EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation, Emory University
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In the News

◆ *EC Lectureship Awards Established*

An Emerson Center Lectureship Award is established recently with approval from the Emerson Center Executive Committee. The purpose of the lectureship is to 1) enhance the visibility of the Emerson Center (EC) and Emory University among international and domestic scholars, 2) bring more domestic and international recognition to the Emerson Center, 3) promote and consolidate the EC subscribers' scientific interests, and 4) help Emory to recruit outstanding students and scholars. Funding of the Emerson Center Lectureship Award are from private and industrial contributions.

The Selection Committee, which includes representatives of five Departments (Biology, Biochemistry, Chemistry, Mathematics & Computer Science, and Physics) as well as the Emerson Center, will select once a year a scientific field and one of the leading scholars of this field for lecture presentation at the Emerson Center, based on the recommendation of EC Subscribers. An annual one-day symposium with participation of students and faculty from neighboring Colleges/Universities will be held; speakers of the symposium will be the lectureship winner and local scholars.

The members of the Selection Committee for 2003-2006 are: Profs. Rustom Antia (Biology), Michele Benzi (Math & Comp. Sci.), Justin Gallivan (Chemistry), Keiji Morokuma (Emerson Center), Kurt Warncke (Physics), and Keith Wilkinson (Biochemistry). Dr. Jamal Musaev, Manager of the Emerson Center, is the Coordinator for the Lectureship.

EMERSON CENTER WELCOMES NEW SUBSCRIBER

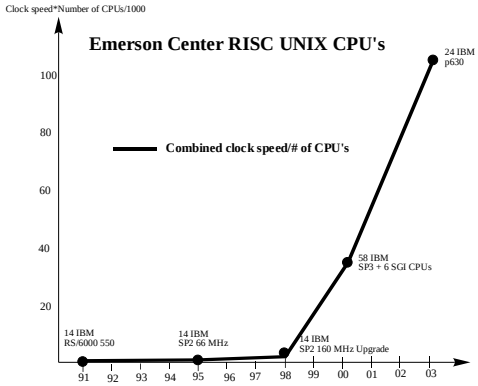
The Emerson Center welcomes Dr. Craig Hill, Goodrich C. White Professor of Chemistry at Emory, as the newest subscriber to the Emerson Center. The general research interests of Dr. Hill are new concepts and inorganic systems in catalysis, materials science, environmentally benign ("green") chemistry and medicine. Much of his research involves the design, synthesis, characterization and development of large molecules including early-transition-metal oxygen anion clusters (polyoxometalates or "POMs") and materials derived from self-assembly of such big molecules into larger arrays. Dr. Hill plans to use the Emerson Center facilities (in collaboration with Drs. Jamal Musaev and Keiji Morokuma) to launch comprehensive and integrated experimental and computational studies to establish the factors and fundamental principles that control reactivity in one of the most intellectually challenging and practically important areas of chemistry–the catalysis of selective (non-radical) reductant-free oxidation of organic substrates by O_2 catalyzed by binuclear (di-metal) complexes. This part of Dr. Hill's multicomponent research programs will be funded by a US Department of Energy grant recently obtained jointly with Dr. Musaev and Prof. Morokuma.

Prof. Craig Hill

A "HOT" SUMMER FOR THE EMERSON CENTER

While many people say the summer of 2003 has been one of the "cool" summers for Atlanta because of the amount of rain we had, the Emerson Center has experienced a very "hot" and busy summer. The Center has had record numbers of Visiting Fellows during the summer. Although some of the visitors stayed with their research collaborator groups, the Center had to find temporary spacing solutions to accommodate all the visitors. Among the visitors are Professors J. Moc and P. Paneth from Poland, S. Boccaletti from Italy, G. Ju and Z. Xu from China, M. Tanaka from Australia, and S. Ducki from England. Please see page 2 and 3 of this newsletter for letters and research reports from some of the visitors.

During the summer, the Center also purchased and upgraded several hardware items and software packages. We have a) acquired a new computing Server including IBM's p-Series (p-630) containing 24 Power4+ RISC processors with 1.2 Ghz, which dramatically increased the computing power of the Center (see chart on left); b) upgraded the File and Mail servers, and significantly improved network communications; and c) upgraded the Biomolecular Modeling facility (based on SGI computers) by adding new RAMs and processors. Please refer to page 4 of this newsletter for more details of the hardware and software updates.



Computer Power at the Emerson Center

Letters from Fellows

From April 1st to May 15th, 2003, I had the great privilege and pleasure of visiting the Cherry L. Emerson Center for Scientific Computation at Emory University in Atlanta. This was a unique experience in my life. From one side, indeed, I had the chance of collaborating with Prof. G. Hentschel at the Physics Department, gathering new scientific knowledge and opening my research to new fields and interests. From the other side, I experienced working in a completely new environment, the beautiful campus of Emory University, that I found so stimulating for scientific as well as for social aspects.

The goal of my stay was to start a collaboration on the dynamics of fracture. In particular, we aimed at developing our understanding of the shape of cracks moving with constant velocity under mode I loading. Such a problem involves high level mathematics, especially in the field of conformal mappings together with a deep analysis of the physical mechanisms giving rise to fractures in materials. Furthermore, solving this problem is likely to initiate a novel field of research analyzing bifurcations and fingering in the crack shapes as the propagation velocity increases.

Dr. Stefano Boccaletti

The skills and expertise I have gained from this visit will be of great importance for my future researches in this area, that will include a permanent collaboration with Emory on this field of research. I am sure my stay at the Emerson Center will spark several important contributions to fracture dynamics, a field of great relevance for industrial and technological applications.

My deep gratitude goes to Prof. G. Hentschel and to all his colleagues at the Physics Department of the Emory University for the many very stimulating discussions I had all throughout my stay, as well as for the help I received in many circumstances. Furthermore, I gratefully acknowledge the Cherry L. Emerson Center for having granted me access to its computational facilities, and especially to Professor Morokuma and his secretary Jianli Zhao for the valuable help and support I received in solving all the practical problems related to my visit.

I look forward for future occasions of visiting such a wonderful place!

Dr. Stefano Boccaletti, Istituto Nazionale di Ottica Applicata, Florence, Italy

Dr. Stefano Boccaletti visited the Physics Department of Emory as an Emerson Center Visiting Fellow from April to May 2003.

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 2004-summer 2005 is February 1, 2004. 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, 2004

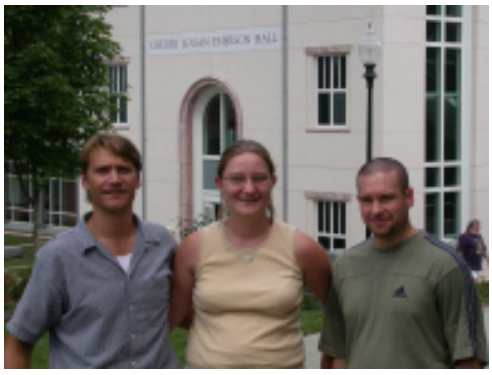
My Stay at the Emerson Center as a Visiting Fellow

Prof. Sylvie Ducki, Centre for Molecular Drug Design

University of Salford, UK

I would like to thank the Emerson Center for giving me the opportunity to work with Professors James P. Snyder and Dennis Liotta. In June 2003, I joined the Liotta-Snyder group to familiarise myself with computational methods used to study protein-ligands interactions. This visit was the outcome of a two-year exchange of emails/ideas between Jim and myself, which was initiated by a common interest in the structure and function of the protein tubulin.

During our stay, my postdoctoral research assistant, Dr. Grant Mackenzie (with the help of Jim Nettles, who I would also like to thank) revealed the location of the colchicine-binding site, using literature data and various molecular mechanics techniques. In the meantime, I carried out a QSAR study of ligands populating this binding site. Using a new Quasar program, we successfully developed a 5D-QSAR model for these agents.



Jim Nettles, Sylvie Ducki & Grant Mackenzie

Although my visit only lasted two months, the discussions with Jim, the support and help of the modelling group, and the excellent computational facilities made this an incredibly pleasant, most educational and very fruitful research visit for me.

With best regards and looking forward to future collaboration.

Dr. Ducki and her postdoc, Dr. Grant Mackenzie, stayed at the Emerson Center from June to August 2003.

Report on Research Activities at the Emerson Center

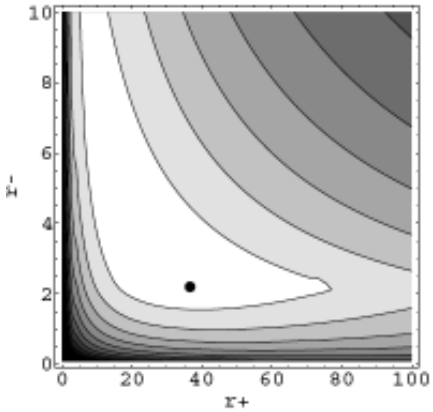
The Emerson Center is supported, in part, by "subscribers" - faculty members, research groups or departments that purchase shares in order to gain access to its resources for their research projects. EC scientific staff members are also encouraged to conduct scientific research in their own areas of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

The Optimal Replication of Poliovirus, a Positive Single Stranded RNA Virus

Mark Tanaka, EC Visiting Fellow, and Roland Regoes, Shane Crotty, Rustom Antia, Biology Dept., Emory University

In recent decades mathematical and computational approaches commonly used in ecology, evolution and epidemiology have been successfully applied to problems in immunology and virology. Mathematical modelling has advanced our understanding of the dynamics of many viruses such as human immunodeficiency virus and hepatitis B and C. Although many studies investigate the interaction between the virus and the cell population within the infected hosts, few focus on viral replication strategies within the infected cells.

We have developed models for the replication of viral RNA within target cells. We focus on poliovirus that -- as a positive single stranded RNA virus -- has a fairly simple life cycle, and for which many dynamical parameters have been estimated. We use our models to understand how far the characteristics of replication of the viral RNA are optimised with respect to the growth rate of the virus within cells. To this end we adopt the framework of classical life history theory, which is concerned with the evolution of traits such as the age of maturity, clutch size, and reproductive investment. Life history traits are often explained successfully in terms of evolutionary optimality given constraints imposed by trade offs between the traits.



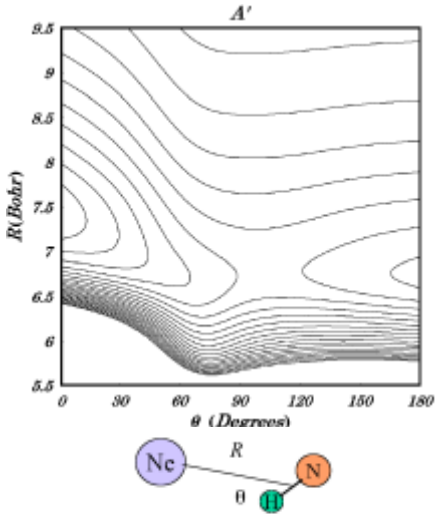
Fitness of virus as a function of the numbers of positive (r+) and negative strands (r-) produced during the replication cycle. The number of proteins produced is set to the optimum. The point indicates the optimum over the three parameters.

In the case of RNA viruses, the replication of the genome involves the translation of the RNA into proteins and the transcription of RNA into secondary strands of RNA, which involve the proteins produced from the translation. The time and resources allocated to translation and transcription determine how fast and how many viral particles are produced within the cell. Hence, investment into translation and transcription trade off against each other and affect the evolutionary fitness of the virus. Using empirically determined parameters for cellular processes, we find that the optimal numbers of (a) proteins, (b) negative strands and (c) positive strands is intriguingly close to what is actually observed in poliovirus.

Theoretical Investigation of the $c^1\Pi$-$\alpha^1\Delta$ Transition of NH-Ne

Galina Kerenskaya, Udo Schnupf, and Michael C. Heaven, Chemistry Department, Emory University

Solvent-solute interactions between an open-shell species and inert solvent molecules (or atoms) influence condensed-phase reaction dynamics. Rare-gas – radical clusters provide model systems for studies of solvation. The most detailed insights can be obtained from studies of binary radical-rare gas atom complexes. A particular point of interest for these systems is the breaking of the orbital degeneracy that occurs when a closed-shell atom or molecule interacts with a radical. The two potential energy surfaces that result from off-axis approach dictate the vibronic energy level structures of bound Rg- complexes. Information about the potential energy surfaces is encoded in the spectrum, but in most instances the spectra are so irregular that they can only be interpreted using guidance provided by theoretical calculations.



Potential energy surface for the A' symmetry component of NH($a^1\Delta$)-Ne. The N-H bond length was frozen at its equilibrium value for this cut through the surface.

In recent experiments we have characterized the NH-Ne complex via the $c^1\Pi$-$\alpha^1\Delta$ transition. High-level theoretical calculations, carried out at the Emerson Center, were an essential component of the analysis of this spectrum. Potential energy surfaces for the upper and lower electronic states were generated using the CASPT2 method. A large basis set (6-zeta quality) was needed to cope with the very weak long-range forces for this system and minimize superposition errors. The figure above shows a 2-dimensional contour plot for one of the NH(a)-Ne potentials. At the deepest point this potential is bound by just 43 cm^{-1}. The energies of vibronic levels supported by the potentials were obtained by numerical solution of the close-coupling equations (another computationally intensive task). Assignment of the spectrum was the accomplished through comparison with the theoretical predictions. The fact that a recognizable facsimile of the spectrum could be generated provides an impressive demonstration of the power of the present generation of theoretical methods. Studies of this kind benchmark our progress in developing high-fidelity models of intemolecular forces for reactive species. However, we find that the level of theory employed was still not sufficient to make quantitative predictions and it is evident that we will need to push on to better methods and larger basis sets.

Recent EC Hardware Acquisitions Boost Computational Power and Improve User Friendliness

Jamal Musaev & Stephan Irle, Emerson Center

The EC has recently acquired new computer hardware to satisfy the ever increasing needs for computational resources of its subscriber groups. 1) Using the remaining funds from its NSF Major Research Instrumentation Grant, an IBM Power4 Scalable Power System was purchased. The purchase of this system more than doubled EC's number crunching power (see Figure on page 1). 2) The EC Biomolecular Modeling Facility was made more powerful by the purchase of a third SGI dual R12000 400 Mhz CPU Octane2 system, plus additional larger disks and more RAM to existing Octane2's. 3) In order to improve user friendliness, a new Power4 server was purchased for interactive login and mailing, and server tasks for essential administrative services were completely redesigned.

1) The IBM Power4 architecture was selected based on the results of benchmark tests for GAUSSIAN and MOLPRO, two frequently used programs at the EC, on IBM Power4, HP Itanium2, and Microway Itanium2 systems. These are all 64-bit platforms, a requirement that was set forth by the members of an EC user meeting that took place in early 2003. At this meeting, the message for EC was loud and clear: To purchase additional high-level supercomputing power for extremely demanding computational tasks which cannot be performed on modern 32-bit Linux based PC's. Among the three alternatives, the IBM Power4 system scored best in both categories: total performance as well as price/performance. Given the very successful history of IBM computers at the Emerson Center, and their long-standing reputation for reliable computer hardware, the choice for the IBM solution was even easier to make. In early June of 2003, the EC installed a 24 processor IBM p630 Scalable eServer consisting of 6 nodes with 4 1.2 Ghz Power4 processors, 8 GB RAM, and 72 GB disk space each. The Power4 architecture is revolutionary in that a single chip contains dual processors with private level 1 cache and a larger shared level 2 cache. In addition, an off chip level 3 cache is shared among all processors of a node. This setup provides an enormous boost for memory-intensive calculations, giving the Power4 architecture a greater speedup over its Power3 predecessor beyond just its higher clock speed rate, in line with the subscribers requirements. Integration into the existing user environment of EC was seamless, with all IBM servers now running AIX5L Version 5.1 of the operating system. From the installation of this Power4 server (individual nodes are called p4p1 to p4p6), CPU usage at the EC has gone up by more than a factor of two, indicating the strong demand for high quality compute cycles among its user community.

2) A third SGI Octane2 400Mhz was purchased to increase the numbers of SGI processors at the EC from 6 to 8. This server features 1.5 GB RAM and 80 GB total disk space, supplementing the LoadLeveler integrated servers for biomolecular modeling at the EC. The Center's other Octane2's were upgraded to 2.5 and 3.3 GB RAM, allowing extremely large systems to be modeled using pro-

Hardware, continued on the right--

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

Space Available at EC Apartment

The Emerson Center has long-term lease on a 2-bedroom/2-bathroom apartment at the Clairmont Campus. The apartment will have some vacancies in the winter and we would like to make it available to other short-term visiting faculty on campus. The apartment is fully furnished with cable TV and internet access. The rent, which includes all utilities and local telephone service, is $690 per room per month, or $35 per day if less than 30 days. Please call 727-0867 or email jzhao@emory.edu for more information.

◆ *Dozens Attended EC Short Course* ◆

The Emerson Center offered a special short course on "Introduction to Practical Computational Chemistry" which was open to everyone on campus. The course started on March 20 and ran continuously for six weeks and was very well received. About 30-40 students and postdocs from various departments attended the short course. Among the lecturers were Drs. Jamal Musaev and Stephan Irle of the Emerson Center, and guest lecturers Dr. Kim Gernert of BIMCORE and Dr. Jim Snyder of the Chemistry Department.

News from the ECEC Meeting

The 16th meeting of the Emerson Center Executive Committee (ECEC) was held on Monday, Sept. 22, 2003. On the agenda were administrative issues, membership, technical reports, and the Emerson Center Lectureship Award. The committee also discussed items on the balance and budget sheet of the Emerson Center operations account, approved a 5% scheduled increase to the per share subscription fee, from $5500/year to $5775/year, and discussed issues related to services to subscribers. The current membership of the Center stands at 16.25 shares. The scientific staff of the center reported in detail the upgrades to the center's hardware equipment and software packages, and raised concerns over space limitations for future expansion/upgrade of the center's equipment. The committee also talked about how the Center can provide service to the Emory community in promoting academic computing on campus.

--Hardware, continued

grams like SYBYL, MacroModel and AMBER.

3) The combined new number crunching compute power naturally required an upgrade of the EC file server, which served for about 5 years and was due to replacement. In an effort to radically increase response time for login sessions, we decided to make our interactive login and mailing server also NFS file server, and purchased an IBM Power4 p615 deskside server for this task. This machine replaced our aging euch4e (a Power3 system), which was reassigned to take over license server duties, formerly handled by one of our oldest systems in the center. Euch4e's high speed internal disks have a total capacity of 144 GB, and therefore released old home directory disk space to be used for temporary user disk space. Per subscription share, 2 GB of new /checkpoint file system was additionally allocated to subscriber groups, and together with the increased disk space of 3 GB/share of backed up /home directories: Now, one subscriber share allows totally 5 GB disk space on EC machines.