Executive Committee Meeting Minutes

Division of Computers in Chemistry
Philadelphia, Pennsylvania
Jeff Evanseck
August 21th, 2004
Convention Center, Room 103B, Convened at 3:00 pm

Present

Michelle Francl (Chair, Councilor), Andy Holder (Chair-Elect, Editor, JGM), Peter Grootenhuis (Past-Chair), Jeff Evanseck (Secretary), Curt Breneman (Treasurer), Peter Gund (Councilor), Peter Jurs (Councilor), Michelle Lamb (Newsletter Editor), Lisa Balbes (Web Master), Wendy Cornell (Program Chair), George Famanii (Guest), Hanneke Jansen (Alternate Councilor), David Spellmeyer (Editor, Annual Reports), Jennifer Miller (Councilor), Jeffry Madura (Alternate Councilor), Kerwin Dobbs (Guest), Alex Tropsha (Alternate Councilor).

1. Chair's and Past Chair's Report (Michelle Francl and Peter Grootenhuis)

- Michelle handed out the agenda (see Attachment 1)

2. Treasurer's Report (Curt Breneman)

- Curt handed out the treasurer's report (see Attachment 2).
- Curt updated the Division's financial status since the Retreat. The report is not much different than previously given.
- The investment pool is down a few percent. However, it is still a 19% increase over the year.
- The assets to expenditure ratio is getting better, but not really a problem.
- Good score on the annual report.
- Speaker reimbursement seems to be a small problem. COMP's policy is that we pay for early registration. Send information to Curt with clear information on reimbursement.

- Councilor's need to send receipts right away. Timing is important, where the ACS will reimburse within a short window of time.

3. Secretary's Report (Jeff Evanseck)

- Jeff gave the Secretary's report.
- The total membership for 2004 is down 131 members as compared to this time in 2003. The total membership was 2663, 2707, and 2620 for 2001, 2002, and 2003, respectively.
- Jeff then presented the election information passed to him by Andy Holder. Due to apparent conflict of interest, Andy will run the election, count all ballots, and report the information back to national ACS. The candidates for Chair-Elect 2005 are Alex Trospha and Jeff Evanseck, for Secretary Hanneke Jansen and Kerwin Dobbs, and for Councilor Christopher Whitehead, Michelle Francl and Carol Parish.
- The election due date is October 1, 2004.

4. Program Chair's and Vice-Chair's Report (Wendy Cornell)

- Wendy handed out the program chair's report and a one page (front and back) description of the Philadelphia programming (see Attachment 3).
- Wendy described the Philadelphia meeting. It has six symposia, two of which are large (Schafer's Birthday and Docking and Scoring).
- The Dock and Scoring Symposium is co-sponsored with CNIF.
- The Emerging Technologies symposium is in conflict with CNIF's Emerging Technologies symposium.
- Curt B. needs one more judge for the Emerging Technology Symposium. He currently has five judges.
- Wendy needs chairs for the general sessions, David S. volunteered.
- She reported that COMP is in good shape for San Diego, and described it as given below.
- The John Pople symposium will be big and well attended. Schlegel and Radom are co-organizing.
- Gaussian and others may fund ~$20K
- The Michael Klein Symposium will possibly be big.
- There will be 4-5 co-sponsored symposia with CNIF.
- There is still room in the schedule for a half day symposium in San Diego.
- The Washington DC is also shaping up well.
- For the Flashmob event, a reporter will be on site for an ACS press release.
- This is a nice tie in with the High Performance Computing Symposium.
- Novartis is a new sponsor, which will be recognized at the Poster Session
- IBM, Schrodinger and Merck contributed to the Docking and Scoring Symposium.
- Alex T. described a proposed Knowledge Discovery/Data mining symposium. It will be co-sponsored with CNIF; two sessions in COMP and two sessions in CNIF. The hidden agenda is QSAR.

5. Local/Regional Meetings Report (Michelle Francl)

- Michelle asked for opinions on supporting for Midwest Award Symposium at the Midwest Regional Meeting to be held October 20-22, 2004 in Manhattan, KS.
- In addition, The Mid Atlantic Region (MARM) has made a request for support of their regional meeting as well.
- Michelle commented that Divisional allocations may be tied to its support of regional meetings.
- If COMP is to make more regional connections, then we need a single person for coordination. The question is if this should be separate or tie to the Chair position. Past Chair of Chair? Should a new person be assigned this responsibility? It could be a three year position, which is appointed and not elected.
- Andy is surprised about the Midwest Region request. He has not heard of this symposium yet.
- After more discussion, the Executive Committee agreed to support the MARM and Mark Gordon conferences for $500 a piece.
- Curt reported that we have supported regional meetings five times since 1996. The Midwest Regional meeting in 1996, the Central Regional Meeting in 1997, and MARM (could not remember date).

6. Workshop Request (Alex Tropsha and Lisa Balbes)

- Alex and Lisa handed out a description of the proposed workshop (see Attachment 4).
- The workshop is “Translating an Academic Background into an Industrial Career”
- It is proposed for the Washington DC national meeting
- It will be co-sponsored by PROF, Department of Career Services, Education.
- It is aimed at early career computational chemists – graduate students and post docs. It will cover from how to find a job, understanding the job you are applying for, and getting the right academic training. Academics who have placed students in industry will speak.
- One of half-day symposium.
- There was discussion if it should be a workshop or symposium.
- Jeff M. said it should be a full day focusing upon careers and critical skills.
- Awareness is the key. You have to manage your own career.
- This would be a good idea for COMP young members.
- The Executive Committee thought it was an excellent idea.
- Peter G. stated that there are not a lot of positions outside of Pharma and Ag.
- Peter G. suggested that this should be co-sponsored with MEDCHEM.
- Maybe this should be posted on the website. Not many graduate students go to the national meetings.
- Michelle F. said we should start simple, and then if successful, we can expand to regional meetings to connect with the younger members.
- Since the FlashMob event is listed as a workshop, this could be scheduled in the same fashion at the national meeting.

- Andy H. said this would be a good way to connect with the local sections.

7. Website (Lisa Balbes)

- Lisa handed out the COMP website report (see Attachment 5)
- The report covered from Jan 1 – July 31, 2004.
- There have been 26,529 visits during this time.
- Average per day visits was 124.
- Again as with the last report, 51% of the visits are from the US.

8. FlashMob Update (Michelle Francl)

- Michelle F. Handed out the flyers for the FlashMob workshop (see Attachment 6).
- The event is getting good press.
- The ACS is providing a room for the workshop.
- We are lacking computers. Michelle has only 8 so far. We will need 48 in total.
- Need non-Mac computers on Wednesday.
- Free tee-shirts to anyone providing a computer.
- Michelle is asking the organizers of symposia to advertise the event.
- Stress the free tee-shirt.
- Also, the speed of computer can be 2 GHz or great, which is slower than originally advertised.

9. By-Laws Update (Michelle Francl)

- Michelle F. Handed out specific changes to the By-Laws (see Attachment 7).
- The By-Laws for electronic elections need to be changed.
- It is better to do it sooner than later. The change will eventually need to be carried out.
- It will need to be in accordance with the national ACS.
- Other changes may be needed.
- David S. stated that the voting membership (Executive Committee) should be confined to the elected officials.
- The Executive Committee voted upon striking the Editor of the Division Newsletter from Bylaw IV, section 3.

10. Annual Reports in Computational Chemistry (David Spellmeyer)

- David S. reported that there are 18 contributors to the first issue of the ARCC. The manuscripts are being converted into the proper format.
- All transfer agreements have been signed.
- Should come out next December or January.
- There will be a website for next year.
- David is already working with section editors for next year.

- David S. constructed a made a poster for the COMP poster night which advertised our sponsors (see Attached 8).

11. Meeting Abstracts on Web (Lisa Balbes)

- Lisa reported that the abstracts may be posted on the web for the next meeting.
- This will saving on mailing costs.
- There will be a password for the abstracts before the meeting, then no password afterwards.
- This can be accomplished by having a hidden link.
- We must send out a postcard.

12. JMGM Report and Related Issues (Andy Holder)

- Andy H. handed out the JMGM report (see Attachment 9)
- In 2004 to date, 51 papers were received and 17 were accepted for publication.
- The Molecular Graphics Society is getting JMGM by buying licenses from Elsevier.
- There are many concerns for COMP. Cannot afford everyone. What is the benefit to the membership, What is the overhead to the Division. There are serious budget concerns. The Executive Committee, says thanks, but no thanks, for now.
- We have been examining this for 5 years. The issue should be moved to the “historical list”.
- Andy informed us that the impact factor for JMGM has moved to 2.93.

13. Councilors (Michelle F., Peter J. and Peter G.)

- Peter J. reported that the ACS will attempt a new publication in Chemical Biology.
- There will be big changes in Publications. There are many retirements and reorganizations.
- CE&News will feature “Reel Science”. Give short description of movies that depict science. It will be a comment on how scientists are portrayed. There will be an annual award for the best movie.
- Peter J. commented upon changes in the U.S. doctoral system.
- It is the 50th anniversary of the PRF.
- For the San Diego meeting, there will be a symposium on environmental chemistry and forensic sciences (co-sponsored with ANAL).
- University of Florida have 700 students in forensic sciences.
- At the Washington DC meeting a green chemistry symposium will be held.

14. Other

- Michelle said the Retreat should be held before the spring meeting, early in 2005. This will be at the beginning of the Chair's tenure.
- Michelle and Andy will need nominations for 2006.