Division of Computational Physics (DCOMP)

Physics Computing News

Spring 1997

Contents:

It is time for our Division to elect members of the *Executive Committee*. Questions regarding the items in this newsletter or suggestions for future issues of *Physics Computing News* should be directed to **Robert E. Peterkin, Jr.**, Newsletter Editor. His address is given at the end of the Roster of the Executive Committee.

NEWS BYTES

APS and DCOMP Home Pages

The Division of Computational Physics has a home page that is available through the APS Divisions, Topical Groups, Sections, and Forums page attached to the APS home page at www address http://www.aps.org/index.cfm . The latter can be reached by using Internet browsers such as NCSA Mosaic, Netscape, and others.

The DCOMP home page provides up-to-date information about the Division's leadership, policies, and activities, including those regularly featured in this newsletter, including 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. Please send your suggestions for how to improve the DCOMP home page to the Newsletter Editor.

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 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** and **Michele Parrinello** (1995),and **Steven Gwon Sheng Louie** (1996).

1997 Aneesur Rahman Prize Winner: Donald H. Weingarten

The fifth Rahman Prize was awarded to **Donald H. Weingarten** of the I.B.M. Watson Research Center. His citation reads: "For his seminal work on lattice quantum chromodynamics including algorithmic innovations, massively parallel computer software development and hardware implementation that led to calculations of hadron masses and the mass and decay couplings of the scalar glueball."

Background:

Dr. Weingarten is a native of Massachusetts. He received his undergraduate degree from Columbia College in 1965 and his Ph.D. degree from Columbia in 1970. From 1969 to 1976 he held research positions at Fermilab (then National Accelerator Laboratory), the University of Copenhagen, the University of Paris, and the University of Rochester. From 1976 to 1983 he was an Assistant Professor, Associate Professor, and full Professor at Indiana University.During the Fall of 1982 and the Spring of 1983 he was on leave at Brown University. In 1983 he joined the Research Division of IBM in Yorktown Heights,New York, where he still works today.

1998 Aneesur Rahman Prize: Call for Nominees

Nominations for the sixth Rahman Prize are still open. Division members who wish to nominate deserving colleagues for the Rahman Prize are encouraged to do so before 1 July, 1997. Announcements will appear periodically in *APS News* over the intervening months.

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: **David P. Landau**, Rahman Prize Committee Chair, Center for Simulational Physics, The University of Georgia, Athens, Georgia 30601. (email: DLANDAU@UGA.CC.UGA.EDU; voice (706) 542-2908, FAX (706) 542-2492).

FELLOWSHIP PROGRAM

In 1997, the Division of Computational Physics had five members elevated to Fellowship in the APS. We congratulate these colleagues on being so honored. The new Fellows are:

1. **Maria Dworzecka**, George Mason University, for co-directing the Consortium of Upper Level Physics Software (CUPS) and co-editing accompanying instructional material for upper level physics classes.

2. **Alex Friedman**, Lawrence Livermore National Laboratory, for innovations in computer modeling of fusion plasmas, laser-plasma interactions and charged particle beams, and design of high space charge accelerator components.

3. **Adrian Lewis Melott**, University of Kansas, for groundbreaking studies of the origin and evolution of cosmic structure.

4. **Gregory Rewoldt**, Princeton Plasma Physics Laboratory, for his authorship of comprehensive codes for linear toroidal eigenmodes with realistic geometry and kinetic effects, and his extensive contributions to the understanding of microinstabilities in tokamaks.

5. **George B. Zimmerman**, Lawrence Livermore National Laboratory, for his creation, and subsequent development, of the LASNEX simulation code, which has been used extensively to guide the development of the National ICF program from its inception, to this day.

The deadline for 1998 nominations is 1 February 1998.

JOURNALS & PUBLICATIONS

Computers in Physics: Call for Educational Software Submissions

Computers in Physics (CIP) is continuing its sponsorship of an annual contest for the best in educational physics software. Since 1991 the winners have included inventive and creative educators and researchers from institutions of all sizes. Entries from the U.S. and from other countries are encouraged. The scope of the contest is broad, with entries from such areas as simulations, demonstrations, microprocessor-based laboratories, and utilities. In addition, there is a prize for the best undergraduate student entry; this software is not limited to pedagogy and may be associated, for example, with a research

project. Submissions for the contest can be in the form of traditional software packages (i.e. something that a student would use on a PC/Mac desktop computer), or World Wide Web pages that demonstrate useful pedagogy in physics.

CIP is seeking submissions for the next contest. Contest information can be found on the World Wide Web page at http://www.aip.org/cip/contest/ . The application form can be downloaded directly from the web. Since the contest inception in 1991, there have been 36 winners. 1996 winners were announced in the Nov/Dec issue of CIP. Submissions for the 1997 prize should be made soon. Questions can be addressed to jhuergo@aip.acp.org via e-mail or to Computers in Physics, One Physics Ellipse, College Park, MD 20740, the old fashioned way.

MEETING ANNOUNCEMENT

International Conference on Computational Physics: PC '97 at the U. California Santa Cruz

PC '97 is the annual meeting of the Division of Computational Physics of the American Physical Society and is sponsored jointly by the Forum on Industrial and Applied Physics (FIAP) of the APS, the European Physical Society, and the International Union of Pure and Applied Physics.

Join your colleagues **25-28 August 1997** at the University of California at Santa Cruz

PC '97 will be held on 25-28 August 1997 in Santa Cruz, California, USA. It will highlight basic and applied computational physics and its applications worldwide to the university, industrial and laboratory communities. Santa Cruz, located 75 miles south of San Francisco along the California coast, offers easy access for travelers from the U.S., Europe and Asia via the international airports at San Francisco and San Jose.

Our Conference Chairman is **Professor Barry M. Klein** of the University of California at Davis. For Conference information, please check the web site:http://www.aps.org/meet/PC97/. If you can't find what you need to know on this web site, you can contact the Conference Secretary: **Ann Lavallee**; e-mail comp97@physics.ucdavis.edu; phone 916-752-4088; fax 916-752-4717. Program Committee co-chairs are **Kenneth Hass** of Ford Motor Company and FIAP, and **Malvin Kalos** of Cornell University and DCOMP. The conference is expected to attract over 300 participants and to facilitate interactions between developers and users of computational methods, as well as to strongly emphasize applications of computational physics to industrial and other practical problems. Our keynote speaker for the banquet on the night of Wednesday 27 August is Paul Horn, VP Research, IBM.

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. These will be announced in June.

The conference will include topics from the following areas:

1. Applications to Industrial Devices, Materials and Processes
    - Device modeling
    - Process modeling
    - Electronic materials
    - Structural materials
    - Polymeric materials
    - Other industrial modelling
2. Applications to Environmental and Geological Phenomenon
    - Petroleum exploration
    - Environmental remediation
    - Seismic and oceanic phenomena
    - Hydrospheric and atmospheric geophysics
    - Other environmental and geological studies
3. Applications to Computational Materials Science
    - Nanostructure materials
    - Bridging the length scales
    - Electronic structure
    - Lattice models
    - ``Soft" materials (e.g., foams, emulsions, colloids, liquid crystals)
    - Other materials studies
4. Applications to cosmology/astrophysics
5. Applications to particle physics phenomena
6. Applications to nuclear physics
7. Applications to plasma physics
8. Applications to fluid dynamics
    - Turbulence modeling
    - Complex-fluid hydrodynamics
    - Rheology
    - Flow through porous media
    - Other fluid dynamic application areas
9. Other application areas
10. Multipole methods
11. Computational fluid dynamics methods
    - Finite-difference & finite-element methods & their variants
    - Spectral and spectral element methods
    - Vortex methods
    - Lattice gases and lattice Boltzmann methods
    - Other fluid dynamic methodologies
12. Object oriented methods
13. Quantum computing methods
    - Computational complexity issues

- Quantum error correction
- Quantum encryption
- Experimental realizations of quantum computers
- Other quantum computation issues

14. Monte Carlo methods
    - Quantum Monte Carlo
    - Monte Carlo simulations of fluids
    - Direct-simulation Monte Carlo
    - Hybrid Monte Carlo
    - Neutral-particle Monte Carlo
    - Lattice Monte Carlo (e.g., lattice fermion models)
    - Detector design
    - Pseudorandum number generation issues
    - Other issues in Monte Carlo simulations
15. Electronic structure methods
16. Other computational physics methods

PC '97 Deadlines

The deadline for submission of abstracts was May 16, 1997, 5:00 p.m. EDT at the APS Headquarters. If postdeadline abstracts are submitted, the organizers intend to include them in a supplementary program. The deadline for submitting conference registration fees and housing reservation forms is July 15, 1997.

PC '97 Tutorials Offered on Sunday, 24 August 1997

A series of six 90-minute tutorials is being planned for the Sunday preceding the conference, 24 August 1997. Advance registration for the tutorials is recommended (as there may be space limitations), but anyone registered for the conference may sign up for as many tutorials as they'd like at no additional charge. Tentative topics for the tutorials include:

1. Materials Modeling -- Stephen Foiles (Sandia, Livermore)
2. Industrial Physics -- Ken Hass (Ford) and others
3. Kinetic Schemes for the Euler and Navier--Stokes Equations -- Ramesh Agarwal (Wichita State U.)
4. Serial and Parallel Code Optimization -- presenter to be determined
5. Simulated Annealing and Related Optimization Methods -- presenter to be determined
6. Object--Oriented Methods -- presenter to be determined.

Additional information will be posted on the web site.

PC '97 housing

Conference housing will be provided on the campus of the University of California, Santa

Cruz. Information on accommodations, as well as the actual housing and registration forms, can be found on the conference web site located at http://www.aps.org/meet/PC97/. Additional information regarding plenary and invited speakers, and the Sunday tutorials will be added to the conference site as it becomes available.

Santa Cruz is home to picturesque coastal scenery, giant redwood groves, historical landmarks and museums which offer sights and activities for the whole family to enjoy. The Santa Cruz Beach Boardwalk, the Roaring Camp and Big Trees railways logging camp, and the nearby Monterey Bay Aquarium are just a few of the attractions that Santa Cruz has to offer. Several half-day trips are being planned.

ROSTER OF EXECUTIVE COMMITTEE

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Term ends 1998; Condensed Matter, Low Temperature Physics

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Term ends 1999; Statistical Physics

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Term ends 1998; Plasma Physics, Condensed Matter Physics

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Term ends 1998; Condensed Matter

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Term ends 1999; Condensed Matter

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Term ends 1996; Plasma Physics

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Complex Systems Group Leader

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Ex Officio; AMO Physics, Fluid Dynamics, Nuclear Physics, Plasma Physics

Robert E. Peterkin, Jr. *Newsletter Editor*

PL/WSQ

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Ex Officio; Plasma Physics, General Relativity

DCOMP ANNUAL ELECTION

In this year's election, we will elect a Vice-Chair and two Members-at-Large for our Executive Committee. The candidates to be elected this year will serve on the Executive Committee of the Division for three years; their terms expire in the Spring of 2000. The Vice-Chair becomes Chair-Elect next year, and the Chair of the Division in two years. The Executive Committee of our Division has a total of six Members-at-Large.

For each of these positions we have two or more candidates. Their biographical information and policy statements are included to help inform you about them. Enclosed is a ballot sheet and a return envelope. Please vote for one candidate for the office of Vice-Chair, and for two candidates among those running to be Members-at-Large.

Mail your ballot in the enclosed envelope to the Secretary-Treasurer of the Division. It must be received by **June 30, 1997** for it to be counted.

INFORMATION ABOUT THE CANDIDATES

Vice-Chair

Gary D. Doolen

Group Leader: Complex Systems Group

Los Alamos National Laboratory

Gary Doolen received his Ph.D. in Physics from Purdue University in 1967. From 1967 to 1969 he was a National Academy of Science/National Research Council-Research Associate at Goddard Space Flight Center. In 1969, he joined the Physics Department at Texas A&M University. At Los Alamos National Laboratory since 1975, he has worked on a wide range of computational research: fluid dynamics, nuclear physics, atomic physics, plasma physics, magnetohydrodynamics, neural networks, nanotechnology, lattice gas and lattice Boltzmann methods, and nonlinear mathematics; he has published about one hundred refereed journal articles and edited five books. He served as Senior Scientific Editor for the Defense Research Review. He was Deputy Director for the Center for Nonlinear Studies in1990, and Acting Director for the Center for 1991-1994. Since 1994, he has been the Complex Systems Group Leader in the Theoretical Division at Los Alamos. In January, 1996, he also became Project Leader for Accelerator-Driven Transmutation Technology.

He was Secretary/Treasurer of the Division of Computational Physics for three years.

Candidate's Statement

Computational Physics is a expanding field. Computers are now used for efficient design, for exploring new parameter regimes, and for creating new understanding that can readily be communicated to others. Physicists discuss ``numerical data" from computer simulations; insights are being being created by computer that cannot be practically measured. We are now in the age of the teraflop computer and it appears that several orders of magnitude increase in speed are technically feasible. Data transfer rates of the order of gigabits/second exist now and rapid increases are anticipated. The computer culture is becoming a world-wide standard, significantly enhanced by the internet, by software development, and by hardware breakthroughs.

My recent experience as a computer user in applied physics indicates that there is much that the APS can do. Bulletin boards, web pages, and two-way video teleconferencing

over the net will become standard in the next decade. Hopefully, all scientific articles will also become available over the internet during this period. For the past few years, I have been involved in APS-funded software development that will make the pre-1995 Physical Review and Physical Review Letters available in a useful form on-line; soon the 1985-1995 PR and PRL will be available over any terminal connected to the net.

There is a definite need for a proactive Division of Computational Physics. With your guidance, advice and assistance, our Division is capable of developing many new ways to benefit its members. If elected, I will do my best to continue the traditional support that the Division has given to its members; I will also work hard to make our Division work better for you.

Vice-Chair

Dalton D. Schnack

Senior Scientist: Applied Physics Operation

Science Applications International Corp.

Dalton Schnack received his Ph.D. in Engineering/Applied Science from the University of California, Davis, in 1977. Prior to entering gaduate school he worked for seven years (1967-1973) at the Pratt & Whitney Division of United Aircraft Corp., where he first became involved in the problems of large scale numerical simulation by computing complex steady flow in rotating machinery. From 1973-1977 he did his Ph.D. research in computational plasma physics under the direction of Prof. John Killeen. From 1977-1980 he was a staff member at the Magnetic Fusion Energy Computer Center (presently the National Energy Research Scientific Computing Center) at Lawrence Livermore National Laboratory. From 1980-1982 he was a staff scientist in the Controlled Thermonuclear Fusion Division of Los Alamos National Laboratory. He joined Science Applications International Corp. in 1982, serving as Manager of the Applied Plasma Physics Division from 1985-1992. He is presently Director of the Center for Space and Laboratory Plasma Physics. He has authored or co-authored over 30 refereed publications and one book in the field of nonlinear computational magnetohydrodynamics (MHD). His current research interests include analysis and simulation of the nonlinear dynamics of space and laboratory plasmas, especially extended MHD models to describe the evolution of very hot plasmas in realistic three-dimensional geometry.

Dr. Schnack has chaired the Fusion Computing Council, and is presently a member of the Sherwood Fusion Theory Executive Committee. He is also Team Leader for the NIMROD Project, a Department of Energy sponsored activity to develop a new simulation capability for advanced tokamak experiments. He is a Fellow of the APS and is currently a member of both the Division of Computational Physics and the Division of Plasma Physics.

Candidate's Statement

Computational Physics is presently undergoing a revolutionary change. For years we have been able to rely on evolution of generation after generation of larger, faster vector supercomputers on which to conduct our ever more complex research. Computer manufacturers actively sought our opinions about hardware and software specifications, and were happy to provide specialized products to cater to our needs. Over the past few years all this has changed with the development of cheap, fast scalar chips that can deliver more flops per dollar than superconducting vector technology. The needs of scientific computing are no longer the driving force in the marketplace; cost is. The age of the vector supercomputer mainframe is near an end. The next generation of large scale computational problems will likely be performed on a collection of these fast processors, configured either as a farm of workstations or as a massively parallel mainframe.

Concurrently, for the first time in decades there may now be a viable, possibly preferred, alternative to Fortran as the programming language of choice for scientific computing. Object oriented languages are now virtually standard in the non-scientific computing world, and their efficacy for scientific problems is presently being debated.

While the questions of the future computing environment have yet to be settled, it is clear that changes in both hardware and software for large scale scientific computing are inevitable. No matter the outcome, the way we compute will have changed dramatically. This change and uncertainty presents a pressing problem for a working computational physicist, because the choice of algorithm for a particular problem is determined by both the physics and the computing environment. The Division of Computational Physics is in a unique position to provide guidance and information to the scientific community to ease the transition. This can be done through special forums held in conjunction with the divisional meeting, through the sponsorship of special purpose workshops, and by issuing informational papers on these subjects. Our organization across all branches of physics allows the experience in many different types and sizes of problems to be brought together. I will work to have the Division become the best source of unbiased information for issues that relate to choices of languages, hardware, and algorithms in these changing times. I see this as the most valuable contribution that the Division can make for the next several years.

Member-at-Large Francis J. Alexander

Research Assistant Professor

Boston University

Frank Alexander obtained his Ph.D. in Physics from Rutgers University in 1991, after receiving his B.S. in Mathematics and Physics from The Ohio State University. From 1991 to 1993 he was a postdoctoral Fellow at the Center for Nonlinear Studies at Los

Alamos National Laboratory, and from 1993 to 1995 at the Institute for Scientific Computing Research at Lawrence Livermore National Laboratory. In 1995 he joined Boston University's Center for Computational Science. His research focuses on statistical mechanics and computational physics.

Candidate's Statement

Though there has been extraordinary growth of computational resources for both scientific and educational purposes, more can be done to reap the advantage of computers as a means of large-scale communication. Accordingly, I propose a number of initiatives to meet the Division's four explicit goals:

1. *To promote research and development in computational physics*, I propose (a) the promotion of a software archive which, much like the existing linear algebra and statistical software archives, (such as LINPACK), would house contributed (well-documented) code on a variety of research areas; and (b) the development of a database of computational physicists and their current research, as well as other scientists interested in computational physics (including those outside of physics).
2. *To enhance the prestige and professional standing of its members*, I propose that the Division sponsor a series of regularly scheduled, interactive, web-based forums. These forums could facilitate the dissemination of scientific and educational developments to an audience, such as high school students and teachers, for whom travel is not an option. These forums could also make known to a world wide audience state-of-the-art results in a variety of computational physics areas.
3. The Division's third goal, *to promote scholarly publication*, seems to have been met based on the phenomenal growth in the number of published papers that fall under the purview of computational physics. However, I suggest that more emphasis and education be devoted to raising the standards in the acquisition and reporting of computational results (for example, the design of numerical experiments and the analysis of results).
4. Proposals included in (1) and (2) would serve to facilitate *the promotion of international cooperation*, the fourth goal of the division.

Member-at-Large

Amy L. R. Bug

Associate Professor of Physics

Swarthmore College

Amy Bug received a B.A. in Physics and Mathematics from Williams College in 1979, and a Ph.D. in Physics from M.I.T. in 1984. She was a postdoc in the Theoretical and

Mathematical Sciences group at Exxon Research and Engineering Co., and in the Chemistry department of Columbia University. She is a computational physicist, and has done work applied to medical physics (cardiac electrophysiology), condensed matter physics (order/disorder transitions), and chemical physics (guest/host properties of microporous solids). During her sabbatical leaves, she's held visiting appointments at the University of Pennsylvania and Boston University. She has taught a dozen different physics courses in her 8 years at Swarthmore, including a mathematical methods course with a numerical methods component, and she has designed labs which feature the computer as a teaching tool, both for simulation and measurement.

Candidate's Statement

We computational physicists are specialists in a multidisciplinary field with its own unique set of strengths, and also frustrations. Our numbers include not only physicists, but people who also consider themselves theoretical chemists, mathematical biologists, ... Our methods and capabilities are of interest to experimentalists in almost every subfield of physics. There is an undeniable excitement in having a specialty with such broad power and appeal, but there is also a frustration inherent in having one's research effort tied to a technology which evolves so rapidly, in a manner which is out of the hands of the individual researcher.

What kind of support would I, a busy teacher and researcher, want from the Division? I suppose it would be to offer guidance in complex issues, the sort that it would take members large numbers of person-hours to investigate alone. I would like the Divisional publications and meeting sessions to keep members current on new hardware technologies, algorithmic developments, and educational software, with ideas about its successful uses. I would like the Division make an effort to solicit and centralize information on meetings across the subdisciplines, and to draw our attention to publications of interest to us. Perhaps the Division can facilitate networking of people with similar needs. As important problems arise, ones which constitute technical challenges, I would like to see the Division put its weight behind the development of a solution, via working sessions at meetings and other types of advocacy and sponsorship. Perhaps the Division can even play a role as an advocate for computational physicists with the computer industry. I realize that this is asking a lot of the Divisional representatives. But as a representative myself, I would try to move in some of these directions; to make the Division function as a good colleague and mentor to each of its members.

Member-at-Large

Adriana Moreo

Associate Professor of Physics

Florida State University

Adriana Moreo obtained her Ph.D. in Physics from the Instituto Balseiro (Bariloche - Argentina) in 1985. Her thesis work was in the context of Lattice Gauge Theory in High Energy Physics. She was a Post-doctoral Research Associate from 1985 to 1988 at the University of Illinois at Urbana continuing her work on Lattice Gauge Theory and problems of Condensed Matter Physics. From 1988 to 1991 she became a Research Associate at the University of California at Santa Barbara specializing in High Temperature Superconductors. She joined the Florida State University faculty in 1992. She is a member of the Theory Group at the National High Magnetic Field Laboratory. Her present research interests are still in Condensed Matter Physics, mainly in the study of strongly correlated electronic systems using numerical techniques. This area includes high-Tc superconductors, quasi-one dimensional compounds, and manganite materials among others. Her research requires the intensive use of computers and analysis of experimental data. She has also incorporated the use of computers in her teaching of Physics at the undergraduate level.

Candidate's Statement

In spite of being a relatively young physicist I already had the experience of working with very different generations of computers. They include somewhat primitive IBM machines in the 80's in Argentina, Vax's and various generations of Cray supercomputers later in my postdoctoral work, and finally clusters of work stations in my more recent research. It is remarkable how much computers have evolved and improved in the last ten years. This has been correlated with the development of Computational Physics as a powerful sub-branch of Science. In particular in my field of expertise, computational work has produced crucial contributions towards the understanding of strongly correlated electrons, and Materials Science. In many contexts where perturbative expansions are doubtful, computers can provide unbiased information that guide the current research in those areas. Experts in my field have the dream that some day we will be able to fully simulate new materials in a computer instead of painfully synthesizing them one by one at the lab! Still there are some colleagues that stubbornly resist computers. Some old guard scientists refuse to believe that computers can produce good science. I believe that it is a duty of our division to show them otherwise by giving visibility to computer work in the APS and other international meetings devoted to different branches of Physics. The message would be that computational physics is here to stay and it is time to make it part of the curriculum of graduate studies in our Physics Departments. Nowadays the computer has also become a tool for electronically communicating new scientific results much faster than it was possible until only a few years ago. Although most of our colleagues use this newly developed tools, several are still not fully aware of their importance. We still need some education process to take place in our ranks, and certainly we also have to educate the general public on these matters as best as we can. If I am elected I will do my best to reach these goals.

Member-at-Large

Robert E. Wyatt

Professor of Chemistry and Biochemistry

University of Texas at Austin

Robert E. Wyatt, a native of Chicago, received his B.S. in Chemistry at the Illinois Institute of Technology. He then received an M.A. and a Ph.D. in Chemistry at the Johns Hopkins University. As an NSF postdoctoral fellow, he did research in theoretical chemistry in England and at Harvard University. He then joined the Chemistry Department at the University of Texas at Austin, where he is currently W.T. Doherty Professor of Chemistry and Director of the Institute for Theoretical Chemistry. He has been a visiting Professor at Shandong University in China, and at the University of Paris, Orsay. In addition, he took a sabbatical in the Theoretical Division of the Los Alamos National Laboratory. He currently serves on review committees at Brookhaven National Laboratory and Argonne National Laboratory. His research interests include quantum mechanical studies of spectra and energy transfer in high energy molecules, and the development and application of algorithms for large eigenvalue problems. He has been an enthusiastic user of both vector and distributed memory parallel supercomputers.

Candidate's Statement

One of the most important challenges facing our division is that of education-- not only for college students, but for the professional scientist. In many areas, excellent algorithms are being used or are under active development. However, information about these developments seeps slowly from each applications community into the other areas. The barriers between our specialties can be high! Our Division should actively promote tutorial sessions and minisymposia on computational and algorithmic issues at APS meetings, in addition to those at the Physics Computing conferences. In addition, the Division should promote symposia at the APS meetings which are focused on broadly useful computational topics.

The Division of Computational Physics should take an activist role in promoting the computational laboratory as the third approach to studying complex scientific problems. The common bridge between members coming from diverse areas of physics is computers, algorithms, and numerical results. The catalytic effect resulting from the members in this Division learning about each other's' methods frequently provides exciting possibilities for further developments. If elected, I will use this position to promote the spread of knowledge about computational methods across the broad spectrum of computational scientists. Finally, there are communities of computational scientists who are not well represented in the Division, although they contribute

significantly to the body of knowledge in this area. We should seek to broaden the membership to include these computational areas.

BALLOT

Vice-Chair: Vote for **one** candidate.

- ☐ Gary Doolen
- ☐ Dalton Schnack

Members-at-Large: Vote for **two** candidates.

- ☐ Frank Alexander
- ☐ Amy Bug
- ☐ Adriana Moreo
- ☐ Robert Wyatt

Please return your ballot in the envelope provided. It must be received on or before June 30, 1997 for it to be counted.