outstanding Achievement Award, and the 1997 DOE-BES award for Sustained Research in Solid State Physics.

2002 Rahman and Metropolis Prizes 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/>.

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 is invited to present his or her work in an appropriate session of the meeting. The award is sponsored by the Journal of Computational Physics.

Details can be found at <http://www.aps.org/praw/metropol>.

2001 NICHOLAS METROPOLIS AWARD: ***John Ernest Pask*** University of California, Davis

Citation:

"For his contributions to computational physics that included the formulation and implementation of a new finite-element-based method for solving the equations of density functional theory"

Background:

Dr. Pask did his undergraduate studies at the University of California, Davis, where he was a recipient of the Edward Frank Kraft Scholarship Prize in 1983, a University Scholarship in 1984; and graduated with honors in 1988 with a B.S. in physics.

After graduation, he went on to a position at the Naval Nuclear Power School in Orlando, Florida, where he taught introductory physics to enlisted students from 1988-1990; and taught mathematics, physics, and reactor dynamics to officer students and civilian engineers from 1990-1994, during which time he was awarded the Navy Achievement Medal and served as Director of the Mathematics and Physics division from 1993-1994. While at Nuclear Power School, Dr. Pask did graduate work at the University of Central Florida, where he completed an M.S. in mathematics in 1994.

In 1994, Dr. Pask returned to the University of California, Davis to pursue a Ph.D. in physics. While there, his graduate work, under Dr. Barry Klein, focused on the development and implementation of a new finite-element based approach to large-scale ab initio electronic-structure calculations. During the latter part of his graduate studies, in 1998-1999, Dr. Pask worked with Dr. Philip Sterne at the Materials Research Institute of the Lawrence Livermore National Laboratory on the extension and application of the finite-element based electronic-structure method to large-scale ab initio positron distribution and lifetime calculations. Dr. Pask completed his Ph.D. in physics in 1999.

In 1999, Dr. Pask was awarded a National Research Council Associateship to continue work on electronic-structure method development and applications with Dr. David Singh at the Naval Research Laboratory in Washington, DC; where he is currently working on the development of the finite-element approach and applications of the linearized augmented planewave method to transition-metal oxide systems.

FELLOWSHIP PROGRAM

This year, the Division of Computational Physics had seven members elevated to Fellowship in the APS. We congratulate these colleagues on being so honored.

The new Fellows are:

Kim K. Baldridge, University of California, San Diego

For her development and application of methods for quantum calculations of molecular structure and reactivity, including her studies of aromaticity which continue the tradition of Maria Goeppert-Mayer.

Glenn Bateman, Lehigh University

For his theoretical and computational research on MHD instabilities and predictive transport modeling of tokamak plasmas, emphasizing detailed comparisons between theory-based simulations and experimental data.

Bruce Michael Boghosian, Boston University

For contributions to mathematical and computational fluid dynamics, lattice models of fluids and soft condensed matter, and leadership and service in the field of computational physics.

Stanley Roderick Deans, University of South Florida

For helping reveal the beauty and power of the Radon transform.

Carl Richard DeVore, Naval Research Laboratory

For his development of a new class of numerical algorithms for magnetohydrodynamic simulations, their wide dissemination in software, and their applications to physics.

Stephen M. Foiles, Sandia National Laboratories

For significant advances in the computational simulation of materials including pioneering work on the embedded atom method and demonstrating the power of simulations to determine important properties.

Mark Alan Novotny, Florida State University

For original algorithm development and applications of computational statistical mechanics to equilibrium and nonequilibrium problems in condensed-matter physics and materials science

The annual deadline for nominations from DCOMP is 1 April.

NPACI-Supported Computational-Physics Bachelor's Degree To Be Offered at Oregon State

In recognition of the exploding demand for university-trained computer specialists, Oregon State University is preparing to offer Bachelor of Science degrees to students majoring in computational physics. Rubin Landau, a physics professor and director of the Computational Physics for Undergraduates (CPUG) program at Oregon State, has received the endorsement of the Department of Physics, the university provost, and the chancellor's office of the Oregon University System for such a program. Rubin is a former member of DCOMP's Executive Committee and currently one of DCOMP's Webmasters. SDSC and NPACI provided one-month summer appointments to help Landau develop his curriculum as well as software and teaching materials. "More than having their financial support, having the personal support of the leaders of a national scientific organization such as NPACI helped me win this authorization."

Landau said the need for his CPUG program has been apparent for years. Technical specialists with baccalaureate degrees in computational-physics are needed by companies that use high-performance computers to model ground-water movement, the atmosphere, and to design cars, aircraft, and other transportation equipment. "Unfortunately, there are not enough IT (information technology) workers to meet the demand," he said. Illinois State University is one of the few, if only other, universities that also offers a bachelor's degree in computational physics. Several other U.S. universities offer bachelor's degrees in physics with minors or specialties in computational physics, said Landau.

Landau has written three physics textbooks, including "Computational Physics: Problem Solving with Computers," and he began offering computational-physics classes to seniors 10 years ago. In 1997, he began offering versions of those classes to freshmen. The courses use physics, computer science, and applied mathematics to solve real-world problems. Students enrolled in computational-physics courses receive computer codes that were previously developed as part of master's and Ph.D. thesis projects at Oregon State. Students make use of Web-based tutorials and demonstrations, textbooks, classes, and a trial-and-error approach in the computer lab. "The students have two to three weeks to get a feel for the research and how to do simulations," he said. "It's a real challenge." Physics students use computer-simulation software such as Maple and MatLab to solve problems, but Landau says they often don't understand the computer science involved.

ROSTER OF EXECUTIVE COMMITTEE

James E. Gubernatis, Chair

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Term as Chair ends 2002

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Condensed Matter Physics
Term as Past-Chair ends 2002

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Plasma Physics, General Relativity, Astrophysics
Term ends 2003

Jerzy (Jerry) Bernholc, Vice Chair

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Condensed Matter Physics, Biological & Chemical Physics,
Material Physics
Term ends 2004

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Condensed Matter Physics, Statistical & Non-Linear Physics
Term ends 2003

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Condensed Matter Physics
Term ends 2003

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Term ends 2002

Estella Blaisten-Barojas, Member at Large

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Term ends 2004

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Condensed Matter Physics
Term ends 2002

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Term ends 2003

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Term ends 2004

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Condensed Matter Physics, Materials Physics
Term ends 2003

Thanks for all the hard work for the Division by the following individuals whose terms on the Executive Committee expired in 2001:

Gary D. Doolen, Chair (1997 - 2000), Past-Chair (2001)

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AMO Physics, Fluid Dynamics, Nuclear Physics, Plasma Physics

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