



# Division of Computational Physics... ...DCOMP

# Physics Computing News

Fall 2002

## 2003 DCOMP Meeting at 2003 APS March Meeting in Austin

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## Message from the Chair

Dear DCOMP Members,

For the past two decades I have thought of myself foremost as a computational physicist. As the years pass, bigger and faster computers continuously become available to us, and we have used them to investigate systems of increasing complexity with increasing fidelity. The class of problems I investigated a decade ago on a Cray Y-MP, I now can investigate on my laptop. The class of problems I investigate now on supercomputers was impossible a decade ago. The news is full of stories about real or anticipated dramatic advances in computational power. The first that comes to my mind is Japan's Earth Simulator that went on line earlier this year with an amazing 40 TeraFLOP/s of peak computational power. It recently achieved an even more amazing 26 TeraFLOP/s sustained performance on a global atmospheric circulation simulation. In an article that appeared in the July 2001 issue of *Scientific American*, Thomas Sterling of NASA's Jet Propulsion Lab and CalTech outlined several possible routes to the trans-PetaFLOP/s level. As computers get bigger, their power and cooling requirements can also grow to excessive levels. Several news organizations (including CNN and the New York Times) picked up on the Supercomputing in Small Spaces project at Los Alamos National Lab (<http://www.sss.lanl.gov>) on constructing a lower-power, low maintenance supercomputer. There is also great interest in the thing called Grid Computing, i.e., the development of a secure infrastructure to allow a large distributed research community access to remote resources (computers and data). (See, for example, the article by Ian Foster in the Feb 2002 issue of *Physics Today*.)

So is computational physics now only about bigger, faster, more efficient computers? What about better algorithms? After all, to achieve a factor of two finer resolution in an explicit 4-dimensional global atmospheric circulation simulation requires approximately a factor of 16 increase in computational resources. Does our extended community have the proper investment ratio of software to hardware development? Francis Sullivan of IDA and Jack Dongarra of ORNL/U.Tenn were brave enough to list their opinion of the top ten algorithms of the 20th century in an article in the Jan.-Feb issue of *Computing in Science and Engineering*. Their chronological list begins with the Monte Carlo method of von Neumann, Ulam, and Metropolis, and ends with the fast multipole algorithm. The Metropolis algorithm is at least 50 years old (and will be celebrated with a 50-th anniversary conference at LANL; see [cnls.lanl.gov/Conferences/MonteCarloMethods](http://cnls.lanl.gov/Conferences/MonteCarloMethods)), and the fast multipole algorithm was invented in the 1980-s. Where are the new great algorithms?

I would argue that a standard way of performing message passing, specifically MPI developed in the 1990-s, ought to be on the list. Quantum Computing, i.e. computing with entangled quantum bits, is an exciting area of research but so far has had more of an impact on the interpretation of quantum mechanics than on the solution to important problems. But, the field is still young. Despite the excitement of performing calculations of unprecedented complexity with today's supercomputers, and the ability to analyze huge distributed data sets with the Grid, is the rate at which we produce great algorithms falling to an unhealthy level, and is our present investment strategy in computational science out of whack? Let me know your thoughts. I'll include the best ideas in a future column.

On behalf of the DCOMP Executive Committee, I welcome DCOMP's newly elected Officers: Barry Schneider, our new Vice-Chair, and new members-at-large Mark Novotny and Peter Reynolds. I am grateful to have worked with outgoing members-at-large David Arnett and David Ceperley. Finally, I want to express my deepest appreciation for the efforts put forth for our Division by our past Chair James Gubernatis. Thanks Jim!

**Robert E. Peterkin, Jr., Chair**

## DCOMP 2002-2003 Committees

### DCOMP Nominating Committee:

**Chair:** Dale Koelling

**Vice Chair:** Elaine Oran

### DCOMP Annual Meeting in 2003:

**Chair:** Jerzy (Jerry) Bernholc [bernhol@ncsu.edu](mailto:bernhol@ncsu.edu)

**Local Organizer:** Jerry Bernholc

The 2003 meeting is discussed in this Newsletter. Specific questions can be sent to [bernholc@ncsu.edu](mailto:bernholc@ncsu.edu)

### Fellowship Committee:

**Chair:** Jim Gubernatis [jg@lanl.gov](mailto:jg@lanl.gov)

**Members:** To be announced.

The 2003 nomination deadline is April 1, 2003.

### DCOMP Rahman Prize Committee:

**Chair:** Priya Vashista [priyav@bit.csc.lsu.edu](mailto:priyav@bit.csc.lsu.edu)

**Vice Chair:**

**Members:** Shiyi Chen  
Michael Creutz  
Richard M. Martin

Information concerning this award is at <http://www.aps.org/praw/rahman/>. The nomination deadline is 1 July 2003.

### Metropolis Award Committee

**Chair:** Bruce Cohen [bcohen@llnl.gov](mailto:bcohen@llnl.gov)

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

The nomination deadline is 31 January 2003. Information concerning this award is at <http://www.aps.org/praw/metropol/>.

### DCOMP International Liaison Committee

**Chair:** Rubin H. Landau [rubin@physics.orst.edu](mailto:rubin@physics.orst.edu)

**Vice Chair:** David Landau

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## 2003 DCOMP Annual Meeting at the APS March Meeting, March 3-7

The DCOMP Annual Meeting will take place in Austin, Texas in conjunction with the APS March Meeting. In order to encourage the participation of those with a particular interest in Computational Physics, the DCOMP sessions are predominantly scheduled for the latter half of the week.

The March Meeting is the largest physics convention in the world, and we can all look forward to a vibrant and stimulating experience. An added attraction this year is the location, Austin, Texas, a thriving, friendly and safe city known as America's capitol of live music.

The DCOMP Program Committee and the Organizers of the various sessions have worked hard to provide high-quality speakers in a variety of interesting areas. As you can see in a separate box, we are sponsoring eight *Invited Symposia* and six *Focused Sessions* for a total of 56 invited speakers. As a demonstration of the broad reach of Computational Physics, four of the Symposia and all the Focused Sessions are co-sponsored with other Divisions.

All committee members and organizers personally request that you come to the DCOMP 2003. Although the Symposia and Focused Sessions are already fixed, you are encouraged to contribute an abstract in any area of computational physics **The deadline for submissions is December 6**, and post-deadline poster abstracts can be received until the end of January. The remaining deadlines, listed on the web site, include reduced fees for early registration (1/3/03). Finally, please take the advice of a 25-year March-Meeting veteran (me), book your hotel room early or your choice will be gone! I already did and am looking forward to seeing most of you in Austin. It will be an exciting meeting!

Jerry Bernholc, [bernholc@ncsu.edu](mailto:bernholc@ncsu.edu)

Chair of the Program Committee and DCOMP Chair-Elect

### DCOMP 2003 Symposia & Focused Sessions

#### **Symposia**

Computational Physics on the Nanoscale  
Computational Geophysics  
Computational Biophysics (+DBP)  
Advances in Monte Carlo Algorithms  
Quantum Computing from a Computational Viewpoint  
Computational Approaches to Time-Dependent Dynamical Problems (+DAMOP)  
Optical and Dielectric Properties of Materials (+DMP)  
Microelectronics Modeling and Simulation (+FIAP)

#### **Focused sessions**

Applications of Pseudopotentials in Materials and Solid State Physics (+DMP)  
Multiscale Modeling of Polymer Systems (+DPOLY)  
Theory and Simulation of Magnetism and Spin Dependent Properties (+DMP & GMAG)  
Simulations of Complex Materials (+DMP)  
Theory of Nanotubes (+DMP)  
Modeling and Simulation of Biomolecules (+DBP)

## Report on the Conference on Computational Physics: CCP2002 Hyatt Regency Islandia San Diego, CA 25-28 August 2002

The 2002 Conference on Computational Physics (CCP2002) took place 25-28 August 2002 in San Diego, California. It was organized by the APS Division of Computational Physics and also served as the annual meeting for our Division. All technical sessions were held at the conference hotel, the Hyatt Regency Islandia, n Mission Bay.

CCP2002 attracted approximately 160 attendees including 50 from outside the US. The three-day technical program had a single plenary session each morning and three parallel sessions each afternoon.

DCOMP continued a tradition by dedicating the first day's plenary session to a series of "Doing it Big" talks from across the spectrum of computational physics. Invited speakers included Uzi Landman (Georgia Tech), Robert Rosner (U. Chicago), Charles Brooks III (Scripps), and Stephen Eubank (LANL). The second day's plenary session focused on "Complexity in Fluids" with talks by Norm Zabusky (Rutgers), Jay Boris (NRL), and Hans Peter Bunge (Princeton). Jerry Brackbill (LANL) then gave a review talk on the PIC method for plasma physics, and Eytan Domany (Weizmann, Israel) gave a talk on cluster analysis of DNA-chip data.

The final day included two sequential plenary sessions. The first on "The World View of Computational Physics" featured talks by Tony Hey (University of Southampton, UK), Akira Ukawa (University of Tsukuba, Japan), and Fran Berman (UCSD). The second session was the DCOMP Award and Prize presentations with talks by the 2002 Metropolis Award winner Nadia Lapusta (Harvard), and the 2002 Metropolis Prize winner David Landau (U. Georgia). DCOMP also recognized its newly-elected APS Fellows.

The topics of the afternoon parallel sessions included condensed matter, complex systems, high energy physics, QCD, plasmas, electromagnetics, material science, computational physics education, statistical mechanics, Monte Carlo methods, non-equilibrium phenomena, the DOD High Performance Computing Modernization Program, and stellar and astro-physics. A popular Poster Session – reception with over 40 posters took place Tuesday evening. The complete program and photographs can be viewed from the conference website:  
<http://www.aps.org/DCOMP/Meetings/meet02/CCP2002.htm>.

CCP2002 was part of the series of international annual meetings that began with PC'89 in Boston, and continued in September 2001 with CCP2001 in Aachen, Germany (<http://www.kfa-juelich.de/ccp2001/>). CCP2002 was sponsored jointly by the American Physical Society, the International Union of Pure and Applied Physics, and the European Physical Society. Future conferences in this CCP series include:  
CCP2003 20-25 July 2003; Xi'an, China (<http://iccp6-ccp2003.iapcm.ac.cn>), and  
CCP2004 1-4 September 2004; Genoa, Italy (<http://www.ccp2004.infm.it>)  
Our Division will again have the opportunity to apply to IUPAP to host CCP2005.

## Report on the 2002 annual business meeting of the APS Division of Computational Physics

The meeting took place Monday evening. About 20 members attended and heard outgoing Chair Jim Gubernatis discuss recent changes to the Division's bylaws that were passed by the membership during the spring election. The new bylaws can be found at [http://www.aps.org/DCOMP/bylaws\\_web/bylaws\\_web.htm](http://www.aps.org/DCOMP/bylaws_web/bylaws_web.htm)

The annual meeting also heard Chair-elect Jerry Bernholc discuss his plans for our Division's participation in the APS March 2003 meeting that will take place 3-7 March in Austin, TX. DCOMP will have several Invited speaker sessions at APS's largest annual meeting, and he and his Program Committee have put together an exciting program in computational physics. Jerry's report on DCOMP's plans for this meeting appear on page 2 of this newsletter.

*Robert E. Peterkin, Jr., Chair*

## 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*, 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 CiSE 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. 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:

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Estela Blaisten-Barojas, [blaisten@gmu.edu](mailto:blaisten@gmu.edu).

## DCOMP Election Results

**Vice chair:** Barry Irwin Schneider  
**Members at Large:** Mark A Novotny  
Peter J Reynolds

We thank all the candidates for their participation.

## **FELLOWSHIP PROGRAM**

In 2001 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

### **Benioff, Paul, Argonne National Laboratory**

For highly original work that first showed quantum computation to be theoretically possible and led to important subsequent advances in quantum communication and quantum computing.

### **DeGrand, Thomas Alan, University of Colorado**

For contributions to our understanding of the strong interactions- particularly for the development of innovative techniques in the numerical study of quantum chromodynamics.

### **Peters, Michael H., Florida State University**

For contributions to the computational physics of aerosols and gas/solids systems and to computational non-equilibrium statistical mechanics of aerosols.

### **Rapaport, Dennis Chaim, Bar-Ilan University**

For innovative contributions to applications, methodology and education in the field of molecular dynamics

### **Rice, Julia Elizabeth, IBM Almaden Research Center**

For pioneering the development of efficient algorithms for the analytic derivative method with electron correlation, and for the calculation of frequency dependent polarizabilities with accuracy comparable to experiment.

### **Rikvold, Per Arne, Florida State University**

For innovative and significant computational studies in statistical and condensed-matter physics, materials science, and electrochemistry, including development of novel algorithms to study the decay of metastable phases of matter.

### **Schmidt, Kevin Edward, Arizona State University**

For his contributions to enhanced high accuracy computational methods and application in the simulation of electronic structure, nuclear matter and quantum fluids.

### **Wu, Ruqian, University of California, Irvine**

For contributions to the understanding of magnetic, electronic, mechanical, chemical and optical properties of compounds, alloys, interfaces, thin films and surfaces using first-principles calculations and for development of the methods and codes for such

### **Zhang, Shengbai, National Renewable Energy Laboratory**

For contributions to the understanding of semiconductor defects, impurities, surfaces, interfaces, and high-pressure phases using first-principles calculations.

## **The Open Source Physics Project**

W. Christian, J. Gould, H. Gould, and J. Tobochnik

Most members of DCOMP have heard of the advantages of object oriented programming and, especially, of its implementation with Java. Just as the switch from procedural to object-oriented programming has caused dramatic changes in commercial software design, so we expect to see similar changes in Computational Physics education and research software.

The advantages of Java include its easy syntax, its excellent graphics and user interactivity, and its ability to run unmodified on most computer platforms and over the Web. However, writing methods to open windows and create buttons or text fields is not only tedious and time consuming, but also goes against the object-oriented spirit of reusable components.

One of the goals of the *Open Source Physics* project is to develop a library of Java classes that perform much of the routine programming tasks that occur when writing educational software. These include: input, output, animation, and user interaction. Accordingly, our application programming interface (based on Swing and Java 1.3x ) includes packages for:

- **Controls:** For building graphical user interfaces and components.
- **Display:** A drawing framework base on the Drawable interface and the DrawingPanel class
- **Display2D:** Visualization tools for 2D data such as contour and surface plots
- **Display3D:** A 3D visualization framework based on Java 3D
- **Tools:** Numerical analysis tools such as ODE solvers.

We usually use these packages to write our programs as applications that can be easily incorporated into Web pages without any modifications.

A beta version of the packages has been released in October 2002 under the *GNU GPL* license for code distribution. Information about the Open Source Physics project is at <http://www.opensourcephysics.org>.

A further goal of the project is to provide an exemplary set of tools for teaching computational physics. Specifically, the third edition of *An Introduction to Computer Simulation Methods* by Gould, Tobochnik, and Christian, should provide such a set (see <http://sip.clarku.edu> for a preview). The OSP library has also been adopted by the *Statistical and Thermal Physics* project of Gould and Tobochnik; *Easy Java Simulations* by Esquembre; and *Tracker*, by Brown.

Partial funding for this work by NSF grants DUE-9752365 and DUE-0126439 (WC), NSF PHY-9801878 (G&T), and NSF DUE-0127363 (G).



Nadia Napusta receives the Metropolis Award at CCP2002

### 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/>.



David Landau receives the Rahman Prize at CCP2002

Thinking about the future, some of the major strengths of DCOMP are the broad interests and the expertise of its members. We would like to make a special effort to make the Annual Meeting attractive to those members whose primary Divisions do not participate strongly in the March Meeting. Your suggestions on this and other topics will be very much appreciated.

### Thanks for all the hard work for the Division by the following individuals whose terms on the Executive Committee expired in 2002:

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## **THE MONTE CARLO METHOD IN THE PHYSICAL SCIENCES**

### **Celebrating the 50<sup>th</sup> Anniversary 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 a conference to celebrate this anniversary and the important role of the Metropolis algorithm and the Monte Carlo method in the physical sciences. The conference will review the use of the Metropolis algorithm and the Monte Carlo method, highlight recent developments, and note the spread of the Monte Carlo method to other fields. It will emphasize algorithms and algorithmic issues. More information about the conference is at

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

or

**Jim E. Gubernatis, [jeg@viking.lanl.gov](mailto:jeg@viking.lanl.gov)**

## ***What's Happening with the Annual Meeting?***

At the beginning of the year, the DCOMP Executive Committee voted unanimously to hold the Division's regular meetings in 2003, 2004, and 2005 at the March Meeting, and in 2005 to hold an additional meeting, most likely that summer, at a place to be determined. For this additional meeting, the Division would seek co-sponsorship by the International Union of Pure and Applied Physics's (IUPAP) Commission on Computational Physics (C20).

The Division's tradition had been to bi-annually host its regular meeting apart from the March Meeting and jointly with the European Physical Society (EPS). In alternate years its regular meeting was at the March meeting and was unsponsored. Several years ago the EPS placed their meetings under IUPAP who initiated a three year cycle of co-sponsoring a computational physics meeting in North America. Our bi-annual tradition was now out of phase with IUPAP.

In 2001 the Division continued the bi-annual tradition of being apart from the March meeting even though it was not time for IUPAP co-sponsorship. In 2002 it was time for co-sponsorship, but with the meeting returning to the March meeting. Because March and the venue were inappropriate for an IUPAP meeting, the Division organized its 2002 meeting apart from the March meeting to maintain its co-sponsorship tradition until it could re-evaluate its traditions for its regular meetings.

If we divorced ourselves from the March meeting, yearly stand alone meetings would be burdensome. Their history includes several poorly attended meetings with significant financial losses. Such meetings however give the Division a clear identity and the opportunity to create a broad program. If we married ourselves to the March meeting, we would not serve those members who do not attend that meeting, and we would lose some control and identity because of the dominance of material science and condensed matter physics at that meeting. On the other hand about 60% of our members are potential participants in that meeting, and because of its large attendance, participation at our invited speaker sessions would increase significantly, and we would be promoting computational physics to many more people. Another problem was moving in-and-out of the March meeting had been placing many of the Division's activities out of phase with the APS. Balls

were being dropped. Do we need to continue seeking IUPAP co-sponsorship? This periodic joint venture addressed a written requirement in our by-laws that the Division promote computational physics internationally.

The vote by the Executive Committee to hold our regular meetings at the March meeting, at least for the next three years, permits a more in-phase approach to executing the Division's APS activities. Deciding now to have a second meeting in 2005 permits better long-range planning and keeps the door open for continued co-sponsorship with IUPAP. Most importantly, the extra meeting allows the Division to maintain a regular Divisional computational physics meeting for those members who do not normally attend the March meeting. By committing to the March meeting for three years, we were also able to negotiate a much larger presence at that meeting. In recent years, we organized only one or two invited sessions at that meeting. For this March we had six to start with, plus we had the promise that we could cluster them together to give certain days a computational physics flavor. Elsewhere in this Newsletter, Jerry Bernholc, our Program Chair for this March, summarizes our sessions for this March. By co-sponsoring some of our invited sessions with other Divisions, there will be ten invited sessions this March with a computational flavor

Our stand alone meetings in 2001 and 2002 were important because we demonstrated that with proper planning we can make money on such meetings even though the two meetings had different planning models, allow budget and low risk one and a higher budget and higher risk one. (Each made about \$10K.) The 2001 and 2002 meetings unfortunately also demonstrated that our meetings can still miss attendance objectives. Our attendance at these meetings was roughly 250 and 160. Our 1900 members account for only about 50% of the attendance. (The Executive Committee and invited speakers accounted for roughly one-fourth and one-third of the attendance at these meetings.) Planning for the 2005 international meeting will begin shortly. Boosting the participation of our members will be an important objective.

Jim Gubernatis, Past Chair

## ROSTER OF EXECUTIVE COMMITTEE

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