

## **NEWSLETTER - SPRING 1991**

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### **PHYSICS COMPUTING '91**

including

#### **The 3rd International Conference on Computational Physics**

Announcement and Second Call for Papers

The Topical Group on Computational Physics has combined forces with the editors of the AIP journal *Computers in Physics* to bring you a full week on the many aspects of the use of computers in physics including the traditional topics of computational physics. The meeting will convene on 10 June 1991 in the San Jose Convention Center and run through 14 June 1991.

San Jose is located some 40 miles southeast of San Francisco at the south end of the San Francisco Bay, and is in the heart of "Silicon" Valley. The universities, national laboratories, and the large assortment of computer hardware and software companies in the region make San Jose an ideal venue for this meeting.

The meeting program consists of plenary, oral, poster, and tutorial sessions, with many invited papers being given in the oral sessions. We are fortunate to have D. Allan Bromley, Assistant to the President for Science and Technology, to give our Keynote Address. Our meeting format consists of several 90-minute sessions arranged such that the plenary sessions do not run in parallel with other sessions and with 3-hour poster sessions held in the exhibit hall. We have arranged 11 plenary and 70-plus invited papers on the methodology of using computers in physics research and education. We are seeking presentations that emphasize computational methodology and discourage papers that only emphasize results. There are presentations with applications to most branches of physics, including acoustics, astronomy, astrophysics, atmospheric physics, atomic physics, biophysics, chemical physics, climatology, condensed matter physics, fluid dynamics, geophysics, high energy physics meteorology, nuclear physics, optics,

physics teaching, polymer physics, plasma physics and vacuum science. Rather than organize sessions by physics specialties, we are arranging them by methodology.

A partial list of these session topics includes few-body problems, Lagrangian methods, visualization in fluid dynamics, spectral and spectral elements methods, finite difference and finite element methods, molecular dynamics, acceleration algorithms, experimental particle physics, gene and protein sequencing, particle methods, fast multipole methods, real time computing, quantum Monte Carlo, parallel computing, visualization, computing environments, artificial intelligence, neural networks, physics education, symbolic computing, signal processing, Monte Carlo methods in statistical mechanics, large matrix manipulations, chemical dynamics, chaos, growth and fractals, and cellular automata.

Monday, June 10th, is being largely devoted to tutorial presentations (mini-courses) each of three hours duration. Classes on topics of interest to the physics computing community are being offered for a separate fee of \$75.00 for each three hour class. Below we give some further details under the heading "TUTORIAL PROGRAM DETAILS." Course notes and other materials will be furnished by the instructors and are included in the fee. Sign-ups may be made on the enclosed pre-registration form or at the registration desk up until the start of each course session. Classes with three or fewer students will be subject to cancellation.

### **CALL FOR PAPERS**

We are soliciting presentations in the areas mentioned above. The cross disciplinary nature of our conference is facilitated by presentations that stress methods so we strongly discourage offerings that emphasize results. In keeping with this authors are encouraged to follow the 10-80-10 rule in apportioning their presentations. This means roughly 10% on the theory or background, 80% on methodology, and 10% on results.

Please send your abstract of approximately 100 words to the Meeting Secretariat:

Ms. Martelle Mays  
P. O. Box 5509 L-561  
Livermore CA 94550 USA  
FAX (415) 422 0435  
E-mail: mmays@llnl.gov

It is not necessary to conform to the usual APS abstract format because we are electronically scanning and retyperetting all of our abstracts. Abstracts may be sent by mail, FAX or electronic mail. Most presentations will be scheduled for poster sessions, which the organizers feel affords the best medium of presentation for contributed papers. Authors preferring oral presentation may indicate this preference at the bottom of their abstract submission. The poster sessions will be held in the large Hall of Exhibits while the contributed oral papers will be given in one of the parallel oral sessions. All abstracts received by the Deadline of May 10, 1991 will be assigned sessions and appear in the Proceedings of Abstracts to be distributed at the Meeting. (Abstracts which we received prior to February 1st will also appear in the Bulletin of the APS.) Post-deadline submissions that are received after May 10th may be scheduled for presentation on a space available basis and will not appear in the proceedings.

### **MEETING REGISTRATION**

Registration for Physics Computing '91 may be accomplished by using the enclosed Pre-registration Form or by registering on-site. Attendees are advised to pre-register, at a discount, by returning the enclosed Pre-registration Form together with payment prior to May 10, 1991. Sign-ups and payment for the Tutorial Sessions may also be done with this form. On-site registration, in the 1st floor lobby of the San Jose Convention Center, will be available from 2PM Sunday June 9th. All registration fee refund requests must be submitted in writing to Lawrence Merrill, Meeting Arrangements Manager, the AIP Special Programs Department, 500 Sunnyside Blvd., Woodbury, NY 11797, no later than 1 June 1991.

### **HOUSING**

Blocks of rooms, at special discount rates, have been reserved for conference attendees and their guests at the Fairmont, the Hotel De Anza, the Hyatt and the Holiday Inn. The Fairmont will be the headquarters hotel for the conference, although all of the technical sessions will be held in the San Jose Convention Center. All hotels are either

within walking distance or 5 to 10 minutes away from the Convention Center by local rail transportation. To ensure receiving the special discount rate, please use the hotel reservation form enclosed here and book your room no later than 15 May 1991.

## SUPPLEMENTARY INFORMATION

### Travel to San Jose

We have made arrangements with AMERICAN AIRLINES for SPECIAL DISCOUNT FARES for those attending the Physics Computing '91 Conference. Discounts from 35% to 45% are available, off regular day coach fares and 5% off most promotional fares. To obtain these rates please call American at 1-800-433-1790 and ask for the travel representative at STAR NUMBER S-0161B3. These special fares are available only within Canada and the USA. You will be informed of the most economical and convenient flights to San Jose.

Hotel shuttle buses are available to each of the conference hotels from the San Jose Airport. Taxis are a reasonable alternative as the hotels are within a few miles of San Jose Airport. Attendees arriving at the San Francisco Airport, which is approximately 35 miles away, can make reservations with Bayporter Express at 415-467-1800 for transportation to San Jose.

### Local Information

The San Jose Convention and Visitors Bureau will be sponsoring a local information booth in the registration area to provide information on restaurants and local attractions.

### Placement Center

The American Institute of Physics will operate a Placement Center as a service to employers and to potential employees. Further information will be available at the Registration Desk.

### Open Business Meeting

On Thursday afternoon from 17:00-18:00 in Ballroom A an informal business meeting will be held for the meeting organizers and attendees to exchange views. We solicit feedback on how to better organize meetings like this in future years. Of particular interest is the question regarding our present plan to hold biannual meetings because there is some interest in having it on an annual basis.

### Town Meeting for NERSC Users

Users of the National Energy Research Supercomputer Center (NERSC) and other interested parties are invited to participate in a Town Meeting where the Users may exchange ideas with Representatives from the NERSC facility. The purpose of this is not only to facilitate communication, but is also to build User Profiles. These profiles are then used in Strategic Planning. The Town Meeting will be held in Ballroom A-1 at 8:00pm on Tuesday, June 11th.

### Exhibit Show

Several vendors of computer hardware and software as well as other organizations will participate in the Exhibit Show, which will be held for three days (11-13 June) in exhibit Hall I. It will be held in conjunction with the poster sessions of the technical program and should provide valuable resources for many of our future computational needs. A partial list of the exhibitors includes:

- Addison-Wesley
- Apple
- American Institute of Physics
- Computer System Architects
- Cray Research
- Daedalon
- Fischer Scientific
- Hewlett-Packard
- Horstmann Software Design
- IBM
- Intelligenceware
- Language Systems
- National Instruments
- Physics Academic Software
- Prescience Corporation
- Soft Warehouse
- Springer-Verlag
- Sun Microsystems
- TriMetrix
- Tutsim Products
- Wolfram Research

### Social Activities

The conference social program includes receptions on Monday and Wednesday evenings which are open to all meeting attendees and companions. On Monday, the 10th of June, a no-host cocktail party will be held at the Convention Center at 5:00 pm. Then on Wednesday evening, following the Keynote Address, a no-host cocktail party will be held at approximately 6:30 pm.

### Companions Program

We have organized a program for Companions as follows:

Tuesday	9:30	Welcoming Reception
Tuesday	11:00	Walking Tour of Historic San Jose
Wednesday	1:00	Bus Tour to Mirassou Winery
Thursday		Self-Guided Train Excursion to San Francisco

A nominal charge will be made for the Tours.

#### NASA Tour

On the afternoon of June 10th we have arranged a bus tour to the NASA Ames Laboratory. This tour is free but a small charge will be made for use of the bus. Space is limited so please sign up in advance at the Registration Desk.

#### Satellite Meetings

Please contact the meeting Secretariat, Ms. Martelle Mays, to make arrangements to reserve rooms for satellite meetings. (Call 415-422-1529 or FAX 415-422-0435 or E-mail mmays@llnl.gov) These can be reserved at any time except that we discourage them during plenary sessions.

#### Audio Visual

All session rooms will have an overhead projector, a 35mm slide projector, a VHS VCR, two color monitors, a screen, pointer, and lavalier microphone. The Plenary session will have a video projector instead of the monitors. If you have additional Audio/Visual requirements, please contact Michael Scanlan, Meetings Manager, The American Physical Society, 335 East 45th Street, NY, NY 10017; (212)682-7341. There may be a charge for additional equipment. Some computers may be available on a limited basis. Please notify Michael Scanlan if you require one for your presentation.

### TUTORIAL PROGRAM DETAILS

#### Monday June 10 8:30am

##### **T1:** *Introduction to Mathematica*, Nancy Blachman, Variable Symbols, Inc.

This tutorial offers a general introduction to Mathematica, interactive software that makes it easy to perform mathematical calculations and manipulations, and graph functions and data. Mathematica can work with numbers, polynomials, power series expansions, matrices, and graphics. Tutorial participants will learn how to use Mathematica interactively, manipulate expressions, and plot functions and data. This Tutorial is intended for those with little or no experience with Mathematica.

##### **T2:** *Autotasking: Parallel Processing of Fortran Codes*, Kim Snyder, Cray Research, Inc.

This tutorial will consider the costs and returns of running a Fortran code on a parallel architecture. We will look at how Cray Research, Inc. addresses parallel processing with its Autotasking compiling system. Some of the issues to be discussed are those of costs of programmer's time, cpu time, memory use, real time performance, system throughput and code transportability. Many of the ideas extend beyond the Cray Research "world" to other parallel machines of the MIMD type.

##### **T3:** *Features of Fortran 90*, Dick Hendrickson, Spackman & Hendrickson, Inc.

This tutorial will present a brief overview, from a physicist's point of view, of how Fortran 90 came into being and its current status. It will describe the major new features of the language - array processing, numeric precision, modules, user-defined data types and operations, memory management, and pointers - and discuss how they impact efficiency, portability, and safety.

##### **T4:** *Networking a Physics Department: Why, How, and the Pitfalls*, Richard W. Cline, University of British Columbia

Computer networking has become increasingly important as the power of personal computers has eclipsed that of yesterday's mainframes. Using our experience installing a network at UBC as the starting point for discussion, this tutorial will focus on 1) why a computer network can be an important addition to a physics department, 2) how to design and install a network (including a comprehensive discussion of networking hardware and software options), and 3) the problems that are likely to arise in developing a network. The aim of the tutorial is to give participants sufficient background to allow them to make informed decisions about installing a network in their own physics department.

#### Monday June 10 1:30pm

##### **T5:** *Introduction to Programming in Mathematica*, Nancy Blachman, Variable Symbols, Inc.

This tutorial offers an introduction to programming in Mathematica. It is intended for people who have used Mathematica interactively and who are interested in learning how to write functions, programs, and packages in Mathematica.

**T6:** *Statistical Mechanics of Data Analysis: Simulated Annealing and Maximum A Posteriori Probability Maximization in NP Complete Problems*, James Cole, Naval Research Laboratory

The problem of picking a solution out of a “very large” and “complicated” candidate solution space can be cast as a constrained energy minimization problem and “solved” by “statistical mechanical analogy” using the simulated annealing algorithm. “A priori” information from a “good” model or previous experiments can be incorporated into the analysis via Bayes’ theorem. As an example, we apply the technique to the restoration of a degraded image. Finally, the “philosophical validity” of this statistical mechanical approach will be discussed. If time permits we will look at a simulated annealing calculation of Feynman path integrals and spin glass relaxation decoding.

**T7:** *Introduction to the DADI Method for Solving PDE’s*, Dennis Hewett and Said Doss, Lawrence Livermore National Laboratory

This tutorial presents the Dynamic Alternating Direction Implicit (DADI) method, a generalization of Alternating Direction Implicit (ADI), for solving multi-dimensional vector partial differential equations. Traditionally, ADI methods have had the advantage of being highly vectorizable - parallelizable and of having low memory requirements, while suffering the disadvantage of slow convergence relative to popular methods such as pre-conditioned conjugate gradient (PCG). We emphasize how the DADI method chooses its acceleration parameter in such a way to give convergence rates that are now competitive and exceeding those enjoyed by the PCG methods.

**T8:** *Object Oriented Programming for Physicists*, Paul Kunz, Stanford Linear Accelerator Center

This tutorial will cover the basic concepts of object oriented programming from the perspective of a FORTRAN programmer. Simple examples will given in the Objective-C and C++ Languages

## HIGHLIGHTS OF TECHNICAL PROGRAM

### Keynote Address:

D. Allan Bromley, Assistant to the President for Science and Technology

### Plenary Talks:

*Computational Quantum Field Theory*, C. DeTar

*Predicting the Structure of Solids*, J. D. Joannopoulos

*3-D Numerics and Computational Cosmology*, Richard A. Matzner

*High Performance Computing and the Grand Challenge of Climate Modeling*, Robert M. Chervin

*Visualization as a Tool for Physics Education*, Robert S. Wolff

*Astronomical Computing in the 1990s: The Bahcall Committee Report*, Larry L. Smarr

*Turbulence Modeling: Physics or Curve Fitting?* J. P. Boris

*The Computational Requirements Associated with Building an Optical Digital Computer*, Alan Huang

*DNA and Protein Sequence Analysis by Dynamic Programming*, Michael Waterman

*Acceleration Algorithms*, Robert H. Swendson

### Technical Program Schedule:

#### TUESDAY MORNING

8:30 Welcoming Remarks. Borchers, Anderson, Hamill. Ballroom A-1.

9:00 AA Plenary Session I. DeTar, Joannopoulos. Ballroom A-1.

10:30 Coffee Break. Convention Center Foyer.

11:00 AB Plenary Session II. Matzner, Chervin. Ballroom A-1.

#### TUESDAY AFTERNOON

14:00 BA Acceleration Algorithms. McCormick, Brower. Ballroom A-1.

14:00 BB Experimental Techniques. Dubois, Larson. Ballroom A-3.

14:00 BC Fractals And Growth. Ziff, Everts, Amar. Ballroom A-4.

14:00 BD Computing Environments. Dyer, Cook, Norman. Conference Room B-1.

14:00 BE Monte Carlo Fluids. McDonald, Feiereisen. Conference Room B-4.

14:00 BF Poster Session I. Exhibit Hall 1.

16:00 CA Eigenvalue Solvers. Gruber, Jones. Ballroom A-1.

16:00 CB Neural Networks. Granger, Hammerstrom. Ballroom A-3.

16:00 CC Boundary Conditions. Moretti, Shankar, Grinstein. Ballroom A-4.

16:00 CD Information Retrieval. Gorry, Mihalas, Kahle. Conference Room B-1.

16:00 CE Few Body Problems. Wiringa, Zhang. Conference Room B-4.

#### TUESDAY EVENING

20:00 NERSC Town Meeting, Ballroom A-1

#### WEDNESDAY MORNING

8:30 DA Plenary Session III. Wolff, Smarr. Ballroom A-1

10:00 Coffee Break. 2nd Floor Lobby

10:30 DB Physics Education. Wilson, Fuller, Risley. Ballroom A-3.

10:30 DC Lagrangian Methods. Trease, Anderson. Ballroom A-4.

10:30 DD Quantum Monte Carlo I. Hamann. Conference Room B-1.

10:30 DE New Fast Transform Methods. Greengard, Coifman. Conference Room B-4.

#### WEDNESDAY AFTERNOON

13:30 EA Visualizations in Fluid Dynamics. Kuwahara, Winkler. Ballroom A-4.

13:30 EB Particle Methods I. Eastwood, Sydora. Conference Room B-1.

13:30 EC Quantum Monte Carlo II. Dagotto, Kilcup. Conference Room B-4.

13:30 ED Turbulent Flow Simulations. Moser, Fischer, Marcus. Conference Room C-1.

14:00 FA Poster Session II. Exhibit Hall 1.

15:30 GA Visualization. Kerlick, Laurel. Ballroom A-4.

15:30 GB Particle Methods II. Reinders, Benz. Conference Room B-1.

15:30 GC Spectral Methods. Karniadakis, Streett, Gottlieb. Conference Room B-4.

15:30 GD Symbolic Computing. Christensen, Hobill. Conference Room C-1.

17:15 Keynote Address. D. Allan Bromley. Ballroom A-1.

#### WEDNESDAY EVENING

18:00 Reception. Ballroom A-3.

#### THURSDAY MORNING

8:30 HA Plenary Session IV. Boris, Huang. Ballroom A-1.

10:00 Coffee Break. 2nd Floor Lobby.

10:30 HB Finite Differences and Finite Volume Algorithms. Colella, Hughes. Ballroom A-3.

10:30 HC Cellular Automata. Doolen, Toffoli. Ballroom A-4.

10:30 HD Molecular Dynamics I. Alder, Tsai. Conference Room B-1.

10:30 HE Time Independent Chemical dynamics. Wyatt, Bacic. Conference Room B-4.

#### THURSDAY AFTERNOON

13:30 IA Inverse Problems I. Berryman, Lynch. Ballroom A-3.

13:30 IB Digital Image Processing I. Hunt, Goodman. Ballroom A-4.

13:30 IC Molecular Dynamics II. Grest, Broughton. Conference Room B-1.

13:30 ID Time Dependent Chemical Dynamics. Gray, Kouri. Conference Room B-4

15:30 JA Inverse Problems II. Frazer, Tolstoy. Ballroom A-3.

15:30 JB Digital Image Processing II. Sherman, Chen. Ballroom A-4.

15:30 JC Thermochemical Nonequilibrium Phenomena. Candler, Sharma. Conference Room B-1.

15:30 JD Real Time Computing. Kolbe, Moore. Conference Room B-4.

17:15 Open Business Meeting. Ballroom A-1.

#### FRIDAY MORNING

8:30 KA Plenary Session V. Waterman, Swendson. Ballroom A-1.

10:00 Coffee Break. 2nd Floor Lobby.

10:30 KB Monte Carlo Methods In Statistical Mechanics. Ferrenberg, Landau. Ballroom A-3.

10:30 KC Parallel Computing. Bhanot, Scott. Ballroom A-4.

10:30 KD Chaos. Dickson, Lakhtakia. Conference Room B-1.

10:30 KE Biological Macromolecules. Skolnick, Benham. Conference Room B-4.

Conference Executive Committee:

David Anderson, Co-Chair  
Robert Borchers, Co-Chair  
Edward Greely, Exhibits  
Patrick Hamill, Local Arrangements  
Martelle Mays, Secretariat  
Larry Merrill, Meeting Arrangements  
Michael Scanlan, Meeting Arrangements

Conference Steering Committee:

Berni Alder  
Jay Boris  
Harvey Gould  
Frank Griffin  
Michael Schluter  
Robert Wolff

Program Committee:

Ben Bacon, Co-Chair  
Elaine Oran, Co-Chair  
David Anderson  
Richard Brower  
Harvey Gould  
Kate Kirby  
John Negele  
Claudio Rebbi  
Robert Wolff

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## 14th INTERNATIONAL CONFERENCE ON THE NUMERICAL SIMULATION OF PLASMAS

The 14th International Conference on the Numerical Simulation of Plasmas will be held on September 3-6, 1991 at Loews Annapolis Hotel in historic and picturesque Annapolis, Maryland, a short drive from Washington, DC.

Annapolis is the capital of Maryland, and was first settled in 1649. Situated directly on the Chesapeake Bay, it is the sailing capital of the United States and home of the US Naval Academy. Loews Annapolis Hotel, one block from the Historic District and less than ten minutes by foot from the waterfront, has guaranteed government rates to all conference attendees.

The conference is sponsored by the Topical Group on Computational Physics of the American Physical Society, and is being organized by the Applied Physics Operation of SAIC and the Plasma Physics Division of NRL. The conference program committee consists of A. Adolf (CEA-CELV), M. Ashour-Abdalla (UCLA), J. Denavit (LLNL), R. Faehl (LANL), I. Haber (NRL), W. Herrmannsfeldt (SLAC), J. Johnson (PPPL), A. Mankofsky (SAIC), and D. Seidel (SNL). The local organizers are I. Haber (NRL) and A. Mankofsky (SAIC).

The program committee invites submissions emphasizing methods of computational plasma physics in areas such as

- magnetic fusion
- inertial confinement fusion
- charged particle beams
- pulsed power
- electromagnetics
- plasma processing
- accelerators
- space and astrophysical plasmas
- free electron lasers
- x-ray generation
- solid state plasmas

Topics which have been addressed in previous meetings include particle-in-cell, fluid, hybrid, and Fokker-Planck calculations as applied to linear and nonlinear equilibrium, stability, transport, and dynamics. Methods presented include explicit and implicit finite-difference, finite-volume, and finite-element techniques, adaptive meshing, spectral techniques, and fast PDE solvers. The focus of the conference is on all relevant aspects of numerical methods,

from model and algorithm development and code optimization for modern computer architectures to visualization and interpretation of results. Participation from related disciplines, such as computational fluid dynamics and meteorology, is also welcome.

As presently planned, the meeting will include plenary talks, oral sessions, poster sessions, and possibly a panel discussion. There will be no simultaneous sessions. A cocktail reception will be held on Tuesday evening for arriving participants, and a banquet is planned in the hotel's atrium on Thursday night.

Deadlines (subject to change) are as follows:

call for papers sent	April 1991
4-page abstracts (to appear as proceedings)	July 15 1991
hotel reservations due	July 15 1991
conference program available	August 15 1991
conference convenes	September 3 1991

If you have not already received the preliminary announcement for the conference, please contact the Conference Secretary or one of the organizers (preferably via Fax or electronic mail) to be placed on the mailing list. We look forward to seeing you in Annapolis.

Anita Mahaffey, Conference Secretary  
Science Applications International Corporation  
(703) 821-4387

Conference E-mail:  
SIMCONF%MCL.SAINETCCC.NERSC.GOV  
SIMCONFCCC.NERSC.GOV  
Fax: (703) 821-1134  
Telex: 362026

Co-Chairmen:

Irving Haber, Naval Research Laboratory, (202) 767-3198  
Alan Mankofsky, Science Applications International Corporation, (703) 734-5596

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#### ANNOUNCEMENT OF PRAGUE MEETING

The 4th International Conference on Computational Physics will be held in Prague, Czechoslovakia during September 1992. It is intended that this meeting will be much like the meeting in San Jose in its scope and emphasis and will solicit presentations in the same areas as described above in the Announcement for San Jose.

It is planned to mail an announcement about this Conference to members of the Topical Group later this year. For further information please contact the Conference Chairman:

Dr. Jaroslav Nadrchal  
Institute of Physics  
Czechoslovak Academy of Sciences  
Na Slovance 2  
18040 Praha 8, Czechoslovakia

42 235 5500 Office  
42 231 23184 FAX

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#### IN MEMORY OF SID FERNBACH

Sid Fernbach, founder of The Topical Group on Computational Physics, died of a heart attack February 15th at the age of 73. He was a true pioneer in many aspects of high performance computing. For three decades, as the Director of the Livermore Computer Center, he challenged the computer industry to produce not only faster computers, but also better peripheral equipment, such as printers and storage devices. He initiated networking and time sharing, some 25 years ago. In 1974 he organized the Controlled Thermonuclear Research Computer Center which was renamed the National Magnetic Fusion Energy Computer Center and more recently the National Energy Research Supercomputer Center. This Center became a model on how to run such a Center on a National scale as exemplified by some of the NSF Supercomputing Centers. He was the founding co-editor of the book series *Methods in Computational Physics* and the *Journal of Computational Physics*. He was a father figure to many young computational scientists. He was a member of many professional societies and consultant to many organizations, but

his honors were relatively few for such a doer and shaker. He was a Fellow of The American Physical Society and was given the Ernest O. Lawrence Award in 1976. He could best be characterized as a visionary with both sandal-clad feet firmly on the ground. He took technological risks and became a prophet in his own time. He saw the future and spent a good part of his life making it come true.

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## TRANSITION TO DIVISIONAL STATUS

During the Winter of 1991 we petitioned the APS Council to approve our request to become the Division of Computational Physics. Under the new APS Constitution, now being ratified, the procedure for a Topical Group to become a Division is almost automatic. Whenever such a group reaches 3% of the society membership, the status of that Sub-unit will change to that of a Division.

Our membership total of 1249 members on June 30, 1990 was used to determine our eligibility for Divisional status and this fell one short of the 1250 members required to pass the 3% level. As a result, the Council of the APS will reconsider our request again during the Fall of 1991 when our membership numbers from June 30, 1991 will be used. Since our membership is already in excess of 1350 we are confident of "passing" the test later this year. Thus it is likely that the Topical Group on Computational Physics will become the Division of Computational Physics near the year's end.

The most important difference between Topical Group and Divisional status is that Divisions are represented at the APS Council while Topical Groups are not. In most other respects, Topical Groups and Divisions are treated alike.

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## FELLOWSHIP NOMINATION PROCESS

The Topical Group will soon be forming a Fellowship Committee to review APS members who are nominated for Fellowship Status who list their principal work as Computational Physics. It is important to realize that the Topical Group does not make the nominations, it simply reviews the list of nominee's collected by the APS Headquarters and makes its recommendations to them.

The procedure for nomination is: Obtain a Fellowship form, often printed in the Bulletin of the APS, and submit it together with a detailed resume plus publication list. These are submitted to the APS Headquarters which then initiates the review and selection process. This form may also be obtained from the Fellowship Office, American Physical Society, 335 East 45th Street, New York, NY 10017-3483, 212 682 7341.

Members who are nominated with their Principal Work given as Computational Physics will have their applications forwarded to the Fellowship Committee of the Topical Group on Computational Physics.

The APS limits the number of persons recommended to be one half of one percent of the Topical Group membership. Of these 75% can be Fully Recommended and the remaining 25% Recommended as Alternates. These Recommendations are forwarded to the APS Fellowship Committee. Those who are Fully Recommended by their Sub-units (read Topical Group) are usually Recommended by the APS Fellowship Committee. The APS Council, in turn, considers these recommendations and elects Fellows of the APS from the Recommendations received.

Each year APS sets January 15th as the deadline for collecting nominations. On the nomination form it is necessary to list the Principal Work as Computational Physics. Based on our present membership, the Group on Computational Physics could find approximately 5 to 6 of its members elevated to Fellowship status next year. If you have further questions please call Dave Anderson (415 422 9818) or Elaine Oran (202 767 2960.)

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## MESSAGE FROM CHAIR

The role of Computational Physics in scientific research is becoming more and more prominent. The program of the forthcoming meeting in San Jose illustrates well the very wide breadth of computational applications: there is hardly any branch of physics which does not profit today from the information and insight that computers provide. The rapid progress in the development of hardware and software is astounding. Desktops capable of 100's of Megaflops

and massively parallel supercomputers delivering Teraflop performance are on the horizon. Everything augurs well for the future of our field. There is even a progressively increasing recognition in Washington of its importance for the National Interest and augmented funding support is likely.

I have been involved in our group since its establishment, due largely to the foresight and initiative of Bernie Alder and Sidney Fernbach, and it has been extremely exciting to follow its progress. The meeting we held in Boston two years ago was the first step in the direction of giving ourselves an identity. The participants brought to it a remarkable enthusiasm and it opened the way for the meeting which will be held this Summer. Organized with the valuable collaboration of Computers in Physics, Computing '91 promises to be an extremely interesting and stimulating conference and I can hardly wait to be there. Many persons have volunteered a lot of time to the planning of the meeting and, more generally, to attending at the business of our topical group, and I would like to thank them all for their help and support. Among these let me mention explicitly our Vice-Chair, Elaine Oran, and Ben Bacon, for their role as Co-chairs of the program committee, our Secretary-Treasurer Dave Anderson for his relentless efforts in making sure that everything functions properly and Michael Schluter for his excellent job as Chair of the nominating committee. Many more people, in our executive committee and in the various committees that have been working since last year for the organization of the San Jose meeting, also deserve special acknowledgements and I do not mention all their names only for reasons of space.

But, ultimately, the real success of our group comes from all its members, and I wish to thank all of you for the enthusiasm in Computational Physics that has brought you to join. I encourage your active participation in all the matters of our group, it is the best measure of its success, and I definitely invite all of you to attend the meeting in San Jose this Summer. We are all looking forward to it as a great opportunity to be together, for all the members of our group.

Claudio Rebbi

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#### OTHER NEWS ITEMS

**Your comments and suggestions are solicited.** Please send your ideas regarding the Topical Group to us. Now is a particularly good time to give us feedback about the Group's activities, mission, structure and finances. The changes in the APS governance through its new Constitution and Bylaws are necessitating changes in our Group's Bylaws. When we make these revisions we will also consider other changes. For those interested we will send relevant information.

**Specialty Conferences encouraged.** In the short history of our Group we have held specialty conferences in the areas of Fluid Dynamics and in Plasma Physics. We think that the computational aspects of chemistry, biological physics, condensed matter physics, high energy physics, atomic physics and other fields are sufficiently developed to warrant specialty conferences in these areas. The Executive Committee of the Topical Group will assist members who want to hold such meetings.

**The Value of Computational Physics to Science and Society.** To serve both our members and science, the discipline of Computational Physics, through the Topical Group, deserves organized representation both within the APS and without. To accomplish this we must develop an articulate statement of what computational physics is, what the realistic opportunities are in the near future for Computational Physics to have an impact on science and society, and what we want the society and the funding agencies to do. Development of this statement is of paramount importance. Your suggestions, text, or supporting information are welcome. Please contact Jay Boris (E-mail: BORIS@LCP.NRL.NAVY.MIL).

**Political Education Efforts.** Although the APS and its Sub-units are prohibited from lobbying legislative bodies, there remains a great deal that the Sub-units and members can do to keep lawmakers aware of the issues facing our research community. We can make ourselves available to Members of Congress and other legislative bodies to give advice and to generally educate our Representatives.

We can follow the lead of the Division of Atomic, Molecular, and Optical Physics. They have sponsored receptions in Washington for Members of Congress and for their Divisional members to facilitate interactions between the Physics community and the Congress. They have given their members instructions in how best to approach legislators- the "do's" and "don't's"- and have encouraged individual physicists to communicate their desires to the Congress.

Even with the restriction against lobbying by the APS, there is no restriction on what individual physicists ask

their representatives so long as they do not act in the name of the APS. If you are interested in participating in our political education efforts please contact David Anderson (E-mail: ANDERSON@CCC.NERSC.GOV).

**Suggestions for a Computational Physics Prize Sought.** Several members of the Topical Group on Computational Physics have suggested that some kind of Prize or Award be established to honor physicists who have made outstanding contributions to this field. We solicit suggestions regarding the name of the prize, the benefactors, the criteria for receiving the prize and about the mode of making the award. Generally, the APS requires an endowment fund from which the interest or dividends are used for the prize and associated expenses. Please communicate your ideas to Elaine Oran who will be organizing a committee to study these questions starting this summer.

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## ROSTER OF EXECUTIVE COMMITTEE

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#### **INSTRUCTIONS FOR VOTING**

We have a slate of four nominees for election to fill two upcoming vacancies on our Executive Committee. For each candidate we have biographical information and a candidate's statement included here to help inform you about them. You will find enclosed a ballot sheet and a return envelope for your use. Please vote for one candidate for each vacancy.

We must receive your ballots by May 8th 1991 for them to be counted.

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## CANDIDATES STATEMENTS

Vacancy 1:

**J. Andrew McCammon**  
*M. D. Anderson Professor of Chemistry and  
Chairman of the Chemical Physics Program  
University of Houston*

J. Andrew McCammon received his B.A. in chemistry from Pomona College, and his Ph.D. in chemical physics from Harvard University, where he worked with John Deutch on biological applications of statistical mechanics and hydrodynamics. In 1976-78, he was a research fellow at Harvard, where he developed the computer simulation approach to protein dynamics in collaboration with Martin Karplus. Since joining the faculty at Houston in 1978, Professor McCammon has developed novel theoretical methods for predicting and interpreting molecular recognition, the rates of diffusion-controlled reactions, and other properties of chemical systems. He is the author with Stephen Harvey of the book "Dynamics of Proteins and Nucleic Acids," published in 1987 by Cambridge University Press, and is the author or coauthor of about 200 papers on a variety of subjects in theoretical chemistry and theoretical biochemistry. He has served on advisory boards for the National Academy of Sciences, the National Science Foundation, the National Institutes of Health, and other agencies. He received the first George Herbert Hitchings Award for Innovative Methods in Drug Design from the Burroughs Wellcome Fund in 1987. His other awards include an Alfred P. Sloan Fellowship, a Research Career Development Award from the U.S. National Institutes of Health, and a Camille and Henry Dreyfus Teacher-Scholar Award. He is a Fellow of the American Physical Society.

### *Candidate's Statement*

Professor McCammon's goals in working with the Topical Group include the encouragement of more undergraduates to pursue graduate studies in computational physics, and the encouragement of chemical and biological physicists to become more involved in the activities of the group.

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Vacancy 1:

**Robert Swendsen**  
*Professor of Physics  
Carnegie-Mellon University*

Robert Swendsen received his B.S. from Yale and his Ph.D. in Physics from the University of Pennsylvania. He was in Germany between 1971 and 1976 at the University of Cologne and the Kernforschungsanlage in Jülich. He then worked at Brookhaven National Laboratory until 1979, when he joined the staff of the IBM Zurich Research Laboratory. Since 1984, he has been a Professor of Physics at Carnegie-Mellon University.

He has served on the Peer Review Board for the Pittsburgh and Illinois Supercomputer Centers and the Editorial Board of the International Journal of Modern Physics. He has helped organize conferences on statistical mechanics in Europe, and was on the organizing committee for the 1986 Conference on Magnetism and Magnetic Materials.

His work has included magnetism, crystal growth, critical phenomena, and the structure of biological molecules. He has helped develop Monte Carlo renormalization group, replica Monte Carlo, and cluster simulation methods.

### *Candidate's Statement*

It is well known that the rapid increases in computational power in recent years have expanded the size and scope of problems we are able to deal with. Beyond that, these quantitative improvements have led to qualitative changes in our methods, which have brought even greater progress. These two parallel developments have opened up extraordinary opportunities for fruitful interdisciplinary collaborations. To realize these opportunities, we need to promote interactions between workers in a wide variety of areas. Continuing support of computational physics at conferences and workshops and increasing awareness at funding agencies of the importance of this work will be crucial for future progress.

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Vacancy 2:

**Harvey Gould**  
*Professor of Physics*  
*Clark University*

Harvey Gould was born in Oakland, California in 1938. He received his B.A. in 1960 and Ph.D. in 1965 from the University of California, Berkeley, the latter under the direction of Hugh DeWitt and Kenneth Watson. He held a NRC postdoctoral fellowship in 1966–67 at the National Bureau of Standards in Washington, D.C. In 1967 he was appointed Assistant Professor of Physics at the University of Michigan, Ann Arbor. He joined the Department of Physics at Clark University as an Associate Professor in 1971 and was promoted to Professor of Physics in 1981. He has been Chair of the Department during 1976–78, 1983–85, and 1988–90. He was a Visiting Associate Professor of Physics at Bar-Ilan University in 1974–75. He received a NSF Faculty Development Fellowship and was a Visiting Scholar at the James Franck Institute, University of Chicago and a Visiting Professor at the Université Pierre et Marie Curie during 1978–79. During 1986–87, he was a Visiting Professor of Physics at Boston University where he continues to have an affiliate appointment.

Gould is a member of the Editorial Board of Computers in Physics, the Pi-net advisory committee of the American Institute of Physics, and a member of the National Steering Committee and the Technical Program Committee of Physics Computing '91.

Gould's research emphasis is on computer simulation studies of the dynamics of first-order phase transitions including crystalline nucleation and the dynamics of glasses. He is the co-author with Jan Tobochnik of a textbook on computer simulation and with Tobochnik edits a column on computer simulation for Computers in Physics. He is a member of the Division of Condensed Matter Physics, the Division of Chemical Physics, the Forum on Physics and Society, as well as the Topical Group on Computational Physics of the American Physical Society and a member of the American Association of Physics Teachers.

#### *Candidate's Statement*

The widespread use and availability of computers and computer networks has led to new ways of thinking about physical systems, new international collaborations, stronger links between physicists working in different areas and between workers in related disciplines, and new possibilities for teaching physics. These rapid and important changes give us an impetus to educate and expand our membership. I would work hard to realize the goal of the Topical Group to become a Division of the APS and to involve workers in all areas of physics in both research and teaching.

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Vacancy 2:

**Ralph Roskies**  
*Professor of Physics*  
*University of Pittsburgh*

Ralph Roskies is Professor of Physics at the University of Pittsburgh, specializing in high energy theoretical physics. He is also a founder and Co-Scientific Director of the Pittsburgh Supercomputing Center (PSC). He is the author of over 60 papers in elementary particle physics. His physics research over the last few years has been in lattice gauge calculations. His earlier work in Pittsburgh included a series of papers applying symbolic computation methods to fundamental problems in electrodynamics done in collaboration with Professor Michael Levine. In 1984, Dr. Roskies helped establish and became the first Director of the Certificate Program in Scientific Computing at the University of Pittsburgh. This program was one of the first in the country to integrate advanced computing techniques with applications programming. That same year, together with Dr. Levine and James Kasdorf from Westinghouse, he wrote the proposal to the National Science Foundation for what was eventually to become the PSC. As Scientific Director at the PSC, he continues to oversee operations, to plan its future course, and to concern himself with its scientific impact.

*Candidate's Statement*

The Administration has made the High Performance Computing and Communication Program a national priority. This program has important implications for computational physicists. At the minimum, we must publicize to the community the funding opportunities supported by this program. We must inform the community of promising directions in high performance computing. And we must also continue to articulate ways in which computational physics helps attack some of the technological challenges facing the nation, in such areas as the behavior of materials, fluid dynamics, plasma physics and biophysics. We must continue to promote interactions between computational physicists in different areas who could benefit from a cross fertilization of ideas.

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## BALLOT

The candidates to be elected this year will serve on the Executive Committee of the Topical Group for three years; their terms expire in the Spring of 1994.

**Vacancy 1:** Vote for one candidate.

- J. Andrew McCammon
- Robert Swendson

**Vacancy 2:** Vote for one candidate.

- Harvey Gould
- Ralph Roskies

Please return your ballot in the envelope provided as soon as you can. We must receive your ballot on or before May 8, 1991 for it to be valid.

David V. Anderson

Secretary-Treasurer

APS Topical Group on Computational Physics