## Fall 2004 Highlights

- FlashMob in Philadelphia to solve problem in anthrax research
- *Annual Reports in Computational Chemistry,* Volume One, in press
- Vote in this year's COMP Election; ballots are due October 1st

Division of Computers in Chemistry

# COMP Newsletter

## Statement from the Chair

*Michelle Francl, COMP Chair 2004, reports recent Division initiatives*

It's hard to believe the fall National Meeting is upon us; summer seems to have just started. Thanks to our program chairs COMP has a number of exciting symposia planned for the fall and for future meetings. After many years, Ralph Wheeler has stepped down as COMP's program chair. We appreciate the terrific job Ralph did recruiting symposia organizers, planning the program and organizing everything from the general sessions to poster sessions, and dealing with the inevitable glitches in programs that included hundreds of papers. We are delighted to have Wendy Cornell as the new program chair; after serving the last several years as vice program chair, Wendy is well acquainted with the intricacies of organizing COMP's semi-annual event. If you have an idea for an interesting symposium topic, would like to organize a symposium or are willing to help chair sessions, contact Wendy.

We know many of our members cannot always attend the national meetings and rely on the abstracts to keep abreast of the presentations. Beginning with the Spring 2005 National Meeting, the abstracts will be available at the COMP web site, rather than mailed as hard copy. We hope this will make it easier for members to archive and search the abstracts, as well as reduce the Division's mailing costs.

COMP is pleased to announce the first volume of Annual Reports in Computational Chemistry will be published early in 2005. David Spellmeyer is the editor, and the first volume will cover a wide range of areas in computational chemistry. All members will receive a volume each year as a benefit of membership.

At the National Meeting in Philadelphia, COMP is hosting a unique event: *Chemistry by FlashMob 2004*. The goal is to link together 48 laptops to build an instant supercomputer. A team from the University of San Francisco previously created FlashMob I and linked more than 200 machines to run a benchmark calculation in a single day (http://www.flashmobcomputing.org/). COMP's event, which Semichem, Inc. is supporting, will mark the first time this approach will be used to solve an actual problem. The spores of *Bacillus anthracis* have been used as a biological weapon, and protection against anthrax infection is a national homeland defense priority. The goal of this FlashMob is to compute the structural motion and necessary transitions in the sequestration of calmodulin by the anthrax edema factor using steered molecular dynamics and the NAMD software. Interested in participating? Sign up to have your laptop participate by sending me an e-mail with the subject "FlashMob 2004 Volunteer". We will have available a CD with software to enable you to set up your own system on the fly. Want to see how it all works? The FlashMob will be set in Convention Center 203A from 10am-4pm—drop by at noon Wednesday, August 25th to see how many GFlops we are getting with the simulation!

Finally, COMP is now supporting the CCL (Computational Chemistry List) and will use it as our official "e-mailing list". All our announcements will be clearly labeled as being from the ACS COMP Division, to permit easy filtering. Subscribe at http://www.ccl.net/chemistry/. And be sure to visit the Division's website for the latest COMP news and information:

http://membership.acs.org/C/COMP/

As always, we welcome your ideas and help. Share your thoughts with me (mfrancl@brynamwr.edu), or our incoming chair, Andy Holder (holdera@umkc.edu). Our executive committee meeting in Philadelphia is open to members. We meet on Saturday in Convention Center 103B at 4 pm for those interested in the program and at 5 pm for the executive meeting. If you're interested in working with COMP, we'd be delighted to see you there!

Michelle M. Francl

## Division Election In Progress

*And you thought this year's most important election was the one coming up in November…!*

*The COMP election for 2005 officers is now underway!* We have a number of key candidates who will continue to make the COMP Division even better. The positions to be filled next year are Chair-Elect, Secretary and Councilor.

Alexander Tropsha and Jeff Evanseck are running for Chair-Elect. Alexander is a Professor of Medicinal Chemistry, Director of the Laboratory for Molecular Modeling in the School of Pharmacy, and Associate Director of the Carolina Center for Genome Sciences at the University of North Carolina at Chapel Hill, where he has been on the faculty since 1991. Alexander received a PhD degree in biochemistry and pharmacology from Moscow State University, Moscow, Russia, in 1986. His research interests include computer-aided drug design, chemoinformatics, structural bioinformatics, and molecular simulations of proteins and peptides. He has been associated with the Executive Committee of the COMP Division in various capacities for the past six years, most recently serving as an Alternate Councilor (2001-2003).

Jeff is the Director of the Center for Computational Sciences and Associate Professor of Chemistry and Biochemistry at Duquesne University, since 2000. He completed his Ph.D. work in physical chemistry at UCLA in 1990. During a post-doctoral experience at Harvard University, he focused upon theoretical biophysics. His research program is based on the integration of molecular dynamics simulations, quantum mechanical methodologies, and algorithm development to address problems in organic and biophysical chemistry. Jeff has been a member of the ACS since 1986. He was elected as the ACS Counselor of the South Florida Section (1996-1999), and became the Chair–Elect of the South Florida Section (1997-2000). Most recently, he has served as the COMP Division's Secretary (2001-2004).

Hanneke Jansen and Kerwin Dobbs are running for Secretary. Hanneke is a native of the Netherlands, where she earned her Ph.D. in computational medicinal chemistry from the Department of Pharmacy, University of Groningen in 1995. Hanneke joined Chiron in December of 1997 and is currently working in the computational chemistry group as a senior scientist. Her responsibilities include support of therapeutic projects from HTS through pre-development using computational technologies, with a strong emphasis on structure-based drug design. Hanneke has been a member of the ACS since April 2000, and has served on the executive committee of the Computers in Chemistry division as alternate councilor for the 2002–2004 term.

Kerwin Dobbs received a Ph.D. in 1986 from the University of California-Irvine. After two postdoc positions, one at University of Texas-Austin and the other at the University of Delaware, in 1990 Kerwin joined DuPont in Central Research & Development. In 1997, he received an appointment as Adjunct Professor in Chemistry at the University of Missouri-Kansas City, and earlier this year, he received an appointment as Visiting Research Professor in Chemistry at Drexel University. Kerwin has been using computational quantum chemistry to solve problems in organic, inorganic, and organometallic chemistry. He has been a member of the ACS since 1977.

Christopher Whitehead, Michelle M. Francl, and Carol Parish are running for Councilor. Christopher completed his Ph.D. in organic chemistry in 1999 at Rensselaer Polytechnic Institute. Since then, he has been a valued member of the Computer-Aided Drug Discovery Group of Pfizer Global Research and Development in Ann Arbor. At Pfizer, he supports therapeutic project teams and seeks to develop and apply new computational techniques to drug discovery problems. He has been a member of COMP division for the last five years.

Michelle Francl is currently a professor of chemistry at Bryn Mawr College, where she has been on the faculty since 1986. Her research area is generally that of *ab initio* molecular orbital theory. Current interests include the structures of topologically intriguing molecules, molecular motions in solids and organoaluminum chemistry. Michelle has served as secretary for the COMP division from 1996-1998 and has been a councilor representing COMP since 1999. She is currently serving as Chair in 2004. As a councilor she has worked on the Divisional Activities Committee (DAC), where she is currently the co-chair of the Divisional Status Committee and secretary for the committee.

Carol Parish is an associate professor of chemistry at Hobart & William Smith Colleges in Geneva, New York where she has been on the faculty since 1997. Her research focuses on understanding the dynamical behavior of interesting molecular systems and her undergraduate research group uses quantum mechanics, conformational searching and free energy simulations to answer questions about the structure, energy and dynamics of these systems. Carol has served on the ACS Women Chemists Committee and is a founding member of the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY).

As the COMP Secretary, I believe that we have outstanding candidates that will make significant contributions to the COMP division. Your vote matters – we typically have a 10-15% turn out. *Please vote as soon as you receive the ballot.* You should see the ballots near the end of August. The vote will be due on October 1, 2004.

Jeff Evanseck

### *Opportunity: COMP Division Newsletter Editor*

Interested in getting more involved with the Division? The Executive Committee is looking for a newsletter editor for 2005-2007 to edit and distribute two newsletters each year and serve as a voting member of the Committee. If you'd like to learn more, contact current Editor, Michelle Lamb.

## Announcing: *Annual Reports in Computational Chemistry*

*First Edition to be shipped to Division members in early 2005*

In order to provide significant new value to COMP members, the Executive Committee has made a commitment to develop a printed annual report covering the most important topics in computational chemistry. Under discussion, planning, and development for several years, the *Annual Reports in Computational Chemistry* is nearly a reality. Elsevier has been selected as the publisher based on their expertise and overall low cost. Sections covered in this volume include Quantum Mechanical Methods (Section Editor: T. Daniel Crawford), Molecular Modeling Methods (Carlos Simmerling), QSAR/QSPR (Yvonne Martin), Applications of Computational Methods (Heather Carlson), Chemical Education (Theresa Zielinski), and Emerging Science (Ralph Wheeler).

- An Introduction to the State-of-the-Art in Quantum Chemistry; *Frank Jensen*
- Time-dependent Density Functional Theory in Quantum Chemistry; *Filipp Furche and Kieron Burke*
- Computational Thermochemistry: A Brief Overview of Quantum Mechanical Approaches; *Jan M. L. Martin*
- Bond Breaking in Quantum Chemistry*; C. David Sherrill*
- A Review of the TIP4P, TIP4P-Ew, TIP5P, and TIP5P-E Water Models; *Thomas J. Dick and Jeffry D. Madura*
- Molecular Modeling and Atomistic Simulation of Nucleic Acids; *Thomas E. Cheatham, III*
- Empirical Force Fields for Proteins: Current Status and Future Directions; *Alexander D. MacKerell, Jr.*
- Non-Equilibrium Approaches to Free Energy Calculations; *Adrian E. Roitberg*
- Calculating Binding Free Energy in Protein-Ligand Interactions; *Kaushik Raha and Kenneth M. Merz, Jr.*
- Computational Prediction of ADMET Properties: Recent Developments and Future Challenges; *David E. Clark*
- Filtering in Drug Discovery; *Christopher A. Lipinski*
- Structure-based Lead Optimization; *Diane Joseph-McCarthy*
- Targeting the Kinome with Computational Chemistry; *Michelle L. Lamb*
- Status of Research-Based Experiences for First- and Second-Year Undergraduate Students; *Jeffrey D. Evanseck and Steven M. Firestine*
- Crossing the Line: Stochastic Models in the Chemistry Classroom; *Michelle M. Francl*
- Simulation of Chemical Concepts, Systems and Processes Using Symbolic Computation Engines: From Computer-Assisted Problem-Solving Approach to Advanced Tools for Research; *Jonathan Rittenhouse and Mihai Scarlete*
- The Challenges in Developing Molecular Simulations of Fluid Properties for Industrial Applications; *Raymond D. Mountain and Anne C. Chaka*
- Computationally Assisted Protein Design; *Sheldon Park and Jeffery G. Saven*

Special thanks go the section editors and to the authors for volunteering their time and effort to make this publication a reality.

We are currently looking for future contributors and ideas on topics that might be of interest to the Membership of the Division. Please contact David Spellmeyer (dcspell@pacbell.net) if you would like to contribute or to suggest a topic or an author.

## 228th National ACS Meeting Philadelphia, PA, August 22-26, 2004

COMP—Co-sponsored Symposia and Related Symposia of Interest

**ANYL**: Chemometrics and Data Analysis

**CHED**: State of the Art – Rational Drug Design, Applications to Teaching

**CHED**: Teaching Bioinformatics in the Undergraduate Curriculum

**CHED**: Molecular Modeling on an Undergraduate Budget – A Symposium in Memory of Professor Wayne P. Anderson

**CINF:** Advances in Virtual High-Throughput Screening

**CINF:** Emerging Technologies in Chemical Information

**CINF:** Forging Leadership Pathways for Women in Science

**CINF:** Herman Skolnik Award Symposium

**CINF**: Graduate Education in Chemical Informatics: Needs and Opportunities

**COLL:** Complex Fluids: Multi-Scale Modeling

**ENVR**: Molecular Modeling in Environmental Chemistry

**INOR**: Computational Chemistry

**INOR**: Bioinorganic Modeling

**PHYS:** Advances in Quantum Chemistry – Theory, Algorithms and Applications

**PHYS:** Quantum/Classical Calculations in Chemistry and Biophysics

## Upcoming ACS National Meetings

Current List of Symposia & Organizers

**San Diego, Spring 2005:**

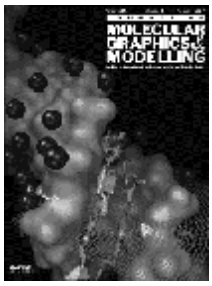
1) ACS Award for Computers in Chemical and Pharmaceutical Research
2) Understanding Protein-Ligand Interactions (C. Reynolds, K. Merz)
3) John Pople Memorial Symposium (B. Schlegel, L. Radom)
4) Safe Exchange of Chemical Information: Can We See the Unlimited Possibilities? (A. Tropsha, T. Oprea)
5) Applications of Information Theory in Chemistry (V. Shanmugasundaram, G. Maggiora)
6) Symposium in Honor of Mike Klein's 65th Birthday (D. Tobias)

## Upcoming National Meetings...

**Washington, Fall 2005:**

1) Emerging Technologies in Computational Chemistry (C. Breneman)
2) Chemistry in the Large – Multiple Processor Computing (T.Windus)
3) Structure-Based Design (S. Rao, A. Nayeem)
4) Translating an Academic Background into an Industrial Career (L. Balbes, A. Tropsha)
5) Computational Chemistry in the Discovery and Development of New Anti-Infective Agents (S. Weston)
6) Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap (S. Mohanty, R. Ross)
7) Knowledge Discovery in Chemical, Biological, and Scientific Literature Databases (A. Tropsha, O. Guner)

## *Journal of Molecular Graphics and Modelling*




*The COMP Division's Journal*

The Journal held an editorial board meeting at the Anaheim National Meeting. We agreed on a number of new initiatives that will be rolled out in the next couple of years. Submissions to *JMGM* remain strong, and we are on a pace this year to almost double the number of papers received last year! I couldn't do it without the help of the referees and editorial board members, the great majority of whom are members of the ACS and COMP. In addition, this spring Elsevier supported the first in a series of COMP symposia. The inaugural event was "Computational Approaches to Problems in Environmental Chemistry", and we are preparing a special *JMGM* issue from that symposium.

Keep the papers coming!

Andy Holder, U.S. Editor, *JMGM*

## Chemical Computing Group Excellence Awardees Announced

CHEMICAL COMPUTING GROUP INC.

*Chemical Computing Group Excellence Awards support travel to Philadelphia meeting*

The ACS Division of Computers in Chemistry and the Chemical Computing Group congratulate the latest recipients of the CCG Excellence Awards for the Fall 2004 National Meeting. Be sure to visit the COMP poster session Tuesday evening to meet the awardees and discuss their research!

Established in 2000, the CCG Excellence Awards are designed to encourage graduate student participation in COMP Division symposia and poster sessions at ACS National Meetings. Awardees are chosen on the basis of the quality and significance of the research to be presented and the strength of the supporting materials.

The following students will receive a one-year software license of CCG's MOE (Molecular Operating Environment) for their academic research groups, in addition to travel funds:

- **Geney, Raphaël**, *State University of New York, Stony Brook*: "Investigations of Salt Bridge Strength in the Generalized Born Water Solvation Model" (COMP 157)
- **Guha, Rajarshi**, *Pennsylvania State University*: "Using Similarity and Classification Methods to Determine Applicability of QSAR Models to Query Set Compounds" (COMP 191)
- **Harriman, David J.**, *University of New Brunswick, Canada*: "'Reverse Docking' as a Computational Tool for the Study of Asymmetric Organocatalysis" (COMP 193)
- **He, Linnan**, *Pennsylvania State University*: "Can a QSAR Model Reliably Predict a Query Compound's Activity" (COMP 76)
- **Hixson, Christopher**, *University of Oklahoma*: "Filling the Gap between Conventional and 'Mean-Field' Molecular Dynamics: Implementing the Exact Approximation" (COMP 152)
- **Mazumder, Devleena**, *University of California, Santa Barbara*: "Computational Study of Hyperthermophilic Indole Glycerol Phosphate Synthase: Structural Alterations at the Active Site with Temperature" (COMP 128)
- **Oloff, Scott**, *University of North Carolina, Chapel Hill*: "COLIBRI: A Novel Method for the Prediction of Complementary Ligands Based on Receptor Information and its Application to Database Screening" (COMP 120)
- **Rajamani, Somianarayanan**, *Rensselaer Polytechnic University*: "Molecular Level Studies of Water-Mediated Interactions Between Ions and their Relevance to Biomolecular Interactions" (COMP 202)
- **Shirts, Michael**, *Stanford University*: "Directly Calculated Ligand Binding Free Energies using Folding@Home" (COMP 208)
- **Zhang, Shuxing (King)**, *University of North Carolina, Chapel Hill*: "ALL-QSAR: A Novel Automated Lazy Learning QSAR Approach and its Application to Experimental Datasets" (COMP 41)

Details regarding the application process for the Spring 2005 meeting in San Diego will be posted on the COMP Division web site. Application materials are due prior to the Division's OASYS abstract deadline, so interested graduate students should plan ahead!

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