EMERSON CENTER Newsletter

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In the News

- ◆ Emerson Center computers switched to the year 2000 without major problems. According to the cCenter's System Manager, Dr. Stephan Irle, the Center's system did run into some minor problems during the transition period, but they were not Y2K related. A full report by Dr. Irle is on Page 4.
- ◆ The Emerson Center has recently purchased more than a dozen reference books to add to its library collection. The new books, along with previous volumes, are available to all subscribers and users. Please see page 4 for a list of new titles.

◆ Emory College has approved the Emerson Center's request to add a third staff member to the Center who specializes in biomolecular modeling and graphics. This is a junior faculty-equivalent position. Hiring for the position will start shortly. This addition will help enhance the center's collaboration with BIMCORE, Biomolecular Computing Resources at Emory, also a subscriber to the Emerson Center.

EMERSON HALL CONSTRUCTION

Ground breaking for Cherry Logan Emerson Hall was held last May 16th. Since then construction of the building has progressed at a rapid rate. The first stage, during June and July, was the construction of an underground vault to handle services - hot water, steam, etc. - which had been located in the Atwood Hall chiller plant. Following that, the chiller plant was demolished and the foundation was begun.

The chiller plant "deconstruction" was carried out by perforating the walls with a small, but obviously powerful battering ram, and then knocking out each weakened section in turn. In order not to delay construction of the building itself, excavation and pouring of the foundation and the first floor columns were carried out simultaneously on the remaining area of the site.

Starting in September, with the chiller plant gone construction of the entire building began. The walls rose rapidly and by the first week in January virtually all of the concrete structure was poured. Perhaps the most remarkable aspect of the "rise" of Emerson Hall is not all of the

modern technology, e.g., laser "leveling", but the rather crude wooden framework that is constructed before the floors are poured. Even before all of the concrete work was done, however, interior installation of ductwork and piping began. At this time construction of the masonry walls is proceeding rapidly and some of the interior "sheet rock" walls on the first floor have been installed. We anticipate that the building will be finished and ready for occupancy in the late fall of this year. The Emerson Center will be occupying the top (5th) floor of Emerson Hall.



Cherry Logan Emerson Hall Construction Site

Update provided by Dr. David Goldsmith, Director, Phys. Sci. Facil. Development and Professor, Chemistry Dept.

BIOLOGY PROFESSOR AS TRIAL SUBSCRIBER

Dr. Christopher Beck, a new faculty member in the Department of Biology, has recently signed up for trial membership at the Emerson Center. Professor Beck's research interests related to the Center involve using genetic algorithms to determine the optimal solutions to questions in behavioral ecology. Since his research uses large population sizes and the simulations must be run for at least 40,000 cycles, the models are computationally intensive. After about one month's test, Dr. Beck said he is very satisfied with the facilities of the Emerson Center and is currently working on a proposal to be submitted to NSF for funding so that he can become a regular subscriber. Please refer to page 3 of this newsletter for a research report by Professor Beck.

PROPOSAL FOR MAJOR EQUIPMENT PURCHASE SUBMITTED

The Emerson Center recently submitted a proposal to the National Science Foundation's Major Research Instrument (MRI) program for the purchase of new computer systems for computational chemistry and chemical physics. Its principal investigator is Dr. Keiji Morokuma, Director of the Center, with co-investigators Drs. Joel Bowman, Michael Heaven, M. C. Lin, Dennis Liotta, James Snyder (Chemistry), Fereydoon Family, George Hentschel (Physics), Stephan Irle and Djamaladdin Musaev (Emerson Center), joined by James Nagy and Vaidy Sunderam of Math & Computer Science. If funded, a system consisting of a mix of clustered workstations and personal computers will be purchased to replace the aging SP2 system of the Center, to be installed at the new Emerson Hall in late 2000 or early 2001.

Letters from Fellows

9 am grateful to Professor Keiji Morokuma for inviting me to spend a month with his group. During this month we have started a joint study in which I have applied the ONIOM method to investigate the



on the thermodynamic stability of Si≡C triplybonded compounds. It turned out that one month was not sufficient to finish the project, and I am continuing the study from Israel, with the help and guidance of Dr. Thom Thom Vreven. has instructed me in my first steps with the ONIOM method, and I am thankful for his patience and help. It

was a privilege and pleasure to work with the people who develop the method and the code and to receive instant help whenever problems arose, and there were many. I would also like to thank Jamal, Robert, Stephan and Dima for their assistance with various computer problems and Jianli Zhao for arranging my visit.

I enjoyed the colorful fall in Emory. The beautiful neighborhood and pleasant weather made my short walks to the department a pleasure, and my stay in Emory a joy.

*Dr. Karni comes to the Emerson Center as a Visiting Fellow from Technion-Israel Institute of Technology, Haifa, Israel. She visited the center from October 1-31, 1999.

 $\mathcal{W}_{\mathcal{V}}$ visit at the Emerson Center in the hot August of 99 was very productive. The possibilities for everyday discussions with Professor Keiji Morokuma and the members of his research group, the excellent



computing facilities and the weekly seminars create an environment that stimulates the emergence of new ideas and ensures rapid progress on their realization. Although I had not thought of this before coming to

Dr. Peter Karadakov

Atlanta, it struck me during the first few days of my visit that Professor Morokuma's ONIOM approach would be the ideal way of including correlation effects into NMR shielding calculations on large molecules. Within the duration of my visit we managed to develop this idea fully and write a paper, which will appear shortly in Chem. Phys. Lett. I would like to thank everybody at the Emerson Center for being friendly and helpful and for making my visit not only productive, but also very enjoyable.

*Dr. Karadakov is Foundation Fund Lecturer at Univ. of Surrey, UK. He stayed at the Emerson Center as a Visiting Fellow in August 1999.

DEADLINE FOR **F**ELLOWSHIPS **E**XTENDED

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. The deadline for Emerson Center Visiting Fellowship applications for summer 2000-summer 2001 has been extended to March 1. 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).

EXTENDED DEADLINE: MARCH 1, 2000

My Emerson Center Days

Prof. David Wardlaw, Queen's University, Kingston, Ontario, Canada

Warm and sunny days, a beautiful campus, a stimulating research environment, and newly discovered colleagues come to mind as I reflect on my month-long stay at the Emerson Center last September. This was a productive and enjoyable part of my sabbatical from Queen's University. The sabbatical is now over but the renewal it provided is tangible.

There are many people who contributed to my positive experience at Emory. The Emerson Center staff were most helpful: Jianli ably steered me through the departmental and university bureaucracy, made arrangements for the apartment, and

directed me to local shops; Jamal and Stephan helped me through all the computer problems I usually encounter when exposed to a new computer system. My host, Prof. M.C. Lin, could not have been more gracious and hospitable. M.C. and I had a number of stimulating scientific discussions. His research group made me feel welcome. My interaction with the group was an important aspect of my visit. Thanks to the efforts of Dr. Park I was able to settle quickly into my office and began using the Lin group computer cluster. Within the Chemistry Department,



Prof. David Wardlaw

I am indebted to my physical and theoretical chemistry colleagues who treated me as part of that group from my first day. I particularly enjoyed the weekly departmental seminars and sharing meals with some of the speakers. Finally, I want to mention enriching scientific discussions with Profs. Keiji Morokuma and Joel Bowman and to thank Joel for including me in several of his group meetings.

My work as a Visiting Fellow was in collaboration with M.C. Lin and concerns theoretical modeling of rate constants for the recombination of radicals (or the reverse dissociation reactions). This type of process plays a major role in atmospheric and combustion chemistry. A distinguishing feature of such association reactions is the absence of a potential energy barrier. The most reliable and widely applied approach for predicting this type of rate constant is Flexible Transition State Theory (FTST). It is a specialized version of variational transition state theory, originally developed by Wardlaw and Marcus in the early 1980s. FTST has been systematically improved, both in a formal sense and in terms of computational appeal, in the 1990s. The stateof-the-art version of FTST is now encoded in a free software package called VariFlex (stands for Variable Reaction Coordinate Flexible Transition State Theory; authors are Dunbar, Klippenstein, Robertson, Wagner, and Wardlaw). The VariFlex package was installed on the Emerson Centre computer system. The package will be updated as new versions become available. I plan to return to these applications in the spring once classes are over.

*Dr. Wardlaw is Professor of Chemistry at Queen's University, Ontario, Canada. He stayed at the Emerson Center as a Visiting Fellow from August to October 1999 collaborating with Prof. M. C. Lin, one of the Center's Subscribers.

Emerson Center Subscribers & their Research Activities

The Emerson Center is supported, in part, by "subscribers" -- faculty members or research groups who purchase shares in order to gain access to the center's resources for their research projects. This section provides information about some of the Emerson Center subscribers and their research activities.

New Code Developed by EC Fellow

Prof. Joel M. Bowman Dept. of Chemistry, Emory Univ.

A code, 'MULTIMODE', which does accurate calculations of vibration/rotation energies and wavefunctions of polyatomic molecules, has been developed in collaboration with visiting Emerson fellow, Stuart Carter. This code is currently being interfaced with electronic structure codes by Dr. Stephan Irle. The first application in progress is to a calculation of vibrational energies of the water dimer using GAUSSIAN 98 at the CCSD(T) level of theory. A web site describing this code has been established. Its URL is www.emory.edu/CHEMISTRY/faculty/ bowman/multimode

BIMCORE & EC Collaboration

Dr. Kim M. Gernert Director, Molecular Modeling Center, Dept. of Biochemistry, Emory Univ.

BIMCORE, the BioMolecular Computing Resource at Emory, has become a subscriber of the Emerson Center to make their software available to our subscribers. The users of BIMCORE Molecular Modeling Center are currently active in a number of protein modeling procedures.

1. Homology modeling - the process of building a three-dimensional model of a protein sequence based on sequence similarity and sequence alignment to a protein of known structure. (Sybyl Composer and Modeller).

2. Threading - the process of aligning a protein sequence onto known structures and evaluating the fit based on amino acid preferences and packing energies. A three-dimensional model for the given sequence is generated based on a statistically significant fit with a known structure. (Sybyl Matchmaker and Threader).

3. Computational mutational analysis of a protein. Prediction of the changes of structure, stability, reaction mechanism and specificity of the protein due to specific amino acid mutations based on a given three-dimensional structure.

4. Prediction of protein - protein interactions based on protein surfaces, geometric fit and matching of chemical properties. (Sybyl FlexiDock, FTDock and Gramm)

5. Direction of development - drug searching, docking and design. Specifically, the design of peptides or peptide mimics to inhibit protein - protein interactions.

As projects proceed and the expertise needed overlaps with that available at the Emerson Center, BIMCORE would like to develop working collaborations with the members of the Emerson Center. For more informaton check out BIMCORE at http://www.bimcore.emory.edu.

Are Older Males Sexier than Younger Males?

Research Report by Prof. Chris Beck Dept. of Biology, Emory Univ.

Currently, I am investigating the effects of both male and female age on female mate choice decisions. In many species in nature, females prefer to mate with older males. The most common explanation for this preference is that older males are of higher genetic quality than younger males, because only high quality males should be able to survive to an old age. As a result, by choosing to mate with older males, a female can increase the genetic quality of her offspring. If females do indeed prefer to mate with older males, this could result in a decrease in the rate of aging for males!

My colleague Dr. Daniel Promislow (Department of Genetics, University of Georgia) and I have been exploring whether older males are of higher genetic quality (i.e., sexier) than younger males by using a genetic algorithm. In our model, the degree

of preference for males of a particular age is determined by the value for a given gene. By using a genetic algorithm, female preference for males of different ages is allowed to evolve over thousands of generations. If older males are sexier than younger males, females should evolve a stronger preference for older males and a weaker preference for younger males. Our preliminary results suggest



Effect of mortality rate on female preference

that when mortality rates in a population are low females prefer to mate with older males (see figure). However, as mortality rate in a population increases, females exhibit a greater preference for middle-aged males.

We are continuing to run simulations to see if the patterns of female preference that we have found previously are maintained over a greater number of generations. The facilities at the Emerson Center have been quite useful in carrying out these simulations. Our algorithm uses populations of 4,000 individuals, and we are currently running simulations for 320,000 generations. As a result, our simulations are quite computationally intensive (they last 24 hours on the SP2) and could not be done without access to a supercomputer.

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.

Y2K: SURVIVING THE BUG

Year 2000 has finally come, and fortunately we are still here, despite government warnings and common fears that the Y2K bug could potentially eradicate the human species. Some people argue that we survived due to the costly procedures of upgrading our computer systems, whereas others say that there was never a real problem at all.

In order NOT to find out what Y2K could do to the Emerson Center we upgraded the operating system and queuing system software of all computers in the summer of 1999. The system was successfully tested, and therefore we felt comfortable that no major glitch was to be expected from the millennium bug (we reported this in our last newsletter). However, feeling comfortable is OK, but feeling safe is of course much better. Therefore, we decided to make a double set of backup tapes from the entire file system (operating system, application software, utilities, and, last but not least, user home directories) in addition to our weekly home directory backups. Who could have known that exactly this Y2K PRECAUTION could lead to what looked like a Y2K PROBLEM? Apparently, the SCSI interface of the backup tape drive did not like to work so hard and decided to bring our file server to a halt. This happened on Dec. 29 during nighttime, and we were unable to bring the system back until we discovered on Jan. 2 that the tape drive had to be removed. After the culprit was disabled, the file server was able to reboot without any signs of the Y2K bug.

Stephan Irle, System Manger

New Features of Molpro 2000.1

A new version of the popular Molpro program, Molpro 2000.1, is now available at the Emerson Center. Compared to version 98.1, it includes the following principal changes and additions:

- 1. There was a fundamental error in the derivation of the spin-restricted open-shell coupled-cluster equations in J. Chem. Phys. 99, 5129 (1993) that is also reflected in the RCCSD code in Molpro version 98.1 and earlier. This error has now been corrected. Fortunately, it is not anticipated that any computed properties will have been significantly in error.
- 2. There was a programming error in the transformation of gradients from cartesian to internal coordinates, which in some cases resulted in slow convergence of geometry optimizations. The error is now fixed.
- Vibrational frequencies formerly by default used average atomic 3. masses, rather than those of the most common isotopes, which is now the default behavior.
- 4. MCSCF second derivatives added (preliminary version, only without symmetry). Frequency and geometry optimization programs are modified so that they can use the analytic hessian.
- New internally contracted multireference second-order perturba-5. tion theory code through command RS2C.
- 6. EOM-CCSD for excited states.
- QCISD dipole moments as true analytical energy derivatives. 7.
- Linear scaling (CPU and Memory) LMP2. 8.
- Improved handling of basis and geometry records. 98.1 dump files can be restarted, but in case of problems with restarting old files, add RESTART, NOGEOM immediately after the file card. Also, if there are unjustified messages coming up in very large cases about "ORBITALS CORRESPOND TO DIFFERENT GEOMETRY" try ORBITAL, record, NOCHECK. (This can happen for cases with more than 100 atoms, since the old version was limited to 100).

Other additions include: reorganization and generalization of basis input; increased basis set library; counterpoise geometry optimizations; important bug fixes for DFT grids, CCSD with paging, finite field calculations without core orbitals, and spin-orbit coupling; adding an interface to the graphics program MOLDEN, which allows visualization of molecular structures, orbitals, electron densities, or vibrations; improved *local* electron correlation methods, and many other internal changes.

As an additional service to the Molpro community, an electronic mailing list has been set up to provide a forum for open discussion on all aspects of installing and using Molpro. In order to subscribe to the list, send mail to majordomo@tc.bham.ac.uk containing the text subscribe

molpro-user; for help, send mail containing the text help. Messages can be sent to the list (molpro-user@tc.bham.ac.uk) and viewed in the archive at http://www.tc.bham.ac.uk/molpro/molpro-user/archive irrespective of whether or not you subscribe to the list. Please do contribute to make this resource mutually useful.

Jamal Musaev, Applications Software Manager

New Book Titles at EC

- 1. Anonymous, . Maximum Security: A Hacker's Guide to Protecting your Internet Site & Network, Indianapolis, IN: SAMS, 1998.
- 2. Arnold, Ken & James Gosling. The Java Programming Language, Reading, Mass.: Addison-Wesley, 1999
- Cannon, Casey, Scott Trent & Carolyn Jones. Simply AIX 4.3, Upper Saddle River, NJ: Prentice Hall, 1999.
- 4. Carasik, Anne. UNIX Secure Shell, New York: McGraw-Hill, 1999.
- 5. DuBois, Paul. Using csh and tcsh, Cambridge: O'Reilly & Associates, 1995.
- Gamble, Jesse & Bill Merrow. AS/400 System Administration Guide, New York: McGraw-Hill, N1995.
- 7. Lafore, Robert. Object-Oriented Programming in C++, 3rd Ed., Indianapolis, IN: SAMS, 1999
- Musciano, Chuck & Bill Kennedy. HTML: The Definitive Guide, 3rd Ed., Cambridge: O'Reilly, 1998.
- Newham, Cameron, & Bill Rosenblatt. Learning the Bash Shell, Cambridge: O'Reilly, 1998.
- 10. Patsis, Peter. UNIX awk & sed Programmer's Interactive Workbook, Upper Saddle River, NJ: Prentice Hall PTR, 1999.
- 11. Pitts, David, & Bill Ball, et al.. Red Hat Linux 6, Indianapolis, IN: SAMS, 1999.
- Pohl, Ira. C++ for Fortran Programmers, Menlo Park, Calif.: Addison-Wesley, 1997.
- 13. Skansholm, Jan. C++: From the Beginning, Reading, Mass.: Addison-Wesley, 1997.
 14. Spainhour, Stephen, & Robert Eckstein. WebMaster in
- a Nutshell, Cambridge: O'Reilly, 1999.
- 15. Witherspoon, Coletta & Craig. Red Hat Linux 6: Fast & Easy, New York: Prima Tech, 1999.

New Tape Library Backup System

The Emerson Center has acquired a new, more powerful backup system to protect the Center's software and user data from being destroyed and to guarantee data security. This tape library provides backup and random retrieval of up to 550 GB* on 8mm DLT tape cassettes. Its backup speed of 6MB/sec. allows for rapid access to the tape and thus enhances our data recovery service. It can be programmed to perform regularly scheduled backups, and we will create our weekly user data backup using this new device. In addition to this, we will back up the entire system every other month (also see the article "Y2K: Surviving the Bug"). If a user loses data or accidentally removes files from his home directory, we will be glad to restore this data upon request, provided the data is on the tape. Please feel free to use this service.

Stephan Irle, System Manger

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