



Executive Committee Meeting Minutes

Division of Computers in Chemistry
New Orleans, Louisiana

March 22nd, 2003
Convention Center, Room 387, Convened at 4:00 pm

Present

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

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.

2. Secretary's Report (Jeff Evanseck)

- Jeff handed out the secretary's report (see attachment 2).
- ACTION ITEM: The 2002 Annual Secretary report was submitted on time, send an electronic copy to Executive Committee.
- Membership for 2002 is down by 5%, or 156 members.
- Total 2002 membership is 2707.
- Michelle stated that the membership across the national ACS is down by ~6%, and that compared to other divisions our decrease is not too bad.
- The data from the D510 disks do not explain reasons for the drop in membership.
- Michelle stated that the D510 membership disks are created from different sources at different times, thus the numbers will not add up.

- ACTION ITEM: 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: Membership demographics were discussed. The data was viewed as important and will be deposited for future use. Jeff will send Lisa the new 2003 graphical data.
- ACTION ITEM: To expand the demographic data beyond 2001, David suggested that Wendy Torosian or Judith Jankowski be contacted.
- ACTION ITEM: Lisa will keep all demographic information on the COMP website, but will create a non-advertised location so that the information is not lost.
- A Stop-Gap gap funding request was made and funded at a reduced rate for 2002. The total amount received was \$1,500. The money was spent to cover expenses from the 2002 Yale Retreat.
- Michelle reported that the Innovative Project Fund for Divisional Enhancement submitted in 2002 was not funded.
- An absence of outreach programs was noted, but it was made clear that the division does not have the resources to engage at local or regional levels.

3. Treasurer’s Report (Curt Breneman)

- Curt handed out the treasurer’s report (see attachment 3).
- From the final 2002 report submitted to the ACS, Curt reported that the COMP division is in good financial shape.
- The status of corporate sponsors was discussed. The divisions of Platinum, Gold, Silver and Bronze have been posted on the web.
- The operational account gained \$5,187 in 2002, primarily due to the new CCG graduate student awards to be given out at the New Orleans meeting.
- 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.
- A new algorithm will determine ACS allocation of funds to divisions. As with the previous method, two main components include the number of presentations and the attendance of the symposia.
- 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.
- The total asset to annual operating budget is 1.29:1, which is lower than last year’s number of 1.7:1. Curt said that this could be a possible “red flag,” where a 2:1 ratio is targeted typically. Michelle said that the ACS would not be concerned unless the ratio dropped below 1.
- Curt believes that the division is virtually clear of previous problems with filing Division’s taxes.

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

- 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 member of the JCICS editor search committee.
- 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.
- Jennifer will get her councilor duties tomorrow.

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).
- C&E News featured COMP symposia, with cover stories, twice in 2002.
- The number of symposia and presentations increased in 2002. The programming continues to grow.
- COMP has four regularly funded symposia. The COMP Awards (Acerlys), Emerging Technologies (Schrodinger), Michael Dewar Symposia (SemiChem), and Elsevier Symposium (Elsevier).
- The New Orleans meeting should set a new record in number of total ACS presentations, along with a record of total COMP presentations.
- The New York meeting will be of a typical or smaller 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 continued fund raising for endowed symposia.
- Ralph said that other divisions need to be reached. In this way broader topics could be established that result in symposia with larger attractions.
- Ralph suggested that we implement unofficial but regular symposia covering certain topics that are of interest to the membership.

- Ralph stated that Anaheim will be his last meeting as Program Chair. He strongly advocated that Wendy take over.
- Wendy Cornell accepted the position starting immediately after the Anaheim meeting.
- ACTION ITEM: Need to identify an assistant program chair.

6. JMGM Report and Related Issues (Andy Holder)

- Andy handed out the JMGM Editor's report (see attachment 5).
- John Essex is the JMGM European Editor.
- Special issues are now less frequent, and regular manuscript publication dominates. The plan is to have one special issue per year, but there is pressure to have more.
- It is likely that the page budget will increase this year.
- MGMS has the Elsevier Symposium in Australia this year; COMP will have it next year.

7. Electronic Journal Access for Members (Peter Grootenhuis)

- Peter stated that he does not see a strong consensus among the executive committee members concerning the issue of electronic journal access.
- He has approached several companies, and is not finding the necessary support for the reoccurring costs for electronic journal access.
- If we decide to proceed, then the money will have to come from an increase in division fees.
- The current economic environment makes the electronic journal access project impossible. If we increased the divisional fees by the required amount, then we would lose too many members.
- Personally, Peter believes that the executive committee should concentrate its efforts on the Annual Reports and remove the electronic journal access from consideration.
- Peter suggested, seconded by Michelle, that the electronic access for COMP membership be removed for future consideration. The vote was unanimous in favor of removing electronic access from consideration.

8. Annual Reports in Computational Chemistry (David Spellmeyer)

- David handed out a description of the annual reports in computational chemistry (see attachment 6). The idea is to prepare the executive committee for discussion during the annual retreat in San Diego.
- The goal is to provide significantly new and sustained value to the COMP membership.
- David is looking for volunteers as section editors.
- The annual reports in medicinal chemistry (ARMC) published by MEDI continues to serve as a model for COMP's efforts.
- The initial thought is to use a similar basic editorial structure as ARMC.

- Each review will be approximately 12 pages, whereas each annual report will be approximately 350 pages.
- David gave the executive committee a homework assignment (see attachment #5)
- The timeline for publication involves papers due by April 1 with publication by October. The expected first issue is 2004, maybe,...

9. Other Business

(a) Elections (Peter Grootenhuis)

- Potential candidates for 2003 COMP elections were discussed. The positions to be filled are Chair-Elect, Councilor and Alternate-Councilor. A few names were mentioned for the positions.
- ACTION ITEM: Peter needs to get the candidates to Jeff so that the election may proceed. According to the by-laws, two names for the chair-elect, 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.
- ACTION ITEM: Does the executive committee want to delay the election again, or stick with the stated schedule above?

(b) Web Site (Lisa Balbes)

- The COMP home page was visited over 6,000 times, since its creation.
- Lisa continues to update and manage the page, as executive committee members provide her with information.

(c) Newsletter Editor (Michelle Lamb)

- Michelle stated that the next newsletter is slated with a June 3rd, 2003 deadline.

(d) 2004 Dues (Curt Breneman)

- Division members dues are currently \$10, students \$5, foreign \$12, and nonmembers \$15.
- Curt suggested that to compensate for the 20% increase in programming that an increase to \$12 and \$14 for full and foreign members, respectively.
- After discussion, the executive committee voted unanimously to accept the fee increase to compensate for the costs incurred by the increase in programming.
- ACTION ITEM: What about the \$5 fee for students and the charge of \$15 for nonmembers? Any increase?

(e) Summer Retreat (Peter Grootenhuis)

- The 2003 annual strategic meeting (June 27-29) in San Diego was briefly described. A number of activities are planned. Peter asked for any ideas to be forwarded to him.

(f) Committee on Science (Peter Gund)

- The COMP sponsored (co-sponsored by COMSCI) program on “Challenges for the Chemical Sciences in the 21st Century will be held in New York City, Fall 2003.
- Nanotechnology will be the theme for the 2004 Anaheim meeting.