EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation
http://www.emerson.emory.edu
Volume 1, March 15, 1998

In This Issue . . .

New!

FREE-TRIAL SUBSCRIPTION!

If you are not sure whether you may benefit from the Emerson Center services and facilities, you may now try the service (hardware, software and consulting) **FREE** for 3 months! It is the newest feature initiated by the recent Emerson Center Executive Committee meeting in an effort to reach out to the university community. Please call the Emerson Center at 727-2380 or email clec@euch3g.chem.emory.edu for details. Also, please make sure you return the enclosed USER SURVEY form for future information updates.

Letter from the Director

HIGH-END COMPUTATIONAL FACILITY FOR YOUR SERVICE

-- Keiji Morokuma --

The Cherry L. Emerson Center for Scientific Computation may not be the best known center on campus, but it surely is one of the most active scientific research facilities. The Emerson Center was established in 1991, with a generous gift of Emory Alumnus, Cherry L. Emerson, and has a dual mission to accomplish: to establish Emory as a world center of computational chemistry and physics, and to provide a high-end of computational services to the Emory research community. It presently owns and operates an IBM9076 SP2 parallel computer with 14 processors, as well as fifteen IBM, HP and SGI workstations. It also offers a variety of application software and consulting services in computational chemistry and physics, in addition to basic mathematical and graphic libraries. With the use of its facility, the Center subscribers have published over 200 scientific papers in the first six years of existence, and have put the name of Emory clearly on the map of computational chemistry and physics.

Mr. Cherry L. Emerson

Prof. Keiji Morokuma, Director, Emerson Center

We are currently expanding the scope of the Center to other disciplines, including computational chemical, physical and biological sciences, and to encompass a much broader base of scientific computing. This newsletter is one of our efforts to reach out to potential users who might need the Center's computing hardware, software and consulting services for their research. Through issues of this newsletter we plan to provide up-to-date information about the Center and its facilities and activities.

If you have a need for high-end computing for your research, please contact the Emerson Center. The Center is easy to reach, via internet web page, e-mail, telephone or visit, whichever is convenient to you.

Meet the Emerson Center Staff:

Dr. Jamal Musaev, Applications Software Manager 7-2382
musaev@euch4g.chem.emory.edu

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Dr. Stephan Irle, System Manager
7-4658 *irle@euch4g.chem.emory.edu*

■

Jianli Zhao, Administrative Assistant
7-0867 *jzhao@euch4e.chem.emory.edu*

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1998-99 VISITING FELLOWSHIP

The Emerson Center offers visiting fellowships in computational chemistry/physics throughout the year. Scientists from academic institutions all over the world who want to perform intensive research in computational chemistry/physics for one to several months are encouraged to apply. We also accept faculty on sabbatical leave. Postdoctoral research associates are not supported through this program. Travel expenses (and stipend for long term stay) are available. Although fully independent research is not excluded, collaboration with a "subscriber" is desirable. Deadline for application is usually Feb. 1 each year, and decisions are made in late February at the Executive Committee meeting of the center.

For the 1998/99 academic year, the Executive Committee has offered 6 fellowships so far for computational research in theoretical and experimental chemistry and physics. The names of awardees and their affiliation are listed below. Additional $15,000 is still available for visiting fellows interested in collaborating with scientists doing mainly experimental research.

The Emerson Center Visiting Fellowship Awardees, 1998-1999

Dr. K. Christoffel, Augustana College, Illinois
Collaborator: Prof. J. M. Bowman, Chemistry
Dr. C. Hu, Academia Sinica, Taiwan
Collaborator: Prof. F. Family, Physics
Dr. J. Moc, Wroclaw University, Poland
Collaborator: Prof. K. Morokuma, Chemistry
Dr. R. Musin, Russian Academy of Sciences, Siberian Branch
Collaborator: Prof. M. C. Lin, Chemistry
Dr. B. Yates, University of Tasmania, Australia
Collaborator: Prof. K. Morokuma, Chemistry
Dr. Y. Osamura, Rikkyo University, Japan
Collaborator: Prof. K. Morokuma, Chemistry

Previous Emerson Center Visiting Fellows

1996/1997

Dr. Stuart Carter
Univ. of Reading, UK
Dr. Kevin Dunn
Hampden-Sydney College, VA
Dr. Viktor Horvath
Eötvös University, Hungary
Dr. Stephen Klippenstein
Case Western Reserve Univ., OH
Dr. Lucas Lathouwers
Univ. of Antwerp-RUCA, Belgium
Dr. Feliu Maseras
Univ. de Montpellier II, France
Dr. Ruslan Minyaev
Rostov University, Russia
Dr. Srihari Murthy
Georgia Tech., GA
Dr. Shogo Sakai
Osaka Sangyo Univ., Japan
Dr. Tamar Seideman
Nat. Res. Council, Canada

1997/1998

Dr. Harold Basch
Bar-Ilan Univ., Israel
Dr. Stuart Carter
Univ. of Reading, UK
Dr. Viktor Horvath
Eötvös University, Hungary
Dr. Nobuaki Koga
Nagoya University, Japan
Dr. Eugene Kryachko
Bogolinbov Inst., Ukraine
Dr. Vladimir Mandelshtam
Univ. of S. California, CA
Dr. Minh Tho Nguyen
Katholieke Univ., Belgium
Dr. Huan-Xiang Zhou
Hong Kong Univ., Hong Kong

The Emerson Center Subscribers

The Center is supported, in part, by "subscribers" or faculty members who purchase shares in order to gain access to its resources for their research projects. IBM workstations are housed in their labs while controlled by the LoadLeveler queuing system. Currently, there are nine subscribers, eight from the chemistry department and one from physics. In addition, there is a Chemistry departmental subscription, providing access to the Emerson Center for class use and occasional users in the department. The following is a list of faculty subscribers and their research interests

Joel Bowman (Phys. Chemistry)
(404) 727-6592
bowman@euch3g.chem.emory.edu
Quantum Calculations of Chemical Reaction Dynamics and Vibrations of Large Molecules

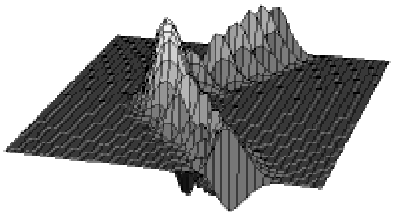
Fereydoon Family (Physics)
(404) 727-4293
phyff@physics.emory.edu
Monte Carlo Simulation and Molecular Dynamics of Models of Material Growth and Other Non-equilibrium Phenomena

Karl Hagen (Inorg. Chemistry)
(404) 727-6556
chemksh@emory.edu
Structural Studies of Supramolecular Model Complexes as Models of Metalloproteins

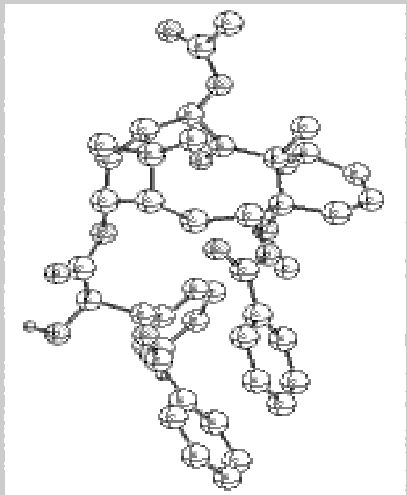
Michael Heaven (Phys. Chemistry)
(404) 727-6617
heaven@euch4c.chem.emory.edu
Calculation of Potential Energy Surfaces for Weakly Bound Systems

M.C. Lin (Phys. Chemistry)
(404) 727-2825
chemmcl@emory.edu
Calculation of Potential Energy Surfaces for Combustion Related Reactions and Reactions on Solid Surfaces

HCN/HNC



Isomerization Wavefunction
Contributed by Joel Bowman



Designed Mimic of the Breast Cancer Agent Taxol
Contributed by Dennis Liotta & Jim Snyder

Dennis Liotta (Org. Chemistry)
(404) 727-6602
dliotta@emory.edu
Computational Approaches for Examining Enzyme/Ligand Interactions; Ab Initio Calculations for Assisting Synthetic Strategies and/or gaining Understanding of Synthetic Results; Effective Core Potentials for Examining the Electrostatics of Ligands Containing Metals

Fred Menger (Org. Chemistry)
(404) 727-6599
Optimization of Molecular Geometry and Energy Calculations for Local/Global Minimum and for Transition States, Calculations of Reaction Pathways, Prediction of Rate Constants for Organic Reactions and Isotope Effects

Albert Padwa (Org. Chemistry)
(404) 727-0283
chemap@emory.edu
Computational Studies in the Area of Heterocyclic Chemistry and Rhodium Catalysis

Keiji Morokuma (Phys. Chemistry)
(404) 727-2180
morokuma@emory.edu
Quantum Chemical Studies of Chemical Reaction Mechanisms: Transition States for Gas Phase Reactions, Organic Reactions, Organometallic Reactions and Enzymatic Reactions

News from the Emerson Center Executive Committee Meeting

The newly formed Emerson Center Executive Committee (ECEC) had their first meeting on Feb. 9, 1998. The committee, appointed by the Provost, consists of three faculty members: Keith Wilkinson (Biochemistry), Michael Heaven (Chemistry), and Al Padwa (Chemistry-will join in fall), and is chaired by Keiji Morokuma, Director of the Emerson Center. It will oversee all matters related to administrative support and operation. At its first meeting, Morokuma reported to the committee on the current status of the Emerson Center and its operations. Technical issues related to hardware and software upgrades were discussed. The committee also reviewed applications for the 1998/99 Emerson Center Fellowship, and selected 6 award winners. (See page 2 of this newsletter for names of award winners.) Additional funds are still available specifically for visiting fellows collaborating with experimentalists.

Also discussed at the meeting are issues related to future operations of the center, subscriber issues, suggestions on how to strengthen collaboration between the Emerson Center and BIMCORE, and how to expand the scope of the center to be of better service to the larger community of the University.

The committee is scheduled to meet monthly.

Hardware & System Software Specifications

The Emerson Center provides powerful computational resources and promotes active computational research in chemistry, physics and related areas. The Center has an IBM9076 SP2 parallel computer with 14 ThinNode-2 units (each is equivalent to an RS/6000 model 39H), a High Speed Switch, 4 GB of total memory and 63 GB of disk space. The operating system of the SP2 is IBM's Unix version AIX accompanied by IBM's parallel system support product (PSSP). In addition, there are 10 IBM RS/6000 model 550 workstations, one 590, and two 350s. These machines are also running under AIX and connected to Emory's ethernet network, whereas internally connected to each other via the Network File System (NFS) and Network Information Systems (NIS). The homogeneity of these AIX machines allows efficient and transparent user access by facilitating an IBM batch queueing system product called LoadLeveler, where the user submits a job to a single queue and the software dispatches the job to the first available CPU for execution. Parallel jobs are executed using message passing parallel programming environments such as PVMe and Linda. In addition to this variety of IBM RISC machines the Emerson Center owns one HP workstation, model 730 and one Silicon Graphics Indy 2 graphics workstation with video-output capabilities. The total computing power of these machines ranges from 0.5 to 1 gigaflop, depending on the application used.

However, due to intensive use of our facilities the capacity limit is already sometimes reached, and therefore we plan to substantially upgrade our hardware in the near future.

-Contributed by Dr. Stephan Irle,
System Manager, The Emerson Center

Application Software Descriptions

The Emerson Center offers basic mathematical, graphical(GL), FORTRAN NAG and IBM's ESSL libraries, along with dozens of extremely powerful software packages, which can be divided into several different categories:

1. Electronic structure codes, such as Gaussian-94, Gamess-96, Molpro-96.4, Cadpac-5.4, Hondo-8.4, Molcas_4.0, Turbomole/ TurboNMR, Mopac_93. These codes allow users to
   (a) optimize the geometry of the molecules,
   (b) search for transition states,
   (c) calculate the energy, transition dipoles, vibrational frequencies, force constants, intensities for vibrations, polarizabilities and hyperpolarizibilities, Mulliken population analysis, multipole moments, natural population analysis, electrostatic potential, atomic charges, thermochemistry using arbitrary isotopes, temperature and pressures.

These packages offer semi-empirical methods (such as CNDO, INDO, MINDO/3, MNDO, AM1, PM3, etc.), Hartree-Fock and various versions of density functional methods, as well as the high level correlation methods such as MCSCF, MR-CISD, CCSD(T), QCISD(T), MP2, MP4. With these codes, users can
   (a) study the potential energy surface of the complex inorganic, organic, organometallic, biochemical reactions, at the both ground and excited electronic states of the reactants, and
   (b) search for the new materials with given physical and chemical properties.

Our message passing parallel environments such as PVM_3.2 and Linda that permits the use of powerful Gaussian-94, Gamess-96 and Hondo-8.4 packages which speed up the calculations with parallel processing.

2. Molecular modeling and molecular dynamic software such as Cerius2, SYBYL, MM3, AMBER, Spartan_4.0, and HyperChem_4.5.

PLEASE VISIT US AT OUR WEB PAGE:

http://www.emerson.emory.edu

The Emerson Center web page gives the most up-to-date information about the Emerson Center operations. You will have access to information about the center's Mission Statement, the current list of the centers subscribers and their research interests, our Visiting Fellows Program updates, software and hardware upgrade information, news on conferences and other programs that the center initiates, tutorials, and links to many other exciting sites.

Software -continued

Such software allow users to use computational methods to predict properties or assist structural analysis using molecular or atomic scale models and rich molecular visualization capabilities. Applications are to polymers, zeolites, catalysts, ceramics, semiconductors, metals/alloys, organometallic, and molecular materials. They are intended to provide a convenient environment to carry out individual molecular mechanics calculations and semi-empirical, ab initio Hartree-Fock and correlated molecular orbital calculations on diverse molecular systems. They also serve to facilitate processing of large numbers of closely-related calculations as might be required to map a conformational energy profile, to screen a set of compounds for a particular property or structural characteristic, or to parameterize a potential function for later use in a molecular mechanics or molecular dynamics calculation.

3. MOLDEN and SciAn. Software for visualization and animation of the research results.

4. Data bases such as QCLDB_97. Quantum Chemical Literature Database, for example, is an on-line application and allows users to search quantum chemical literature. This database includes all quantum chemical papers published up to 1996.

The Emerson Center also offers Morate_4.5 and Polyrate_7.0 for calculations of the rate-constants of reactions. Additional software are added continuously upon requests from subscribers according to their research needs.

-Contributed by Dr. Jamal Musaev,
Applications Software Manager, The Emerson Center

Cherry L. Emerson Center
for Scientific Computation
Atwood Hall, 1515 Pierce Dr.
Atlanta, Georgia 30322
Phone: (404) 727-2380
Fax: (404) 727-6586
Email: clec@euch3g.chem.emory.edu
http://www.emerson.emory.edu

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