

EMERSON CENTER Newsletter

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IN THE NEWS

*The Sun Linux Opteron Cluster

The Emerson Center has added a new flavor to its mix of UNIX compute servers: The 54 CPU Linux-based AMD Opteron 2.2 GHz server manufactured by Sun Microsystems under the company's official name "V20z Fire". And this computer is truly hot: Combined, this Linux cluster delivers about the same number of FLOPS compared with the center's 24 CPU IBM Power4 server, which runs the AIX operating system. With the new "Fire" cluster, users can now take advantage of the popular Linux operating system for sequential CPU intensive jobs, and parallel benchmarks using the AMBER and VASP programs are showing very good performance for about 4 CPU parallel jobs. See Page 4 for details.

*EC Sponsors Math/CS Symposium

The Emerson Center was proud to be one of the sponsors for the "2005 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Scientific and Industrial Applications", May 19-21, 2005, chaired by Prof. Michelle Benzi of the Math/CS Department, Emory. Math/CS Dept. is a departmental subscriber of the Emerson Center.

EMERSON CENTER SYMPOSIUM A SUCCESS

The second Emerson Center (EC) Lectureship Award Symposium on the "Computational and Mathematical Modeling in Biological Sciences" concluded successfully on May 4, 2005. More than a hundred people, including faculty, students and postdocs from colleges and universities in Georgia, Alabama and South Carolina attended this one-day event.

Dr. Earl Lewis, Provost of Emory University, opened the event by emphasizing the importance of this Symposium for the Emory community in bringing together fine scholars with different scientific backgrounds and helping the promotion of cutting-edge research activities at the university. Prof. Lanny Liebeskind, Senior Associate Dean of Emory College, expressed his gratitude to the EC Lectureship Award Selection Committee for their marvelous job in selecting excellent research topics and speakers for this Symposium.

This year's keynote speaker was Prof. George Oster of Berkeley, whose talk highlighted recent advances in mathematical modeling of myxobacteria (which are rod-shaped bacteria that 'glide' over surfaces. They hunt in large swarms by secreting enzymes that digest much faster moving bacteria) and protein motor. Four other invited speakers gave talks on their respective area of research. Dr. Mark Borodovsky of Georgia Tech talked about the modeling and recognition of functionally important regions in Biomolecular Sequences. Dr. George Hentschel of Physics Dept. of Emory described computational approaches to the early stages of skeletal development in the vertebrate limb in which mesenchymal cells, the precursors to cartilage cells. Dr. Bruce Levin of the Emory Biology Dept., talked about the role of mathematical and lesser models in experimental population and evolutionary biology. Dr. James Snyder of Chemistry Dept. at Emory beautifully reviewed latest computational approaches to Cytoskeletal Proteins, Molecular Motors and the Action of Small Molecules.

The poster session, organized for the first time within the EC Lectureship

--continued on page 4



J. Musaev, G. Oster, and K. Warncke

ECEC MEETING MINUTES

The 20th meeting of the Emerson Center Executive Committee (ECEC) was held on Tuesday, September 6, 2005. On the agenda were administrative issues, membership, technical reports, computer upgrade, and the Emerson Center Lectureship Award Symposium. The committee also examined and discussed items on the balance and budget sheets of the Center operations account, approved the budget and the per share subscription fee to stay at \$6000/year (\$1500/year per unit). The membership shares have remained stable at 14.50 shares. Reports were presented to the ECEC on the EC Lectureship budget/expenses as well as preparation for next years symposium. The scientific staff of the center reported on the upgrades to the Center's hardware equipment and software packages, as well as the CIRF-MU proposal submitted to the NSF for the center's major computer upgrade.

Letters from Fellows

I spent part of the Spring 2005 as an Emerson Center Visiting Fellow hosted by Professor Fereydoon Family in the Dept. of Physics carrying out research in collaboration with both Prof. Family and Prof. H.G. E Hentschel on pattern formation during the nanoindentation and nanoscratching of solid surfaces.



Dr. Jacques Amar

While I was familiar with both the Physics Department and the Emerson Center from my earlier stay at Emory University as a Postdoctoral Research Associate and Research Assistant Professor, it had been almost 8 years since I had spent any significant time at Emory University. I was therefore quite pleasantly surprised by the enormous expansion in the Emerson Center computational facilities which had occurred since then. During my stay I was able to use the computational facilities at the Emerson Center to carry out large length-scale and long time-scale molecular dynamics simulations of the nanoscratching of metal surfaces. I also enjoyed discussions with Stefan Irle of the Emerson Center as well as with other members of the Dept. of Physics & Astronomy including Stefan Boettcher and Stephan Koehler. I would also like to thank the members of the administrative staff of the Physics Department and Emerson Center for their kind assistance during my visit.

Jacques G. Amar
Associate Professor of Physics & Astronomy
University of Toledo



Dr. Jacques Amar visited Emory as an Emerson Center Visiting Fellow from February to April 2005.

EMERSON CENTER VISITING FELLOWSHIP

The Emerson Center offers visiting fellowships to interested scientists throughout the year. Scientists from academic institutions all over the world who want to perform intensive research in computational chemistry, biology, physics, and math & computer sciences for one to several months are encouraged to apply. Travel expenses and stipends are available. Although fully independent research is not excluded, collaboration with an EC subscriber is desirable, and EC subscribers are encouraged to make recommendations. The deadline for Emerson Center Visiting Fellowship applications for summer 2006-summer 2007 is February 1, 2006. To formally apply, please submit:

- 1-2 page research proposal
- CV including publication list
- Amount of financial support needed
- Length of stay with an approximate start/end date

Applications should be submitted to the Emerson Center (address on p. 4).

APPLICATION DEADLINE: February 1, 2006

My Visits to the Emerson Center as a Visiting Fellow

Stuart Carter, Ph.D., C.Sci., FRSC, University of Reading, England

My first experience of Atlanta was my arrival at Hartsfield one steamy night in August, 1996 - Olympic Year. My only connection to the Emerson Centre was a scrap of paper with the address of an apartment written on it - somewhere in N. Decatur Road. I finally arrived there around midnight, without key of course, and so I had to awaken the inhabitants in order to be let in. Jim Coxon (an Emerson Fellow from N. Zealand) finally appeared somewhat bleary-eyed and did the honours. We (my wife & I) were "sort of" expected, but unfortunately we wouldn't have a bed since another Japanese Fellow had had complications with his return ticket, and had decided to stay an extra night in order to sort it all out. . .

We returned in 1997, and were introduced to our new accommodation in an apartment on Clifton Road, where we have spent many an enjoyable visit. This had the grand title of "Carriage House", and turned out to be an apartment built over a four-car garage with incredibly noisy remote-controlled doors, most frequently used around 6.00 am. I soon used this feature to my own advantage however, as it served as my wake-up call for morning coffee down at Caribou, where I had fallen in with a fine cross-section of Atlantans, thus forming a regular "Coffee Club" (we once celebrated a "member's" birthday at 6.00 am, complete with cake, candles, hooters and party streamers - I shudder to think what the neighbours must have thought!).

The Emerson Center apartment has since moved to its beautiful location on the Clairmont Campus and I have been coming back with my wife twice a year ever since, both in Spring and Autumn. These visits are the highlights of our year, not only for the incredible floral displays in Spring, the rich Autumnal colours and the beautiful climate that Atlanta has to offer at these times of year, but it gives us the chance to meet up with all the friends we have made, both in and out of the Department. We have also "discovered" Savannah, one of the few places on earth where I find I can totally unwind, and which we visit each time we come. And, by the way, I've been able to do quite a lot of useful research with Joel Bowman during my visits to Emory, to whom I am enormously indebted for inviting me in the first place.

Work or play...it's all been great fun, and we just can't get enough of it!



A frequent/yearly visitor to the Emerson Center, Dr. Carter was awarded Visiting Fellowships from the Center in 1996, 1998, 2000, and 2005.



Dr. Stuart Carter

Report on Research Activities at the Emerson Center

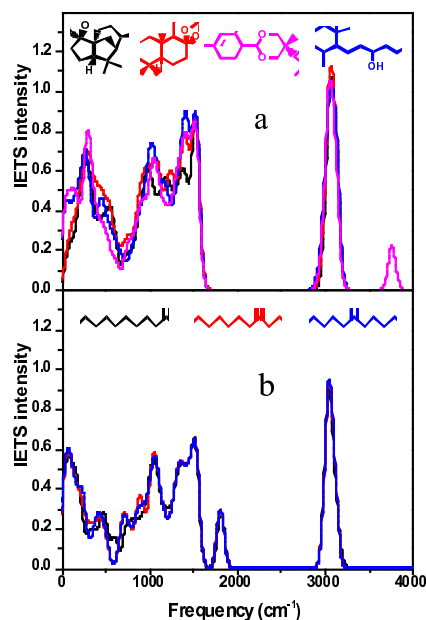
The Emerson Center is supported, in part, by "subscribers" - faculty members, research groups or departments that purchase shares in order to gain access to its resources for their research projects. EC scientific staff members are also encouraged to conduct scientific research in their own areas of specialty. The following are two research reports from the Emerson Center.

Can Inelastic Electron Tunneling Account for Human Smell?

Tiao Xie, Shubin Ling and James P. Snyder
Department of Chemistry, Emory University

For decades, researchers have been applying their chemical knowledge to understand the molecular mechanisms behind smell. Various theories have emerged, the two most popular being the structure based theory and the vibrational theory. Both approaches fail a variety of tests. Recently, Luca Turin proposed a biostructural mechanism for smell, which combines elements of both previous theories including electron transport and suggests the odor receptors work as inelastic electron tunneling spectrometers (IETS).

To support his theory, Turin calculated approximate IET spectra for several sets of molecules.



Some share similar structures, but impart very different odors; and some involve very different structure, but smell similar. Employing the semi-empirical PM3 method, Turin determined similarities and differences in the spectra by visual inspection. Two weak points in Turin's study are the use of PM3, well known to only poorly describe molecular vibrations, and the comparison of IET spectra without a quantitative measure. To test Turin's novel idea, we initially re-examined two sets of molecules. Geometry optimization and

vibrational analyses were performed using DFT (Becke3LYP) with a 6-31G* basis. Mulliken, natural bond orbital (NBO), and electrostatic potential (ESP) charges were used to calculate IETS intensities. The resulting stick spectra were then convolved with a Gaussian function of width (FWHM) 100 cm⁻¹.

Fig. (a) shows the IETS of four molecules with the same amberggris odor but different structures, while in Fig. (b) we compare the IETS of three molecules with similar structures, but different odors. The IETS in Fig. (a) were claimed by Turin to be much more similar than those in Fig. (b). For a rigorous comparison, we calculated the root mean square deviation (RMSD) of the spectra within each group. Surprisingly we find the RMSD for Fig (a) is about three times that of Fig (b). The results from this rather limited test dataset completely conflict with Turin's conclusions. Further analyses are underway to determine if this observation is general.

Contribution from the Snyder-Liotta group.

Nobel Metal-oxo Compounds. Realization of Compounds Proposed and Sought for Half a Century

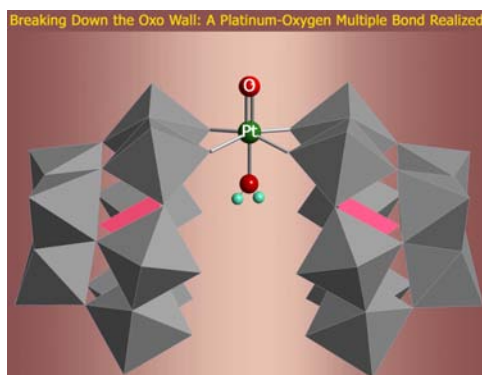
Craig L. Hill
Department of Chemistry, Emory University

When oxygen (O₂ from air) combines with noble metals in a host of technologies that range for all automobile catalytic converters (Pt or Pd + O₂), fuel cell electrodes (Pt + O₂), air-based CO and organic oxidations under very mild conditions (Au + O₂) and several major industrial oxidations (Ag or Au + O₂), it has been proposed that terminal metal-oxo complexes may be key intermediates. These complexes contain a single

oxygen atom bound to the metal. Metal-oxo species are well known for the early transition-metal elements but become progressively less stable as one traverses the periodic table from left to right. For the noble metals (Pt, Pd, Au, Ag, etc.), metal-oxo species were unknown despite sizable and continual efforts by synthetic chemists and heterogeneous catalyst investigators (physical chemists and chemical engineers) to make and study them for more than 40 years.

In late 2004, our group (Travis Anderson later joined by Rui Cao) using large multi-metal ligands with empty d orbitals of appropriate symmetry (polytungstates), prepared the first noble-metal-oxo complex, a Pt-oxo complex, L₂Pt=O, L = polytungstate ligand (figure). This was followed rapidly by 6 other complexes in the intervening year.

The electronic and physical structures of these complexes are as ground breaking and unusual as the complexes themselves. As a consequence, we are probing these features and the fundamental reactivities of this new family of compounds in collaboration with Jamal Musaev, Keiji Morokuma and their colleagues in the Emerson Center.



Structure of $K_7Na_9[O=Pt(H_2O)L_2]$, $L = [PW_9O_{34}]^{9-}$ (1-Pt with cations omitted for clarity) from liquid He (30K) X-ray and neutron diffraction crystal structures. (*Science*, 2004, 306, 2074-2077.)

Installation of Sun Linux Opteron Cluster

Stephan Irle, Emerson Center

(Sun Systems, continued from page 1)

The Sun Linux Opteron cluster system was officially put in service at the EC on April 15, 2005. It consists of 26 dual 2.2 GHz AMD Opteron CPU nodes with 4 GB RAM and 73 GB 15K RPM SCSI hard drives in each node, plus a dual CPU master node with 600 GB SCSI main hard disks. The fast hard drives are perfect even for medium I/O demanding jobs, and offer 28 GB scratch space per job. Although the Sun Fire line came out about 1 year ago at its first release, due to the slow development of dual core Opteron CPU's, this server is currently among the very fastest in the 64-bit Linux-based computing market place. The Gigabit Ethernet switches attached to the system have 48 and support MPI based parallel applications in distributed parallel mode. Downtime of the nodes has been essentially zero, only interrupted by one rare air condition outage earlier this year. For the first time, we are offering the capability to run jobs for 4 days, facilitated by the 10 "fire4" queues, while all nodes can routinely handle "fire2" and "fire1" two- and one-day jobs, respectively.

The operating system of the cluster is SuSE Linux, and the nodes are tightly integrated into our existing setup using LoadLeveler as main queueing system, with the popular and very robust OpenPBS as local queueing system, which is invisible to the end user. Usernames, passwords, and home directories are transparent throughout the entire EC hardware architecture, integrating IBM, SGI, and Sun Linux architectures into a single, high-performance compute platform.

Installed application software on the Sun Fire cluster includes mainly GAUSSIAN 03, MOLPRO 2002.6, MATLAB R14, AMBER 8, VASP 4.6, GAUSS 2.0, TINKER 4.2, NWChem 4.3, DeMon 1.1, and visualization software. We are working to install more software as

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demand for the server increases. The master server "fire.chem.emory.edu" has all standard software packages from SuSE installed, and graphical output can efficiently be remotely displayed on any X11 emulation desktop program, such as Apple's Mac OS X X11, or cygwin under MS Windows, using the 'ssh -X' remote login protocol.

(Lectureship, continued from Page 1)

Symposium, featured latest research findings of more than 25 students/postdocs from the Emory, Georgia Tech and Georgia State University. Two cash awards for \$100 each was awarded to this year's best poster presentations: Martina Kaledin of Emory University and Burcu Bakir of Georgia Tech.

Both Dr. Jamal Musaeov, Manager of the Emerson Center and Lectureship Coordinator, and Prof. Kurt Wancke, Chair of the EC Lectureship Committee, expressed their appreciation to all EC Subscribers for their support, to all Lectureship Selection Committee members for their marvelous work, to 2005 Award Winner Prof. George Oster and to all speakers and poster presenters for their beautiful presentations. Dr. Cherry L. Emerson, Emerson Center's benefactor, attended to all presentation and gave a short speech during the special dinner honoring Prof. George Oster.

The EC Lectureship will be awarded annually and the award symposium next year is schedule for beginning of April 2006 at Emory.



EC 2005 Lectureship Symposium Speakers, left to right, G. Oster, M. Borodovsky, B.R. Levine, H.G.E. Hentschel, J. Snyder



From left to right, Social among participants including Dr. Emerson; Poster Session Discussions; Lecture Room Audience