

EMERSON CENTER Newsletter

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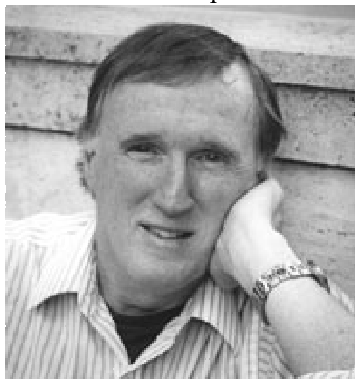
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◆ REPORT FROM THE ECEC MEETING

The Emerson Center Executive Committee (ECEC) members met on Friday, January 28, 2005 for their 19th meeting. Present were committee members R. Antia, D. Lynn, K. Morokuma, V. Sunderam, and K. Wilkinson, as well as Emerson Center staff members. On the agenda were administrative report, technical report, lectureship symposium, and the selection of the 2005-2006 Emerson Center Visiting Fellowship Awards. Out of about 30 applications received, the 2005-2006 EC Visiting Fellowships were awarded to 11 scientists and scholars residing in regions including Germany, Japan, Poland, Russia, Taiwan, Thailand and the UK (list on page 2). The committee also approved a 20% increase to the stipend award to visiting fellows, which had remained unchanged for the past 10 years. The scientific staff members of the Center reported on the dismantling of the old SP2 server and the purchase of a new server from Sun Microsystems. Details can be found in the hardware and software report section on page 4 of this newsletter.

OSTER WINS 2005 EC LECTURESHIP AWARD

The 2005 Emerson Center Lectureship Symposium has taken on an excellent start. Topic-wise, the Lectureship Selection Committee (Profs. K. Warncke (Chair), R. Antia, M. Benzi, J. Gallivan, K. Morokuma, and K. Wilkinson) has selected “Computational and Mathematical Modeling in Biological Sciences” as the broadly defined field for the Symposium. From a half dozen nominees, the Committee has chosen Prof. George Oster of UC Berkeley as the recipient of the 2005 Emerson Center Lectureship Award. Prof. Oster is a prominent scholar and professor of cell



Prof. George Oster

& developmental biology and of environmental science, policy and management at the Department of Molecular & Cellular Biology, University of California, Berkeley. We are delighted that Prof. Oster has accepted our invitation and will visit Emory on May 4th to present a lecture on the “Myxobacteria Motors and Morphogenesis” at our one-day symposium.

The Emerson Center Lectureship Award Symposium will be held on May 4, 2005, in Room 360, Atwood Chemistry Center. The Symposium will consist of a morning poster session, from 9am to 12pm, and an afternoon oral presentation session, from 1pm to 6pm. To encourage student participation, two cash prizes have been set up for best student posters, and the winner will be announced at the Symposium. In addition to Prof. Oster, the afternoon session will include four well-known local speakers in the area. Symposium participants will include students, postdocs, and professors from Emory and the neighboring universities and colleges of Georgia, Alabama, Florida, South Carolina and Tennessee. Please mark your calendar for this exciting scientific event. We would appreciate professors encouraging students and postdocs to attend the symposium and to participate in the poster presentations.

EMERSON CENTER SAYS “GOOD-BYE” TO OLD SP2 AND WELCOMES THE NEW OPTERON-SERVER

In order to provide better service and more computing power for Emerson Center's Subscribers and Users, the Center's Technical Committee recommended the purchase of a new Server from Sun Microsystems Inc, containing 27-nodes with dual 2.2 GHz Opteron-248 Processors. The 54-CPU Sun Fire cluster will consist of 27 nodes with 4 GB RAM and 73 GB 15K RPM SCSI hard drives, plus a master node with 600 GB SCSI main hard disks. The Gigabit Ethernet switches will have 48 ports. The cluster will run under SuSE Linux (please see page 4 for more details). The system will be delivered in early March and will replace our dismantled SP2-server.



Report on Research Activities at the Emerson Center

The Emerson Center is supported, in part, by “subscribers” - faculty members, research groups or departments that purchase shares in order to gain access to its resources for their research projects. EC scientific staff members are also encouraged to conduct scientific research in their own areas of specialty. The following is a research report from one subscribing group at the Emerson Center, Prof. J. Thursby of the Economics Department, and a report from one Emerson Center Visiting Fellow discussing his research related experience during his stay at the Emerson Center.

A New Set of Tools for an Old Experimentalist

Prof. Edward Rosenberg, Dept. of Chemistry
Univ. of Montana, Missoula, Montana

I have always had a tremendous amount of fun doing organometallic chemistry, but I would say that my semester at the Emerson Center was one of the most enjoyable and rewarding periods of my thirty five years as an academic scientist. I came to the Center with no hands on experience in computational chemistry and when I left I had a new set of tools to apply to the mechanistic questions I had been asking for many years. I now have at least a rudimentary working knowledge of the Density Functional Theory (DFT) method. More importantly, with the expert comments and critiques of Dr. Jamal Musaev and Professor Keiji Morokuma I was able to understand some of the limitations of the method and to learn what questions could and could not be answered. I learned a tremendous amount from my daily interactions with Jamal. Some of my former and current coworkers have applied DFT to the metal cluster systems that we work with but there were some serious flaws in the ways in which the methodology was employed and interpreted. On my return to Missoula I was able share the insights I had gained and help my graduate students get on the right track with the computational projects we were engaged in. I came to the Center with a veritable “laundry list” of questions that I could not answer experimentally and left with a remarkable number of them answered and with an enthusiasm for computational chemistry that I never expected. I must especially acknowledge the help of graduate student Taraneh Nowroozi whose patience, daily help and computational expertise made the progress we made on our joint project possible. I hope I was able to contribute a little to her growth as a scientist.

The technical knowledge gained was only part of my Emerson Center experience. The Morokuma group, with whom I was associated, is engaged in a broad range of projects covering the fields of organic, biological, inorganic and materials chemistry. The weekly group meetings exposed me to areas of chemistry at the cutting edge of current research and I am sure that I will bring new insights to the upper division undergraduate and graduate courses that I teach as a result of this exposure. It was great to be in an environment where the primary objective was using computational science to deepen our understanding of real chemical problems. Of course, there is an entirely separate group of investigators in the Morokuma group engaged in developing new computational methods and I was impressed with how many of these young scientists tried to make their work comprehensible to a “pot boiler.”

The administrative staff did everything to make my stay comfortable with a minimum of bureaucratic hassles and I am indebted to Jianli Zhao for all her help.

I cannot imagine a better way to have spent the first part of my sabbatical than as an Emerson Fellow.

Emerson Center Research Report

Prof. Jerry Thursby, Dept. of Economics, Emory Univ.
Prof. Marie Thursby & Ms. Swastika Mukerjee
College of Management, Georgia Tech

A prominent issue in the debates over faculty involvement in university licensing is whether financial incentives associated with licensing have diverted faculty from basic toward applied research. In earlier work we provide empirical support for the view that increased disclosure activity is more reflective of an increased willingness of faculty to engage in commercial activity than a change in research profile. To date, however, there has been a scarcity of theoretical work that explores the link between sources of income and work effort. In part, that scarcity has arisen due to the intractability of the necessary modeling.

In our current work, we present a life cycle model of faculty research that allows us to examine this and related issues.

In our model, the faculty member can engage in applied and/or basic research and can earn income both as current salary and license income. Both types of research have consumption value and both



Left to right, S. Mukerjee, Jerry & Marie Thursby

contribute to income since publications are rewarded in salary. Thus, there is a consumption motive for research that does not decline over the life cycle and a financial motive that does. In our case, however, there is an additional motive for applied research, and this motive does not decline over the life cycle. Applied work that is licensed provides a future income stream that continues regardless of work effort.

The model is a continuous time dynamic model that we are unable to solve analytically, thus we resort to simulations. Our goal is to solve the model over multiple sets of parameters in order to determine “typical” life cycle patterns and how those patterns relate to underlying parameters related to individual preferences, university policies, research production functions and rates of depreciation of knowledge. To date results have been encouraging in that they conform to empirically observed behavior.

EC HARDWARE REPORT

Drs. Jamal Musaev & Stephan Irlle, Emerson Center

◆ Decommissioning of EC's 10-year old 14-node IBM RS/6000 SP2 system

As veteran users of the Emerson Center may remember, the 1995 purchase of an integrated, distributed parallel computer with (at the time) ultrafast interconnect between compute nodes represented a significant step forward for the Center towards becoming a serious competitor among nationally recognized supercomputing facilities. IBM's Scalable Parallel (SP) hardware solution provided at the time the greatest computing power with the potential for being systematically upgraded as the Center's computing demands were expected to increase over the years. The system was very popular with our user community for its speed and ease of use. To satisfy the growing users' appetite for number-crunching power, after 3 years all of its 14 Power2 RISC CPUs were replaced by nearly three times faster CPUs (166 MHz in 1998). The system remained stable in this configuration throughout its life-time until early February this year. During the years, as the Center moved forward in increasing its computational resources by adding successors of the SP2, namely a 58-CPU IBM SP3 in 2000 and a 24-CPU IBM SP4 system in 2003, the original SP2 became less attractive for numerically highly intensive applications, and was mostly used for teaching and educational purposes. In order to make room (space, power, and air conditioning) for our latest addition, a Sun Opteron based system (see the next chapter), we decided to dismantle the EC's first true supercomputer, which served the Center's users for 10 long and very successful years. An estimated total of about 600 scientific papers published by our subscribers resulted from the use of this facility.

◆ Purchase of an AMD Opteron-based 54-CPU Sun Fire V20z compute node cluster

So far, the Emerson Center has undertaken major upgrades of computing resources in regular time intervals, from the purchase of the original IBM RS/6000 Power1 cluster in early 1990's over the purchase of the above mentioned SP2 in 1995 to the IBM SP3 system in 2000. However, since progress in computer architecture leads to doubling of CPU speed every 1 1/2 years (according to Moore's Law), and naturally users' demands also increase as their research progresses, we have in the past added more computer power in between with lower-number CPU systems such as an SGI cluster and the 24 CPU SP4 system. Up until now, IBM has been one of the strongest competitor in our purchases, but recently Sun Microsystems has been aggressively pushing sales in the academic computing market, promoting their Sun Grid Engine. Additionally, AMD's Opteron 248 (2.2 GHz) CPU has been a tremendous success price/performance wise, and Sun has packaged a turnkey-solution ready with Gigabit ethernet connections between dual nodes at the most competitive price/performance ratio the EC technical committee could find. Besides price/performance issues, the EC technical committee wanted to establish a significant presence of a Linux system at

Hardware, continued on the right--

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*This issue of the Emerson Center Newsletter
is designed and edited by Jianli Zhao*

Hosting a Short-Term Visitor?

The Emerson Center may be able to help you house your short-term visitor. We have a long-term lease on a 2-bedroom/2-bathroom apartment at the Clairmont Campus for the Center's visiting fellows. The apartment has vacancies from time to time and we would be happy to make the space available to other short-term visiting faculty on campus. The apartment has easy shuttle access to campus and is fully furnished with cable TV and internet access. The current rent, which includes all utilities and local telephone service, is \$710 per room per month, or \$40 per day if less than 30 days. Please call 727-0867 or email jzhao@emory.edu for more information.

--Hardware, continued

the Emerson Center. The now ordered 54-CPU Sun Fire cluster will consist of 26 dual CPU nodes with 4 GB RAM and 73 GB 15K RPM SCSI hard drives, plus a dual CPU master node with 600 GB SCSI main hard disks. The Gigabit Ethernet switches attached to the system will have 48 ports which leaves room for future addition of nodes if desired. The cluster will run under SuSE Linux, and if possible will be integrated into our existing setup using LoadLeveler as the main queueing system. Usernames, passwords, and home directories will be transparent throughout the entire EC hardware architecture, integrating IBM, SGI, and Sun architectures into a single, high-performance compute platform. An image of the Sun Fire V20z cluster to be delivered is shown on page 1.

SOFTWARE ADDITIONS & UPDATES

We installed VASP 4.6 (The Vienna Ab Initio Package Simulation) program for use on our IBM computers. VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. The approach implemented in VASP is based on a finite-temperature local-density approximation (with the free energy as variational quantity) and an exact evaluation of the instantaneous electronic ground state at each MD-step using efficient matrix diagonalization schemes and an efficient Pulay mixing. These techniques avoid all problems occurring in the original Car-Parrinello (CPMD) method (also installed at the Emerson Center), which is based on the simultaneous integration of electronic and ionic equations of motion. The interaction between ions and electrons is described using ultrasoft Vanderbilt pseudopotentials (US-PP) or the projector augmented wave method (PAW). Both techniques allow a considerable reduction of the necessary number of plane-waves per atom for transition metals and first row elements. Forces and stress can be easily calculated with VASP and used to relax atoms into their instantaneous ground state equilibrium geometries. In order to run VASP at the Emerson Center, please use the script provided in /libs/scripts/vasprun. We are currently working to parallelize the code for 4 CPUs.

EMERSON CENTER LECTURESHIP AWARD SYMPOSIUM

Computational and Mathematical Modeling in Biological Sciences

Cherry L. Emerson Center for Scientific Computation, Emory University



Dr. Cherry L. Emerson

Wednesday, May 4, 2005

Location: 360 Atwood Hall, Emory University

AWARD WINNER & KEYNOTE SPEAKER:



George Oster

*Professor of Cell & Developmental Biology and of Environmental Science, Policy & Management
Department of Molecular & Cellular Biology, University of California, Berkeley*

Myxobacteria are rod-shaped bacteria that 'glide' over surfaces. They hunt in large swarms by secreting enzymes that digest much faster moving bacteria. When food is scarce they aggregate into fruiting bodies containing the spores that will seed the next generation. During this aggregation they pass through several developmental stages characterized by elaborate collective behaviors, including spiral wave patterns, and culminating in multi-armed fruiting bodies. Their collective behavior is a consequence of an internal cell 'clock' and an intercellular communication system that depends only on direct contact; no diffusible morphogens have been detected. Some of the patterns they form are unlike any other in biology, chemistry or physics. Investigating these humble organisms reveals many puzzles whose solution sheds light on

similar phenomena in the cells of higher organisms. I will discuss how mathematical modeling has produced answers to several mysteries: How do these cells propel themselves? How do they communicate with each other? And how does their internal 'clock' steer their collective morphogenetic patterns?

INVITED SPEAKERS:



Mark Borodovsky
*Schools of Biology &
Biomedical Engineering,
Georgia Tech., Atlanta*



H. G. E. Hentschel
*Department of Physics,
Emory University,
Atlanta*



Bruce R. Levin
*Department of Biology,
Emory University,
Atlanta*



James Snyder
*Department of
Chemistry, Emory
University, Atlanta*

SCHEDULE OF EVENTS:

9:30 - 12:00

POSTER PRESENTATIONS

12:00 - 1:00

LUNCH (and tour of Emory and Emerson Center)

1:00 - 1:15

OPENING CEREMONY & AWARD PRESENTATION

1:15 - 2:15

Prof. George Oster (UC-Berkeley, Biology), *Myxobacteria Motors and Morphogenesis*

2:15 - 3:10

Prof. Bruce Levin (Emory, Biology), *The Role of Mathematical & Lesser Models in Experimental Population & Evolutionary Biology*

3:10 - 3:30

COFFEE BREAK

3:30 - 4:25

Prof. Mark Borodovsky (Georgia Tech, Biology), *Modeling & Recognition of Functionally Important Regions in Biomolecular Sequences*

4:25 - 5:20

Prof. George Hentschel (Emory, Physics), *The Morphogenesis of Skeletal Pattern Formation in the Vertebrate Limb*

5:20 - 6:15

Dr. James Snyder (Emory, Chemistry), *Cytoskeletal Proteins, Molecular Motors & the Action of Small Molecules*

6:15 - 6:25

Closing

7:00 - 8:30

DINNER (by invitation only)

REGISTRATION AND CONTACT INFORMATION:

Email: clec@euch4e.chem.emory.edu

<http://www.emerson.emory.edu/conferences/index.html>

Abstracts of invited talks are available at the website.

Registration is free, but you must register to attend.

The Emerson Center Lectureship Award was established in the fall of 2003 to recognize distinguished achievements by scientists in computational sciences and to facilitate collaboration among different disciplines of computational sciences. On the board of the Emerson Center Lectureship Award Selection Committee are Professors Kurt Warncke (Physics, chair), Rustom Antia (Biology), Michele Benzi (Math & Computer Science), Justin Gallivan (Chemistry), Keiji Morokuma (Emerson Center), and Keith Wilkinson (Biochemistry) of Emory University. Dr. Jamal Musaev (Emerson Center) is appointed as the Lectureship Coordinator.



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