COMP Executive Committee Meeting
March 24, 2007
Chicago, IL

Present: Curt Breneman, Wendy Cornell, Jeff Madura, Ralph Wheeler, Hanneke Jansen, Emilio Esposito, Carlos Simmerling, Adrian Roitberg, Orlando Acevedo, Jeff Evanseck, Peter Jurs, Michelle Francl

Guests: Dan Ortwine, George Purves, Rommie Amaro

Programming Meeting

Chicago: 318 papers total
General oral: 14 total sessions
Reception at Yvonne Martin's symposium is the only major reception for this meeting.

Boston, Fall meeting: Oasys deadline is April 2nd.
Separate poster session in connection with Bill Goddard's birthday symposium on Sunday evening (expect around 300 posters).

HP award: have money for this Spring meeting and a promise to go ahead for the Boston Fall meeting. Hope to go year-by-year, with billing in advance of the meeting. Need to be more pro-active to get applications. Jeff Madura will add wording to the Newsletter to point this opportunity out. There will also be a call for applications on Tuesday when the Award is presented.

CCG and HP awards deadline is April 6th (including letters of support).

New Orleans, Spring 2008
Joint meeting with AICHE.
Bill Schneider is organizing a joint symposium between AICHE and COMP.
Jeff puts forward a request for symposium ideas and people to step up and organize.

Executive Committee Meeting
(Agenda: Appendix 1)

Chair report: Overview of the Strategic Plan meeting (February 2007) and associated actions

Attendees fleshed out mission (similar/same to what we started with) with goals and action items. The hope is that this gives direction and continuity to our work as division leaders.

Goal 1: Strengthen the community of computational chemical scientists by providing opportunities for networking and career growth and by enhancing outreach.

Action 1: Mentoring structure
Point people: Rommie & Wendy

Organizing mentoring lunches with small groups of students and 2 mentors for this Spring Meeting (Chicago).
Academic focus: Heather Carlson, looking for partner on Tuesday (Ralph and Michelle are available).
Industrial focus: Marty Head (also Tuesday) and Dan Ortwine.

Practicalities: Signs outside meeting rooms and sign-ups on a first come, first served basis. No more than 10 students per group.
Rommie & Wendy will finalize signs and sign-ups

Proposal that COMP pays the lunch for the mentors if they require assistance. Students will have to pay for themselves.
Post-meeting notes: no requests for assistance have been received. GSK & Pfizer paid for everybody's lunch in the group with the industrial focus.

Action 2: Evaluate/enhance COMP website
Pressing issue: need new Web Maven/Master. Lisa wants to turn responsibilities over. She has been doing this for free for the last few years to free funds for the ARCC initiative. With a new person, we may have to consider paying again.

Note that ACS has a big web initiative and we should look into getting assistance/templates from them. The committee should discuss how much we should (or want to) make sure that divisions have similar look-and-feel between them and with ACS national.

Michelle has a contact who worked on "The chemical forums". He is a grad student who developed this social networking site. She will get his contact information to Hanneke who will follow up in the context of expanding tools available to our members on the COMP website.

Specific web site change request: we should post pictures (w/o alcohol) for everybody listed on the officer's page.

Everybody is encouraged to email Ralph with further ideas on website and recommendations for a new Web Master or Web Maven

Goal 2: Develop and deliver premier activities, products and services for computational chemical research and education.

Specific examples:
Activities: programming, awards
Products: ARCC, JMGM discount

Services: providing opportunities for networking, social networking applications

Action 1: Flyer for national meetings
At the retreat, Adrian volunteered to create a flyer with COMP news and benefits of COMP membership. This did not happen for Chicago. He did connect with David Spellmeyer and got previous issues to use as a template. He will work on the Boston issue.

Action 2: Powerpoint for dead time with COMP news
Wendy is almost done with the Powerpoint presentation for dead time during symposia. She will add sponsors (information from Curt) and deadlines for awards. She will then email to symposium organizers.

Action 3: Simplify sign-up, catch new members at the national meeting.
Some discussion on how we can we sign up members during the national meetings. One approach would be to print & hand-out the online form that needs to be sent to ACS. Post-meeting note: Ralph got verification during the Chicago meeting that the Membership Desk at national meetings is able to accept dues payment for those wishing to join COMP at a national meeting.

Action 4: Webcast/movie on how to create flashmob
Michelle has some material and will initiate this. From there, we can define how to create webcasts in more general terms.

Action 5: Podcasting and electronic availability of presented material
ACS is pushing and COMP wants to be on the forefront. ACS is starting to post PDF's of posters electronically, with access only for registered people.

Michelle has experience from teaching a course that is electronically available. She will find out who we can talk to in ACS for help & guidelines. Proposal is to try this at the Boston meeting, for example for the "Emerging Technologies" symposium.

Goal 3: Refine divisional administration and implement operational processes to utilize time and financial resources for enhanced member benefit.

Action 1: Split job of Secretary and get Treasurer-assistant

Treasurer assistant:
Annual report preparation (using Quicken) and help with reimbursements after national meetings (especially collecting all the information from symposium organizers).

Secretary tasks:
1) Elections: are easy to separate; proposal to install an Election Chair.
2) Minutes & Action items: twice a year and possibly at the retreat. Could be shared with an assistant.

3) Archive: moving to electronic format. Need to extract from email and scan historical paper archive. This is currently back-logged but should be caught up by the end of current Secretary's term (EOY 2007). Once the archive is up-to-date, responsibility could be shared with or moved to an assistant.

4) Membership: download of monthly rosters, review before national meetings, requests for official mailing lists from ACS (ARCC, election, surveys). Could be moved to or shared with an assistant.

5) Annual report: Will be Secretary's responsibility, but an assistant could help with specific sections.

Proposal to get an Election Chair and an Assistant to the Secretary. The latter's responsibilities will be defined based on skills and interest from the list above.

These positions (Assistant to the Treasurer, Assistant to the Secretary, Election Chair) will be appointed positions with a one-year term; they can be re-appointed.

Ralph will email the committee with descriptions of the duties of these additional positions to facilitate recruiting. We will also ask for volunteers on the Powerpoint (shown during symposium dead-time) and in the newsletter. People who are interested should contact Ralph and people who have recommendations for others should send them to Ralph who will then follow up. We will not put a deadline up on these first announcements. If there are no takers, we will post again with a deadline.

Motion put forward to provide financial support for the Assistant to the Secretary at $500 per meeting/$1000 annual level (as Secretary). The motion was seconded and approved unanimously.

Action 2: Update & maintain Procedures manual

Currently, we only have updates from the Chair and Web Maven. We should have information on positions that matter, in a format that is useful. This is especially important since ACS does not always remind us in timely manner. Positions of particular importance are Chair, Treasurer, Secretary, Program Chair.

Everyone is encouraged to write up tasks in an Excel format, including position, task, deadline, notes.

Chair report: Division business

1) Letterhead: Should be renewed annually, at the beginning of the calendar year and list all elected officials plus program chair.

2) Accelrys Award Sponsorship
This sponsorship has to be arranged annually.
Ralph will call Andy to find out current status and get a recommendation on how to proceed. If anyone has an existing relationship with Accelrys that could be used for

contacting them, they should let Ralph know. If there is no such relationship, then Ralph will contact Accelrys.

3) Indirect cost (IDC) charged to sponsors: policy was voted on by the executive committee through email (vote called on January 23rd) and sets a 15% level for indirect costs charged to sponsors. The Chair informed the executive committee on January 29th that the proposal passed. Text of the proposal that was approved by the email vote:

1) All donations in support of COMP Division symposia will include 15% indirect costs.
2) All potential donors and symposium organizers must be informed in advance of the policy to charge indirect costs.
3) All commitments prior to January 25, 2007 will be "grandfathered" and will not be charged IDC.

Commitments made after Jan 25, 2007 are subject to IDC. The new policy is effective immediately regardless of the meeting where sponsorship will occur.

Everybody who contacts a sponsor should remind them of this policy and point out some of the things that happen with the money. One aspect of the operational cost that COMP incurs is the reimbursement of one registration fee per ½ day symposium. It should also be noted to sponsors that by going through COMP, the sponsorship counts as a tax deduction.

Symposium organizers should be made aware of how valuable it is to have their activities be an official ACS/COMP function. This includes the advertising in the program (with our logo), as well as the fact that COMP has the skills and experience to organize things well and interact efficiently with the ACS organization.

Other ways to make up for operational costs would be to recruit more aggressively (make sure that all symposium organizers are members of COMP) or take away the reimbursement of one registration per ½ day symposium.

4) Member dues
We increased dues twice in the past 4 years to cover start-up costs for ARCC. There does not appear to be a current need to increase further. Check under Treasurer report for details.

5) Committee reorganization
The Program Chair recently appointed 3 Assistant Program Chairs. These 3 individuals assist in programming with a focus on general oral sessions:
Emilio Esposito: Molecular Mechanics & posters
Adrian Roitberg: Quantum Mechanics
Irache Visiers: Drug Discovery
They can be listed in the program, even though their positions are not specified in the Bylaws. The system appears to be working well, and no Bylaw changes are required.

Need point person for Recruitment & Retention efforts: Wendy will do this as part of her Chair-Elect duties. Proposal that every new Chair-Elect presents a plan for recruitment & retention at the Spring meeting (to be added to the procedures manual). Wendy will do this for the Fall meeting.

6) Need contributions for Newsletter, Flyer, and dead-time Powerpoint: send reminder for Boston.

For recruitment purposes, enlarge the flyer to become a COMP information poster at the poster session. Adrian will create the flyer, and Jeffry will check on a poster board.

Wendy will update the dead-time Powerpoint presentation for Boston.

Secretary report

1) Reimbursement Policy review. Current version posted on website. Will add "Assistant to the Secretary" as mentioned above. Discussion on travel support for Assistant Program Chairs, since we now have three appointments, rather than one. We will leave this as is (providing support for one assistant) under the assumption that no more than one additional person will be granted full support. The Program Chair will monitor this and discuss with the finance committee if exceptions are necessary.

2) Procedures manual was discussed above.

3) Election: slate nearly complete, but need candidates for Secretary. Ralph reports current slate:
Chair: Hanneke Jansen, Adrian Roitberg
Councilor: Andy Holder, Rommie Amaro, Emilio Esposito
Since Hanneke is a candidate, we need an independent Election Chair to run the election. Post-meeting note: Lisa Balbes volunteered to become the Election Chair and was appointed by the Chair.

3) Membership
Recruitment & retention really are necessary! A slight drop in membership is observed. Year-end numbers for 2005 and 2006 were virtually identical at 2,511 and 2,508 respectively. The number on the February roster was 2,393, which is surprising given the expected increase due to registration for the Spring meeting. ACS is not helping in this respect: members not getting invoices, but receiving delinquent notices; members receiving a survey including a question what they thought of their anniversary gift, without having received such a gift. As a division, we should reach out and be more welcoming/supportive. We also should think about increasing the member-only benefits.

Treasurer report
See appendix 2 (snapshots from a few days before the meeting).

No red flags. Things are looking good!

Assets are up, but note that this is a snap shot and some money is due to flow out (for example the gift funds associated with the Honig symposia). Real growth has happened, and is due to a larger Division Allocation than in previous years (due to a change in the formula used to determine allocations). This growth offsets the ARCC costs and means we do not need another dues increase, nor do we need to take money out of the investment pool. ARCC can now be considered self-sustaining !

Investment pool is up 8.3%

The HP Award program appears to be a commitment from HP. We don't have that in writing, but billing is done in advance.

Programming
All covered in the Programming meeting (see above).

ARCC
Volume 3 is heading to the publishers in early April with an expected 12-15 papers.
Financially now break-even, which is a great accomplishment.
Congratulations to David for all his hard work!

Back copies are stored at Duquesne. Jeff Evanseck estimates that we have 100-150 copies of volume 2 and 20-30 copies of volume 1. We could use these for recruitment. For example, bring them to Boston and hand them to people who sign up on the spot.

Decision that anybody who requests a back copy should get one, regardless of membership qualification. Anybody who gets a request should pass it on to Jeff Evanseck who will mail the requested book(s).

Hanneke will resend the 3 names of people who presented a coupon for ARCC-1 at the Fall 06 poster sessions to Jeff, who will mail them copies of that volume.

Awards Committee
Divisional Service Award: We need to find out what happened with the latest committee that was installed for this purpose in 2005. Hanneke will contact Jennifer Miller about this. Ralph will subsequently install a new committee.

Councilor reports

Michelle Francl: "nominations & elections" committee deals with mostly confidential information, so no report.

Michelle has written a document on how we ran our first electronic election, which will be available for other divisions. She asks if Jeff Evanseck is willing to be a contact person for questions; Jeff agrees.

This is the last year as a councilor for Michelle and the committee expresses a heartfelt "thank you" for all her hard work!

Peter Jurs: also on "nominations & elections", with no report.
In addition, Peter is a consultant on the publications committee. He reports that both "Journal of Chemical Theory and Computation" and "Journal of Chemical Information and Modeling" will be monitored in the next half year by that committee. This is a process to ensure high quality of publications.

Carlos Simmerling: not on any committee (yet)

Unforeseen

Angela Wilson joined the meeting. She is on the committee on science and asks that people contact her with ideas for thematic programming.

Michelle asks for COMP moral support for a Flashmob international effort in developing countries. This fits well with Goal 1 of the Strategic Plan "Strengthen the community of computational chemical scientists by providing opportunities for networking and career growth and by enhancing outreach." The Division extends full moral support!

Meeting adjourned at 6.40 pm

Respectfully submitted,
Hanneke Jansen
COMP Secretary