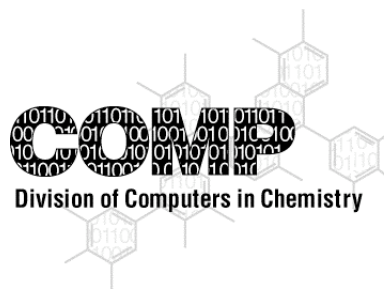


## Spring 2005 Highlights

- All Week in San Diego: John Pople Memorial Symposium and Michael Klein 65<sup>th</sup> Birthday Symposium
- Peter Willett to be Honored Tuesday Afternoon with ACS Award for Computers in Chemical & Pharmaceutical Research
- Division's CCG Excellence Awards will be Presented to 10 Students



# COMP Newsletter

## Statement from the Chair

*Andrew Holder, COMP Chair 2005, reports on the Division status*

It's a good time to be a computational/theoretical chemist! Our unique approaches and methods impact almost every aspect of chemical technology and we are becoming as essential to modern chemical research as the NMR or GC/MS operator. This is immediately obvious in the breadth and scope of technical programming at the two National Meetings. The number and quality of the various types of presentations has steadily increased through the years and is now at a historical high. Thanks to Wendy Cornell, our excellent programming chair, for a job well-done.

It's not just about numbers, though. It's also about vision, innovation and trying new ways of doing old things. The Division sponsored (along with Semichem, Inc.) a "Chemistry by Flashmob" event at the Philadelphia National Meeting that saw more than 20 laptop computers clustered together as a temporary supercomputer. This "flashmob" worked to solve a molecular dynamics problem using the NAMD package that related to *Bacillus anthracis*, a potential biological weapons vector. While we don't think laptop clusters are the wave of the future in computational chemistry, the event was an

excellent proof-of-concept demonstration on how all of those wasted cycles in the ether can be harnessed for something (at least) as useful as the Search for Extra-Terrestrial Intelligence.

With new technology comes changing ways of carrying out our mission. If you are reading this and are a member of COMP, you have probably already received a postcard directing you to the Division's website for two important items: this newsletter and the abstracts for the San Diego National Meeting. In previous years, we have mailed out paper copies of both of these at considerable expense and effort. Given virtually universal access to the internet, we think it's time to invest your money in more services and benefits, as well as make your life more convenient by providing these online. You will get a similar postcard at least twice each year directing you to the website for this and (we hope soon!) for an electronic version of our elections. Enjoy, and let us know how you think such access might be improved.

If you haven't already, you will soon receive by mail your first copy of *Annual Reviews in Computational Chemistry*, a new benefit of COMP membership! I've had a chance to look through the page proofs and I am really impressed with the collection of topics and authors that the editor (David Spellmeyer at IBM) has been

able to assemble. In its first issue, it is a classic reference that will find a home on every one of our shelves. And it's free to you as a member of COMP! Enjoy, and be cooperative with David when he calls asking you to write an article.

Just as a side note, the Division and ACS itself are very concerned with protecting your contact information. Please rest assured that we take every reasonable precaution when we provide our mailing list to outside entities. We regularly turn down requests for access and we *never* sell the list in any form.

As always, please feel free to contact me or the other officers with your suggestions and ideas. The Executive Committee and Programming Committee meetings are open to all members and will be held on Saturday afternoon, March 12. Send me an email or give me a call if you would like to attend.

Andy Holder

## Statement from the Past Chair

*Summary of COMP Division activities in 2004*

It was a pleasure to serve as Chair of the COMP Division last year. Last year COMP continued to work toward this

spring's launch of the Annual Reports in Computational Chemistry. I'd like to thank all of the members of the executive committee over the past 3 years, as well as the section editors, for all the efforts they have put into this project. In particular, ARCC's editor David Spellmeyer deserves a great deal of the credit for not only getting the project underway, but in making sure both the big picture and necessary details are well tended.

COMP's executive committee met in Bryn Mawr this past summer for its annual retreat. We fine-tuned plans for the ARCC, developed new strategies for communicating with our members and hatched plans for a unique event at the Fall 2004 ACS meeting in Philadelphia. In conjunction with the symposiums organized by Wendy Cornell and Vijay Pande on High Performance Computing in Computational Chemistry, COMP, with support from Semichem, built an *ad hoc* supercomputer, used it for a large MD simulation and took it apart – all in a single day!

The continued support of the Chemical Computing Group enabled us to recognize the work of 20 students this year, funding not only travel to the National Meetings, but also celebrating their accomplishments at a dinner. Thanks to Wendy Cornell and her legion of symposium organizers, COMP continues to have a strong presence in the technical program at the National Meetings, hosting the presentation of more than 500 papers last year.

I'd like to express the Division's appreciation to Michelle Lamb, who has done such a terrific job of overseeing the creation of the Division newsletter twice a year. We will miss her work, but are happy to welcome Orlando Acevedo who will be editing the newsletter beginning with this issue.

I'm delighted to turn over the leadership of the Division to Andy Holder, confident in the Division's strength and am looking forward to its continued growth under Andy's care.

Michelle M. Francel

### ACS Award for Computers in Chemical & Pharmaceutical Research

Professor Peter Willett of the University of Sheffield is the winner of the 2005 ACS Award for Computers in Chemical and Pharmaceutical Research for his contributions to the field of Cheminformatics.

Willett received his B.S. degree in chemistry and his M.S. and Ph.D. degrees in information studies from the University of Oxford. He joined Sheffield as a lecturer and has remained there throughout his career, becoming a professor in 1991 and receiving the D.Sc. in 1997. In 2000, Willett established an M.S. program in Cheminformatics at Sheffield, the first of its kind in the world.

Professor Willett has elected to present his address before the COMP Division. The day-long award symposium takes place on Tuesday and features morning presentations from Bill Town, Wendy Warr, John Delaney, and Stephen Pickett. The afternoon session will include Bob Clark, Jason Cole, and Eric Vangrevelinghe, culminating with the award address entitled "Molecular Similarity Approaches for Chemoinformatics." This award is generously sponsored by Accelrys.

### Letter from the Program Chair

#### *Highlights in San Diego and upcoming symposia preview*

The COMP program for the Spring 2005 National Meeting in San Diego features a near record 357 total papers organized into six invited symposia, three contributed symposia, and the poster session. The total number of papers was higher only at the Spring 2003 meeting in New Orleans. Anchoring the program are the John Pople Memorial Symposium, honoring the late Nobel Prize winner, and the Michael Klein 65<sup>th</sup> Birthday Symposium, each of which begins on Sunday morning and runs through Thursday afternoon. Other invited symposia include Understanding Protein-

Ligand Interactions, Applications of Information Theory in Chemistry, and Safe Exchange of Chemical Information.

The high number of submissions for the General Oral contributed symposia is particularly noteworthy and permits the scheduling of three specialized symposia: Drug Discovery (two sessions), Quantum Chemistry (three sessions), and Molecular Mechanics and Simulation (four sessions). At 103, the number of papers is over twice that submitted for any recent National Meeting. We hope to see this trend continue as it allows us to program stronger General Oral sessions. Anyone willing to chair one of these sessions should contact the Program Chair. Computational chemists at all levels of their career are welcome, including graduate students.

The poster session also breaks Division records with 110 submissions. Graduate student recipients of the CCG Excellence Awards, sponsored by Chemical Computing Group, will be recognized in a special ceremony during the poster session. Novartis Institutes for Biomedical Research will provide financial support to fund refreshments at this popular event.

The program for the Fall 2005 National Meeting in Washington, D.C. promises to be quite strong with symposia planned on the following topics:

- Emerging Technologies in Computational Chemistry
- Chemistry in the Large – Multiple Processor Computing
- Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap
- Visualization and Interpretation of Computational Models
- Computational Chemistry in the Discovery and Development of New Anti-Infective Agents
- Structure Based Design
- Translating an Academic Background Into an Industrial Career

The Fall meeting runs from August 28 through September 1 and the deadline for abstract submission is April 25, 2005.

Wendy Cornell

### Chemical Computing Group Excellence Award Recipients Announced



*Ten Students to Receive CCG Excellence Awards Tuesday Evening*

The COMP Division and the Chemical Computing Group are pleased to present CCG Excellence Awards to ten outstanding graduate students recognizing the quality their research as part of the COMP program. Awards subsidize travel expenses to the San Diego meeting and provide a one-year license for the CCG Molecular Operating Environment (MOE) software (<http://www.chemcomp.com/>).

The awardees, in alphabetical order, are:

- Anastassia Alexandrova: "Ab Initio Genetic Algorithm-based Elucidation of Multiply Aromatic Clusters", *Utah State University*
- Biggi Albrecht: "Uncovering Networks within Protein Structure", *Cambridge University*
- Dechuan Zhuang: "Consensus Descriptor Selection under Multiple Objectives using Linear Support Vector Regression", *Rensselaer Polytechnic Institute*
- Hanbin Liu: "On the Convergence of a Hybrid Parallel Tempering Tsallis Statistics Monte Carlo Algorithm", *University of Pittsburgh*
- John Mongan: "Discrete State Constant pH Molecular Dynamics in Generalized Born Implicit Solvent", *University of California, San Diego*
- Matt Sundling: "PEST vs CoMFA: A Comparative Study of two 3D QSAR Technologies", *Rensselaer Polytechnic Institute*
- Melinda Harrison: "A QM/QM' Approach to Modeling the Zn(II)/Cu(I) Core of a Protein", *Duquesne University*
- Scott Yockel: "Structures and Energetics of Small Third-Row Molecules with Correlation-Consistent Basis Sets", *University of North Texas, Denton*
- Xianlong Vincent Wang: "Ab Initio Studies of Methyl and t-Butyl Group Internal Rotation in Aromatic Molecular Crystals", *Bryn Mawr College*
- Zunnan Huang, "Trajectory-randomized Replica Canonical and Microcanonical Ensembles Simulations and Limitations of MD simulations", *University of Oklahoma*

Applications for Awards to attend the meeting in Washington D.C. in August consist of an extended abstract, vitae, personal statement, and a supporting letter from the student's advisor and are **due to Curt Breneman before April 11, 2004**. Please see the COMP website for more details.

### Journal of Molecular Graphics and Modelling

*The COMP Division's Journal*

It has been a good year to be COMP's Editor for the *Journal of Molecular Graphics and Modelling*. JMGM saw more papers submitted and published than at any time in recent years. The *Journal* is healthy and widely cited, as indicated by an impact factor (a measure of how many times papers published in the *Journal* are cited in other publications) for 2003 that puts it in the top **four** Journals in computational chemistry. It has become a publication venue of choice for many of your colleagues. As always, we love to

publish papers from COMP members, and can promise rapid and expert review of your research findings.

We have a number of new initiatives on the way in the near future. These include a better, more streamlined online submission system (that will include electronic refereeing) and a series of seminal review articles in various aspects of our field.

As always, thanks to you and the Editorial Board for your help and support.

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

### *What do chemists need to know about computers and computing?*

The Division of Chemical Education (CHED) and the Division of Computers in Chemistry are organizing an electronic meeting on the topic of what chemists and chemistry students need to know about computers and computing. The meeting, part of the CONFICHEM series that CHED has run since 1993, is planned for fall 2006 or winter 2007. COMP would like to encourage members, particularly those working in industry, to consider contributing a paper and joining the conversation. Look for more details in the Fall 2005 newsletter. For more information about CONFICHEM, see <http://www.ched-ccce.org/confchem/>.

### Supercomputing in a Flash(Mob)

*Volunteers use Laptops as a Supercomputer to Solve Large Problem*

At the Fall National ACS meeting in Philadelphia, COMP joined forces with the organizers of FlashMob I to build an instant supercomputer and use it to do chemistry, live, at the Convention Center. FlashMob computing ([www.flashmobcomputing.org](http://www.flashmobcomputing.org)) was born at the University of San Francisco, the brainchild of computer scientists Patrick Miller, Greg Benson and John Witchel. In April of 2003, they managed to convince the owners of more

than 700 computers to show up at USF's gym in an attempt to build a one-day supercomputer that would rank among the world's 500 fastest ([www.top500.org](http://www.top500.org)). Volunteer's machines were booted off of a special CD that ran LINUX. The originally installed operating system was left untouched. The USF group succeeded in running the LINPACK benchmark, achieving 77 Gflops on 100 processors. While this was only about one third the speed required to break into the ranks of the top 500, it was enough to prove the concept was viable. You don't need a dedicated cluster and all that is required for its maintenance are volunteers – and some software that will help them to talk to each other.

“Chemistry by FlashMob”, COMP's event at the August ACS meeting was the first time the FlashMob software had been used to solve an actual scientific problem. Twenty-eight meeting attendees volunteered their laptops, Bryn Mawr College lent a fast switch and USF sent four dozen cables along with a FlashMob wizard, Dr. Patrick Miller. Semichem produced the software on CD and t-shirts to mark the occasion. Over the course of an hour or so, the volunteers wandered in and were wired into the growing machine.

### **Instant Supercomputing!**

Join COMP in building a wireless supercomputer at the ACS Fall National Meeting. Interested? Send an e-mail to [chemismom@verizon.net](mailto:chemismom@verizon.net) to be added to the mailing list!

By lunchtime, all the machines were cabled into the switch and running. The goal was to compute the structural motion and necessary transitions in the sequestration of calmodulin by edema factor (EF) using steered molecular dynamics for Jeff Evanseck's lab at Duquesne. We succeeded in running 50,000 timesteps of the solvated system with NAMD in about 40 minutes on the ad hoc cluster. In less than an hour, the last of

the laptops had gone back to its mundane solitary existence and the cluster was no more.

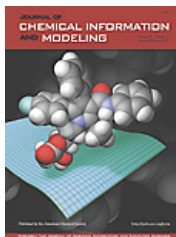
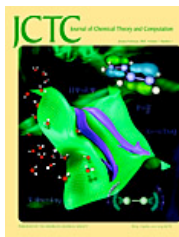
Recently, Grace Chou, a graduate student at MIT, ran a workshop on using FlashMob to build a temporary supercomputer. COMP hopes to encourage and support more of these ventures, doing chemistry for a live audience, both at National and Regional events. If you are interested, contact Michelle at [mfrancel@brynmawr.edu](mailto:mfrancel@brynmawr.edu).

The FlashMob software can be used to run any NAMD problem, so if you have a large system you'd like to run, and no easy access to a cluster to run it on, download the original version of the software at [http://www.cs.usfca.edu/~pjmillier/Chemistry\\_By\\_FlashMob.iso](http://www.cs.usfca.edu/~pjmillier/Chemistry_By_FlashMob.iso), invite your friends over by pizza and ask them to bring their laptops. Or, just steal computer lab cycles at night!

A new and improved version with better scaling, a much faster launch speed, and Macintosh compatibility is available for beta test. Contact the author at [patrick.miller@gmail.com](mailto:patrick.miller@gmail.com) if you would like a copy.

Michelle M. Francel

### **ACS Introduces New Computational Journals**



New in 2005, the ACS introduces the *Journal of Chemical Theory and Computation (JCTC)* to provide a focal point for publications based on new theories, methodology, and/or important applications in quantum chemistry, molecular dynamics, and statistical mechanics. Many in the COMP Division have believed for a long time that these

topics should be represented in a dedicated ACS journal, and now the ACS has responded. Your submissions are invited through the on-line Paragon system.

Starting in 2005 as well, the title of the *Journal of Chemical Information and Computer Science (JCICS)* has been revised to the *Journal of Chemical Information and Modeling (JCIM)*. The name change is intended to better reflect the evolving contents of the Journal, while still emphasizing the Journal's preeminent position in chemical informatics. In particular, papers reporting new methodology and/or important applications in the fields of chemical informatics or molecular modeling are appropriate for submission to JCIM.

For more detailed information on JCTC and JCIM please visit the ACS publications website, <http://pubs.acs.org>.

William L. Jorgensen, Editor

### **228<sup>th</sup> National ACS Meeting San Diego, CA, March 13-17, 2005**

#### **COMP Sponsored List of Symposia...**

- 1) ACS Award for Computers in Chemical and Pharmaceutical Research
- 2) John Pople Memorial Symposium (PHYS)
- 3) Michael Klein 65<sup>th</sup> Birthday Symposium (PHYS)
- 4) Understanding Protein-Ligand Interactions
- 5) Applications of Information Theory in Chemistry (CINF)
- 6) Safe Exchange of Chemical Information: Can We See the Unlimited Possibilities? (CINF)

#### **... and Co-sponsored in Other Divisions**

- 7) ADME/tox Informatics (CINF)
- 8) Safe Exchange of Chemical Information: Can Relevant Chemical Information be Exchanged Without Disclosing Chemical Structures? (CINF)

## **Computer Aided Drug Design**

Gordon Research Conference  
Tilton School, Tilton, NH  
July 31-August 5, 2005

<http://www.grc.org/programs/2005/ca/dd.htm>

Sessions Include: Scoring Docking Poses, Cheminformatics, Energetics of Molecular Recognition, Modeling GPCRS, Protein Modeling, New Technologies, Case Studies

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