



Executive Committee Meeting Minutes

Division of Computers in Chemistry
New York, New York

Jeff Evanseck

September 6th, 2003

Jacob K. Javits Convention Center, Room 2D10, Convened at 3:00 pm

Present

Peter Grootenhuis (Chair), Michelle Francl (Chair-Elect, Councilor), Bill Jorgensen (Past-Chair), Jeff Evanseck (Secretary), Curt Breneman (Treasurer), Peter Gund (Alternate Councilor), Peter Jurs (Councilor), Michelle Lamb (Newsletter Editor), Ralph Wheeler (Program Chair), Lisa Balbes (Web Master), Wendy Cornell (Assistant Program Chair), Hanneke Jansen (Alternate Councilor), Dominic Ryan (Guest), Andy Holder (Editor, JGM), David Spellmeyer (Editor, Annual Reports), Chris Whitehead (Guest), Alex Tropsha (Alternate Councilor).

The Program Committee was scheduled to meet at 2:00 pm, instead it started at 3:00 pm.

0. Summary of Action Items

- **ACTION ITEM 1:** Wendy needs to identify an assistant program chair.
- **ACTION ITEM 2:** Dave will talk with publishers, ACS, Wiley, Elsevier, etc. concerning ARCC publication.
- **ACTION ITEM 3:** Peter needs to contact Scott Kahn at Acceryls to see if they will continue to sponsor the ACS COMP award.
- **ACTION ITEM 4:** Michelle needs to get the 2004 candidate names to Jeff so that the election may proceed. According to the by-laws, two names for the chair-elect, two names for secretary, three names for councilor and alternate-councilor positions must be submitted to Jeff by April 15th. The ballots are to be mailed out by June 1st and the election deadline in July 15th. The Chair-elect should be from academics this year.

- **ACTION ITEM 5:** It was decided that a “Welcome Letter” to new memberships should be sent. A letter written by Peter and Jeff will be constructed and mailed. This will be done every two months when membership data is received.
- **ACTION ITEM 6:** Construct a post card for election reminder (Jeff). This card is to be sent out two weeks before the election deadline (July 1st).
- **ACTION ITEM 7:** Lisa should check into how the organic division conducts their electronic elections.

1. Chair’s and Past Chair’s Report (Peter Grootenhuis and Bill Jorgensen)

- Peter welcomed everyone, covered the agenda (see attachment 1) for the meeting and had introductions, since Chris Whitehead was attending.
- Bill acknowledged the effort and good work that David Spellmeyer has put in for the Annual Reviews in Computational Chemistry.
- Peter thanked Bill for his contributions over the last three years; this is Bill’s last official executive committee meeting.

2. Secretary’s Report (Jeff Evanseck)

- Jeff handed out the secretary’s report (see attachment 2).
- Jeff presented a comparison of membership statistics since 1994. Note discrepancy from the last report in New Orleans. The 2001 total membership is 2663, not 2863. Consequently, the 2002 membership is up 2% compared to 2001. It is also of interest that our current membership is up 2% compared to the same time in 2002.
- Micelle Francl commented that most divisions were down 5-10%, so the simple fact that we are growing in a positive sign. See attachment 2 for more details.
- Jeff then reported on the elections. There was a total of 355 votes or a 13.3% turn out.

2004 Chair-Elect

Andy Holder, 189, 2004 Chair-Elect

Bill Swope, 166

2004 Councilors

Peter Jurs, 183, 2004 Councilor

David Spellmeyer, 147, 2004 Councilor

Ralph Wheeler, 128, 2004 Alternate Councilor

Jeffry Madura, 96, 2004 Alternate Councilor

Whitehead, 73

Dominic Ryan, 65

- For the 2004 election, we will need candidates for the Chair-Elect, Secretary, Councilor and Alternate Councilor.
- As promised from the San Diego retreat, Jeff made a graphical presentation of the division’s demographics. A comparison between 2001 and 2002 has been made and will be posted on the web by Lisa.

- Different than decided at the retreat, there will be no password to view the demographics.
- Several people questioned if there was a problem in posting the information. After some discussion, it was decided to post the information.
- It was also suggested to designate where the data was taken from. Lisa will post that the data comes from the ACS 2002 annual and bimonthly reports.

3. Treasurer's Report (Curt Breneman)

- Curt handed out the treasurer's report (see attachment 3).
- Curt reported that 2003 has been a good year so far.
- The operating budget has increased from \$82,505 to \$103,276 this year. The increase is due to an increase in donations and associated program services.
- There was a 12% drop in the pool investments, which is not unreasonable in light of the performance of many equity funds over last year. However, the market is back up 8% in the last 8 months. This is good news!
- The total asset to annual operating budget is 1.29:1, which is lower than last year's number of 1.7:1. We will run between 1:2 and 1:3 in the near future. Curt claims not to worry unless the ratio drops below 1.

4. Councilor's Report (Michelle Franci, Peter Jurs and Jennifer Miller)

- Michelle reported that the division allocation passed.
- Michelle went into more detail concerning how allocations to local sections and divisions will be made. Both the divisions and local sections will receive more money next year.
- The new allocation systems, determined by a complex formula, will bring the division financial allocation closer to that provided to the local sections.
- Even though the allocations are more equal, the power of the divisions remains weak compared to the local sections.
- The funding will be made by increasing the national membership fees. The national fees will increase by \$5-\$10. The increase will be phased in over a three-year period.
- COMP will get approximately \$5,000.
- Bill pointed out that we are getting only a fraction of the increased amount that national will receive from the increased membership fees. Roughly, 2,700 COMP members times a \$5 fee increase results in \$13,500, much less than the \$5,000 that the division will get. Should we back this?
- Peter Jurs said that backing the fee increase would be good for the division in the long run.
- Peter reported that JCICS will have an editor change. The change is to support more computational chemistry away from chemical information. Additionally, the current editor is not research active.
- Curt Breneman was suggested as a possible editor.
- JCICS is not in trouble; the journal is doing well.

- The archive of electronic material was discussed. There is on-going debate on how the electronic archives should be made to its membership. It is possible that electronic material may involve a fee only in the first year, and all other material may be free. Several people questioned this proposal.

5. Program Chair's and Vice-Chair's Report (R. Wheeler and W. Cornell)

- Ralph handed out the program chair's report (see attachment 4).
- Chemical Engineering and News chose to feature two COMP symposia in 2003: "Computational Nanotechnology" (Mario Blanco) and "Teaching Medicinal Chemistry for Undergraduate Majors" (Phil Bowen)
- The number of symposia and presentations significantly increased from 2000 to 2003. The programming continues to grow.
- There are now four regularly scheduled symposia. The ACS COMP Award (Accelrys), Emerging Technologies (Schrodinger), Michael J. S. Dewar Symposia (SemiChem), and Elsevier Symposium (Elsevier).
- Semichem will fund the M. J. S. Dewar Symposium entirely by the end of 2004.
- The New York meeting will be of a typical size. A few reasons involve the cost of staying in NY (cheapest rates will start at \$200/night), the inconvenience of traveling, and the fact that September 11 is the last day of the conference.
- Ralph stated that we need to increase the diversity of topics.
- Ralph said that he has heard complaints that we overlap with other divisions. However, he made it clear that overlap is hard to avoid and that we are serving the COMP members well. Thus, we should not worry. We have a good relationship with PHYS, CNIF is a little bit more difficult. The PHYS theory subdivision claims that COMP is serving their members.
- Ralph encouraged Wendy to coordinate with other divisions.
- **ACTION ITEM 1:** Need to identify an assistant program chair.

6. JMGM Report and Related Issues (Andy Holder)

- 34 papers have been received by the US Editor's office, 7 have been forwarded to Elsevier for publication.
- 22% rejection rate in 2002, and 29% rejection rate in 2003.
- 28% papers were submitted on-line in 2002, while 74% were submitted on-line in 2003.
- The impact rose from 1.21 in 2002 to 2.29 in 2003.
- ACS-CAS, ACS publications and Elsevier have agreed to link their services for scientists. The database connection will be made by the end of 2004.

7. Annual Reports in Computational Chemistry (David Spellmeyer)

- Eight sections in ARCC.
- The Application Section has two editors.
- David has all but one section editor.
- On track for publication next year (2004).

- **ACTION ITEM 2:** Dave will talk with publishers, ACS, Wiley, Elsevier, etc. concerning ARCC publication.

8. Review of COMP Division Annual Report

- Peter stated that each category is graded by “+”, “0” and “-“. Overall the COMP division is strong. Should not try to satisfy categories unless it is in the best interest of the membership. COMP should stay on track.
- Leadership 4(+)
- Planning 4(+)
- Outreach 2(+); 1(0); 1(-)
- Programming 3(+); 1(0)
- Communications 4(+)
- Councilors 4(+)
- By-law violation: election late.
- Treasurer 4(+)
- Membership 3(+); 1(0)
- Web site 4(+)

9. Awards

- Graham Richards is the 2004 ACS COMP award winner.
- The Acceryls contract will expire next year. If they decide to drop it, will IBM be willing to sponsor the award?
- **ACTION ITEM 3:** Peter needs to contact Scott Kahn at Acceryls to see if they will continue to sponsor the ACS COMP award.
- CCG Excellence Awards will be presented at Tuesday dinner. 10 awards and t-shirts will be presented at dinner.

10. Awards

(a) Elections (Jeff Evanseck)

- **ACTION ITEM 4:** Michelle needs to get the candidates to Jeff so that the election may proceed. According to the by-laws, two names for the chair-elect, two names for secretary, three names for councilor and alternate-councilor positions must be submitted to Jeff by April 15th. The ballots are to be mailed out by June 1st and the election deadline in July 15th. The Chair-elect should be from academics this year.
- **ACTION ITEM 5:** It was decided that a “Welcome Letter” to new memberships should be sent. A letter written by Peter and Jeff will be constructed and mailed. This will be done every two months when membership data is received.
- It was brought up that the division can save nearly \$3,000 by switching to electronic elections. Two ideas were discussed and formed into action items.
- **ACTION ITEM 6:** Construct a post card for election reminder (Jeff). This card is to be sent out one month before the election deadline.

- **ACTION ITEM 7:** Lisa should check into how the organic division conducts their electronic elections.

(b) Web Site (Lisa Balbes)

- The COMP home page is visited 300 times per month on the home page.
- Lisa continues to update and manage the page, as executive committee members provide her with information.
- Change by-laws from “chairman” to “chair”

(c) Newsletter Editor (Michelle Lamb)

- Michelle needs information for the next newsletter.