EMERSON CENTER Newsletter

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

◆ ***Dr. Jamal Musaev promoted to Principal Scientist and Manager of EC***

Dr. Djamaladdin G. Musaev, Application Software Manager of the EC since 1993, has been promoted to Principal Scientist and Manager of the Emerson Center. This promotion was effective September 1, 2000. In addition to his continued responsibilities on application software, Dr. Musaev will take up some administrative and supervisory duties and will be mainly responsible for day-by-day operations of the EC. The Center and its user community look forward to Dr. Musaev's continued outstanding service.

IBM($625K) & NSF($300K) Provide New Supercomputer to Emerson Center

IBM recently announced a prestigious Shared University Research (SUR) Award to the Emerson Center for equipment for a retail value of approximately $625,000. The SUR Awards are provided to selected institutions to support research projects that are dedicated to research areas of mutual interest.

With a $300,000 Major Research Instrument grant from the National Science Foundation and the IBM SUR Award, supplemented with the Emerson Center Equipment Fund endowed by Dr. Cherry Emerson, the Center recently purchased and received the delivery of a new IBM supercomputer system consisting of 58 CPUs as well as 32Gigabtes of memory. With this new system, the Center's computing power has increased by about a factor of 8. The system has been installed and has been placed in service for research in computational chemistry, physics and biology since January 22.

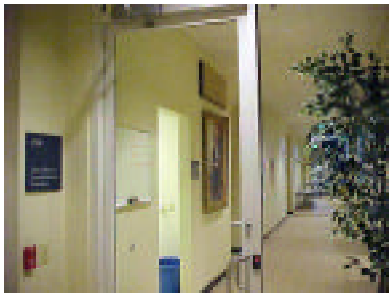
The EC is also in process of improving its graphics capability for molecular and biological modeling by purchasing graphics workstations with powerful computing and graphics engines.

Newly Purchased SP at EC

NEW EC EXECUTIVE COMMITTEE APPOINTED

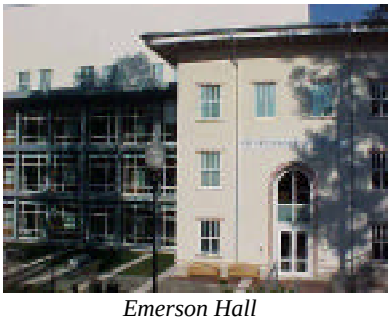
The new Executive Committee of the Emerson Center (ECEC) was appointed recently by the University Administration for a three-year term. Continuing as members are Profs. Keiji Morokuma (Emerson Center Director, Committee Chair), Michael Heaven (Chemistry) and Keith Wilkinson (Biochemistry). Newly appointed members are Profs. George Hentschel (Physics) and David Lynn (Chemistry), with Chemistry Dept. Chair Jay Justice serving as an ex officio *member. Acknowledgement is due to the leaving members who served the first three years on the Executive Committee: Profs. Joel Bowman and Al Padwa (both Chemistry). Please refer to page 2 of this newsletter for meeting minutes of the first meeting of the new ECEC.*

EMERSON CENTER MOVED TO EMERSON HALL



Entrance to the New EC

The Emerson Center was the first to move into the newly completed Cherry Logan Emerson Hall right after Christmas of 2000. The Center occupies about 80% of the fifth floor of Emerson Hall, and houses offices for three computational chemistry professors, three scientific staff and two administrative/secretarial staff members, graduate student/postdoctoral research laboratories, offices for visiting fellows, as well as computer rooms, a graphic laboratory and a seminar room. Next to Emerson Center are offices and laboratories for two Math/Computer Science faculty members.



Emerson Hall

Letters from Fellows

I would like to thank the Emerson Center for giving me the opportunity to spend two months in the Group of Prof. Heaven this past summer. My stay at the Emerson Center was incredibly pleasant and most educational in many ways. The excellent computational facilities made my stay at the Center very productive.

Coming from a small University in the South I enjoyed it very much having so many enthusiastic people around to talk with, who share my interest in theoretical chemistry. In particular I enjoyed the many quiet hours in the library reading up on the progress in my field, and not to forget my daily lunches and discussions with Prof. Heaven.

Dr. Udo Schnupf

I wish to express my deepest gratitude to Prof. Heaven for his guidance, his time, and his seemingly never-ending encouragements. My special thanks goes to Dr. Irle for his constant willingness to help, and for his resourcefulness in making Molpro work for my applications. In addition, I like to thank Dr. Eisfeld with whom I had so many stimulating discussions. Finally, I would like to thank the remaining members of the Emerson Center and Prof. Heaven's group for being so helpful in making my stay so enjoyable and fruitful.

**Dr. Schnupf is Assistant Professor at Dept. of Chemistry, Troy State University in Alabama. He visited the Emerson Center in June and July 2000.*

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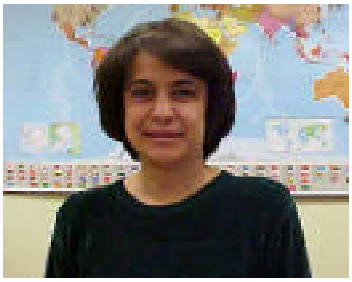
I arrived in Atlanta with the ambitious project to elucidate the role of divalent metal ions in the catalysis by RNA molecules. Catalytic RNAs, called now ribozymes, were first discovered in the 1980s. The concept of RNA as a catalyst raises the intriguing possibility of an "RNA world", one where RNA enzymes predated protein enzymes (which for many years were considered the sole catalytic moieties in the cell) and catalyzed all biochemical reactions.

My really exciting project quickly revealed itself a computationally formidable task - I was hardly able to handle even the smallest possible model system in a reasonable time. As usually computational problems of this size are considered the realm of QM/MM calculations, I performed, in collaboration with Prof. Keiji Morokuma and Dr. Thom Vreven a series of benchmark calculations to explore the applicability of ONIOM to RNA hydrolysis and the results brought my happiness back - now I can model the reaction mechanism much faster. And after the upgrade of the PC cluster and the quick installation of the new 58 CPU SP Computing server in January, for which special thanks are due to Drs. D.Musaev, S.Irle and D.Khoroshun, the computing



Dr. Snezhana Bakalova

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Emerson Center Visiting Fellowship Awards for 2001-2002

Dr. Valentine P. Ananikov , ND Zelinsky Inst. of Organic Chemistry, RUSSIA
Prof. Kaori Ando , University of Ryukyus, JAPAN
Dr. Snezhana M. Bakalova , Bulgarian Academy of Sciences, BULGARIA
Prof. Feliu Maseras , University of Barcelona, SPAIN
Prof. Jerzy Moc , Wroclaw University, POLAND
Dr. Laszlo Nemes , Hungarian Academy of Sciences, HUNGARY
Prof. Ilkay Oren , University of Ankara, TURKEY
Prof. Udo Schnupf , Troy State University, USA
Prof. Jonathan E. Stevens , University of Detroit Mercy, USA
Dr. Rongshun Zhu , Chinese Academy of Sciences, CHINA

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.

News from the Executive Committee Meeting

The newly appointed Emerson Center Executive Committee (ECEC) met on Friday, February 9 from 2:00pm to 3:30pm at the newly completed Emerson Center Conference Room on the top floor of Emerson Hall. After introducing the new committee members, Prof. Keiji Morokuma, Director of the center, gave a detailed administrative report about the center, including membership, budget issues, the EC newsletter, and search status of the third staff member for the EC. Prof. Morokuma also introduced to the committee Dr. Jamal Musaev, who has recently been promoted to Principal Scientist and Manager of the Emerson Center. Dr. Musaev then reported on the technical aspects of the center, including status of the new Primary Server System and other secondary systems, and on recent activities of the Technical Subcommittee for Graphic Server System purchase. The ECEC also approved at the meeting the 2001-2002 EC Visiting Fellowship Awards to 10 applicants from 9 different countries. Award details are listed above.

ECEC members, from left to right, Profs. J. Justice, M. Heaven, K. Morokuma, G. Hentschel, D. Lynn, and K. Wilkinson (not in picture).

power is increased several times and optimizations run much faster.

In my opinion the Emerson Center Fellowships program gives visitors the wonderful opportunity to use up-to-date computer facilities to work on their own projects. At the same time one enters a really pleasant working environment and has the opportunity for helpful and stimulating discussions with all the members of the group.

Finally I would like to say THANK YOU to Prof. Morokuma and all the colleagues who make my stay so enjoyable and useful.

**Dr. Bakalova has been staying at Emory as an EC Visiting Fellow since Oct. 1, 2000 . She is also Research Fellow at the Institute of Organic Chemistry at the Bulgarian Academy of Sciences.*

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. EC technical staff members are also encouraged to conduct scientific research in your own areas of specialty. The following is research report from one of the center's staff members.

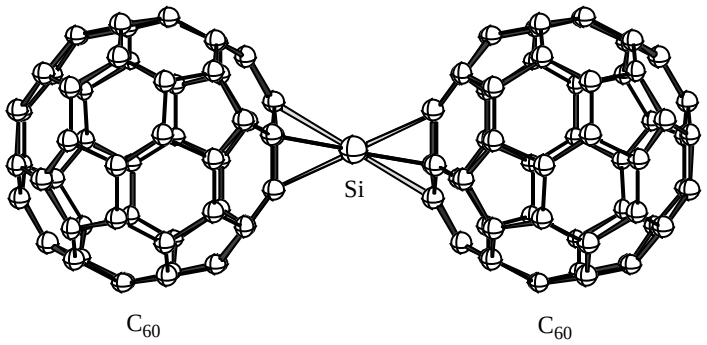
Exploring the World of Nanotechnology and Molecular Science by Means of Quantum Chemical Methods

Research Report by Dr. Stephan Irle
Associate Scientist
Emerson Center, Emory University

Until perhaps two decades ago, carrying out computational chemistry was certainly not as comfortable as it is today, given the enormous amount of time that was required for calculating even just the wave function of very simple molecules (not to mention geometrical parameters). Luckily, my research career in Theoretical Chemistry fell together with the advent of more and more powerful workstations and supercomputers, easier program inputs, and sophisticated algorithms (like gradient optimizations and "direct" methods) which allow to treat complex large systems within a reasonable amount of computational time and available storage space. Thus, it was possible for me to finish a detailed ab initio study on the conduction mechanism of doped organic conjugated polymers within the time frame acceptable for a Ph.D. thesis. Nowadays, nanotechnology has become a rapidly growing area of tremendous importance in electronics and micro engineering. This exciting research field brings together physics, chemistry, mechanical engineering, and computer science, and new applications of molecular structures emerge in all these areas on an almost daily basis.

Due to the enormous size of these systems, mostly classical molecular mechanics approaches have been employed in the past. However, in order to investigate e.g. binding energies of substrates on nanostructures, it is crucial to use electronic structure methods in order to describe bond formation/breaking processes. The ONIOM method (developed at Emory by Prof. Morokuma's group) allows to partition large systems into two or more parts or layers, where the interesting or difficult part(s) of the system (the inner layer) is treated at a high level of theory and the rest of the system (the outer layer) is described by a computationally less demanding method. I (in collaboration with Prof. Keiji Morokuma) am carrying out several studies in this exciting new field of material sciences, including 1) functionalization of carbon nanotubes by [2+2]- and [2+4]-cycloaddition reactions, 2) chemically controlled insertion of metal atoms into C_{60}, 3) investigation of interaction energies between probe molecules and data atoms on C(111) and S(111) surfaces in the context of binary data storage, and 4) investigation of binding mechanisms between silicon atoms and buckyballs as recently proposed structures based on mass spectroscopic data (see figure). Our work is carried out in collaboration with other theoretical and experimental groups, such as Prof. Yves Rubin (UCLA), Dr. Charles Bauschlicher (NASA), and Prof. Michel Broyer (Université C. B. Lyon, France).

But my research interest is not exclusively restricted to large molecular systems. Small molecule reactions are a fascinating field where theory can accompany experimental research very fruitfully. In another collaboration with Prof. Morokuma, I have studied gas phase chemical reactions of $CH_4 + O_2^+$ (J. Chem. Phys., in press), $C_2H_2^+ + CH_3OH$ (J. Chem. Phys. **111**, 3978 (1999)), and the photodissociation of propane (J. Chem. Phys. **113**, 6139 (2000)). Experimental collaborators in this area include Dr. Albert Viggiano (Air Force) and Prof. Scott Anderson (University of Utah).



In a collaboration with Emerson Center subscriber Prof. Joel Bowman, I have performed the direct ab initio variational calculation of vibrational energies of the water···Cl^- complex (J. Chem. Phys. **113**, 8401 (2000)), and we were able to distinguish between two sets of conflicting experimental data sets. Currently we are working on a highly accurate 4-dimensional PES for the protonated water dimer in order to shed light on the controversial infrared spectrum of its O···H···O fragment. For the future, I am looking forward to carrying out more fruitful collaborations especially with our Center's subscribers, and to attack exciting problems together with experimental groups here at Emory.

Want to Be a Subscriber?

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.

Technical Aspects of Emerson Center's Computing Resources

Jamal Musaev, Principal Scientist & Manager
Stephan Irle, Associate Scientist & System Manager
Emerson Center

As you may already know, the Emerson Center has moved into a new building, Emerson Hall, and has recently purchased a new Computing Server (see also page 1 of this newsletter). We have installed our old and new computational equipment at their new location and made them available to our user community. The following is a summary of our computer resources:

I. Our old workstations consists of 15 machines total, including euch2c, euch2d, euch3g, euch3h, euch3f, euch4c, euch4d, euch5c, euch5m, euch6i, fractal, euch3e, euch4e, euch6h and euch5m. Three of them (euch3e, euch4e and euch6h) will be used for special purposes rather than computing power.

II. Our old SP2 (referred to as SP2 below) has 14 nodes/processors with a 160 MHz speed and POWER2 Superchip. Each of these nodes has 256MB memory and 3GB disk space, except pp5 and pp6, which has 512MB memory. We have called these nodes ppx.chem.emory.edu, where x=1-14. All nodes are connected with a high performance switch.

III. The newly purchased IBM RS/6000 SP3 system consists of fifteen thin nodes in a single frame. We have called these nodes spx.chem.emory.edu, where x=1-15. Fourteen of the nodes are equipped with four 375 MHz POWER3 SMP CPU's and a total of 2GB RAM each, and one node (sp2.chem.emory.edu) for memory intensive applications contains 2 CPU's of the same type with a total of 4GB RAM. Each of the fifteen nodes are equipped with a total of 32 GB disk on two separate 10,000 RPM SCSI hard disks for better performance. The nodes are connected to the new control workstation, a powerful RS/6000 44P Model 170 with one 350 MHz POWER3 CPU. Nodes and control workstation operates at a network speed of 100Mbps. No IBM SP switch is needed for the new system, because the nodes with a SMP type architecture already provides enough capability for parallel processing on individual nodes for typical applications in quantum chemistry. Therefore, our old SP2 system and the new system are separate computer systems, with the new system being overall about 8 times more powerful than the old one. However, to the users they appear as a single computational resource, accessible by the center's LoadLeveler batch queueing system.

EC File Server

In order to utilize these different resources efficiently, we reorganized the queueing system and implemented the following rules regulation access to the system:

I. On the old workstations: There is no limit and each user group can submit as many jobs as they want. We have set up the following classes for these workstations: "fast" - up to 1h calculations; "quick" - up to 6h calculations; "normal" - up to 24h calculations; "slug" - up to 48h calculations, and "bigfoot" for euch3f, which has more memory than other workstations. Recommended features (scratch disk space) are "small", "medium", and "big".

II. On the old SP2: We propose to keep the existing share system, e.g. 1 job submission for each 0.25 share, 2 job submission for 0.5 share, 4 job submission for 1 share, and so on. Recommended classes for this system are: "fastp2" - up to 1 hour calculations, "quickp2" - up to 6 hours calculations, "onedayp2" - up to 24h calculations and "twodayp2" - up to 48h calculations. All nodes have 2GB scratch disk space and there is no need to specify "feature" in your loadleveler command (.cmd) files. Five machines have been set up for "twodayp2" class, thirteen machines can run "onedayp2" class, and all fourteen can pick up "quickp2" and "fastp2" classes.

III. On the new SP3: We propose to have EIGHT job submission per share (TWICE compared to old SP2), which is equivalent of 2 job submission per 0.25 share, 4 job submission for 0.5 share, 8 job submission for 1.0 share, and so on.

Left: Old SP2; Right: New SP3

Two nodes, sp5 and sp6, are dedicated for parallel jobs with the following classes: "fparallel" - up to 30 min calculations, "qparallel" - up to 3 hours calculations "hparallel" - up to 12h calculations and "oparallel" - up to 24h calculations. Since each node has very large disk space, there is no need to set up "feature" in your loadleveler command files. We have assigned only one job per node.

Node sp2 with 2 processors and 4GB RAM are assigned for TWO special queues with one processor and 2GB memory each. The classes assigned for these special calculations are "fspecial" - up to 2 hour calculations, "qspecial" - up to 24 hour calculations, "hspecial" - up to 48 hour calculations and "ospecial" - up to 96 hours calculations. Again, there is no need to specify the "feature" in your calculations.

Other nodes (with a total of 48 processors) are assigned for sequential calculations: e.g. one process – one job. NO parallel jobs are allowed. Classes assigned for these calculations are: "twodayp3" - up to 48h calculations, "onedayp3" - up to 24h calculations; "halfdayp3" - up to 12h calculations, "quickp3" - up to 6h calculations, "fastp3" - up to 1h calculations. Each Node is going to run FOUR jobs (job/per processor). Again, since we have plenty of disk space on these nodes, there is no need for specifying "feature" on your .cmd files. There is a total of 12 processors assigned for "twodayp3" calculations, 32 processors assigned for "onedayp3" class, 44 processors assigned for "halfdayp3" class, and all 48 processors assigned to pick up "quickp3" and "fastp3" jobs.

In conclusion, after the new SP3 was put in operation, the number of job submissions per share has been increased by MORE THAN THREE TIMES, and computing power of our subscribers is increased by more than SIXTEEN TIMES !!!

Our observation on the operations of the new system indicates that the current system utilization is already about 80% on the average, which means that the purchase of new SP3 system was anxiously awaited for by our user community.

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