Fall 2005 Highlights

- COMP Division is a finalist for a ChemLuminary Award; Ceremony takes place on Tuesday, August 30th
- Vote in this year's COMP Election; ballots are due October 1st
- FAQ for organizing a COMP symposium for an upcoming ACS meeting

COMP Newsletter

Statement from the Chair

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

The Division is healthy and moving forward. That's been the real emphasis of our Executive Committee's work this year: "How can we provide greater benefit to our members?" We have spent a lot of time asking ourselves what we can do for you to make you a more effective and well-informed professional. We have picked up on some ideas from other Divisions, but are always eager to hear your thoughts.

We have taken some real steps forward this year as we continue to offer extended programming and activities. Our Division is recognized by ACS as being one of the most active and innovative in the entire Society! This is clearly evidenced by our nomination for a coveted ChemLuminary award for our instant super-computer "flashmob" in Philadelphia last year (see the article in the Spring 2005 Newsletter for details). Kudos to Michelle Francl (Past Chair) for wrangling this! Even better, we're doing it again, so send an e-mail to FlashMob@brynmar.edu to be added to the mailing list.

We are reaching beyond the borders of the US and supporting the 13th Brazilian Symposium on Theoretical Chemistry (see http://www.sbqt.net/english/ for details). There is a large computational chemistry presence in Brazil and we are pleased to partner with The Division of Physical Chemistry (PHYS) to offer travel support to and from the meeting. A $500 travel stipend is available for a US scientist to make an oral presentation. To apply, send a CV and abstract of your proposed presentation to me (holdera@umkc.edu) by September 15th.

We are also co-sponsoring an electronic meeting with the Division of Chemical Education (CHED) on the topic of what chemists and chemistry students need to know about computers and computing. The meeting, part of the CONFCHEM series, is planned for Fall 2006 or Winter 2007. We'd like to encourage members, particularly those working in industry, to consider contributing a paper and joining the conversation. For more information about CONFCHEM, see http://www.ched-ccce.org/confchem.

As I mentioned last time, we are now using electronic newsletters (you probably already know that!). Hopefully next year we will also use electronic elections, which we expect will make the process easier and increase participation. One of the items on the ballot for THIS year includes changes in our Bylaws to make this possible.

We plan to send out postcards a couple of times per year to remind you to look at our website for updates and to log in for the election. Also, COMP is now a proud sponsor of the Computational Chemistry List (CCL) at http://ccl.net/. Information about upcoming COMP events will be distributed via this list, with "COMP:" in the subject line.

The first edition of *Annual Reviews in Computational Chemistry* was a rousing success. Thanks to David Spellmeyer for serving as editor. This will be an annual benefit of membership and I'm sure David would be happy to hear from you about it.

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, August 27. Send me an email or give me a call if you would like to attend.

It's an exciting time to be a Computational Chemist!

Andy Holder

Reduced Dues!

COMP Division student membership yearly dues have been reduced in half to $7.50!

Newsletter of the COMP division of the ACS
Fall 2005, Washington D.C.

Division Election in Progress

Every vote counts!

COMP members will receive a paper ballot in their mailbox some time in August. This ballot is your opportunity to influence the composition of the COMP Division's Executive Committee, as well as approve some changes to our Bylaws that may make this the last paper ballot in your mailbox.

The positions to be filled this year on the Executive Committee are Chair-Elect and Councilor.

- The Chair-Elect serves one year in 2006, followed by a year as Chair in 2007 and a year as Past Chair in 2008. The Chair directs and leads the general activities of the COMP Division. Candidates for this position are Lisa Balbes and Ralph Wheeler.

- The Councilor serves a three-year term starting in 2006 and represents the Division on the governing body of the ACS. Candidates for this position are Kerwin Dobbs, Jennifer Miller, and Chuck Reynolds.

Biographical sketches of our candidates can be found online at:
http://membership.acs.org/C/COMP/bios.html
We have a wonderful group of individuals who are volunteering their time and talents to promote all aspects of Computers in Chemistry. Please support their commitment to the Division and vote as soon as you receive your ballot!

The proposed changes to our Bylaws can be found online at:
http://membership.acs.org/C/COMP/bylaws_amend.pdf and include amendments that will allow for greater efficiency and cost savings in the areas of balloting and distribution of abstracts for the National Meetings. In both cases, the Division is moving to electronic means of communication. If the amendments are approved, this year's ballot will be the last paper ballot you fill out for the COMP division, so make sure you enjoy the occasion. We count on your support for the proposed changes!

Please note that all ballots must be postmarked no later than **October 1, 2005** in order to be considered valid. If you have any questions, please contact me at Hanneke_Jansen@chiron.com

Hanneke Jansen

ChemLuminary Awards

For the second year in a row, the COMP division is a finalist for a ChemLuminary Award. The ChemLuminary awards recognize outstanding and innovative efforts of local sections and divisions to serve their members and the public. Last year, we were nominated for our awards program, which spans the career paths from graduate students to eminent researchers, and for the work to produce the inaugural edition of the *Annual Reports in Computational Chemistry* (ARCC). This year we have been nominated for both the ARCC project and for the Chemistry by FlashMob event at the 2004 Fall National Meeting in Philadelphia (see http://pubs.acs.org/cen/coverstory/8239/8239computers1.html).

Award winners will be announced Tuesday, August 30 at a ceremony at the upcoming Washington, DC national meeting. Wish us luck!

Michelle M. Francl

Letter from the Program Chair

Highlights in Washington D.C. and upcoming symposia preview

The Fall 2005 meeting in Washington, D.C. has proved to be a popular one with COMP symposium organizers, with a total of eight special topics symposia appearing on the schedule. In addition, we have the usual complement of General Oral symposia for Drug Discovery, Molecular Mechanics and Simulation, and Quantum Chemistry, as well as the recurring Emerging Technologies symposium.

- Advances in Data Mining and Analysis: Computational Perspective (*Alex Tropsha, Osman Guner*)
- Chemistry in the Large: Teraflop Computing and Beyond (*Theresa Windus, Bert de Jong*)
- Computational Chemistry in the Discovery and Development of New Anti-Infective Agents (*Scott Weston*)
- Computers and Computer Algebra Systems in the Chemistry Classroom: A Tribute to Drs. Joseph Noggle and Sidney Young (*Jeffry Madura, Theresa Zielinski*)
- Emerging Technologies in Computational Chemistry (*Curt Breneman*)
- General Oral – Drug Discovery (*Chaya Duraiswami, Lewis Whitehead, Wendy Cornell*)
- General Oral – Molecular Mechanics and Simulation (*Fiona Case, Peter Krouskop, Jeffry Madura*)
- General Oral – Quantum Chemistry (*Thomas Dick, Ian Gould, Jeffry Madura*)
- Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap (*Rick Ross, Sanat Mohanty*)
- Modeling Water in Protein-Ligand Interfaces (*Leslie Kuhn, Michael Feig*)
- Structure Based Design (*Shashidhar Rao, Akbar Nayeem*)
- Translating an Academic Background Into an Industrial Career (*Lisa Balbes, Alex Tropsha*)
- Visualization and Interpretation of Computational Models (*Andrew Smellie, Anton Filikov, Rocio Palma*)

The poster session will take place as usual on Tuesday night and is once again generously sponsored by Novartis Institutes for BioMedical Research. The CCG sponsored Excellence awards will be presented to the students at that time.

A number of symposia are in place for the Spring 2006 meeting in Atlanta, but there is still room for more. Please contact us if you are interested in organizing a symposium. Symposia scheduled for the Spring 2006 meeting in Atlanta include:

- ACS Award for Computers in Chemical and Pharmaceutical Research (*Curt Breneman*)
- Docking (*Lakshmi Narasimhan*)
- Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday (*Weitao Yang, Paul Ayer*)
- General Oral – Drug Discovery (*Wendy Cornell*)
- General Oral – Molecular Mechanics and Simulation (*Jeffry Madura*)
- General Oral – Quantum Chemistry (*Jeffry Madura)*
- GPCRs (*John Woolfrey, Irache Visiers*)
- Kinases (*Chung Wong*)

The strength and quality of our programming derives primarily from the efforts of our symposium organizers. We thank all of the organizers for their excellent efforts! For those of you who may be thinking about organizing a symposium for an upcoming meeting, we provide a FAQ in this issue.

Finally, I'd like to welcome on board the new Assistant Program Chair -- Jeffry Madura of Duquesne University. Feel free to contact either one of us with questions, comments, or suggestions regarding COMP programming.

Wendy Cornell

FAQ for COMP symposium organizers

Q: What is the official process for proposing my symposium?
A: There is no formal application process – potential organizers should simply contact either Wendy Cornell (Program Chair) or Jeffry Madura (Assistant Program Chair). We normally decide within a few days based on such criteria as whether the topic was recently covered and how full the schedule already is for a particular meeting.

Q: How much lead time is required to organize a symposium?
A: OASYS opens for abstract submission about 6 months before each national meeting and the final deadline for authors to submit abstracts is about 4 months before the meeting.

Q: How long can/should my symposium be?
A: Symposia can be as short as half a day or as long as the entire week.

Q: Can my symposium be scheduled early in the week?
A: ACS has Even Programming Rules which require each division to spread their programming evenly across the week. We attempt to accommodate scheduling requests, however we cannot guarantee when a symposium will be scheduled. We are committed to having strong programming throughout the week and our recent Thursday symposia have been well attended.

Q: How do I identify speakers for my symposium?
A: Most symposium organizers start out by inviting a core group of speakers, usually people who are well known in the field. Calls for papers in C&E News and listservers will help to identify additional speakers. Organizers are encouraged to open their symposium to contributed (non-invited) abstract submissions. The organizers can review these abstracts in OASYS, select any of interest to the symposium, and direct the remainder to the appropriate General Oral session.

Q: Is funding available for my symposium?
*A: The COMP division provides funds in the amount of the price of **one registration per half-day session** at the early member rate (currently $295). These funds can be used for speakers, session chairs, or symposium organizers. PRF offers grants to cover partial costs for foreign based speakers up to a maximum of $1200 per speaker and $3600 per symposium. Another good source of funding is industry. Members of the COMP Executive Committee can often help out by providing contact information.*

Chemical Computing Group Excellence Award Recipients Announced

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

Ten Students to Receive CCG Excellence Awards Tuesday Evening

Chemical Computing Group (CCG) and the American Chemical Society's Division of Computers in Chemistry (COMP) are pleased to present ten CCG Excellence Awards to outstanding graduate students, recognizing the quality and relevance of their research. The awards subsidize travel expenses to the Washington D.C. meeting and provide a one-year software license for the CCG Molecular Operating Environment (MOE). (http://www.chemcomp.com/).

The awardees, in alphabetical order, are:

- Manoj V. Athawale: "Osmolyte (TMAO) effects on the strength of hydrophobic interactions: Origin of osmolyte compatibility", *Rensselaer Polytechnic Institute*
- Barun Bhhatarai: "Digging the past for a clue: A novel in-silico approach for new leads on 4-OH-pyran-2-ones HIV protease inhibitors", *Clarkson University*
- Elaine R. Chan: "Multiscale modeling and simulation of polymer-tethered silsesquioxane assemblies", *University of Michigan*
- Jun Cui: "Accurate calculations of interaction energies of H-bonded clusters", *University of Pittsburgh*
- Jason DeChancie: "Origins of the high affinity binding of the biotin-(strept)avidin complex", *University of California, Los Angeles*
- Christopher B. Harrison: "Unraveling the role of (6-4) Photolyase in DNA repair through

homology modeling, consensus docking, and MD simulations", *University of Notre Dame*

- Benjamin Mintz: "Reduction of computational requirements and trends for high accuracy description of molecular properties", *University of North Texas*
- Jeremy M. Moix: "A phenomenological model for surface diffusion: Diffusive dynamics across stochastic potentials", *Georgia Institute of Technology*
- Kun Song: "A simulation study of the binding modes of formamido-pyrimidine bound to DNA containing 8-oxo guanine", *Stony Brook University*
- Nicholas J. Wright: "Forward-backward semiclassical dynamics", *University of Illinois*

Applications for Awards to attend the meeting in Atlanta, GA in March 2006 consist of an extended abstract, CV, personal statement, and a supporting letter from the student's advisor and are **to due to Curt Breneman by November 2, 2005**. Submissions are restricted to North American students. Please see the COMP website for more details.

ACS ProSpectives Conference

ACS ProSpectives
Where chemistry crosses disciplines to advance science

Please join us for the rare opportunity to hear Structural Biologists, Computational Chemists, and Medicinal Chemists discuss how their work is being integrated & successfully applied to drug discovery.

At this conference, leading academic and industrial researchers will describe the latest methods in experimental determination of target structures and modeling the protein-ligand interactions that are responsible for drug binding. Other topics covered include structure-based ADME-Tox and homology modeling.

In addition, a distinguished group of medicinal chemists who have used structure-based design to deliver new drugs to market will discuss its use in driving a medicinal chemistry program.

Advances in Structure-Based Drug Discovery

Oct 16-19 in Philadelphia, PA

Go to http://www.acsprospectives.org to obtain the most complete, up-to-date information available on topics, speakers, schedule and venue. Questions email acsprospectives@acs.org or call 1 (800) 227-5558.

Highlights of the program include:
Keynotes from two pioneers:

- **Irwin "Tack" Kuntz** of UC/San Francisco, who helped create the field of computer-aided drug design with the development of docking methods
- **Sir Tom Blundell** of Cambridge University, one of the foremost leaders in the application of crystallography to structure-based drug design

On Structural Biology:

- **Lance Stewart** of deCODE Genetics will describe advances in the area of membrane bound proteins
- **Chaohong Sun** of Abbott will outline their use of NMR to help discover potent antagonists of anti-apoptotic IAP proteins
- **Prof Robert Kaptein** of Utrecht University will present his recent NMR studies of the Nisin-Lipid II system

On Computational Chemistry:

- **Prof William Jorgensen** of Yale University will give an overview of modeling in structure-based drug discovery
- **Debbie Loughney** of BMS will share practical insights into the use of fragment-based drug design
- **Prof John Moult** of the Center for Advanced Research in Biotechnology will describe recent progress in protein structure prediction

On Medicinal Chemistry:

- **Joe Vacca** of Merck will describe the role of structure in the discovery of potent BACE inhibitors for the treatment of Alzheimer's disease
- **Bruce Maryanoff** of J&J PRD will outline the development of a new class of serine protease inhibitors that emerged from structure-based design
- **Jack Baldwin** of Vitae Pharmaceuticals will share his experience running structure-based medicinal chemistry programs at both big pharma and small biotech companies.

Chemistry by FlashMob 2005

In June, the COMP division and the Philadelphia Local Section, headed by Deborah Cook, received a grant from the Local Section Activities and Divisional Activities committees to run another FlashMob supercomputing event. Our first FlashMob event, held at last year's fall national meeting was a grand success.

A FlashMob is a unique way to assemble a temporary (yes temporary!) supercomputer out of laptops and desktops that you just have "laying around the house." Unlike computer clusters that are permanently assembled and need highly trained staff for their care and feeding, a FlashMob cluster is assembled by simply rebooting a collection of computers with a special CD to run one problem. When the problem is done, you take out the CD and the notebooks and desktops go back to their mundane, day-to-day existence.

"Chemistry by FlashMob 2005" is a hands-on event. Attendees will be creating a supercomputer out of 48 ordinary laptops to run a NAMD molecular dynamics problem. Take the disk home, collect some computers in your laboratory, and build your own supercomputer too!

Dr. Patrick J. Miller from Lawrence Livermore National Labs, one of the developers of the FlashMob, will be talking about how to build and run these ad hoc clusters. We will also be doing live

science, running two NAMD simulations for local researchers.

Instant Supercomputing!

Join COMP in building a wireless supercomputer from laptops laying around the house. The event will take place September 15th in Philadelphia.

Bring your laptop on Thursday, September 15 between 5:30 and 6:30 to be part of the simulation and learn to set up your own ad hoc cluster. You must be willing to leave your laptop and its power adapter in the cluster from the set-up until after dinner. The laptops will be attended throughout the event and we will have security systems in place to assure that you and your laptop will be reunited at the end of the event. Your hard drive is never touched; everything runs from RAM. Laptop volunteers will get a t-shirt and everyone is welcome to take home the CD. We will have a practice corral up for anyone wishing to practice setting up an ad hoc cluster.

The event will be held at Bryn Mawr College's Thomas Great Hall on September 15, 2005 from 5:30 to 9pm. Dinner will be available at a nominal cost. For further information, directions, to volunteer to be a FlashMobster, or to make dinner reservations, contact: FlashMob@brynmawr.edu. Join COMP for this event!

Michelle M. Francl

Journal of Molecular Graphics and Modelling

The COMP Division's Journal

The *Journal of Molecular Graphics and Modelling* (JMGM) has again seen a steady increase in the number of papers submitted and published over previous 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 you and your colleagues. As always, we certainly solicit papers from COMP members, and can promise rapid and expert review of your research findings.

As always, thanks to you and the Editorial Board for your help and support. It's a pleasure to serve as COMP's editor for JMGM.

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

Upcoming ACS Short Courses

Computational Chemistry and Computer-Assisted Drug Design: Practical Approaches. August 26 - 27, 2005 at the Washington DC Convention Center.

Computational Chemistry - Concepts, Methods, and Practical Approaches. Monday - Tuesday, September 26 - 27, 2005, University of North Carolina, Greensboro.

Computer-Assisted Drug Design - Concepts, Methods, and Practical Approaches. Wednesday - Friday, September 28 - 30, 2005, University of North Carolina, Greensboro.

Registration for all courses is available on-line. More information is available via the COMP website at http://membership.acs.org/C/COMP/.

Mailing Address Corrections

Do you have a bad address?

If you are a COMP member and you have not received the Fall COMP postcard or the COMP election ballot by the end of August, your address may be labeled as a "bad address". Please contact Member & Subscriber Services at service@acs.org and provide them with a valid address, including zip code. This will ensure that you will receive any future mailings, in particular your copy of *Annual Reports in Computational Chemistry* (ARCC) Volume 2 which will be sent (upon publication in 2006) to all COMP members who have paid dues for 2005 and for whom we have a valid address.

National Chemistry Week

Fun-Filled Opportunities are Available Celebrating National Chemistry Week: "The Joy of Toys"

All individuals dedicated to enhancing the public's awareness of the contributions of chemistry are invited to support National Chemistry Week (NCW), October 16-22. The 2005 theme is "The Joy of Toys". The annual NCW celebration unites ACS local sections, industries, schools, and individuals in communicating the importance of chemistry to the quality of life.

Volunteers are needed for the following NCW assignments:

1. Event Coordinator
2. Volunteer recruiter
3. Activities coordinator
4. Industrial interaction coordinator
5. Safety officer
6. Refreshments coordinator
7. Financial advisor
8. Publicity coordinator (could be designated Public Relations chair)

If you are interested in volunteering, please visit http://chemistry.org/ncw/.

If you will be attending the 230th ACS National Meeting in Washington, DC, visit the members of the Committee on Community Activities and the Office of Community Activities at booth #1019 at the DC Convention Center, Monday and Tuesday, Aug. 29 and Aug. 30, from 9 a.m.-5 p.m. and Wednesday, Aug. 31, from 9 a.m.-1 p.m. There will be a community outreach workshop on Monday, August 29 from 1 – 3:30 p.m. in the Ashlawn North room of the Wyndham Hotel.

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