EMERSON CENTER Newsletter

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In the News

◆ ***Professorship Award***

Dr. Jamal Musaev, Principal Scientist and Manager of the Emerson Center, has been awarded a Visiting Professorship at the Univ. of Tokyo for the 2002-2003 academic year.

◆ ***New Software***

Mathematica_4.1, IDL_5.5 and several parallel tools have recently been added to the Emerson Center's software collection and are available to all users. Please refer to page 4 of this newsletter for details.

◆ ***Hardware Upgrade***

The Emerson Center's mail and front-end server, euch4e, has recently been updated. The server is now much faster and more reliable. The Center has also added a new disk drive (RAID) with a capacity of 160 GB to the File Server, which allows for mirroring of the whole /home file systems. In the event of a disk hardware failure, normal operation will no longer be affected. Details on page 4.

PHYSICS & MATH/CS DEPARTMENTS JOIN EC AS SUBSCRIBERS

The Department of Physics and Department of Mathematics & Computer Science at Emory College have joined the Emerson Center as the newest departmental subscribers starting from the fall semester of 2001. Departmental subscription allows all the members of the department to use the Emerson Center services including hardware, software, visiting fellowship, lectures and consulting. These services can be used not only for research carried out in the department but also for undergraduate and graduate courses that require computational facilities. Other current departmental subscribers to the center include the Department of Chemistry and BIMCORE (Biomolecular Computing Resource).

Representing the Math/CS Department, Professor Vaidy Sunderam talks about the department's decision to become a subscriber.

Prof. Vaidy Sunderam

"The Emerson Center is a unique entity that facilitates the confluence of multiple research groups with mainstream or incidental computational interests. As such, it provides Emory with a complementary setting for interdisciplinary endeavors with computing as the common locus. Thus, although the leading-edge hardware and software resources that the Emerson Center provides are the tangible motivations for subscriptions, the sense of community and opportunities for exploring synergies in computing as a research paradigm are the center's real strengths."

In addition to usual hardware and software services, the Emerson Center plans to provide platform for Math/CS faculty members to test their ideas on efficient parallel computing. In a recent meeting, the center's Executive Committee also selected one Emerson Center Visiting Fellow who will be collaborating with Prof. Sunderam.

Prof. George Hentschel

Physics Professor George Hentschel, a long time EC subscriber and member of the Center's Executive Committee, describes why the department became a subscriber.

"Our reasons for doing so are multifold. In the Physics Department at present our main computer hardware are PCs, Macs and personal Workstations such as the Silicon Graphics O2. We expect, however, with the growth of our Department (we are searching for two new faculty in 2002 and 2003) to increase our computing needs substantially. In addition, we are actively developing our graduate program, and we hope soon to have students whose thesis work will involve a substantial component of high end parallel computing. Several of our faulty are involved in research with a strong computational component. Eric Weeks, an exciting new hire in our Department, is using the EC facilities for data analysis of aging and jamming in colloidal systems, and has a student who is developing software for this purpose."

--Continued on page 2

NEWS FROM THE ECEC MEETING

A recent meeting of the Emerson Center Executive Committee (ECEC) was held on Friday, February 8, 2002. On the agenda were administrative issues including membership and the recent scientific staff salary review. Two new departmental subscribers have been added to the EC membership list (details on this page). A technical report was presented by the Center's scientific staff about updates on the hardware condition and software requisition at the Center. The ECEC also approved Visiting Fellowship Awards to eight scientists from various parts of the world. Please refer to page 2 of this newsletter for a list of visiting fellowship recipients and their affiliation.

Letters from Fellows

Achieving reliable results in modern chemistry requires having access to computational technology that is in demand but available for few. It is the Emerson Center staff that made it possible, maintaining perfectly tuned software and hardware resources and fulfilling rigorous state-of-the art standards.

Some of the tasks can be solved using existing tools, while the others stand in need of new algorithm development, thus implying continuous training and learning. That is another point one may be really impressed with even after a short stay under the EC visiting fellowship program.

Dr. Valentin Ananikov

Collaboration is everything in nowaday science, and the benefit becomes clear as soon as one is allowed to work in a friendly and stimulating atmosphere. I came with a demure project on transition metal reactivity in catalytic reactions based on the experimental observations. The theoretical work carried out in collaboration with Dr. Jamal Musaev and Prof. Keiji Morokuma allowed us not only to accomplish planned mechanistic investigation, but also to resolve puzzling questions in a practical and important area of synthetic chemistry.

I would like to thank the EC for giving me the opportunity to work on the project and for making the time equally enjoyable and productive. Special thanks to Jianli Zhao, who can solve everything one step before it appears in front of EC fellows.

With best regards and looking forward to future collaboration,

Dr. Valentin Ananikov
Zelinsky Institute of Organic Chemistry,
Russian Academy of Sciences, Moscow

Emerson Center Visiting Fellowship Awards for 2002-2003

Dr. Yann Bouret, University of Paris VI, FRANCE

Dr. De-Cai Fang, Beijing Normal University, P. R. CHINA

Dr. Roger J. Loader, University of Reading, UNITED KINGDOM

Dr. Boon H. Loo, University of Alabama in Huntsville, USA

Dr. Marek R. Lozynski, Poznan University of Technology, POLAND

Dr. Jian Wan, Central China Normal University, P. R. CHINA

Dr. Li Jie Wang, University of Saskatchewan, CANADA

Dr. Han Zuilhof, Wageningen University, The NETHERLANDS

The Emerson Center offers visiting fellowships to interested scientists throughout the year. Please refer to the Emerson Center homepage at http://www.emerson.emory.edu for application details and deadlines, or send email to clec@euch4e.chem.emory.edu.

My Stay at the Emerson Center as a Visiting Fellow

Dr. Rongshun Zhu, Dept. of Chemistry, Emory University

I would like to thank the Emerson Center for giving me the opportunity to work in the group of Prof. M. C. Lin. During my stay here, I have been working on the NCO + NO, NCN + O_2, CH_3 + (O_2, HO_2), HO + ClO_x etc. reaction systems. Their reaction mechanisms and variational/canonical rate constants have been studied on with the help of the Emerson staff and the excellent computational facilities in the center. I wish to express my deep gratitude to Prof. Lin for his guidance. I have learned a great deal about RRKM theory and related experimental background about my project from our daily discussions. This has been an enjoyable, fruitful and unforgettable period in my academic life.

Dr. Zhu at his office at Emory

-- Physics & Math/CS, continued from page 1

"I am personally carrying out several projects in computational biology which may involve the need for high end computing. For example, with Andrea Campos, a PhD graduate student from Sao Paulo, we are studying cytoskeletal growth by simulating actin polymerization at the intracellular surface of a cell; while with a second graduate student Tilmann Glimm from the Mathematics Department, we are studying cellular condensation and chondrogenesis (the early stages of skeletal formation) using biologically based reaction diffusion models of growth and differentiation."

"Fereydoon Family interests have also turned to Nanobiology. He organized an important International Conference on the subject last October at the Emory Conference Center and is now studying the dynamics of several molecular motors in collaboration with Professor Arizmendi from Mar del Plata in Argentina. In summary it is being more and more apparent that one strand of research in the Physics Department will involve a major computational component."

"The new acquisition of the latest version of Mathematica should also prove very useful for the Physics Department. In conclusion, we are hopeful that a very productive collaboration will emerge between the Physics Department and the Emerson Center."

The Emerson Center looks forward to very fruitful collaborations with these departments. If you feel that your department/program/institute may benefit from the services of the Emerson Center, please contact Dr. Jamal Musaev, the EC Manager, at 7-2382 or dmusaev@emory.edu, for information and consultation.

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 two subscriber groups of the Emerson Center.

Reduced dimensionality quantum calculation of acetylene-vinylidene isomerization

Reported by Prof. Joel M. Bowman
Department of Chemistry

Joel Bowman and graduate student Shengli Zou have completed a reduced dimensionality quantum calculation of acetylene-vinylidene isomerization, a topic of long-standing and current interest in spectroscopy. This is the first such calculation done at sufficiently high energy to determine vibrational wavefunctions that exhibit characteristics of vinylidene. They chose a novel set of coordinates, shown below, which facilitates the description of vinylidene,

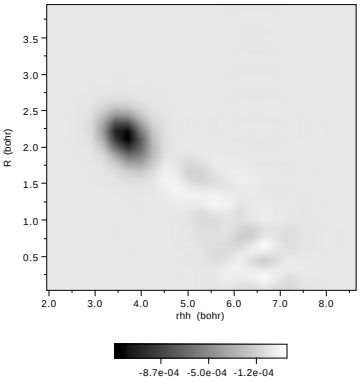
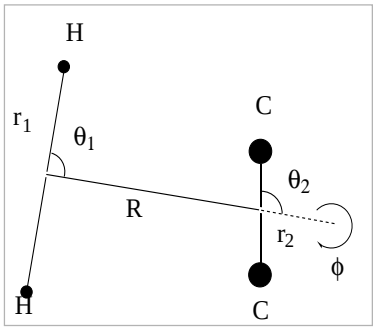


Image plot of a vinylidene state in the radial coordinates r1 (the HH-stretch) and R.

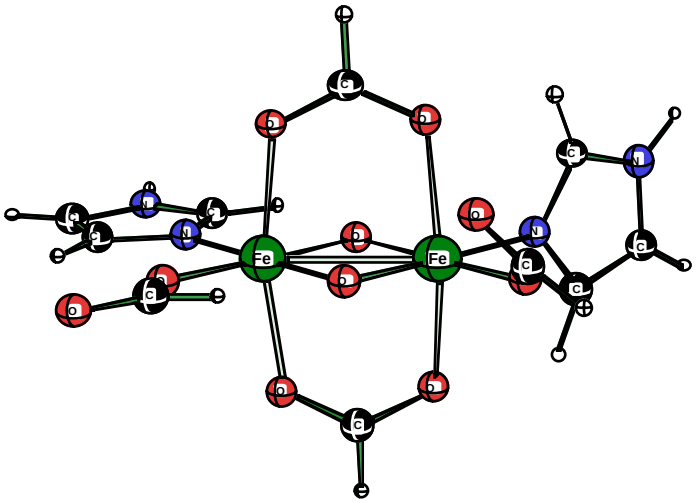
A contour plot of a very high energy wavefunction that exhibits the characteristics of a ground vibrational state vinylidene wavefunction (but with wisps of amplitude everywhere) is shown below. Note that in acetylene r_{HH} is 6.28 bohr but at the vinylidene minimum it is 3.54 bohr.



Theoretical Approaches to Metalloenzymes

Research Report by Dr. Jamal Musaev
Emerson Center

In the past few years, I have been actively working on the problems of metalloenzymes (such as MethaneMonoxygenase (MMO), Fe-only Hydrogenase, Nitrogenase, Cytochrome P450, etc.). The latest upgrade of the Emerson Center s computational facilities, as well as active developments on the hybrid and integrated methods have significantly advanced my research. As a result, papers have been published (on the metalloenzymes alone!) in leading journals during the last two years. For example, recently and in collaboration with Profs. K. Morokuma (Emory University) and H. Basch (Bar Ilan University, Israel), I have studied the mechanisms of the hydrocarbon hydroxylation by MMO. In our calculations we have used the model system, cis-(HCOO)(Imd)Fe(m-O)$_2$(h^2-HCOO)$_2$Fe(Imd)(HCOO), (Imd = Imidazole), **1**, given in the figure. Our studies have demonstrated that the reaction starts by coordination of the substrate molecule to the bridging oxygen atom, O^1 of **1**, an Fe(IV)-Fe(IV) complex, followed by the H-atom abstraction at the linear (O-H-R) transition state leading to the bound hydroxy alkyl intermediate of Fe(III)-Fe(IV) core. In the next step, the exothermic coupling of alkyl and hydroxy groups occurs to give the alcohol complex of Fe(III)-Fe(III) core, from which alcohol dissociates. The H^b-atom abstraction (or C-H bond activation) barrier is found to be a few kcal/mol lower for C_2H_6 and CH_3F than for CH_4. The calculated trend in the H^b-abstraction barrier, CH_4 (21.8kcal/mol) > CH_3F (18.8kcal/mol) ≥ C_2H_6 (18.5kcal/mol), is consistent with the C-H^b bond strength in these substrates. Thus, the weaker C-H^b bond, the lower the H^b-abstraction barrier. The calculated H-abstraction barriers and obtained trends are in excellent agreement with available experiments. The epoxidation of ethylene by complex **1** is found to proceed without barrier and is a highly exothermic process. In other words, the only product of the reaction of ethylene with complex I is expected to be ethylene oxide. We were able to explain several difficulties experienced by experiments.



New EC Software Specifications

Jamal Musaev & Stephan Irle, Emerson Center

Mathematica_4.1.0, IDL_5.5 and new parallel tools are available at the Emerson Center.

I. Mathematica_4.1.0.

You can use it either from our machines or from your labs. To use it from your labs, you should have a workstation running the X windows system. If you have no IBM and SGI computers in your lab, the Emerson Center staff can help you install the software to your PC's, Sun's etc. For detailed instructions on how to use the software from different platforms, please refer to our website: http://www.emerson.emory.edu/local/Frequent/Software_user.htm or contact one of the EC's staff members.

II. IDL, the Interactive Data Language, is the ideal software for data analysis, visualization, and cross-platform application development. IDL integrates an array-oriented language with numerous mathematical analysis and graphical display techniques. The IDL manual states: "Using IDL, tasks that require days or weeks of programming with traditional languages can be accomplished in hours." Users can explore data interactively using IDL commands and then create complete applications by writing IDL programs. Here are just a few features of IDL:

(a) IDL offers a host of built-in-multi-threaded algorithms for performance gains on multi-processor systems. These include many of the core operators and mathematical functions, along with many image processing, array manipulation and type conversion routines;
(b) It allows two- and three-dimensional gridding and interpolation functionality;
(c) It supports the reading and querying of the MrSID files. MrSID is an image formatted based on wavelet compression licensed by LizardTech;
(d) IDL has a convenient multiple-document interface called the IDL Development Environment that includes built-in editing and debugging tools.
(e) IDL has flexible input and output capabilities allowing you to read and write virtually any data format.
(f) IDL allows digital signal processing,
Manuals are available at the Emerson Center.

III. New Parallel Tools.

The Emerson Center now offers a variety of compilers and libraries for program development in a parallel environment both for shared memory and distributed parallelism based models. While our SGI machines (2 CPU's per workstation) only allow for SysV SHM shared memory type calls, our SP3 provides support for programs based on either shared memory type models or PVM, MPI, MPICH (a public domain version of MPI), and IBM's own High Performance Fortran compiler called "xlhpf". In addition to these new features, a parallelized version of IBM's ESSL (Engineering and Scientific Software Library) version 2.2 (based on the scalar ESSL library 3.2) software is available on all machines of the Emerson Center. Currently, we have reserved two nodes for parallel operation, sp5 and sp6. At present, only shared memory type parallelism is offered using the four CPU's within each of these nodes. However, the Center will be glad to extend our parallel capabilities upon specific request by our subscribers.

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

Hardware Improvements & Replacements

Stephan Irle, Emerson Center

The Emerson Center is pleased to report that a new 44P 170 type RS/6000 model has been purchased to significantly improve our user community's interactive network traffic, email services, and disk space requirements for email attachments. It is equipped with 512 MB RAM, 9 GB disk space, and most importantly with a 100Mbps network connection. All software packages required for email, LoadLeveler job management, compilers, and others have been installed on euch4e, and we strongly encourage all subscribers and users to use euch4e from now on as our front-end server. Job submission from euch3f will no longer be supported officially by the Center.

We are also very glad that upon consent with IBM we were able to replace the faulty hard drives in our new SP3 with more reliable ones. Both old and new model disks are the same size (18 GB) and have the same spinning speed (10,000 RPM), but IBM tells us that the new (slightly older) drives are much more reliable than the ones which were purchased with the new SP3 system. The replacement was done on two different days during December and January in order not to interrupt completely the operation of the SP3 main computational power of the Emerson Center. The disk replacement led to a much smoother operation of the SP3 supercomputer, and no node has been shutdown ever since this major operation.

At the same time we used those outages to install an additional 160 GB SCSI RAID disk storage subsystem in place. It is equipped with nine 18.2 GB 10,000 RPM Ultra SCSI drives and a complete match for our current SCSI RAID array. Like the previous array, it has redundant power supply, fans, and in addition it has redundant cabling to the file server, euch6h. This disk subsystem is used to mirror any file in home directories and application software at real time. It means that user files are now physically present on two physically different disk subsystems at the same time in real time, and additionally provide space for reinstalling from backup tapes if necessary. In case of a disk hardware failure, normal operation will not be affected due to this redundancy which is now built into our system to protect our users' valuable data.

--Software, continued

(a) SysV SHM calls. This is the simplest way of accessing SMP type memory. The communication works via sockets, and simple C-library system calls mediate the interprocessor communication.
(b) PVM and MPI/MPICH. These are parallel libraries included in IBM's parallel environment 3.1 and LoadLeveler 2.2. They provide internode parallelism over IBM's high performance SP switch based on TCP/IP as well as SMP type parallelism. Currently, the only LoadLeveler class supporting these applications is called "poetest" and the job_type needs to be called "parallel" in order to run such jobs.
(c) XLHPF. This is IBM's implementation of the High Performance Fortran Forum's specification for interprocessor communication using specific directives understood by the compiler. It is very flexible and allows for platform-independent development of parallel software at an easy-to-use level of syntax within standard FORTRAN programs.
(d) Parallel ESSL. The popular ESSL library used for matrix manipulations and linear algebra has been parallelized for the IBM SP3 model using either shared memory or distributed parallelism. Linking to Parallel ESSL subroutines is done with standard 'ld' UNIX linker software using the –pessl command line option.

Other parallel software: In addition to the libraries mentioned above, we have installed an IDL to PVM link software based on Dynamic Loadable Module technology, Emory's Prof. Sunderam's PIOUS parallel I/O system for PVM3, and a C++ wrapper for (allegedly 1-minute) development of C++ applications called EasyPVM.