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Fifteen Years of the Car-Parrinello Method in Physics and Chemistry

Michele Parrinello (Max Planck Institute) and Roberto Car (Princeton University), center left and center right, are presented plaques by the conference organizers Sokrates Pantelides (Vanderbilt University), left, and James Chelikowsky (University of Minnesota), right.

A workshop to honor the originators of the Car-Parrinello Method and to review major accomplishments and cutting-edge developments within the general area of molecular dynamical simulations was held March 18–19, 2000, at the University of Minnesota Supercomputing Institute for Digital Simulation and Advanced Computation.

The Car-Parrinello method, introduced in 1985 by Roberto Car (Princeton University) and Michele Parrinello (Max Planck Institute), has dramatically influenced electronic structure calculations for solids, liquids, and molecules, and initiated the field of quantum molecular dynamics among physicists. Molecular dynamics is a simulation method wherein the trajectories of individual atoms or molecules are integrated, usually using Newtonian dynamics. These simulations have provided us with great insights into the dynamical and structural properties of matter, such as the microstructure of the liquid state and the diffusion of impurities in crystals.

A key ingredient in this formulation is the description of interatomic forces. Prior to the invention of the Car-Parrinello algorithm, one typically constructed interatomic potentials either from experimental data or from other indirect theoretical methods. These

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classical methods often worked quite well for some systems (e.g., inert gases), but were not generally reliable for systems with complex bonds (e.g., covalent or partially covalent bonds where the interatomic potentials are inherently many-body ones).

The Car-Parrinello method deals directly with a quantum description of the electronic structure for the system of interest. In the Car-Parrinello algorithm, the electronic degrees of freedom are simultaneously evolved quantum mechanically along with the nuclear degrees of freedom, which are treated by a classical description. Within the Car-Parrinello algorithm the resulting interatomic interactions are fully quantum mechanical in nature—no ad hoc assumptions need be invoked.

Norm Troullier (University of Minnesota), José Martins (Instituto Superior Técnico, Portugal), and Renata Wentzcovitch (University of Minnesota) discuss the presentations during a break. Morel Cohen (Exxon Research and Engineering) and Richard Martin (University of Illinois, Champaign-Urbana) stand in the background to the right.

The Car-Parrinello method has led to an explosive growth and interest in accurate modeling and simulating a wide variety of condensed matter systems. Applications of this approach can be performed on liquids (both metals and insulators), clusters, disordered solids, biological systems, defects, and surfaces. It has also led to the development of a number of related algorithms for handling large and complex systems.

Ursula Röthlisberger (ETH Zentrum, Switzerland) and Sandro Scandolo (International School for Advanced Studies) during the workshop's reception.

Roberto Car and Michele Parrinello have both received a number of awards and recognition for their work; for example, the 1995 American Physical Society Aneesur Rahman Prize for Computational Physics was awarded to Car and Parrinello for the development of their algorithm. Aneesur Rahman, for whom the prize is named, was instrumental in the development of the molecular dynamics method. He performed the first realistic molecular dynamics computations and was a professor of physics at the University of Minnesota in the 1980s.

The Supercomputing Institute and IBM sponsored this meeting and it was endorsed by the American Physical Society. Over 80 distinguished scientists attended the workshop, including 24 from 11 countries outside the United States.

The meeting began with a plenary talk by Roberto Car. He spoke on using simulation methods for optimizing multivariable functions. This is a generic, fundamental problem in many fields. For instance, one might want to minimize a complex energy functional by varying a large number of parameters. These parameters might correspond to both electronic and nuclear degrees of freedom. Car outlined a new and novel approach using what he called quantum annealing.

In the following talks, Marvin Cohen (University of California at Berkeley) spoke about the contributions of pseudopotential theory to ab initio molecular dynamics. In particular, he noted that pseudopotential approach allowed one to focus only on the chemically active electrons and made it possible to compute accurate interatomic forces. This observation established the starting point for the Car-Parrinello algorithm. Giulia Galli (Lawrence Livermore National Laboratory) spoke about recent ab initio simulations of water under high pressure. This work extracted unexpected and complex microstructures

Giulia Galli (Lawrence Livermore National Laboratory) and Alfredo Pasquarello (IRRMA, Switzerland) enjoy a few minutes between presentations.

present in a relatively simple liquid. Leonard Kleinman (University of Texas at Austin) followed this theme by outlining the properties of liquid metals such as sodium obtained using ab initio molecular dynamics. Michiel Sprik (Cambridge University) used a similar technique to examine reactions in aqueous solutions. The last speaker in the morning session was Paolo Carloni (International School for Advanced Studies, Trieste). He presented an overview on recent applications of the Car-Parrinello algorithm to understand complex biological molecules. A long-range application of this work would involve drug design and gene therapy.

In the afternoon session, Sokrates Pantelides (Vanderbilt University) discussed extensions of the Car-Parrinello method to excited state systems, applications which can be observed in the absorption of light and the propagation of electronic current through micromolecules, among other examples. Jerzy Bernholc (North Carolina State University) followed his talk, discussing simulations of nanotubes and their mechanical properties using molecular dynamics. Nanotubes are microscopic tubes of carbon that have novel electronic and structural properties. Chris Van de Walle (Xerox) gave an overview of defects and impurities in semiconductors such as gallium nitride. These systems are highly relevant for work within the electronics industry. Ursula Röthlisberger (ETH Zentrum, Switzerland) gave examples of Car-Parrinello simulations in the area of biochemistry, for example, the study of enzymatic reactions. Her talk also illustrated how one could combine molecular mechanical descriptions of these systems with quantum forces. J. Woods Halley (University of Minnesota) concluded the session by discussing water interacting

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with metal surfaces. This is an important system for electrochemical processes.

Michele Parrinello started the second day of the meeting with a plenary talk on spectroscopic properties of disordered and liquid systems using Car-Parrinello molecular dynamics. He addressed fundamental issues involved in predicting the low frequency response functions for amorphous semiconductors and water. The following talks focussed on silica and related materials. Don R. Hamann (Lucent, Bell Labs) outlined a computational method based on adaptive coordinates for examining the electronic and structural properties of pure and doped silica. Peter Blöchl (IBM Zürich Research Laboratory, Switzerland) spoke on zeolites. Zeolites are complex silicates used for catalytic processing as seen in the petroleum industry. He illustrated the Car-Parrinello method by considering methanol and water in zeolitic systems. Alfredo Pasquarello (Institut Romand de Recherche Numerique en Physique des Materiaux, Switzerland) talked about the silicon-silica interface, which plays a crucial role in all electronic devices using silicon wafers.

Don R. Hamann (Lucent, Bell Labs) and Peter Blöchl (IBM Zürich Research Laboratory, Switzerland) compare their research during a break between presentations.

The morning session ended with talks on materials of interest in earth science and geology, as well as the behavior of matter under extreme conditions. Renata Wentzcovitch (University of Minnesota) outlined how ab initio molecular dynamics can be used to predict the elasticity of materials as a function of pressure and temperature. Her work has direct relevance for describing the earth's interior and constructing seismological models. (See article on p. 6.) Sandro Scandolo (International School for Advanced Studies also considered simulations to describe the behavior of matter under pressure and temperature; however, his work focused on non-terrestrial systems such as the planet Neptune.

The afternoon session was comprised of four talks. Richard Martin (University of Illinois at Champaign-Urbana) presented the first, examining methods for improving the efficiency of the Car-Parrinello method to large systems. Most quantum calculations scale in time as some power of the number of atoms considered. For example, if there are N atoms in the system, the computational load might typically scale as N^3 for a quantum simulation, whereas a classical simulation would scale linearly with N. Martin's work focused on developing algorithms for quantum systems that scale as classical systems. David Vanderbilt (Rutgers University) presented some simulations for surface dynamics. In particular, he illustrated how Al atoms move on the surface of the metal. Matthias Scheffler (Max Planck Institute) also examined surface diffusion for semiconductors such as GaAs and related growth methods for these systems. Wanda Andreoni (IBM Zürich Research Laboratory, Switzerland) presented the last talk of the meeting. She used Car-Parrinello simulations to examine the optical and electronic properties of complex inorganic and organic salts on metal surfaces such as gold. ■

Text Mining Workshop

Text mining is a new interdisciplinary field. It is related to data mining, a relatively mature technology, typically applied to the analysis of data stored in structured databases. Text mining seeks to apply some of the same types of analysis, such as knowledge discovery, or trend analysis, to unstructured textual data that data mining applies to structured data. Text mining combines the disciplines of data mining, information extraction, information retrieval, text categorization, probabilistic modeling, linear algebra, machine learning, and computational linguistics to discover structure, patterns, and knowledge in large textual corpora.

Part of the "Hot Topics" Workshop Series presented by the Institute for Mathematics and its Applications (IMA), the workshop on Text Mining was organized by James Allan of the University of Massachusetts, Vipin Kumar of the Army High Performance Computing Research Center at the University of Minnesota, and Paul Thompson of the West Group. It was sponsored by the Army High Performance Computing Research Center, the Supercomputing Institute, and the West Group.

Advances in computational resources and new statistical algorithms for text analysis have helped text mining develop as a field. This two-day workshop brought together leading researchers in this new field, representing its various constituencies, including computer science, mathematics and statistics, information retrieval, and artificial intelligence. Within the text mining community, there is still no consensus when it comes to an exact definition for text mining. One of the purposes of this workshop was to help the community come closer to such a consensus. More generally, it provided an opportunity to share research among the diverse groups represented at the workshop.

Chris Wolff of the West Group started off the program by talking about Extensible Markup Language (XML) and the role it plays in the West Group. Other talks of the day included Dharmendra Modha of IBM Almaden, Daniel Boley of the University of Minnesota, Michael W. Berry of the University of Tennessee, Inderjit S. Dhillon of the University of Texas at Austin, George Karypis of the University of Minnesota, Marti Hearst of the University of California at Berkeley, Michael Steinbach of the University of Minnesota, Thomas Hoffman of Brown University, David Lewis of AT&T Labs, and Ralph Weischedel of BBN Technologies.

Isabelle Moulinier (West Group), Jaime Carbonell (Carnegie Mellon University), and Dan Melamad (West Group) discuss a point raised during Carbonell's talk.

The second day started with a talk by Jaime Carbonell of Carnegie Mellon University. Carbonell spoke of prospecting for novelty in text mining and measures of novelty including maximal marginal relevance in multi-document summarization. Other speakers included Lucy T. Nowell of Battell/PNNL, Breck Baldwin of Baldwin Language Technologies, David Jensen of the University of Massachusetts–Amherst, Peter Jackson of the West Group, Henry Lieberman of MIT, and Eui-Hong (Sam) Han of the University of Minnesota. ■

First-Principles Thermoelasticity of Earth's Mantle Materials

The last decade has witnessed rapid progress in seismological observations of the three-dimensional structure of the Earth's mantle. The deep interior has been revealed to be approximately isotropic and radially symmetric, reflecting the dominant role of gravitational self-compression and depth-dependent variations in temperature and bulk composition. Deviations from the spherically averaged radial profile, though small, are significant because they are intimately linked to geodynamical processes. For example, the seismic anisotropy may be produced by the shear deformation associated with mantle flow, whereas the lateral heterogeneity presumably reflects lateral variations in temperature as well as in phase assemblage and bulk composition.

Seismological observations help address fundamental questions such as compositional stratification, geotherm, mantle dynamics, and the relation between deep mantle with surface plate tectonics, which ultimately bear on our understanding of the history and genesis of the earth itself. Such promise can only be fulfilled if there are advances of similar magnitude in understanding the physics of mantle minerals. A combination of seismology and mineral physics is often taken as a powerful probe of the deep interior. For instance, comparisons of elastic wave velocities of likely mineral assemblages with the seismic data help to ascertain which mineralogical model can best reproduce the seismic structure of the mantle and represent the composition of this region.

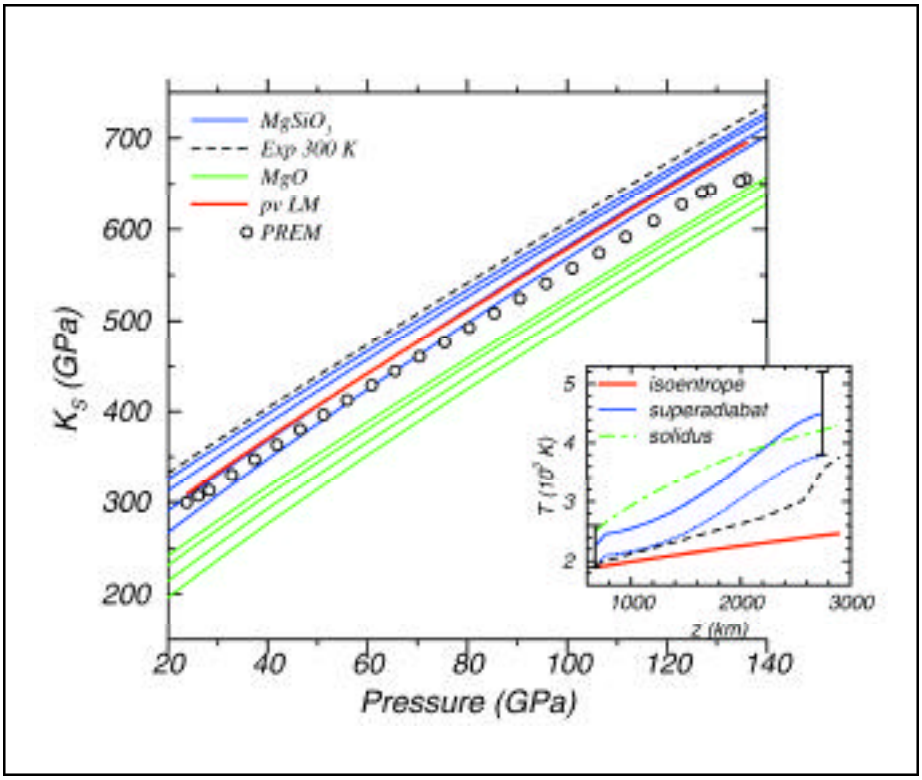

Figure 1: Temperature dependence of the coefficient of thermal expansion α of $MgSiO_3$ perovskite along isobars at 0, 25, 50, 100, and 150 GPa (solid lines from top to bottom). Experimental values of α $\{T_1–T_2\}$ averaged over different temperature ranges are represented by circles at zero pressure, by diamonds in the 47 to 52 GPa range, and by triangles in the 88 to 94 GPa range.

Towards providing a firm basis to relating the seismic features to geodynamical process and to the thermal and chemical state of the deep interior, Professor Renata Wentzcovitch (Chemical Engineering and Materials Science, and Supercomputing Institute Associate Fellow), and her post-doctoral associate and Supercomputing Institute Research

Scholar, Dr. Bijaya Karki (Chemical Engineering and Materials Science), study important geophysical properties such as phase relations, thermal equations of state, elastic wave velocities of the major silicate and oxide phases of the mantle at the extreme pressure-temperature conditions (P to 136 GPa and T to 4000 K). They apply first-principles approaches within the framework of density functional theory. Their recent work focusses on temperature-dependent properties by calculating full phonon dispersions of minerals to include the thermal contribution of the crystal free energy within the quasi-harmonic approximation. These calculations offer crucial results of geophysical interest, including the thermal expansivity (Figure 1) and elastic moduli. The results show an excellent agreement with available experimental data in a limited range of pressures and temperatures.

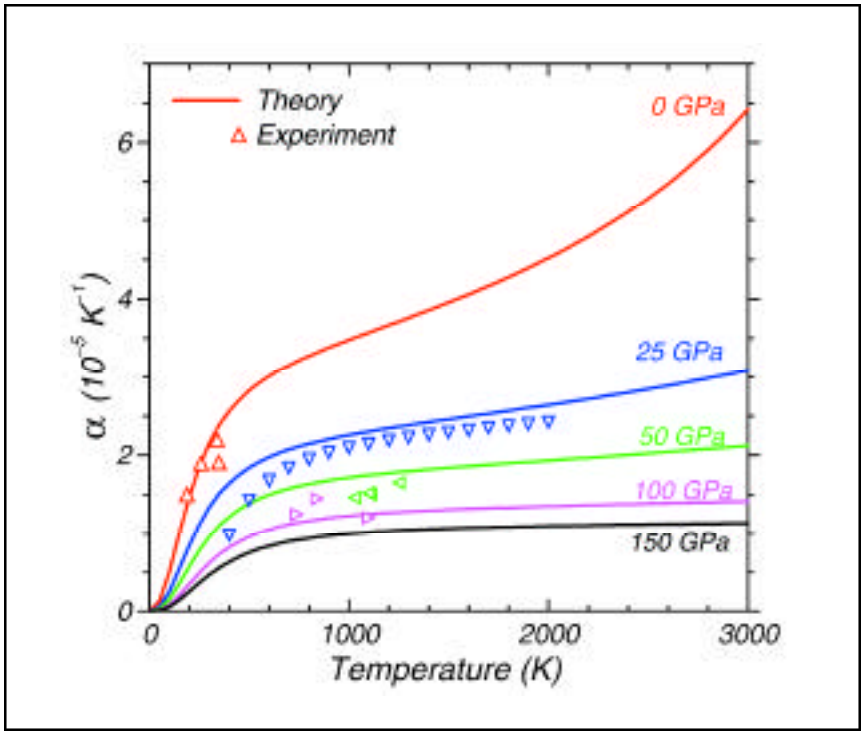

Figure 2: Pressure variations of the calculated adiabatic bulk modulus (K_s) of $MgSiO_3$ perovskite (solid lines) and MgO (dotted lines) along 300, 1000, 2000 and 3000 K isotherms (from top to bottom). The grey line represents K_s of a 100 V% perovskite lower mantle along the calculated isentrope (thick grey line in the inset). The symbols are the seismic data from preliminary reference Earth model. The dashed line is the 300 K bulk modulus of perovskite derived from experiments. The inset shows the temperature-depth ($T(z)$) profiles inferred for pure perovskite (solid line) and pyrolite (dotted line) lower mantle model by comparing the calculated bulk modulus with seismic data. An earlier super-adiabatic geotherm is shown by a dashed while an earlier adiabatic geotherm is indistinguishable our isentrope. The lower mantle solidus line appears as a dash-dotted line.

Direct comparison between the predicted adiabatic bulk modulus of $MgSiO_3$ perovskite, thought to be the most abundant phase of the lower mantle, with the seismic radial profile provides enlightening information (Figure 2). It suggests that an adiabatic and homogeneous compositional model is incompatible with the lower mantle. A 100% perovskite model would require temperatures near or above the solidus, and thus, a pyroxene-type composition (perovskite + MgO) appears to be more appropriate. This is direct evidence for the composition of the lower mantle, which is of central importance to earth science. The results also indicate that the origin of the observed seismic lateral velocity heterogeneities can be attributed to a great extent to lateral variations of temperature. Investigation of the full elastic constant tensor in perovskite is now important to verify the elastic wave velocities and the anisotropy of this mineral. This research is performed in collaboration with Professor Shun-i Karato from the Department of Geology and Geophysics.

Monte Carlo Calculations for Alkanes, Alcohols, Water, and Their Mixtures

The partitioning of a solute molecule, a drug, or a pollutant between a polar aqueous environment and a non-polar organic environment—for example, a biological membrane or soil—is often the critical step in biological, environmental, and geological processes. The 1-octanol/water partition coefficient, K_{OW}, and the corresponding Gibbs free energy of transfer

$$\Delta G_{OW} = -RT \ln K_{OW}$$

for a given solute are therefore widely used in quantitative structure-activity relationships and have been used to correlate or predict a plethora of solute properties, including the pharmacokinetic characteristics of drug compounds in biophases (membranes, adipose tissue, and body fluids) and the toxicity and transport of pollutants in soil/groundwater systems. The 1-octanol molecule consists of a hydrophilic head and a lipophilic tail leading to a microheterogeneous solvent phase which has been found to mimic particularly well the complexities of biological membranes. It has been estimated that experimental K_{OW} are now available for more than 18,000 solutes, but this number is much less than the number of possible drug molecules or possible pollutants that can be synthesized.

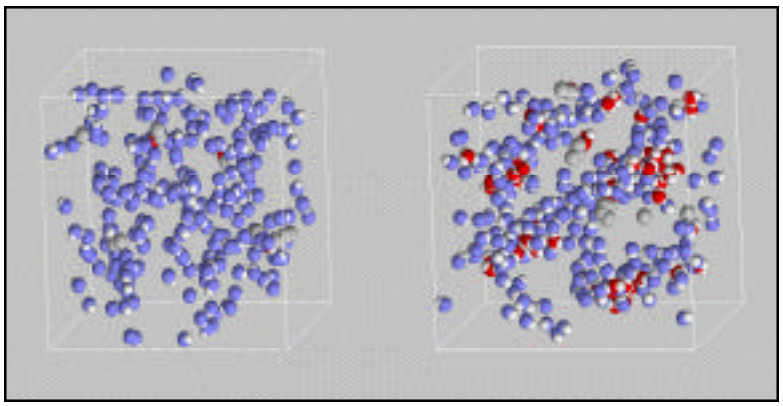

Figure 1: Using the computing resources of the University of Minnesota Supercomputing Institute, graduate student Bin Chen and Professor J. Ilja Siepmann (Department of Chemistry and Supercomputing Institute Fellow) have carried out Monte Carlo simulations to investigate the partitioning of normal alkane and primary alcohol solutes between water and l-octanol phases. These illustrations are snapshots of the dry (left) and water-saturated (right) 1-octanol phase. The gray, blue, red, and white spheres depict alkyl groups of solute molecules, oxygen atoms of 1-octanol, oxygen atoms of water or solute molecules, and hydrogen atoms, respectively. The alkyl tails of 1-octanol are omitted here for clarity.

Using computer resources provided by the Supercomputing Institute, graduate student Bin Chen and Associate Professor J. Ilja Siepmann (Department of Chemistry and Supercomputing Institute Fellow) have carried out Monte Carlo simulations to investigate the partitioning of normal alkane and primary alcohol solutes between water and (dry or wet) 1-octanol phases. These simulations make use of the MC3S (Monte Carlo for Complex Chemical Systems) molecular modeling package and of the TraPPE (Transferable Potentials for Phase Equilibria) force field which are both under development in the Siepmann research group. Configurational-bias Monte Carlo simulations in the Gibbs ensemble allow for the determination of ΔG_{OW} from the ratio of the solute number densities in the two coexisting phases. Comparison of the partitioning between a helium vapor phase and dry and wet 1-octanol established that water saturation has a much larger effect on the partitioning of polar solutes, than on alkane partitioning. Analysis of the structure of the wet 1-octanol phase (Figure 1) shows preferential partitioning of short alcohols (methanol and ethanol) into the water-rich regions of the solvent, whereas

1-butanol solutes are found preferentially at the boundary of hydrogen-bonded clusters.

Mixtures of alkanes and alcohols are of great importance for the petrochemical industries. However, the prediction of their phase behavior is difficult because hydrogen bonding can result in non-random mixing and a departure from ideal solution behavior. Graduate student John Stubbs has investigated the self-aggregation of 1-hexanol in *n*-hexane-rich binary solutions at ambient conditions (Figure 2). The 1-hexanol molecules prefer to self-assemble in clusters with 4 or 5 molecules consisting predominantly of cyclic structures, similar to those found in gas-phase water clusters. Approximately one in six 1-hexanol molecules is found a free monomeric species, and the fraction of dimers is very low. The strong preference to form hydrogen-bonded clusters is also reflected in the unusually large first and second peaks in the oxygen-oxygen radial distribution functions (Figure 3).

In addition to the two research projects described above, other members of the Siepmann research group are working on many related problems. Supercomputing Institute Research Scholar Jeffrey Potoff is investigating mixtures of non-polar and quadrupolar molecules, such as the ternary phase diagram of propane/dinitrogen/carbon dioxide. Graduate student Collin Wick is studying the effects of interfacial adsorption on the retention characteristics of alcohols and alkylbenzenes in helium-squalane gas-liquid chromatography. Graduate student Ling Zhang explores the influence of semifluorinated hydrocarbons on the solubility of alkanes in perfluoroalkanes. This research receives support from the National Science Foundation, Divisions of Analytical and Surface Chemistry and of Chemical and Transport Systems.

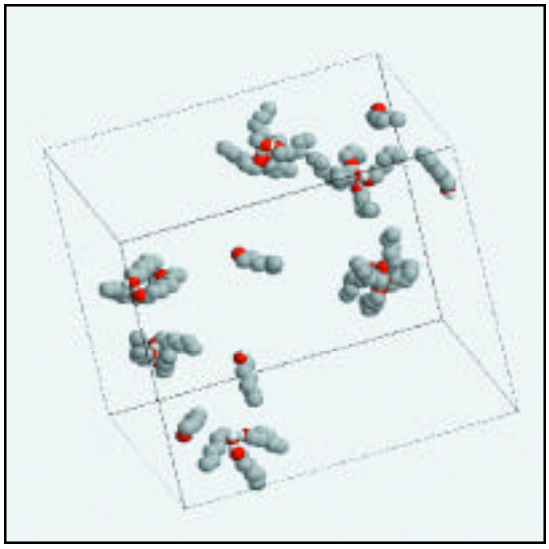

Figure 2: Self-aggregation of 1-hexanol in a 5% solution in *n*-hexane. The gray, red, and white spheres depict the alkyl groups, oxygen and hydrogen atoms of 1-hexanol molecules. The *n*-hexane molecules are omitted for clarity.

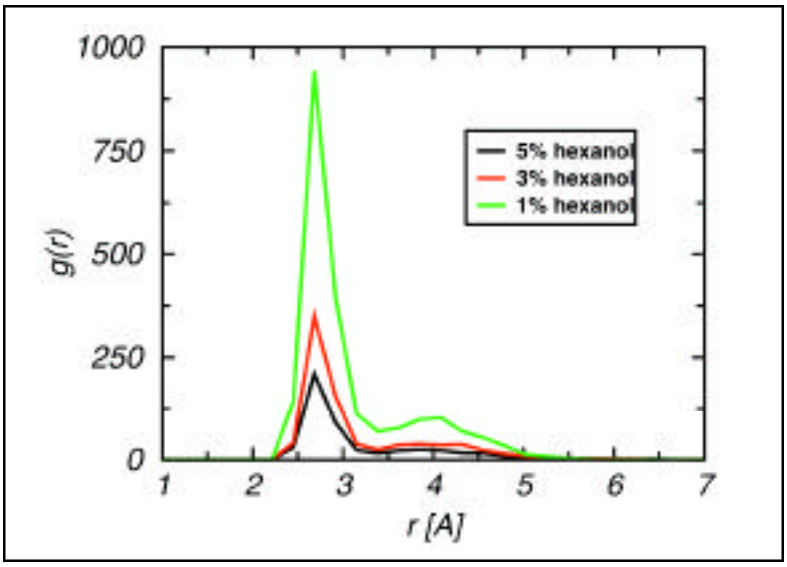

Figure 3: Oxygen-oxgyen radial distribution functions for dilute solutions of 1-hexanol in *n*-hexane.

2000 Midwest Thermodynamics and Statistical Mechanics Conference

The 2000 Midwest Thermodynamics and Statistical Mechanics Conference (May 14–16) brought together researchers in the areas of experimental, theoretical, and computational thermodynamics and statistical mechanics to exchange ideas and recent research results. The conference is designed in particular as a platform for young researchers (graduate students, postdoctoral researchers, and junior faculty members) to present and discuss their ideas and research accomplishments. Invited speakers also provide in-depth presentations of their research areas.

Sessions focussed on phase equilibria, adsorption and transport, macromolecules and colloids, and biological systems. The invited speakers and the titles of their talks were:

- J. Richard Elliott, Jr., University of Akron, "The Discrete World of Discontinuous Potential Modeling"

Chris Lubbers, Gaurav Arya, and Jindal Shah (all affiliated with Chemical Engineering Department of the University of Notre Dame) discussing the day's presentations before a session begins.

Richard McClurg (University of Minnesota) and Christopher M. Sorensen (Kansas State University) during a break in the conference.

- Christian M. Latoskie, Michigan State University, "Stochastic Modeling of Microbial Chemotaxis"
- Christopher M. Sorensen, Kansas State University, "Formation of Nanocrystal Superlattices from Colloidal Solutions"
- David L. Tomasko, Ohio State University, "Adsorption of Supercritical Carbon Dioxide on Microporous Materials"
- David T. Wu, Colorado School of Mines, "Gibbs Ensemble Monte Carlo for Solids"

In addition, there were 21 contributed talks, most of which were presented by graduate students or post-doctoral researchers.

Several of the invited and contributed talks presented experimental findings in adsorption, biochemistry, colloid science,

microbiology, polymer science, and supercritical fluid behavior.

The construction of intermolecular potentials remains a major research focus for several of the groups represented. Discussions of discrete, transferable, electrostatic, and mesoscopic potentials for gases, liquids, crystalline solids, and polymers wove their way through each of the sessions. As simulation techniques become ever more sophisticated, it appears that more accurate force fields are required as input. This will remain a challenge for the foreseeable future.

The conference was organized by Richard B. McClurg (Chemical Engineering and Materials Science) and J. Ilja Siepmann (Department of Chemistry and Supercomputing Institute Fellow), and it was sponsored by the Supercomputing Institute, IBM, and the National Science Foundation.

J. Richard Elliott Jr. (University of Akron) discussing his talk with Paul Van Tassell (Wayne State University).

Christian M. Latoskie (Michigan State University) and J. Ilja Siepmann (University of Minnesota) enjoying some conviviality at the reception for the conference.

Esam Hamad (King Fahd University of Petroleum and Minerals, Saudi Arabia) and Upma Sharma (Princeton University) following Dr. Hamad's lecture.

QFS 2000—International Symposium on Quantum Fluids and Solids

The University of Minnesota hosted this year's International Symposium on Quantum Fluids and Solids on June 6–11. The event took place on the East Bank of the University of Minnesota campus in Minneapolis, and was sponsored by the International Union of Pure and Applied Physics, the National Aeronautics and Space Administration and the Jet Propulsion Laboratory, the Theoretical Physics Institute of the University Of Minnesota, and the Supercomputing Institute. Additional support was provided by the Division of Materials Research of the National Science Foundation, and by the following University of Minnesota offices: the School of Physics and Astronomy, the Institute of Technology, the Office of the Vice President for Research, and the Office of the Senior Vice President and Provost. The co-organizers were Professors Charles E. Campbell and William Zimmermann, Jr., of the School of Physics and Astronomy.

Hiroshi Fukuyama (University of Tokyo) and Douglas Osheroff (Stanford University) take a moment to discuss the symposium.

David Lee (Cornell University), Brian Anderson (JILA, University of Colorado), John Reppy (Cornell University), and Charles Campbell (University of Minnesota) enjoy a moment during the outdoor reception.

The symposium represented the fifth such meeting held under the title since 1992; a number of other, similar symposia devoted to the same topics have been held over the past two decades. Organization of present and future symposia in this series is under the auspices of the Quantum Fluids and Solids Steering Committee; Campbell is an outgoing member and Zimmermann an incoming member of this committee.

The central topics of these symposia have traditionally been liquid and solid ^{3}He and ^{4}He, and their mixtures, but other topics, such as liquid and solid hydrogen and, most recently, the Bose-Einstein condensed phases of alkali atom and spin-aligned atomic hydrogen gases have been included in these meetings. These quantum fluids and solids are characterized by the presence of macroscopic quantum effects, including superfluidity, quantized vorticity, and the failure of most such systems to freeze even as a temperature of absolute zero is approached. The alkali atom systems and spin-aligned hydrogen are extremely low density, metastable gas phases, achieved by spin polarization in a large magnetic field followed by optical and magnetic trapping,

which have been observed to share the property of Bose-Einstein condensation. This property is widely believed to be the key feature that produces the exotic properties of superfluids.

More than 200 participants from around the world heard more than fifty oral presentations in plenary sessions and viewed approximately 140 poster presentations.

As in recent symposia, refereed proceedings will be published as an issue of the *Journal of Low Temperature Physics*. The symposium program was structured to include as broad a range of topics within the field as possible, including fundamental investigations and applications.

Theoretical and simulation research involving large-scale computation provided a strong component of the program. Much of this research is concerned with quantum fluids in confined and constrained geometries. Maria Carmen Gordillo (UPC Barcelona) described her recent simulations of quantum fluids adsorbed in carbon nanotubes. Srecko Kilic (University of Split, Croatia) described work on helium dimers and trimers in confined geometries. David Ceperley (University of Illinois, Champaign-Urbana) reported on path integral simulations of liquid helium droplets, and Birgitta Whaley (University of California–Berkeley) described simulations of superfluid solvation and molecular rotation in helium droplets. Eckhard Krotscheck (Johannes Kepler University, Linz) discussed the theory of the dynamics of ^{4}He in restricted geometries. Susana Hernandez (University of Buenos Aires) presented recent research on trapped fermions at very low densities, and Henry Glyde (University of Delaware) reported on simulations of Bose-Einstein condensation of trapped bosons. Allan Griffin (University of Toronto) provided an overview of the theoretical situation in the trapped boson systems and the relationship to superfluid ^{4}He, including the theory of superfluid hydrodynamics in the former.

Several reports presented at the symposium were on recent research with cosmological implications. Yuri Bunkov (CNRS-Grenoble) presented his "Aurore de Venise" model, a cosmological scenario of the A-B phase transition in superfluid ^{3}He. Peter McClintock (Lancaster University) discussed the question of why the Kibble mechanism seems not to work in liquid ^{4}He. Grigory Volovik (Helsinki University of Technology) gave a wide ranging talk on "Vortices Observed and to be Observed."

E. Dwight Adams (University of Florida), and Takao Mizusaki (Kyoto University) during a pause in the symposium.

Possibly the most stimulating presentation was given by Humphrey Maris (Brown University) under the title "Theoretical and Experimental Studies of Electron Bubbles in Liquid Helium." This was the first public presentation of this controversial research. As described by *The American Institute of Physics Bulletin of Physics News,* Number 501, September 7, 2000, Maris proposes that "a split-up of electrons into two or more fragments would best explain decades of puzzling results in liquid helium experiments." (Available online at http://www.aip.org/enews/physnews/2000/physnews.501.htm .) Maris's report on this research may be found in the August 1, 2000 volume of the *Journal of Low Temperature Physics*.

The next International Symposium on Quantum Fluids and Solids will be held in July 2001 at the University of Konstanz, Germany (http://www.uni-konstanz.de/qfs2001/).

34th Midwest Theoretical Chemistry Conference

The 34th Midwest Theoretical Chemistry Conference (MTCC) is being held October 5–6, 2001, at the University of Minnesota in Minneapolis.

The following is a list of people who have made early commitments to present their work at the conference:

- Daniel M. Chipman, University of Notre Dame
- Christopher Cramer, University of Minnesota
- Larry A. Curtiss, Argonne National Laboratory
- Ernest Davidson, Indiana University
- Michael Davis, Argonne National Laboratory
- Janet Del Bene, Youngstown State University
- Jerry R. Dias, University of Missouri at Kansas City
- Clifford Dykstra, Indiana-Purdue University at Indianapolis
- Jiali Gao, University of Minnesota
- J. Daniel Gezelter, University of Notre Dame
- Rainer Glaser, University of Missouri at Columbia
- Joseph Golab, Amoco Corporation, Naperville, IL
- Mark Gordon, Iowa State University
- Stephen Gray, Argonne National Laboratory
- Christopher M. Hadad, Ohio State University
- Lawrence B. Harding, Chemistry Division, Argonne National Laboratory
- William Hase, Wayne State University
- Katharine Hunt, Michigan State University
- Jan Jensen, University of Iowa
- Steven R. Kass, University of Minnesota
- Nancy Makri, University of Illinois at Urbana-Champaign
- Todd Martinez, University of Illinois at Urbana-Champaign
- Glenn Martyna, Indiana University
- Anne McCoy, Ohio State University
- Piotr Piecuch, Michigan State University
- Mark Ratner, Northwestern University
- George Schatz, Northwestern University
- H. Bernhard Schlegel, Wayne State University
- J. Ilja Siepmann, University of Minnesota
- James Skinner, University of Wisconsin
- Donald G. Truhlar, University of Minnesota
- Peter Wolynes, University of California at San Diego
- Arun Yethiraj, University of Wisconsin at Madison
- Darrin York, University of Minnesota

This event is being sponsored by the Supercomputing Institute for Digital Simulation and Advanced Computation, IBM, and SGI.

Additional conference information will be provided as conference planning progresses. For more information, visit the MTCC's Internet site:

http://www.msi.umn.edu/general/Symposia/MTCC/

or contact the conference administration:

Mr. Michael Olesen
MTCC Conference Administrator
University of Minnesota
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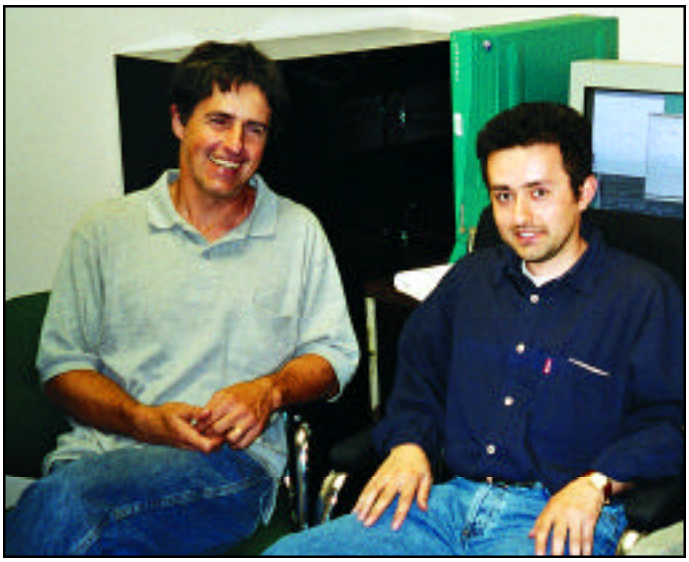
Minneapolis, MN 55415

phone: (612) 624-1336
fax: (612) 624-8861
email: olesen@msi.umn.edu

Pre-registration is required to attend this conference.



Antonio Lamura, right, of the Institute for Solid State Research, Forschungszentrum Jülich, Germany, visited the Supercomputing Institute for three weeks in June to collaborate with Daniel M. Kroll (left) of the Department of Medicinal Chemistry and his research associate Thomas Ihle. While here, Dr. Lamura utilized a new particle-based mesoscopic simulation technique being developed by Dr. Kroll to study Poiseuille flow and vortex shedding around a square object in a planar channel.

Mesoscopic simulation techniques such as the lattice-Boltzmann method, lattice-gas cellular automata, dissipative particle dynamics, and the new particle-based method being developed at Minnesota have recently attracted a great deal of interest because their coarse-grained nature and comcomitant efficient treatment of the hydrodynamic degrees of freedom make them ideally suited for studies of complex fluids—with their widely differing length and time scales—as well as flow and dispersion in complex geometries. The work started by Dr. Lamura during this visit is the first step in a longer collaboration which will utilize and further develop this simulation technique to study colloids and polymeric degrees of freedom in solvent.

Maria Luz Sánchez, far right, and José Corchado, center (standing), visited the Supercomputing Institute in July and August; pictured with them are graduate student Paul Winget, far left, and Patton Fast of Supercomputing Institute User Support (seated). Drs. Sánchez and Corchado—visiting researchers from the Department of Chemistry at the University of Extramadura in Badajoz, Spain—carried out a semi-classical simulation of the oxidation of methylamine to formaldehyde and ammonia by methylamine dehydrogenase in collaboration with Cristobal Alhambra, Jordi Villa, Jiali Gao, and Donald G. Truhlar. The multidimensional dynamics calculations for this project were carried out using the CHARMMRATE module of CHARMm as developed by the collaborators.

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