COMP Division
Program Meeting and Executive Committee Meeting
Philadelphia
Saturday, August 21, 2004

Location: Convention Center 103B

4 pm Program Meeting Wendy Cornell, program chair

5 pm Executive Committee Meeting Michelle Francl, chair
- Treasurer Report, Curt Breneman
- Secretary Report, Jeff Evanseck
- Programming, Wendy Cornell
    o Abstract/newsletter notification via web/postcards
- Requests for support of local meetings
    o Support for Marc Gordon symposium (Midwest Regional Meeting, to be held October 20-22, 2004, in Manhattan, KS)
    o MARM May 2005
- Web report, Lisa Balbes
- Dues raise?
- Bylaws update to prepare for electronic election
- FlashMob update
- ARCC progress, David Spellmeyer
- Retreat planning for early 2006
- Report from councilors
- JMGM/access via Elsevier
- Nominations for 2006 posts ← Carlos *Adrian Roitberg Simmerling*

7:15 pm Dinner ~~Joseph Poons Asian Fusion~~
Sosanna Fu.

COMP
Division of Computers in Chemistry

American Chemical Society

Division of Computers in Chemistry

38 Carlyle Ave
Troy, NY 12180

ACS COMP Executive Committee
American Chemical Society
Washington, D.C.

Re: Treasurer's Report - Fall 2004

Overview of Income and Expenditures - General Operating Fund

The Computers in Chemistry Division of the American Chemical Society funded many successful symposia, awarded twenty CCG Excellence Awards to support graduate student travel and hosted several social events for COMP members at both ACS National Meetings in 2003. Expenses were somewhat higher than expectations, partially due to additional valuable program planning events. The operating account showed a loss of $6,312, but this is due in part to the timing of deposits relative to expenditures near the end of the year and is nicely offset by the large gain in the ACS Investment pool value from $85,762 to $101,984 (a 19% increase) over the year, but down 2% from the Spring report. The COMP Division operating budget has continued to grow from $104,260 per year to $116,059 (an all-time high) due to a moderate (11%) gain in Donations, Gifts and Program Services.

Grants and Funded Activities

The COMP Division was again able to provide rich programming at the National Meetings, including special symposia receptions and poster sessions. Due to generous donations and successful grant applications, the Division increased its funding of National Meeting programs by 11% compared to last year. Due to previous successes in Executive Committee retreats, a planning session and retreat was held during the summer of 2004 at Bryn Mawr, and it again yielded good ideas and implementation plans. Additional planning evens were held during the New York and Anaheim meetings.

Assets of the Division and Long Range Planning

The Division currently maintains one operating account, two CDs and an Investment Pool account. While interest rates were stable over much of FY2003, the CDs earned only 0.7% interest throughout the year. The Investment Pool market value was up 19% from last year – not unreasonable in light of the performance of many equity funds over the same period. No additional funds were invested in the Pool during FY2003 or Spring 2004. Including an expected payment of $23,000 from CCG (at this meeting) for continued funding of the CCG Excellence Award, the ratio of Total Assets ($191,380 including the pledge) to Annual Operating Budget is now 1.64 – up from 1.59 in the Spring, and up from 1.29 last Fall.

Balances as of 8/18/04 – Total Assets: $168,380

Respectfully Submitted,

Operating Account:	$42,452
American Century CD:	$7,688
M&T CD:	$16,256
ACS Investment Pool:	$101,984

Prof. Curt M. Breneman
RPI Department of Chemistry
Treasurer, ACS Comp Division

AGENDA

ACS Division of Computers in Chemistry

Program Meeting

Wendy Cornell, Program Chair

August 21, 2004

1) **Fall 2004 meeting**

    a) **COMP symposia**

    b) **Other symposia of interest**

2) **Media requests**

    a) **Flash Mob event**

    b) **High performance computing symposium**

    c) **Other?**

3) **Social events**

    a) **Poster session Tuesday 6:00-8:00 p.m.; new sponsor**

    b) **Docking and Scoring symposium reception Monday 5:00-7:00 p.m.**

4) **COMP symposia scheduled for future meetings**

    a) **Spring 2005 (San Diego)**

    b) **Fall 2005 (D.C.)**

5) **Operational requests**

    a) **Need chairs for General Sessions**

        i) **Sun a.m. and p.m., Wed a.m., and Thu a.m.**

    b) **Need someone to oversee program on Thursday**

6) **Symposium on Translating an Academic Background into an Industrial Career**

ACS Division of Computers in Chemistry
Symposium List

	Philadelphia, Fall 2004	Organizers	Days
1	Emerging technologies in computational chemistry	Curt Breneman (RPI)	0.5
2	Docking and Scoring	Georgia McGaughey (Merck) Neysa Nevins and Greg Warren (GSK)	3.0
3	Symposium in honor of Henry F. Schaefer's 60th birthday	Paul von Rague Schleyer (U of GA) Ernest Davidson (U of Washington) Weston T. Borden (U of Washington)	4.0
4	3-D Visualization Technology for Teaching Chemistry	Steve Fleming (BYU) Paul Savage (BYU)	1.0
5	High Performance Computing	Vijay Pande (Stanford) Wendy Cornell (Novartis)	0.5
6	Symbolic Computation	Michael Barnett (Princeton)	1.0

	Sun	Mon	Tue	Wed	Thu
Flash Mob				AM, PM	
Emerging Technologies	PM				
Docking and Scoring	AM, PM	AM, PM	AM, PM		
Schaefer Birthday		AM, PM	AM, PM	AM, PM	AM, PM
3-D Visualization for Teaching Chemistry			AM, PM		
High Performance Computing				AM	
Symbolic Computation					AM, PM
General Sessions	AM, PM			AM	AM

OTHER SYMPOSIA OF INTEREST:

Academic Employment Initiative (see *AEI*, Mon)

Advances in Virtual High-Throughput Screening (see *CINF*, Wed, Thu)

Emerging Technologies in Chemical Information (see *CINF*, Sun)

Forging Leadership Pathways for Women in Science (see *CINF*, Sun)

Graduate Education in Chemical Informatics: Needs and Opportunities (see *CINF*, Mon)

Diversity and Chemogenomics (see *MEDI*, Mon)

Molecular Modeling on an Undergraduate Budget - A Symposium in Memory of Prof. Wayne P. Anderson (see *CHED*, Wed)

State of the Art - Rational Drug Design, Applications to Teaching (see *CHED*, Sun)

Teaching Bioinformatics in the Undergraduate Curriculum (see *CHED*, Sun)

Molecular Modeling in Environmental Chemistry (see *ENVR*, Sun)

Computational Chemistry (see *INOR*, Wed)

Computational Chemistry (see *INOR*, Sun)

NSF Sponsored Center for Workshops in the Chemical Sciences and the Impact of the Workshops on Curriculum Development (see *CHED*, Wed)

Integration of Analytical and Experimental Data into Enterprise-Wide Systems (see *CINF*, Mon)

	San Diego, Spring 2005	Organizers
1	ACS Award for computers in chemical and pharmaceutical research	
2	Understanding Protein-Ligand Interactions	Chuck Reynolds (J&J) Kennie Merz (Penn State Univ)
3	John Pople Memorial Symposium *Co-sponsored by PHYS*	Bernie Schlegel (Wayne State Univ) Leo Radom (University of Sydney)
4	Safe exchange of chemical information: Can we see the unlimited possibilities? *Will also do half day in CINF. Primary sponsor not known at this point.*	Alex Tropsha (Univ of North Carolina) Tudor Oprea (University of New Mexico)
5	Applications of Information Theory in Chemistry *Will also do half day in CINF. Primary sponsor not known at this point.*	Veerabahu Shanmugasundaram (Pfizer) Gerald Maggiora (University of Arizona)
6	Mike Klein 65th Birthday *Co-sponsored by PHYS*	Doug Tobias (UC Irvine)

	Washington D.C., Fall 2005	Organizers
1	Emerging technologies in computational chemistry	Curt Breneman (RPI)
~~2~~	~~Computational Study of Liquids and Liquid Interfaces~~	~~Liem Dang (PNL)~~ ~~Gregory Schenter (PNL)~~ ~~Bruce Garrett (PNL)~~
2	Chemistry in the Large – Multiple Processor Computing	Theresa Windus (PNL)
3	Structure Based Drug Design	Shashi Rao (Schrodinger, Inc) Akbar Nayeem (BMS)
4	Translating An Academic Background into an Industrial Career	Lisa Balbes (Balbes Consulting) Alex Tropsha: Univ of North Carolina
5	Computational Chemistry in the Discovery and Development of New Anti-Infective Agents	Steve Weston (South University)
6	Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap	Dr. Sanat Mohanty (3M) Dr. Rick Ross (3M)
7	Knowledge Discovery in Chemical, Biological, and Scientific Literature Databases *2 sessions in CINF and 2 in COMP*	Alex Tropsha (U of North Carolina) Osman Guner (Accelrys)

"Translating An Academic Background into an Industrial Career"
Organized by Alex Tropsha and Lisa Balbes

Proposed Workshop for Washington DC ACS meeting, August 28 - September 1, 2005
Sponsored by COMP
Co-sponsored by PROF, Department of Career Services, Education, YCC?

This session is aimed at early career computational chemists, who are interested in professional development. Industry speakers will share their opinions as to what skills and knowledge (especially non-technical skills) many new graduates are missing, and how to get them. Academicians who have helped numerous students transition into industry will share the qualities of a successful student. Any computational chemist interested in improving their chances of getting a job and/or advancing at the workplace should attend.

Industry doesn't have time to train people, and universities have been set up to train more university professors. If industry can communicate what they want students to know, perhaps universities can start to include it in the curriculum.

Solicit input from committee members with industry experience regarding key factors to succeeding in an industry career in COMP, and people qualified to speak on them. For example:

1. Knowing how to find a job (recruiters and what they can do for you, CCL, C&E News)
2. Understanding the job you are applying for
    a. List and describe different industry jobs and the available career paths.
    b. How is industry different from academia?
    c. How are pharma and biotech different?
    d. Can you transition from biotech to pharma? From a vendor to pharma or biotech?
3. Having the desired academic training
    a. Are certain areas of comp more sought after? (yes!)
    b. Do you need to do a postdoc?
        (depends on your Ph.D. topic and how competitive the job market is)
    c. Is breadth or depth prefered? (don't sacrifice depth for breadth)

Possible types of speakers
    People from industry who hire lots of modelers - Marti Head or Cathy Pieshoff
    Academics who successfully place students - Peter Jurs, Phil Bowen, Tack Kuntz
    Moved rom another field into COMP in industry - who?

    1. Pharma/biotech hiring manager
    2. Pharma/biotech modeller
    3. Patent analyst or lawyer

4. IBM (Glenn Martyna? He was in academia for 8 years before joining, David Spellmeyer/Bill Swope/Jed Pitera)

5. National Lab (Anne Chakra from NIST? Malin Young or Diana Roe, Sandia National Labs. Admittedly not industry but an alternative to industry and academia)

6. Software vendors

    (e.g. Anthony Nicholls or George Vacek from OpenEye or Ramy Farid from Schrodinger?)

7. Independent contractor or consultant?

8. Recruiters (Merry Ambos/Allen Richon)

9. HR reps

    a. How do they evaluate candidates during an interview?

    b. What training is available?

        (big pharma offers leadership, communication, finance, etc)

10. Academic research advisors

11. Other?

Philadelphia ACS National Meeting
Computers in Chemistry Programming

COMP — Division of Computers in Chemistry

SUNDAY - August 22

MORNING

8:00 AM-12:10 PM
Molecular Modeling in Environmental Chemistry
Cosponsored with Division of Geochemistry
Loews — Commonwealth D

8:20 AM-12:20 PM
Computers in Chemistry General
Section B Pennsylvania Convention Center — 104A&B

9:00 AM-12:20 PM
Docking and Scoring
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 109B

AFTERNOON

1:30 PM-4:35 PM
Emerging Technologies in Computational Chemistry
Section C Pennsylvania Convention Center — 106A&B

1:30 PM-4:45 PM
State of the Art - Rational Drug Design, Applications to Teaching
Cosponsored with Division of Chemical Education
Section B Loews — Congress B

1:30 PM-5:20 PM
Docking and Scoring
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 109B

1:30 PM-5:30 PM
Computers in Chemistry General
Section B Pennsylvania Convention Center — 104A&B

MONDAY - August 23

MORNING

9:00 AM-12:20 PM
Docking and Scoring
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 109A

9:00 AM-12:30 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

AFTERNOON

1:30 PM-4:20 PM
Docking and Scoring
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 109B

1:30 PM-5:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

3:00 PM-4:00 PM
Integration of Analytical and Experimental Data Into Enterprise-Wide Systems
Cosponsored with Division of Chemical Information
Section C Pennsylvania Convention Center — 106A&B

EVENING

8:00 PM-10:00 PM
Sci-Mix
Section A Pennsylvania Convention Center — 202B

TUESDAY - August 24

MORNING

9:00 AM-12:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

9:00 AM-12:20 PM
Docking and Scoring
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 109B

9:00 AM-12:30 PM
3-D Visualization Technology for Teaching Chemistry
Cosponsored with Division of Chemical Education, and Division of Chemical Information
Section C Pennsylvania Convention Center — 106A&B

AFTERNOON

1:30 PM-4:30 PM
3-D Visualization Technology for Teaching Chemistry
Cosponsored with Division of Chemical Education, and Division of Chemical Information
Section C Pennsylvania Convention Center — 106A&B

1:30 PM-4:50 PM
Docking and Scoring
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 109B

1:30 PM-5:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

EVENING

6:00 PM-8:00 PM
General Poster Session
Pennsylvania Convention Center — Hall D

Philadelphia ACS National Meeting
Computers in Chemistry Programming

COMP
Division of Computers in Chemistry

WEDNESDAY - August 25

MORNING

8:20 AM-11:30 AM
Advances in Virtual High-Throughput Screening
Cosponsored with Division of Chemical Information
Pennsylvania Convention Center — 110A&B

8:30 AM-12:10 PM
Computers in Chemistry General
Section B Pennsylvania Convention Center — 109B

9:00 AM-12:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section A Pennsylvania Convention Center — 104A&B

AFTERNOON

1:30 PM-4:45 PM
NSF Sponsored Center for Workshops in the Chemical Sciences and the Impact of the Workshops on Curriculum Development
Cosponsored with Division of Chemical Education
Section B Loews — Congress B

1:30 PM-5:00 PM
Advances in Virtual High-Throughput Screening
Cosponsored with Division of Chemical Information
Pennsylvania Convention Center — 110A&B

1:30 PM-5:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

1:30 PM-5:10 PM
High Performance Computing in Computational Chemistry
Section A Pennsylvania Convention Center — 109B

THURSDAY - August 26

MORNING

8:20 AM-12:00 PM
Computers in Chemistry General
Section C Pennsylvania Convention Center — 103C

8:30 AM-11:30 AM
Advances in Virtual High-Throughput Screening
Cosponsored with Division of Chemical Information
Pennsylvania Convention Center — 110A&B

8:30 AM-11:55 AM
Symbolic Calculation in Chemistry
Section A Pennsylvania Convention Center — 109A

9:00 AM-12:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

AFTERNOON

1:00 PM-2:30 PM
Advances in Virtual High-Throughput Screening
Cosponsored with Division of Chemical Information
Section A Pennsylvania Convention Center — 110A&B

1:15 PM-5:05 PM
Symbolic Calculation in Chemistry
Section A Pennsylvania Convention Center — 109B

1:30 PM-5:00 PM
Symposium in Honor of Henry F. Schaefer's 60th Birthday
Cosponsored with Division of Physical Chemistry
Section B Pennsylvania Convention Center — 104A&B

Preliminary Upcoming COMP
ACS National Meeting Programming

San Diego, CA
March 13-17, 2005

ACS Award for Computers in Chemical and Pharmaceutical Research, *Andy Holder and Wendy Cornell*

Understanding Protein-Ligand Interactions, *Chuck Reynolds and Kennie Merz*

John Pople Memorial Symposium, *Bernie Schlegel and Leo Radom and Co-sponsored by PHYS*

Safe Exchange of Chemical Information: Can we See the Unlimited Possibilities? *Alex Tropsha and Tudor Oprea*

Applications of Information Theory in Chemistry, *Veerabahu Shanmugasundaram and Gerald Maggiora*

Washington, DC
August 28 - September 1, 2005

Emerging Technologies in Computational Chemistry, *Curt Breneman*

Chemistry in the Large – Multiple Processor Computing, *Theresa Windus*

Structure Based Drug Design, *Shashi Rao and Akbar Nayeem*

Translating An Academic Background into an Industrial Career, *Lisa Balbes and Alex Tropsha*

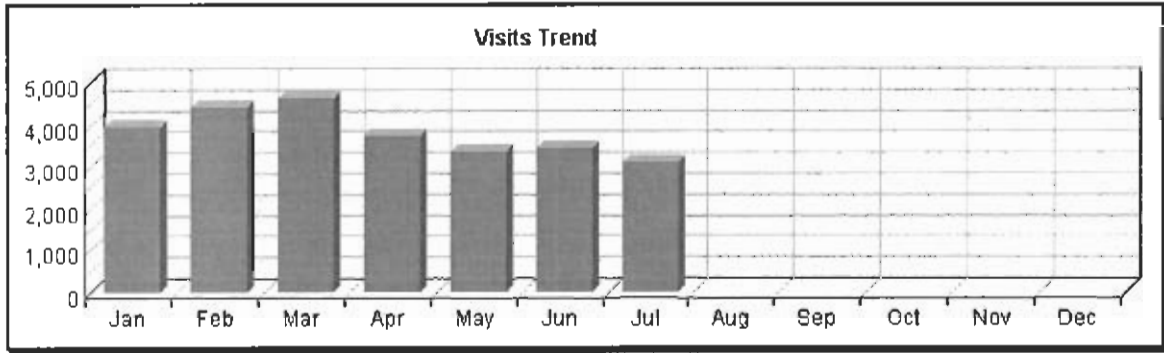Computational Chemistry in the Discovery and Development of New Anti-Infective Agents, *Steve Weston*

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap, *Sanat Mohanty and Rick Ross*

Final Programming and calls for papers are published in C&EN. To participate, contact the organizer and/or submit abstracts through the OASys Online System at http://oasys.acs.org/

Interested in volunteering to organize a symposium or want to see a symposium on a particular topic? Contact *Wendy* Cornell, Program Chair at wdcornell@yahoo.com!

COMP Web Site Report
01 Jan 04 – 31 July 04

Visits Trend

Visit Summary	
Visits	26,529
Average per Day	124
Average Visit Length	00:06:29
Median Visit Length	00:00:50
International Visits	48.59%
Visits of Unknown Origin	0.17%
Visits from Your Country: United States (US)	51.24%

33.75% from Google, 20.72% no referrer, 5.52% google.acs.org

Most frequently downloaded files
 http://membership.acs.org/C/COMP/pastprograms/sp01.pdf - 6194
 http://membership.acs.org/C/COMP/pastprograms/sp02.pdf - 3050
 http://membership.acs.org/C/COMP/pastprograms/fall02.pdf - 1823
 http://membership.acs.org/C/COMP/pastprograms/fall03.pdf - 1640
 http://membership.acs.org/C/COMP/newsletters/fall03.pdf - 434

COMP Workshop

Division of Computers in Chemistry

Wednesday, August 25 at the PA Convention Center, 203A

Workshop: Build your own supercomputer

The FlashMob I (http://www.flashmobcomputing.org/) organizers and the COMP division are teaming up to build an ad-hoc 48-node supercomputer in a day and use it to solve an interesting chemical problem. A FlashMob is a unique way to assemble a temporary (yes temporary!) supercomputer out of laptops, desktops, and the like 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. For "Chemistry by FlashMob 2004," we will be creating a one-day 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!

10 am – noon create a FlashMob cluster
noon – 1:30 pm run NAMD simulation
10 am – 4 pm practice corral open

Bring your laptop at 10 am and be part of the simulation – volunteers get a t-shirt!

Participating laptops must have 2.0 GHz or better P4 or Celeron, 128 M or better RAM. You must be willing to leave your laptop and its power adapter in the cluster from the morning set-up until after lunch. 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.

Questions or want to sign up? Contact Michelle Francl at mfrancl@brynmawr.edu.

COMP thanks Semichem for their support of this workshop.

Bylaw III:

Section 4. Members of this division shall have the privilege of

c) purchasing at reduced rates the **bound** sets of abstracts of papers given at national   meetings of the SOCIETY;

Bylaw IV:

Section 3. The Executive Committee:

   a)   The Executive Committee shall consist of the officers of the Division, the immediate Past Chair, the Editor of the Division newsletter, Councilors, Alternate Councilors, Program Chair, and the Chair of any existing Subdivisions.

Expand?   Assistant Chair — unanimous vote.

Section 4. Elections

(c) The Chair-Elect, Secretary, and Treasurer, shall be elected by a plurality of the ballots cast by members of the Division, as determined by **mail** ballots sent out by the Secretary no later than the June I most closely preceding the commencement of their respective terms of office. To be counted, marked ballots must be received by the Secretary on or before July 15.

(e) In the event of a tie vote for an officer, Councilor or Alternate Councilor, the winner shall be determined by a plurality of the ballots cast by members of the Executive Committee of the Division, as determined by **mail** ballots sent out by the Secretary no later than the August 1 immediately following the tie vote. To be counted, marked ballots must be received by the Secretary on or before September 15. In the event of a tie vote by the Executive Committee of the Division, the Chair of the Division will decide the winner by a coin flip witnessed by the Secretary of the Division or by a person designated by the Secretary of the Division, on or before October 1 following the tie vote by the Executive Committee.

Bylaw XI

Section 1. Amendments to these bylaws may be proposed by the Executive Committee, or by petition of the Division members, provided that 5% of the members sign the petition. The bylaws may be amended at the annual business meeting of the Division by a 2/3 affirmative vote of the members present, provided one month's notice of the proposed amendment with the text thereof has been sent to the members of the Division. Amendment by **mail** ballot is permissible provided that the deadline for receipt of ballots be fixed at not less than one month after the text of the proposed amendment and the ballot have been mailed. A 2/3 affirmative vote of those voting is necessary for amendment by mail ballot.

Computers in Chemistry

COMP
Division of Computers in Chemistry

Chemical Computing Group Excellence Awards
for Graduate Student Travel
2004 Fall National Meeting in Philadelphia

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

Raphaël Geney	SUNY at Stony Brook
Rajarshi Guha	Penn State University
David Joseph Harriman	University of New Brunswick
Linnan He	Penn State University
C. Adam Hixson	University of Oklahoma
Devleena Mazumder	UC Santa Barbara
Scott Oloff	UNC-Chapel Hill
Somianarayanan Rajamani	Rensselaer Polytechnic Institute
Michael Shirts	Stanford University
Shuxing (King) Zhang	UNC-Chapel Hill

Each awardee will receive reimbursement for travel expenses to the ACS Meeting and a license for MOE, the Molecular Operating Environment. Please check the COMP website for information about Future Awards at this URL: http://membership.acs.org/C/COMP/CCG/ccg.html

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We Thank Novartis Pharmaceuticals for Sponsoring the COMP Poster Session Refreshments at the Philadelphia National Meeting

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Preliminary Programming
at Upcoming ACS National Meetings

Final Programming and calls for papers are published in **C&EN** and on the CCL Computational Chemistry e-mail list. To participate, submit abstracts through the **OASys Online System at http://oasys.acs.org/**

Interested in volunteering to organize a symposium or want to see a symposium on a particular topic? Contact Wendy Cornell, Program Chair at wdcornell@yahoo.com!

MJS Dewar Memorial Symposium Series
Sponsored by Semichem

Semichem

Semichem has provided a seed endowment of $25,000 to support a continuing symposium series in computational chemistry to be administered by the Computers in Chemistry Division of the ACS.

Timothy Clark organized the innagural MJS Dewar Memorial Symposium at the 227th ACS Meeting in San Diego. This symposium covered 8 sessions, included over 40 presentations, and was co-sponsored with the Physical Chemistry Division

Other donors are welcome to enhance this seed gift in support of the symposium.

ACS Award for Computers in Chemical and Pharmaceutical Research
sponsored by Accelrys

accelrys

2004	W. Graham Richards
2003	Kendall N. Houk
2002	Irwin D. Kuntz
2001	Martin Karplus
2000	Donald G. Truhlar

Since 1984, The ACS Award for Computers in Chemical and Pharmaceutical Research has annually recognized outstanding individual achievement for the use of computers in education, product development, or research in the chemical and biological sciences.

We thank Accelrys for their continuing sponsorship for this prestigious ACS Award!

2004 Symposium on Emerging Computational Technologies

$1000 prize awarded at the ACS national meeting
Philadelphia, August 2004
Sponsored by:

SCHRÖDINGER

The Computers in Chemistry Division (COMP) of the ACS expects to hold the fourth annual Symposium on Emerging Technologies in Computational Chemistry at the American Chemical Society National Meeting, Philadelphia, USA, August 22-26, 2004. The objective of the symposium is to stimulate, reward, and publicize methodological advances in computational chemistry.

The talks will be evaluated by a Panel of Experts based on the impact the research will have on the future of computational chemistry and allied sciences. The symposium will be ideal for presenting your latest and best research on new techniques and software development.

COMP Sponsors CCL

The American Chemical Society Division of Computers in Chemistry (COMP) is pleased to support the CCL. We will be posting occasional announcements about our activities on this list, hoping to reach our members, as well as other interested colleagues.

All our announcements will be prefaced with "ACS COMP Division:" to facilitate filtering.

CCL.NET
computational chemistry list

Volunteer Opportunities for the COMP Division

The COMP Division is run entirely by volunteers who dedicate their time to providing and building membership value for the >2,600 members of the Division.

Perhaps the most visible volunteers for the Division are the Symposium Organizers, Presiders, and Presenters, both oral and poster. You can volunteer to present your work by submitting an abstract online. You can volunteer to organize a symposium or chair a session by contacting Wendy Cornell, the COMP Program Chair.

The Division Officers run the Division. There are a number of positions, each with distinct functions. Most require a three year commitment and most are positions elected by Division membership. Please contact one of the Division Officers for more information about how the Division functions or if you would like to volunteer to be an Officer.

Low level of commitment:
Chair a Symposium session
contact Symposium Organizer
or Wendy Cornell, Program Chair
Give an Oral or Poster presentation of your work
submit an abstract online to the appropriate symposium

Mid-level of commitment:
Organize a Symposium for a National Meeting
contact Wendy Cornell, Program Chair

Higher level of commitment:
Serve as Divisional Officer
contact Michelle Francl, Division Chair, or another Officer

2004 Divisional Officers
Chair	Michelle Francl
Chair-Elect	Andy Holder
Past-Chair	Peter Grootenhuis
Treasurer	Curt Breneman
Secetary	Jeff Evanseck
Councilors	Michelle Francl, Peter Jurs
	Jennifer Miller, David Spellmeyer
Alternate Councilors	Ralph Wheeler, Peter Gund
	Hanneke Jansen, Jeffry Madura
Program Chair	Wendy Cornell
JMGM Liaison	Andy Holder
Website	Lisa Balbes
Newsetter Editor	Michelle Lamb

Annual Reports in Computational Chemistry

In order to provide significant new and sustained 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 coming close to being a reality.

An Editor and Section Editors have been selected. Manuscripts from numerous authors have been received. Elsevier has agreed to publish the *Annual Reports*. All is in line to ensure that the Innagural Edition will be delivered to members near the beginning of the year. The Editors and the authors all are volunteers. We thank the *Chemical Computing Group* which has agreed to sponsor the series for 3 years to help defray publication and distribution costs.

Topics Covered include:
Advances in Quantum Mechanical Methods
    Section Editor: T. Daniel Crawford
Advances in Molecular Modeling
    Section Editor: Carlos Simmerling
Advances in QSAR/QSPR
    Section Editor: Yvonne Martin
Applications of Computational Methods
    Section Editors: Heather Carlson and Jeffry Madura
Chemical Education
    Section Editor: Theresa Zielinski
Emerging Science
    Section Editor: Ralph Wheeler

Journal of Molecular Graphics and Modelling

In 1998, the Computers in Chemistry Division of the American Chemical Society (COMP) partnered with Elsevier Science and affiliated with the Journal of Molecular Graphics and Modelling (JMGM). Andy Holder serves as the COMP-appointed Editor.

COMP members are encouraged to use JMGM as a forum for their publications. Articles describing research of substantial merit are invited. All articles are subject to standard refereeing in the interest of constructively improving the papers. A special low subscription rate of $65/year is available for COMP members (6 issues).

15% Discount on "Reviews in Computational Chemistry" for COMP division members.

Why Should I Join the COMP Division?

Individuals interested in the use of computers as tools to solve problems in chemistry and related physical and biological sciences are invited to join the COMP Division. Although the primary focus of the Division is theoretical and computational chemistry, the scope of the Division is broad and interdisciplinary.

COMP includes: artificial intelligence, experimental design, and molecular modeling in the fields of agrochemicals, materials science, medicinal and organic chemistry, pharmaceuticals, polymers and theoretical chemistry.

The Division monitors developments in computer hardware, software, and networking and keeps its members informed of new applications in chemistry via symposia and workshops at the National Meetings. The Division promotes undergraduate and graduate student participation and in particular provides travel grants for graduate students to present their work at National Meetings. The COMP division currently has almost 3,000 members.

Benefits of Membership include:
- Copy of *Annual Reports in Computational Chemistry*
- Discount on *Journal of Molecular Graphics and Modelling*
- Discount on *Reviews in Computational Chemistry*
- CCG Graduate Student Travel Awards Competition at each National Meeting
- Emerging Technologies Symposium at each Fall National Meeting
- COMP provides financial support for technical programming
- COMP provides financial support for career development and related programming
- Access to abstracts of papers presented at National Meetings
- Career advancement through professional development and networking opportunities
- Opportunity to present papers at National and Divisional Meetings
- Recognition for your contribution to the advancement of chemistry
- Educational and professional opportunities
- Access to the latest trends in areas of special interest
- Opportunity to participate in technical programming

Become a new COMP Division member or change your membership status by using the on-line form at:
http://membership.acs.org/C/COMP/

Membership dues are:
    ACS Member $15.00
    Student Member $10.00
    Retiree $10.00
    Division Affiliate $17.00
    National Affiliate $17.00
    Outside US , add $3.00 for postage

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❖ To date for 2004, 51 papers have been received in the US editorial office and 17 have been forwarded to Elsevier for publication. This compares to a total of 48 papers in all of 2003.

❖ The US editorial office rejected 11/50 papers in 2002 (22%), 20/48 papers in 2003 (42%) and 15/51 (28% so far) in 2004. Eighteen MSs are in various stages of review.

❖ Elsevier Science and JMGM are sponsored a symposium at the Anaheim meeting providing $3,000 in support. The selected symposium was "Computational Approaches to Problems in Environmental Chemistry", organized by Douglas Tobias.

❖ JMGM's impact factor was 2.93 in 2003, a 25% jump from 2002.

❖ JMGM had an Editorial Board meeting at Anaheim and it as decided to solicit well-known chemists and important papers from the those folks known to the Board. We will offer expedited review and publication by keeping reviews among Board members.