

COMP Executive Committee Meeting
August 18, 2007
Boston, MA

Present: Curt Breneman, Wendy Cornell, Jeff Madura, Ralph Wheeler, Hanneke Jansen, Emilio Esposito, Carlos Simmerling, Adrian Roitberg, Michelle Francl, Peter Jurs, Chuck Reynolds, Phil Bowen

Guests: Rigoberto Hernandez (DAC), Lee Herman (BAGIM), Angela Wilson (ComSci)

Programming Meeting

Boston: 13 symposia with a total of 496 papers.

The “general oral” symposium series were renamed by ACS to “molecular mechanics & simulation”, “drug discovery”, and “quantum chemistry” without the “general oral” prefix.

The NSF supercomputing symposium will be videotaped. This will not be a “live” broadcast but the expectation is that it becomes available through NCSA. There may also be an opportunity to put it as a link on the COMP webpage. Jeffry will coordinate that.

There is an additional poster session on Sunday evening related to the Bill Goddard symposium.

New Orleans: Oasys is up but not yet accessible (expect open early September, close in October). This meeting is a joint meeting with AICHE. COMP is doing 3 symposia with AICHE (computational catalysis, computational evaluation of rate constants, computational Bayes equilibria). There are joint organizers for these. All talks in ACS and AICHE (whether or not they are joint) will be accessible for anybody with an ACS badge.

Wendy brings up a proposal to add an overview of recent literature/developments in the field as a first talk in for example a general oral drug discovery session. The presenter of such a talk would be a senior researcher in the field. Rigoberto adds the suggestion to make it a keynote talk and find sponsors to endow this. Wendy will come with a more detailed proposal, including some of the current discussion and bring it to Jeffry.

Jeffry reports on the multidisciplinary program planning group (MPPG) which coordinates and promotes thematic programming and has representatives from each division. These representatives are chosen by each Division’s Chair. Meetings of this group are expected to take place during national meetings. The steering committee for this contains the top 5 divisions based on attendance, with additional representatives chosen and voted on. Appointments are for 3 years.

Themes for Philadelphia programming have been set and include a drug discovery component. Jeffry expresses a desire for some long range planning with respect to programming. This could be part of an annual retreat agenda.

Procedural note for organizers that if you reject a poster or paper for some award that you move these posters/talks to the general sessions with a note describing the reason for this move.

Executive Committee Meeting

(Agenda: Appendix 1)

Chair report (Ralph Wheeler)

Strategic Plan, Goal 1: networking, career growth, outreach

Mentoring lunches: good feedback from the Chicago participants. The committee definitely wants to continue growing this initiative. Lunches in Boston are planned with Academic and Industrial mentors.

Post meeting note: Mentors were Carlos Simmerling (Stonybrook University) & Adrian Roitberg (University of Florida) and Wendy Cornell (Merck), Marcus Gastreich (BioSolveIt) & Xinjun Hou (Pfizer).

Proposal put forward to have COMP sponsor or fund these lunches and give students a year free COMP membership (currently at \$7.50). Operationally, the mentors would have to bring forms to the luncheon, have students fill them out, return to Curt, who then can send them to ACS with a check for the membership.

Motion to pay for student mentor lunches and give a year free COMP membership to students. Seconded. Passed unanimously.

Logistics have to be worked out between Curt (treasurer), Wendy (mentor lunch coordinator for Boston), Hanneke (secretary).

Electronic elections: Thanks to Lisa for running the elections, which went smoothly. ACS wants to use us as an example. Cautions: several people did not get the invite and some glitches at the start leading to a few restarts (confusion about how many votes for councilor). Some spam filters may eat the links. These issues need to be addressed next time we run. Michelle will communicate this to ACS and use Lisa's write-up for the procedures manual on the Election Chair position. Election results will be formally communicated to ACS when we get their form.

Elected were: Hanneke Jansen as Chair-Elect, John Woolfrey as Secretary, Andy Holder as councilor, and Emilio Esposito as alternate councilor. Note that Emilio had previously been elected alternate councilor for the term 2007-2009. The executive committee voted

by email that the next highest vote-getter, Rommie Amaro, would fulfill Emilio's original term and will be alternate councilor 2008-2009.

Electronic communication: Polling members. Question is raised whether it is getting to be time to poll our members again. Last turn-out was very low and we need to first figure out what we want to learn. This could be tied to the electronic vote. The issue needs more consideration before we take action.

Electronic communication: List serve. A poll of people present shows that this is not being used. Motion that list serve be discontinued. Motion was seconded and passed unanimously.

Electronic communication: CCL support. There was a gap in our support because we didn't receive an invoice. This was rectified and we're back on the list as a sponsor (COMP logo will be shown). The original intent of this support was to use CCL as a communication tool to members. Question is how many of our members subscribe to CCL. This could be a question on a poll. Major use is for announcements like awards, COMP election, and symposia (requesting submission of abstracts). Motion that we keep CCL sponsorship at \$1,000. Motion was seconded and passed unanimously.

Electronic communication: What can we do around concepts of social networking, forums, blogs. Is there anything in this realm that could be developed as a member benefit? Michelle suggests we check out Chemblogs and Chemicalforums.com.

Electronic communication: Michelle will follow up on the topic of Pod-casting of symposia. Jeff states that videotaping and broadcasting is generally OK with ACS but technical questions remain. We will learn from some of the events at this Boston meeting.

Strategic Plan, Goal 2: Activities, products, services
Deferred

Strategic Plan, Goal 3: Divisional Administration

Still looking for an Assistant to the Secretary (working on a couple of leads).

Announcement that Lisa Balbes may be willing to serve as Assistant to the Treasurer. This is an appointed post. Motion to appoint Lisa Balbes as Assistant to the Treasurer with signature authority. Motion was seconded and passed unanimously.

Note post-meeting: Lisa Balbes did not accept this appointment.

Webmaven/Webmaster position: Allen Richon has been recommended. Ralph will contact Allen and solicit quotations, both for redesign and maintenance. Proposals will be communicated by email to the executive committee and Ralph will solicit an email vote.

Status of Award sponsorship (ACS Award for Computers in Chemical and Pharmaceutical Research): Ralph will check with Andy Holder on terms of commitment (1-year or 3-year) and status of this sponsorship (most recently by Accelrys).

Indirect cost charge: Observation that some sponsorship is going outside COMP and question whether that is because of the indirect cost element ? It appears to have raised concerns, but we have no real data. Our ACS allocation has gone up and we could maybe consider that that covers a lot of the indirect costs. An alternative cost-saving measure would be to limit or eliminate the number of free registrations (currently 1 per half day session). It is clear that more data is needed and the issue will be revisited later (strategic planning meeting).

Decided to table the discussion on recruitment & retention.

Secretary report (Hanneke Jansen)

Minutes from Chicago (Spring 07) approved.

Procedures manual: We have up-to-date documents for the Chair (by Jeff Evanseck), Web Maven (by Lisa Balbes) and Election Chair (by Lisa Balbes). The Secretary is also gathering miscellaneous and new tasks in Excel as they come up. Updates and/or new documents are needed for other positions (Secretary, Treasurer, Program Chair, Councilor, Newsletter editor, ARCC editor).

Election: Already reported above.

Membership: Membership numbers are slipping a bit. EOY 2005 and EOY 2006 are the same (2,517/326 UD for 2005; 2,508/360 UD for 2006), but current numbers are lower (2,409 with 329 UD). Recruitment & retention are important!

Discussion about making COMP membership a requirement for certain benefits, like Awards (currently only specified as a requirement for the HP Award) and maybe even eligibility for the ½ day free registration. We definitely need to think about creative ways to grow membership (strategic planning meeting).

Treasurer report (Curt Breneman)

Financial Report, Appendix 2: The Division is in good shape with growing income, especially because of a change in the ACS allocation. It should be noted that the timing of this report and an ACS lag in billing have resulted in inflated numbers. The estimate of outstanding liabilities is \$10,000.

Programming (Jeffrey Madura)

Presented in Programming Meeting.

ARCC (Ralph Wheeler)

Volume 3 has just gone to the printer and will be mailed later this Fall. Invitations for volume 4 will go out soon. The contract with Elsevier has to be renegotiated with special attention to be paid to the number of copies in relationship to the Division's membership numbers; Ralph and David Spellmeyer are involved in this effort. The CCG sponsorship for the outside back cover expires after volume 3. Ralph will contact sponsors for this opportunity. It has been confirmed that we can also recruit sponsors for the inside back pages and Ralph will pursue that as well. Note that we have no intention for ARCC to go beyond self-supporting status.

Reports from Councilors

Michelle Francl: Nominations and Elections Committee. Michelle provided input from the COMP electronic election experiences into general ACS guidelines for elections.

Peter Jurs: Nominations and Elections Committee. Some changes upcoming regarding for example immediate run-offs which will be more efficient and cheaper (no second mailing required). Rules on campaigning are being rewritten.

Peter Jurs: Committee on Publications. The committee has a new president. Recent review of journals has included JCIM and JCTC which were both judged to be doing well. A new ACS website will be coming up shortly (in September).

No report from Chuck Reynolds or Carlos Simmerling.

Unforeseen

Angela Wilson (Committee on Science) reports that thematic programming is continuing. There is a continuing theme on "energy" with symposia and workshops that could be of interest to COMP.

Rigoberto Hernandez (liaison from DAC, Committee on Divisional Activities) reports that ACS members will soon have an opportunity to pay membership for 1, 2, or 3 years upfront. Divisions can decide if they want to give members that option too. Note: no life-membership (yet). The 2006 Annual Report was well-received (Rigoberto will send feedback to Chair, Secretary, Treasurer).

Lee Herman (Chair BAGIM, Boston Area Group for Informatics & Modeling) would like a connection between BAGIM and ACS. The ACS entity to connect with could be either the local section for their area (North-Eastern) or COMP (so forming a subsection or a subdivision). They want BAGIM to be an informal group but they need things like a bank account and a PO box so they can for example accept checks to cover food. Note that in other cases, subdivisions are conceptual rather than geographical. Questions that are raised during discussion are whether this could be an affiliation other than a subdivision, whether "affiliates" are defined in COMP bylaws, and whether we could consider a

subdivision for “local opportunities”, so it could host other areas as well. The committee would like to see a more concrete proposal from Lee Herman who will work with Ralph Wheeler on this.

Jeffry Madura announces that he will attend P2C2. There is an opportunity for someone to attend the though leaders summit, Nov 2-4, 2007 (same date as P2C2).

Final note: some Secretariats are asking to become a Division which would mean that the Secretariat concept gets eliminated.

Summary of motions

- Motion to pay for student mentor lunches and give year free COMP membership to students. Seconded. Passed unanimously.
- Motion that COMP list serve be discontinued. Seconded. Passed unanimously.
- Motion that we keep CCL sponsorship at \$1,000. Seconded. Passed unanimously
- Motion to appoint Lisa Balbes as Assistant to the Treasurer with signature authority. Seconded. Passed unanimously.
Note post-meeting: Lisa Balbes did not accept this appointment.
- Minutes from Chicago (Spring 07) approved.

Adjourned at 6.16 pm