

EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation
<http://www.emerson.emory.edu>
Volume 4, September 1, 1999

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In the News

◆ The Emerson Center has successfully performed Y2K tests recently in compliance with Emory's ITD recommendations (<http://www.emory.edu/ITD/YEAR2000>). We are happy to report that all our systems are ready for the new millennium!

◆ Dr. Jamal Musaev, Applications Software Manager of the Emerson Center, was invited to present a talk at the recent ACS meeting in New Orleans, Aug. 22-26. The topic of Dr. Musaev's talk was "Search for new and alternative catalysts for ethylene polymerization processes: Theoretical Studies."

◆ An international scientific conference dedicated to the 65th birthday of Prof. Keiji Morokuma, Director of the Emerson Center, was held at Emory on May 21-22, 1999. The conference, entitled "In the Frontiers of Quantum Chemistry & Chemical Reactions", was attended by distinguished invited speakers from all over the world and many professors and graduate students from US universities. John A. Pople, 1998 Nobel Laureate in Chemistry, was one of the invited speakers. Pictures on page 3.

NEW HOME FOR EMERSON CENTER

The Emerson Center will move to its new home, Cherry Logan Emerson Hall, in the fall of 2000. Groundbreaking for the Cherry Logan Emerson Hall took place on May 13, 1999, and construction is scheduled to be completed by the fall of 2000. The building is named for Dr. Cherry Emerson, a distinguished alumnus and longtime benefactor of both the sciences and the arts at Emory. The Emerson Center, founded in 1992 based on a generous donation from Dr. Emerson, will occupy the top floor of the new building. Emerson Halls top floor will also house research groups of three computational chemistry faculty members and two research groups from the Mathematics/Computer Science Department at Emory. Laboratories for the Chemistry Department and two physics professors will occupy the rest of the building. When it opens in fall 2000, Cherry Logan Emerson Hall will be the first new component of the Emory Center for the Physical Sciences. The faculty, staff and students affiliated with the Emerson Hall are grateful to Dr. Emerson. His vision and commitment to Emory University will be a continuing inspiration to all who have the opportunity to participate in the science programs at Emerson Hall.



Artists' Sketch of Cherry Logan Emerson Hall
Looking to the Northwest

EMERSON CENTER PARTICIPATES IN GIFT PROGRAM

The GIFT teacher program (Georgia Industrial Fellowships for Teachers) is run by Georgia Tech in conjunction with local business and university partners such as Emory. The program provides Georgia middle and high school teachers with professional development opportunities during the summer. The Emerson Center offered a research position to one GIFT participant, Ms. Jormell Bland, a chemistry teacher at Booker T. Washington High School in Atlanta. Ms. Bland spent two months at the Emerson Center during the summer under the guidance of Prof. Keiji Morokuma, Emerson Center Director, and Dr. Jamal Musaev, Application Software Manager of the center. For a report of Ms. Bland's research at the center, please refer to page 3 of this newsletter.

A NEW POSITION IN THEORETICAL/COMPUTATIONAL CHEMISTRY Affiliated with the Emerson Center

A new position in theoretical/computational chemistry at the tenure-track Assistant Professor level has been created at the Department of Chemistry, Emory University. This position is one of several that will be made in the next few years in the areas of biological and materials chemistry, as part of expansion of the department into the new 40,000 square foot Cherry Logan Emerson Hall. This position will be affiliated with the Cherry L. Emerson Center for Scientific Computation. Applicants should send a curriculum vitae, a research proposal and a short statement on teaching interest, and make arrangements to have three letters of recommendation sent directly to: Theoretical/Computational Search Committee, Department of Chemistry, Emory University, Atlanta, GA 30322. Review of applications will begin on October 15, 1999.

Letters from Fellows

It was of my delight to be invited as a fellow at the Emerson Center in collaboration with Prof. Keiji Morokuma and Dr. Jamal Musaev. Although it was only for 2 months, I really had a great time. It was also my honor to be part of the great symposium, "In the Frontier of Quantum Chemistry & Chemical Reactions" dedicated to the 65th birthday of Prof. Morokuma. Visiting at the Emerson Center gave me an opportunity to carry out portions of my ongoing research, "The reaction of artemisinin antimalarial drug with heme". Several spin states of heme with ammonia as proximal ligand complexing



Prof. Vudhichai Parasuk

with artemisinin were studied at high level of accuracy. Applying ONIOM method, theoretical study of the reaction between derivatives of artemisinin and heme could be carried out. Another highlight of my visit was the weekly Morokuma group meetings. I've achieved what I expected and learned a great deal more. I would like to express my appreciation to Prof. Morokuma, Jamal, Stephan, Mori-san, Jianli and all other people who helped me during my stay.

Vudhichai Parasuk

*Dr. Parasuk is an Assistant Professor of Chemistry at Chulalongkorn University, Thailand. He stayed at the Emerson Center as a Visiting Fellow from April to June 1999

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I would like to thank the Emerson Center for offering a good opportunity and Prof. Lin for a kind acceptance of me. Also I would like to give thanks to Ms. Zhao for making my life at Emory easier and Dr. Park for many computer-related help. Of course, I thank all of you in Prof. Lin's lab too. I found that



Prof. Deok-Kee Choi

the people here were very nice and hard working, so no wonder they have been on the leading edge over many years. A state-of-the-art facilities alone cannot make or produce any progress but it is people who are attributed. In the same fashion, with high-performance facilities and excellent people here I don't see any problem in EC's marching ahead. I myself really enjoyed staying at the center and learned a lot from the people. I am very positive to say that this would be one good progress which I have ever made. I hope everything in EC goes well and prosper.

May God bless you all.

Deok-Kee Choi

*Dr. Choi is an Assistant Professor at Dept. of Mechanical Engineering at Dankook Univ., Korea. He spent 2 months at the Emerson Center in the summer of 1999 collaborating with Prof. M. C. Lin, one of the Emerson Center subscribers.

2000-2001 Visiting Fellowship Announcement

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, physics, and other sciences 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 stipends for long term stays) are available. Although fully independent research is not excluded, collaboration with an EC subscriber is desirable, and EC subscribers are encouraged to make recommendations. To formally apply, please submit:

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

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

APPLICATION DEADLINE: FEBRUARY 1, 2000

1999-2000 EC VISITING FELLOWSHIP AWARDS

Prof. Martina Bittererova, Slovak Technical Univ., Slovakia

Prof. Deok-Kee Choi, Dankook Univ., Korea

Prof. Gerhard Erker, Univ. Münster, Germany

Prof. Takayuki Fueno, Osaka Univ., Japan

Prof. Peter B. Karadakov, Univ. Surrey, UK

Prof. Takako Kudo, Gunma Univ., Japan

Dr. Xin Lu, Xiamen Univ., China

Prof. Vudhichai Parasuk, Chulalongkorn Univ., Thailand

Prof. Jonathan E. Stevens, Univ. of Detroit Mercy, USA

Prof. David Wardlaw, Queen's Univ., Canada

Distinguished Visiting Fellow (Jan. - Jun. 2000):

Prof. William H. Miller, Univ. of California, Berkeley

My Stay at the Emerson Center

Prof. Jerzy Moc, Wroclaw University, Poland

It is incredible how fast the six months of my stay at the Emerson Center passed, and, please believe me that I enjoyed every single day of it. Thus, I am really indebted to Prof. Keiji Morokuma for giving me this opportunity. Needless to say I benefited a lot by the computer facilities and the quantum chemistry software available here. Nearly equally important was a stimulating interaction with the other Emerson Center visitors and the Morokuma group. I suppose that the diversity of chemical projects being carried out at the Center impressed not only me.

I have been intensively and extensively involved in the project concerning adsorption of molecular hydrogen on Pd_n clusters of increasing size, including reaction mechanisms for activation of the first, second, ..., H₂ by these clusters. This topic could actually keep me scientifically busy for the next couple of years, but of course we had to terminate "n" at some digit (at least for now).

Last but not least I would like to thank the remaining members of the Emerson Center "crew", i.e., Jamal, Stephan and Jianli for being so helpful, each in a different way.



Prof. Jerzy Moc

J. Moc

*Prof. Moc was a Visiting Fellow at the Emerson Center from Mar. 1 to Aug. 31, 1999.

Report on Research Activities at the Emerson Center

The Emerson Center is supported, in part, by "subscribers" -- faculty members or research groups who purchase shares in order to gain access to its resources for their research projects. The following are research activity reports from one subscribing group of the Emerson Center, and reports from one of the GIFT program participants who did research at the Emerson Center during the summer.

Use of Spartan in Secondary School Chemistry Courses

Research Report by Jormell Bland
Booker T. Washington High School, Atlanta

Students are facing the twenty-first century with the computer as the backbone of the World. Therefore, educators must prepare students by a thorough investigation of computer applications in all academic areas including chemistry. Progresses in the development of theory, computer technology, and software have created sophisticated systems for performing simple to complex calculations on various chemical compounds.

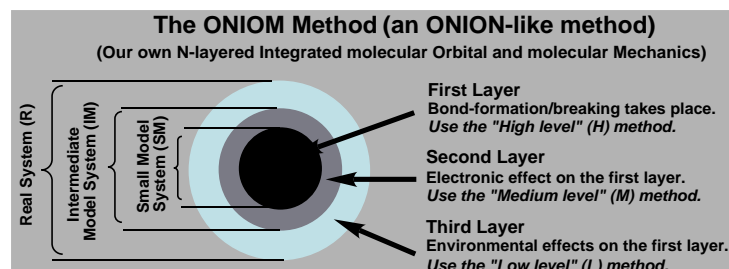
Spartan is a software program that can assist the teacher in explaining the fundamentals of molecules. Many students have difficulties in visualizing molecular shapes, bond lengths, bond angles, dipoles, and polarity. Through the use of Spartan a student can easily build a molecule and rotate the molecule. In addition, the program can display the molecule in different types of models. Spartan provides automatic calculations of energy, dipole moment, charges on specific atoms, and much more. Also, Spartan provides color-coded densities of specific atoms of a molecule, and vibrations of a molecule through the use of colorful and detailed graphics. This study of Spartan applications will include simple calculations and graphics of general molecules that students may investigate.

Development & Applications of the ONIOM Method for Simulation of Large Molecular Systems

A Report from Prof. Keiji Morokuma's Lab
Department of Chemistry, Emory Univ.

Computational chemists have developed a variety of theoretical methods for simulation of chemical problems of different size; from a very accurate but expensive (computer time-demanding) method for small systems (like photochemical decomposition of NO_2 , an air-pollution gas) through various levels up to a very approximate but fast method for large systems (like the folding of proteins). However, the new demand now is for accurate calculations for large systems, which is impossible with the existing technology. In order

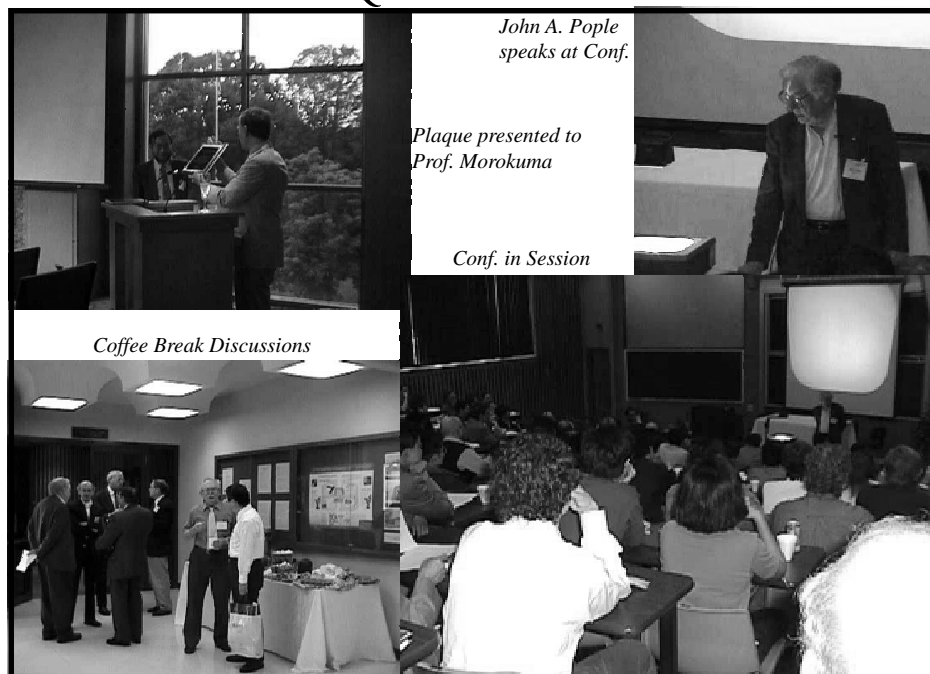
to achieve this goal, in the last few years we have developed a method called ONIOM. The ONIOM method allows, in the "on-ion"-like fashion, the outer layer (the least important part) treated with a least accurate method, while the inner layers are handled with progressively more accurate methods, as shown in the Illustration.



The method turned out to be ideal for theoretical simulation of chemical reactions of large molecular systems. Involving chemical bond formation and breaking, chemical reactions usually require a very accurate and expensive theoretical method. In ONIOM, adopting less expensive methods for bulky substituents and solvent molecules, accurate calculations now can be achieved even for large molecules. For instance, the bond dissociation energy in C_{60} was calculated accurately for the first time.

The ONIOM method is being used for the theoretical design of new catalysts, for instance, for polymerization of ethylene and for harnessing the air-polluting gases for useful products. We are also using ONIOM for the theoretical simulation of the mechanism of reactions of enzymes, such as methane monooxygenase and nitrogenase. The use of the Emerson Center computer facilities is essential for the present project.

* PICTURES FROM THE QUANTUM CHEMISTRY CONFERENCE *



Want to Be a Subscriber?

Try it **FREE** for 3 months or
try the **Introductory Offer**

The Emerson Center offers an introductory subscription of \$1250 per year, which gives the subscriber access to all Emerson Center research resources, both hardware and software, except for the privilege of hosting visiting fellows.

A no-cost 3-month trial subscription to the Emerson Center is also available for those who want to try out the benefit of subscription. For further information, please contact Dr. Musaev (7-2382, musaev@euch4g.chem.emory.edu) or Dr. Irle (7-4658, sirle@emory.edu) at the Emerson Center.

Software:

NAG FORTRAN LIBRARY

New Version now available at EC

A new version, Mark-18, of the NAG (Numerical Algorithms Group, Inc) Fortran Library is now available at the Emerson Center.

Those who have organized computing services are well aware of the two main problems that face the users of computing machines in scientific computation. First, considerable experience is needed before the user can transform a given algorithm into a very efficient program. Second, our users need knowledge of the principles and techniques of numerical analysis, however efficient they might be at program construction, before they can reasonably guarantee to have an efficient algorithm which is as free as possible from numerical instability and which gives results in economic time. Both the cost of computation and the ever-present desire for quick results make obligatory at least a partial solution to these two problems.

Many computing labs and computing services have made some attempts at a solution by constructing libraries of computing programs, but only in the last few years has it been possible to develop really comprehensive schemes by Numerical Algorithm Group Inc. (NAG).

Now, at the Emerson Center, we have the latest version of these libraries, Mark-18. At Mark-18 of the Fortran Library, a variety of new facilities have been introduced and improvements made in existing areas. The Library now contains a total of 1108 documented routines, of which 35 are new at the Mark-18. These extend into areas of ordinary differential equations (ODEs), partial differential equations (PDEs), interpolation, optimization, sparse linear algebra and operations research (OR).

Coverage in the differential equations chapters has been extended as follows:

- Simple driver interface for the integration of a system of first order ODEs using a fixed order Runge-Kutta method until a user-specified function is zero.
- New approximate and exact Riemann solvers for 1-D Euler equations
- Solution of time dependent second order PDE's in 2D using adaptive mesh refinement.

New routines for generating and evaluating interpolants to 2D and 3D scattered data sets (using a modified Shepard interpolant) are included in the interpolation chapter.

The most significant additions to the optimization chapter are as follows:

- New routines to solve sparse LP and QP problems;
- New routines for unconstrained minimization with an extended parameter list to replace existing routines with reserved names
- A new reverse communication routine for constrained minimization using a sequential quadratic programming method.

Coverage in the sparse linear algebra chapter has been extended to provide interactive methods and preconditioners for real nonsymmetric linear systems of equations.

A new routine for finding the shortest path through a network is included in the operations research chapter.

For details, please see the new manual for Mark-18 at the Emerson Center.

Jamal Musaev, Applications Software Manager

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

Hardware Upgrades

In the last issue of the Newsletter we mentioned plans for the main fileserver upgrade at the Emerson Center. We are pleased to inform our user community that we have acquired an IBM 43P RS/6000 Power3 machine which has exactly the desired bandwidth and transmission speed as needed. In the future it will be possible to connect this machine directly to the SP2 via a 400MB/s fast "SP Switch Router" which eases file access tremendously.

In addition we bought a new 160GB RAID storage system which formally increases user disk space 5 times (the exact segmentation will be released and made available by the time this newsletter is in press). This additional equipment will make it more convenient to use the computational power of our new and upgraded SP2 system and will resolve disk space problems for users and the system management of the past.

Stephan Irle, System Manager

Having a place for Rent?

The Emerson Center is seeking accommodations for its Distinguished Visiting Fellow, Prof. William H. Miller of the University of California, Berkeley. Prof. Miller and his wife will be at the Emerson Center from Jan. 15 through mid-June 2000. They are interested in a furnished two-bedroom house or apartment close to Emory. If you have space for rent, please contact the Emerson Center at (404) 727-2380.

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*This issue of the Emerson Center Newsletter
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