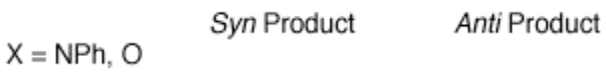

COMP 109 Simulations of Liquid/Vapor Interface for Water and Methnol From First Principles
I-Feng W. Kuo, Chemistry and Material Science, Lawrence Livermore National Laboratory, L-370, PO BOX 808, Livermore, CA 94551-9989, Fax: 925-423-0909, kuo2@llnl.gov, Christopher J. Mundy, Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Matthew J. McGrath, Department of Chemistry, University of Minnesota, and J. Ilja Siepmann, Departments of Chemistry, Chemical Engineering and Materials Science, University of Minnesota

Interfaces are crucial to the understanding of many phenomenons in atmospheric chemistry and biology. We will present results from recent simulations on the liquid/vapor interface of water and methanol from first principles simulations obtained from CPMD and CP2K. We will compare and contrast the structural, dynamical, and electronic properties differences from water and methanol liquid/vapor interfaces. In addition, similarities and differences in structural properties between ab initio interfaces and those modeled using common empirical force fields will be discussed.

COMP 110 Large-scale Monte Carlo simulations for aggregation, self-assembly, and phase equilibria
J. Ilja Siepmann[1], John M. Stubbs[2], Ling Zhang[3], Matthew J. McGrath[3], Neeraj Rai[3], and Collin D. Wick[4]. (1) Departments of Chemistry, Chemical Engineering and Materials Science, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455, Fax: 612-626-7541, siepmann@chem.umn.edu, (2) Department of Chemistry, Grinnell College, (3) Department of Chemistry, University of Minnesota, (4) Chemical Sciences Division, Pacific Northwest National Lab

This presentations will describe the use of efficient Monte Carlo algorithms and open ensembles to explore processes in complex chemical systems that occur on time scales too long to make them amenable for direct molecular dynamics simulations. In particular, aggregation, self-assembly, and phase equilibria for systems containing water, alkanes, alcohols, and/or perfluoroalkanes will be discussed.

COMP 111 Spanning scaling regimes with the SPEAD model
JRichard Elliott, ZNevin Gerek, and Neil H. Gray, Chemical Engineering Dept, University of Akron, Akron, OH 44325-3906, Fax: 330-972-5856, jelliott@uakron.edu

Discontinuous molecular dynamics (DMD) and thermodynamic perturbation theory (TPT) are combined to form the Step Potentials for Equilibria And Dynamics (SPEAD) model. Stripping the simulation to the repulsive core accelerates the dynamics by ~two orders of magnitude. Equilibrium results now permit rapid transition from molecular design (~nm) to chemical process plant design (~1km), especially for small molecules (MW<300). 10 ns molecular simulations over 21 densities are completed in ~8 hours on a 21x3GHz PC cluster. TPT gives the temperature effect, yielding a complete equation of state(EOS). EOS parameters for the repulsive reference systems and perturbation terms of n-alkanes approach asymptotic limits at NC~40. Simulations of tangent sphere chains through the entanglement threshold reproduce the findings of Smith et al. for diffusivity and extend the observations to viscosity and thermal conductivity. Thermal conductivity approaches an asymptote at relatively short chain length. Accurate results for transport properties over wide length scales suggest that SPEAD can be used to calibrate mesocale models.

COMP 112 Strategies for Monte Carlo simulations using quantum chemical energetics
K. D. Jordan[1], R. A. Christie[2], and J. Cui[2]. (1) Dept. of Chemistry and Center for Molecular and Materials Simulations, University of Pittsburgh, Pittsburgh, PA 15260, jordan@imap.pitt.edu, (2) Department of Chemistry, University of Pittsburgh

This talk considers two applications of Monte Carlo simulations coupled with electronic structure calculations. The first involves an n-body decomposition procedure for carrying out MP2-level parallel tempering Monte Carlo simulations of water clusters, and the second involves a novel QM/MM approach for characterizing excess electrons attached to water clusters. In both cases, parallelization of the code is crucial for the success of the simulations.

COMP 113 Watching crystals grow: Determining microscopic behaviour from nanoscale simulation
Julian D. Gale and Stefano Piana, Nanochemistry Research Institute, Department of Applied Chemistry, Curtin University of Technology, PO Box U1987, Perth 6845, Australia, Fax: +61 8 9266 4699, julian@power.curtin.edu.au

Crystal growth is of fundamental importance in many areas of science from minerals processing to pharmaceuticals. Although extensive work has been performed on predicting the morphology of crystals, the direct simulation of surface growth has proved much more challenging since the timescale involved exceeds that usually available to molecular dynamics. Furthermore, the critical nucleus size is also usually too large to access. In this presentation, it will be demonstrated that it is possible to simulate both the dissolution and crystal growth of urea for all of the key surfaces, thus leading to a microscopic understanding of the processes occuring. Through classification of the distinct pathways, it is possible to directly determine the rate constants for these steps and utilise them as input for kinetic Monte Carlo simulation. In this way, it is feasible to simulate crystal growth at length /timescales within an order of magnitude of those observed experimentally.

COMP 114 Current challenges in molecular docking and virtual screening
Richard David Taylor, Computational Chemistry, Astex Technology, 436 Cambridge Science Park, Milton Road, Cambridge CB4 6BZ, United Kingdom, Fax: +441223226201, r.taylor@astex-technology.com

Thymidine Kinase (TK) is a good example to illustrate the current challenges in protein-ligand docking and virtual screening. There is a degree of protein flexibility, the ligands can exist in more than one charge/tautomer state (C/T state) and there are three water molecules in the binding site that can either be displaced by the ligand or Gln125, or that can mediate binding.

Using the protein-ligand docking program GOLD, we were able to predict the ligand C/T state, protein conformer, whether a water is mediating or displaced and the ligand binding mode for most of the complexes in a TK test set. The results from a virtual screening experiment using TK will also be presented. The enrichment graphs for retrieving actives from a database of compounds with similar 1D properties will be discussed along with the effect of protein conformers, water mediation/displacement and ligand C/T states on virtual screening of TK.

COMP 115 Lead optimization via high-throughput molecular docking
Diane Joseph-McCarthy, Chemical and Screening Sciences, Wyeth Research, 200 CambridgePark Drive, Cambridge, MA 02140, Fax: 617-665-5682, DJoseph@wyeth.com

The design and optimization of an existing lead compound can be a time consuming and expensive process. Computational approaches increase the efficiency of the process by reducing the number of compounds that need to be synthesized to achieve a desired potency and property profile. In structure-based design, molecular docking techniques are used predict the binding of a set of proposed compounds. Accurate molecular docking of small molecules to a target structure requires adequate sampling and accurate scoring of each proposed ligand in the target binding site. The use of Monte Carlo docking for the optimization of a lead series for an infectious disease target as well as a metabolic disease target will be presented. In addition, the development of a new automated approach for lead evolution will be discussed.

COMP 116 Structure based lead optimization of isosteric analogues
Roger Sayle, Robert Tolbert, Anthony Nicholls, and A. Geoffrey Skillman, OpenEye Scientific Software, 3600 Cerrillos Road, Suite 1107, Santa Fe, NM 87507, Fax: 505-473-0833, roger@eyesopen.com

"Docking is like a singles bar; its all about posing and scoring". In conventional docking protocols, it's the need to "pose" or orient a ligand within an active site than makes the task of "scoring" the resulting protein-ligand interaction much more difficult. Docking scoring functions for compound screening face the conflicting requirements of soft potentials for radius of convergence against the need to capture complex effects such as desolvation, conformational strain, protein flexibility and entropic terms. Scoring for lead optimization, rather than lead discovery, is a significantly more tractable problem. By effectively (re)using the information from a known crystal (or NMR) structure of a protein-ligand complex, it's possible to rank virtual libraries of isosteric analogues far more accurately than zero prior knowledge docking protocols, that are commonly misused for this application. This talk presents recent advances in the enumeration and

accurate binding energy evaluation of isosteric analogues for lead optimization.

COMP 117 Structure-based design of focused drug-like combinatorial libraries

Peter S. Shenkin[1], Leah L. Frye[1], Robert B. Murphy[1], Matthew P. Repasky[1], Daniel T. Mainz[1], Mark Reboul[1], and Richard A. Friesner[2]. (1) Schrödinger, 120 W. 45th Street, New York, NY 10036, shenkin@schrodinger.com, (2) Department of Chemistry and Center for Biomolecular Simulation, Columbia University

Combinatorial chemistry techniques make it possible to generate orders of magnitude more compounds than can be practically prepared or screened. Therefore, there is a need to develop methods to rationally select the optimal library members for synthesis. Combinatorial library design has recently shifted toward small focused libraries that are biased toward a specific target and exhibit optimal ADME properties. We will describe the development of CombiGlide, a new computational method based on the docking algorithm in Glide that performs rapid screening of libraries to eliminate unpromising compounds upfront. The centerpiece of the approach is a sophisticated selection protocol that rapidly determines which members of the virtual library have the highest likelihood of binding well to the target protein. These compounds are then enumerated and docked. We will present case studies that illustrate various strategies for selecting the optimal reagents for library synthesis based on docking results and predicted ADME properties.

COMP 118 Novel scoring functions for *in silico* database screening: Binding response and pose-based scaling

Shijun Zhong, Department of Pharmaceutical Sciences, University of Maryland, School of Pharmacy, 20 Penn Street, Baltimore, MD 21201, Fax: 410-706-5017, szhong@rx.umaryland.edu, and Alexander D. MacKerell Jr., Department of Pharmaceutical Sciences, University of Maryland

In computer-aided drug design an important tool is *in silico* database screening by which a million or more compounds are virtually tested for binding to a pre-determined site on a target protein. Two novel scoring functions based on a combination of interaction energy and binding pose are introduced to improve the current energy-only criteria which may select ligands positioned at the edge or located completely out of the binding pocket. The first descriptor, the binding response can be used to compare different binding sites to select the ideal site for screening. Another descriptor, the pose-based scaling factor, provides a refined score for selecting well-docked ligands.

COMP 119 Realizing teraflops computing, striving for petaflops computing

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We are presently in the midst of a revolution in computing technologies with an order of magnitude increase in computing capability every three to five years. However, this increase in "peak performance" is not so easily captured in the performance of chemistry applications. What must we do to harness the power of high-end computing technologies to solve the most critical problems in chemistry? First, we must continue to seek advances in the theoretical and mathematical sciences that lead to computational models of ever increasing predictive power and fidelity. Second, we must establish close collaborations among theoretical and computational chemists, computer scientists, and applied mathematicians to translate these advances into scientific applications, computing environments, and analysis and visualization tools that can realize the full potential of high-end computers. Third, we must educate a new generation of chemists in the application of these new tools for scientific discovery. The situation will become even more challenging as we strive for petaflops computing, for new computing technologies will come into play and the gap between "peak" and "realized" performance could grow even larger.

COMP 120 Parallel DFT calculations with ADF: A software vendor's perspective on code optimization

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The Amsterdam Density Functional (ADF) code is a DFT program commercialized by Scientific Computing & Modelling (SCM). All major parts of ADF have been optimized and parallelized for a variety of computer platforms. SCM maintains the ADF code and takes charge of further serial and parallel optimizations. This

includes trying out different compilers, compiler options, and performance libraries, changing algorithms and tweaking code. Results will be shown that can now be routinely achieved with ADF due to these efficiency improvements. The talk will also address some serious challenges faced by software vendors when aiming for efficient massively parallel usage. These challenges include the desire to refrain from platform-specific or vendor-specific solutions, the economic need to concentrate on the wishes of the average user, the limited testing possibilities, and the need to generate correct results for all program options. Optimization for a thousand-CPU machine therefore remains an interesting challenge.

COMP 121 High performance computational chemistry in the 21st century
Theresa L. Windus, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 902 Battelle Boulevard, P.O. Box 999, MSIN: K8-91, Richland, WA 99352, Fax: 509-376-0420, theresa.windus@pnl.gov

High performance computational chemistry has made many advancements, but there is still much to be accomplished. This talk will describe some of the future challenges and new and needed computational methodologies applied to chemical theories to advance computational chemistry to meet the needs of these challenges.

COMP 122 Leadership computing and chemistry
Robert J. Harrison, Computer Science & Mathematics Division, Oak Ridge National Laboratory, Computational Chemical Sciences Group, Oak Ridge, TN 37831-6367, harrisonrj@ornl.gov

"Leadership" computers, the top of the supercomputing pyramid, are motivated by the potential for fundamental scientific advance, in the same spirit as a light or neutron source. To realize this potential, computational chemistry must face up to the challenges (technical, communal and strategic) posed by near-term 100+ TFLOP/s and PFLOP/s computers, as well as the exploding diversity of future computer architectures.

COMP 123 Large scale computing with GAMESS-UK
Joop H. Van Lenthe[1], Martyn F Guest[2], Huub J.J van Dam[2], Ian J. Bush[2], Paul Sherwood[2], Jens M.H. Thomas[2], Remco W.A. Havenith[1], Joost N.J. van Lingen[1], and Marc de Jonge[3]. (1) Theoretical Chemistry Group, University of Utrecht, Padualaan 8, 3584 CH Utrecht, Netherlands, Fax: +31 30 2537504, joop@chem.uu.nl, (2) Computational Science and Engineering Department, CCLRC Daresbury Laboratory, (3) MolMo Services BVBA

The Quantumchemical program GAMESS-UK has known a long history of parallelisation. As machines with more then 500 processors and Gigabytes of memory have become available, it has become relevant to establish the current limits of the program and the scaling behaviour. We will discuss some of the recent developments in GAMESS-UK, which help exploiting the current capability machines. We will discuss the approaches utilised in parallellising the HF/DFT, Ci and Valence Bond modules. We will demonstrate the ability to perform HF/DFT calculation on large (bio)molecules, with more then 3000 atoms and 11000 basis functions in calculations of molecular potentials and densities, meant as input for Computer Aided Drug Design endeavors. We will show DFT Hessian calculations on molecules with more than 400 basis functions and over 50 atoms which are being used to elucidate the structure of heterogeneous Vanadium catalysts, by analysis of their infrared and Raman spectra.

COMP 124 What can we use a Teraflop computer for?
Edoardo Aprà, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352, edoardo.apra@pnl.gov

We describe obstacles, pitfalls and successes relative to the implementation and use of quantum chemistry methods on massively parallel hardware. This is going to be illustrated by using examples of algorithms from NWChem, a computational chemistry software developed in the William R. Wiley Environmental Molecular Sciences Laboratory. Benchmark of scalability of the code on various parallel computers are used to test the efficiency of the simulation software. Finally, we present how NWChem was used on teraflop hardware to study water and transition metal clusters.

COMP 125 BioSimGrid: A distributed environment for archiving and the analysis of biomolecular simulations

Stuart E Murdock[1], Kaihsu Tai[2], Muan Hong Ng[3], Steve Johnston[3], Bing Wu[4], Hans Fangohr[3], Jonathan W Essex[1], Paul Jeffreys[4], Simon Cox[3], and Mark S.P. Sansom[5]. (1) School of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, United Kingdom, Fax: +44 (0)23 8059 3781, s.e.murdock@soton.ac.uk, (2) Department of Biochemistry, University of Oxford, (3) e-Science Centre, University of Southampton, (4) e-Science Centre, University of Oxford, (5) Laboratory of Molecular Biophysics, University of Oxford

The comparison of simulations carried out by different packages or in different labs is logistically difficult due to high volumes of data, proprietary data formats, variety of tools available to analyse the data, and lack of sharing of the data. The Biosimgrid project is developing a software environment to address these issues. With Biosimgrid we provide not only a distributed repository in which we store these large trajectories but also a common environment where they may be analysed with a range of system-supplied or user-supplied tools. The trajectories may be queried by other workers on the basis of their associated metadata. We have developed routines to automate deposition of trajectories from NAMD, Charmm, GROMACS and Amber. We demonstrate the strength of the Biosimgrid environment by analysing different biosimulation trajectories using our standard toolkit. The results may be displayed in a variety of different formats to allow their easiest possible interpretation.

COMP 126 Automated QSPR by competitive workflow

David E. Leahy, J. Cartmell, S. Enoch, D. Krstajic, and J. Bowen, Cyprotex PLC, 13-15 Beech Lane, Macclesfield, Cheshire SK10 2DR, United Kingdom, d.leahy@cyprotex.com

The successful application of an autonomous QSPR modeling process to three previously studied ADME datasets, for solubility, human plasma protein binding and P-glycoprotein substrates is described. The process is implemented using a novel software architecture, Competitive Workflow, which implements workflow as a distributed and competitive multi-agent system. The autonomous QSPR system allows exhaustive exploration of descriptor and model space, automated model validation and continuous updating as new data and methods are made available as well as the prediction of properties of novel structures by an ensemble of models.

COMP 127 Building predictive models using fuzzy biological data: Data mining of the docking results of GSK-3 inhibitors using artificial intelligence approaches

Pavel A. Petukhov, Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, 833 S. Wood St. 539, Chicago, IL 60612, pap4@uic.edu, and Ae Nim Pae, Biochemicals Research Center, Korea Institute of Science and Technology

Virtual screening is one of the ways to effectively improve the hit finding rate in drug discovery. Numerous successful docking, scoring, and ranking approaches have been developed. Despite the significant diversity and dramatic increase in speed of the virtual screening algorithms, the predictive power of these methods is still far from ideal. Among many other challenges, there are two that occur in the majority of the drug discovery projects: (1) what is the best way to analyze incomplete or collected under different experimental conditions biological (a.k.a. fuzzy) data and (2) what is the best way to correlate computed scores with the experimental biological data.

A set of 146 GSK-3 inhibitors collected from eight different publications was docked to the ATP binding site of GSK-3 kinase. For each ligand in the dataset FlexX, DOCK, GOLD, PMF, and ChemScore scores were generated and correlated with the biological activity of the ligands. Depending on the source of biological data, the scaffolds of the ligands, and the experimental conditions, several training and test sets were generated. The virtual scores and biological data of the ligands were analyzed using Self-Organizing Maps (SOM), Free Forward Neural Networks (FFNN), linear regression (LR), and a consensus of the scoring functions (CSF) approaches. We demonstrated that, in general, the SOM and FFNN performed better than the LR and CSF methods. Moreover, the SOM and FFNN methods were much more successful in analyzing fuzzy biological data than the LR and CSF methods. The details of the approach and its application to design of novel highly active GSK-3 inhibitors will be presented.

COMP 128 Modeling Polymer Sorption

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Values of the sorption parameter for liquids of the type PhX and EtX by poly(Sty co DVB)were sucessfully correlated with a form of the IMF equation that included the segmental steric parameterization. Values the sorption parameter for liquids of the type RX where X is constant and R is an alkyl group were corelated with the simple branching equation. Our results show as expected that sorption is a function of intermolecular forces and steric effects.

COMP 129 Computational Chemistry Robots

Joe A Townsend, Peter Murray-Rust, Simon M. Tyrrell, and Yong Zhang, Unilever Centre for Molecular Science Informatics, University of Cambridge, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom, jat45@cam.ac.uk

Millions of compounds are now Openly available (e.g. PubChem) and we describe the automatic computation of their geometries and properties. Using completely automatic procedures, based on modular components and workflow technology (Taverna) we can:

* extract structures from 3D databases or crystallographic publications

* determine a cost-effective level of theory

* optimise ground state geometry and calculate properties

* disseminate the results Openly.

Although error rates are low their management must be completely robotic.

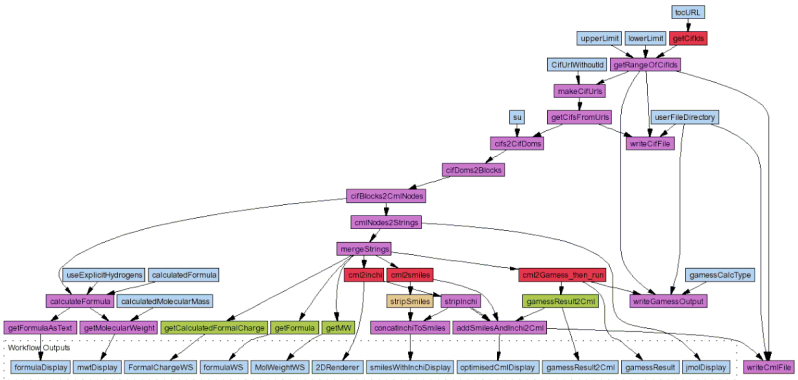
By using spare capacity (Condor) we have calculated 250,000 molecules at PM5 (MOPAC) and over 10000 at B3LYP/63-1G* (GAMESS), and analysed the data robotically, including:

* variability between crystallographic experiment and levels of theory

* geometric variability within instances of a given functional group

* detection of molecular features that give rise to serious errors or pathological computation.

The results in our WorldWideMolecularMatrix (WWMM, http://wwmm.ch.cam.ac.uk) are Openly available in our DSpace repository (http://www.dspace.cam.ac.uk/handle/1810/724).



COMP 130 Assessment of model protein structures using an entropic metric of dihedral-angle correlation

Shi Zhong, Stephen Quirk, and Rigoberto Hernandez, School of Chemistry and Biochemistry, Georgia Institute of Technology, 770 State Street, Atlanta, GA 30332-0400, Fax: 404-894-7452, shi.zhong@chemistry.gatech.edu

New metrics for validating and interpreting model protein structures are needed to sift through the

exponentially growing databanks of structures in the post genomics era. The dihedral angle distribution about a given amino acid residue, the phi-psi plots, and that between any of the 400 possible amino acid residue pair combinations, the psi-phi plots, have been used directly for structure validation and modeling by various groups. In this work, an information-theory based entropy, that takes advantage of high quality phi-psi and psi-phi plots (recomputed herein), has been developed and implemented to observe the range of its values throughout the Protein Data Bank (PDB). This entropy leads to a new metric that uses the relative likelihood of a particular entropy to assess the compatibility of a given model structure to the ensemble of experimentally derived structures in the PDB. The utility of this metric is demonstrated by its use in the analysis of experimentally and theoretically derived structures in the PDB

COMP 131 Modelling the thermal decomposition of large molecules and nanostructures
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Reactive Molecular Dynamics holds the promise of becoming a key tool for capturing the phenomena and rates of reactions in nanometer-scale materials. As in the kinetics of small, gas phase molecules, the covalent bonds that form or break are about 0.1 to 0.2 nm long, and their energies are rooted in local electronic structure. Unfortunately, computational quantum chemistry, ideal-gas statistical mechanics, and statistical reaction rate theories - so powerful for gas kinetics - are much more limited when the bonds are in condensed-phase molecules like synthetic or natural polymers that extend across nanometers and tens of nanometers. The crucial difference is that the dynamics of bond making and breaking may be affected by energy transfer and motion constraints that are some distance from the bond in question. Traditional molecular dynamics simulations are effective for describing nonreactive interactions that do not affect electronic structure of molecules, and ab initio molecular dynamics methods are valuable for modeling nanoscale and larger structures of metals and certain other condensed phases. However, there are few tools for modeling reactions in nanoscale condensed-phase populations, which have large length scales relative to bonds.

Reactive Molecular Dynamics (RMD) captures both the effects of electronic-structure changes and physical interactions. Our previous work on polymer decomposition shows new types of chemical steps that happen because of this coupling between reaction and large-scale physical effects. An important part of our ongoing work, therefore, is to extend our Reactive Molecular Dynamics methods by using more sophisticated new reactive force fields, testing and exploiting these tools using small molecule kinetics, polymer nanodomain and nanoparticle decomposition, and nanoparticle surface kinetics.

In this talk, we will present the theory and implementation of RMD using examples from recent simulations of the thermal decomposition of polymers.

COMP 132 Multiscale simulation of ultraviolet absorber function in polymers
Michael L. Greenfield, Department of Chemical Engineering, University of Rhode Island, 205 Crawford Hall, Kingston, RI 02881, Fax: 401-874-4689, greenfield@egr.uri.edu

Polymer systems (e.g. paints) exposed to sunlight often experience photodegradation and are protected via additives. Ultraviolet light absorber molecules prevent chemical degradation of polymer matrices by converting incoming UV radiation into heat. Absorption occurs in a fixed molecular geometry; conversion to heat has been linked to an intersystem crossing, with out-of-plane rotations about inter-ring torsion angles. Here we apply a sequence of molecular simulation techniques over different length scales to study how this process is related to accessible volume that surrounds an *in situ* UV absorber. Configuration interaction singles calculations were used to estimate the conformation dependence of the absorption energy. Classical molecular simulations were then used to calculate the fraction of absorber molecules in conformations likely for absorption. Simulations of polymer/absorber mixtures revealed the effect of polymer environment on this distribution. Geometric analysis calculations were used to relate absorber position and inter-chain packing. We found that absorber molecules in polymers are surrounded by little accessible volume and they modify the extent of local chain dynamics.

COMP 133 Using Nanoconfinment to Tailor Semiconducting Polymers

Michael L. Drummond[1], Bobby G. Sumpter[1], Michael D. Barnes[2], William A. Shelton[1], and Robert J. Harrison[1]. (1) Computer Science & Mathematics Division, Oak Ridge National Laboratory, Computational Chemical Sciences Group, Oak Ridge, TN 37831-6367, Fax: 865-574-0680, drummondml@ornl.gov, (2) Department of Chemistry, University of Massachusetts-Amherst

Semiconductors and other inorganic crystals are the basis for electronics and other technologies, but their chemical properties are fairly inflexible. Soft materials such as polymers, on the other hand, have almost unlimited possibilities, as the chemical repeat groups can be modified to suit a particular application. However, commonly used techniques capable of producing the needed types of soft-material structures, such as thin-film or self-assembly processes, suffer from substrate and other molecular interactions which may dominate or obscure the underlying polymer physics. In order to minimize these complexities, we have recently explored ink-jet printing methods for producing polymer particles with arbitrary size and composition. By combining experimental measurements, observations and developments with extensive computational chemistry studies we have found substantial evidence indicating the production of highly ordered rod-shaped structures for single molecule MEH-PPV (2-methoxy-5-(2'-ethyl-hexyloxy)-p-phenylenevinylene) and CN-PPV (2,5,2',5'-tetrahexyloxy-7,8'-dicyano-p-phenylenevinylene) systems. Results clearly show that chain organization is crucial to the photophysical properties, which can be controlled to a large extent by the solvent. For toluene and THF solvent preparations of MEH-PPV and CN-PPV, the resulting single molecule nanoparticle structures show a very high level of organization consisting of π-stacked folded chains. This leads to nanoparticles that are organized into a core-shell system, where the inner core is a self-solvated PPV system with inter-chain distances ~0.3 Å closer than the surrounding chains. Since there is orbital overlap throughout the system, facile fluorescence resonant energy transfer without the emission of a photon can occur to the core emission site. Altered fluorescence lifetimes occur for this type of molecular organization and confinement which are partially due to classical electromagnetic interactions resulting from vacuum fluctuations that are altered from boundary reflections, and also fluorescence quenching is reduced by the shell providing a protective layer to oxidation.

COMP 134 Mean-field prediction of block copolymer phase behavior and structure in selective solvent

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A given block copolymer can self-assemble in the presence of a selective solvent to form a variety of thermodynamically stable phases with structures that include ordered arrays of spherical, cylindrical or planar assemblies. Research activities in our group are directed toward the utilization of such self-assembly for the formulation of complex systems [US Patent 6,503,955] and synthesis of nanomaterials [Langmuir 2004, 20, 8426]. Information on the thermodynamics of block copolymer self-assembly in selective solvents is crucial to this end. We have thus investigated the effects on phase behavior and structure of solvent quality and block copolymer molecular features by means of small angle scattering experiments [Macromolecules 1995, 28, 7700; 1997, 30, 6788; 1998, 31, 6935; 2000, 33, 5574; 2001, 34, 5979; 2002, 35, 4064; 2004, 37, 912] and mean-field lattice theory [Macromolecules 1999, 32, 637; Eur. Phys. J. E 2003, 10, 45; Langmuir 2003, 19, 4483; Polym. Mat. Sci. Eng. 2003, 89, 402]. The presentation will highlight modeling results on the concentration-temperature stability and internal structure of ordered phases formed by ABC triblock copolymers as affected by the copolymer block sequence and length.

COMP 135 Computer simulation studies on mechanisms of poration for hydrolytically degradable diblock copolymer membranes

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Dissipative particle dynamics computer simulations are proposed to give a molecular understanding to the application of aqueous diblock copolymer systems to drug delivery. The use of a hydrolysable monomer as the hydrophobic block leads to a destabilization of the vesicle membrane due to the increase in the hydrophilic molecular weight fraction (fEO) of the chains, which makes them prefer high curvature

conformations such as worm-like and spherical micelles. Experimental work suggests that aggregation of these micelle forming chains provokes a local phase transition to the micellar state, causing poration of the membrane with eventual release of the encapsulated hydrophilic drug and disintegration of the vesicle. In this study, free-energy techniques are employed to examine the microdomain formation by high fEO chains, leading to poration, by using a coordination number reaction coordinate. Additionally, results from atomistic studies on percolation of water into the membrane hydrophobic core will be reported for PLA.

COMP 136 Development of small molecules designed to modulate protein-protein interactions

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Protein-protein interactions are essential to most biological processes, and offer attractive opportunities for therapeutic intervention. Developing small molecules that modulate protein-protein interactions is widely considered to be difficult, owing to issues such as the large size of protein-complex interfaces and the lack of crevices and pockets for small-molecule binding. Here, we discuss a general strategy based on the "privileged-structure hypothesis" - that any organic scaffolds mimicking protein surface structures (such as alpha-helices, beta-strands, reverse turns and etc.) are potential privileged structures as protein-complex antagonists - for addressing the challenges inherent in the discovery of small-molecule inhibitors of protein-protein interactions. A succesful design can lead to a novel comformational template for a combinatorial library that are tremendously useful in targeting multiple, unrelated therapeutic targets.

COMP 137 Decoupling torsional and Cartesian alignment: Applications to pharmacophore alignment problems

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We have recently developed a new ligand-alignment technology that decouples the identification of pharmacophorically similar conformations of flexible molecules from the superposition of those molecules in 3D space. Efficient and effective alignment in torsional (inner coordinate) space is through a novel genetic algorithm that makes use of a multi-objective scoring function based on consensus among pharmacophore and steric multiplets as well as on energy. Subsequent alignment in Cartesian space is carried out by an extension of the LAMDA rigid-body alignment technique (N.J. Richmondet al., J. Mol. Graph. Model. 2004, 23, 199-209) to pharmacophore features. The practical effects of this decoupling will be discussed in the context of several literature data sets that have frustrated analysts in the past.

COMP 138 Induced-fit docking to account for receptor flexibility

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We present a novel protein-ligand docking method that accurately accounts for both ligand and receptor flexibility by iteratively combining rigid receptor docking with protein structure prediction techniques. While traditional rigid-receptor docking methods are useful when the receptor structure does not change substantially upon ligand binding, success is limited when the protein must be "induced" into the correct binding conformation for a given ligand. We provide an in-depth description of our novel methodology and present results for 21 pharmaceutically relevant examples. The average ligand RMSD for the 21 pairs is 1.3 Å; the RMSD is <1.5 Å for 17 of the cases. In contrast, traditional rigid-receptor docking yields an average RMSD of 5.5 Å. This methodology represents a considerable advance in the state of the art of induced-fit prediction, combining excellent accuracy with computational efficiency for a wide range of test cases.

COMP 139 Physics-based methods in virtual screening: Factors impacting practical application

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The success of physics-based approaches to estimate binding free energies of protein-ligand complexes has been well documented. Previously we have presented the successful application of the MM-GBSA and Linear Interaction Energy (LIE) methods to estimate the binding free energies of docked complexes of thymidine kinase (TK). This study has been extended to include a third approach, MM-PBSA, which has been used by researchers with some success in past studies. In this presentation, we examine the impact of initial pose selection, entropic contributions, bound waters, and sampling. In order to utilize these methods in a virtual screening protocol, it is critical that the role of specific components and criteria is well understood as we seek to identify an appropriate balance between the quality and cost of results. Observations from our studies are presented as well as suggestions for the application of these methods as part of a discovery program.

COMP 140 Direct calculation of absolute free energies of ligand binding without knowledge of the bound state

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We calculate the absolute free energy of binding for eight ligands to the FKBP12 protein with full atomistic molecular dynamics simulations and explicit water. We not only calculate the free energies from binding modes modeled from crystal structure, but also calculate these binding free energies without any knowledge of the binding site using multiple docked ligand configurations. These extensive, all-atom explicit water absolute binding calculations are made possible by both the new application of very efficient free energy methods and the use of worldwide distributed computing on tens of thousands of processors. We have obtained binding free energies with clear predictive value, with RMS from fit of approximately 1 kcal/mol, despite the magnitude of the sampling problem for this system and the lack of force fields parameterized to experimental condensed phase free energy data. These calculations point the way to much more directly physical methods of drug design.

COMP 141 Large scale first principles simulations for problems in earth and planetary science (ion hydration) and biochemistry (phosphoryl transfer signaling reactions)

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A major limitation to modeling complex materials is the accurate representation of the many-body forces for large systems that lead to their interesting chemical properties. Recently progress has been made in the development of simulation methods based on forces calculated directly from the electronic Schrödinger equation. We discuss two problems which require such methods. The description of the finite temperature properties of ionic solutes in aqueous solutions is of great importance to earth and planetary science. For highly charged ions accurate representations of interparticle interactions are not available. Large numbers of waters (128) must be included to simulate chemical processes in the hydration region. Simulation times of several ps are required to sample the system. Our results agree well with the measured hydration properties of Al3+. The octahedrally coordinated waters in 1st shell are trigonally coordinated to 12 waters to form a tightly structured 2nd shell. The emergence of tetrahedral bulk water coordination occurs by the third shell. While there is no transfer of waters between the 1st and 2nd shells on the ps time scale, there is transfer between the 2nd and 3rd shells via an associative mechanism. For high T the transfer of protons in the solvation shells leads to a five coordinated hydrolysis species. The 2nd problem area concerns the computational analysis of a protein kinase an important class of enzymes that catalyze the transfer of the gamma-phosphoryl group of ATP to serine, threonine, and tyrosine residues. This reaction is an important signaling mechanism in cells. In order to obtain reliable results we had to include roughly 150 atoms in a full B3LYP calculation coupled with an additional 54,000 molecular mechanics atoms representing the protein environment. Our calculations support a dissociative mechanism for the reaction process with a late proton transfer to a catalytic base residue.

COMP 142 Million-to-Billion Atom Simulation of Chemical and Mechanical Processes

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Ultrascale simulations of chemical and mechanical processes in materials require hierarchical simulation methods, algorithms, and parallel computing and visualization techniques. We have designed O(N) embedded divide-and-conquer (EDC) algorithms for 1) first principles-based parallel reactive force-field (P-ReaxFF) molecular dynamics (MD), and 2) density functional theory (DFT) on adaptive multigrids for quantum mechanical MD, based on a space-time multiresolution MD (MRMD) algorithm. To map these O(N) algorithms onto parallel computers, we have developed a hierarchical cellular decomposition (HCD) framework, including 1) wavelet-based computational-space decomposition for adaptive load balancing, and 2) octree-based probabilistic visibility culling for interactive visualization of billion-atom datasets. Preliminary tests on 1,920 Itanium2 processors of the NASA Columbia supercomputer have achieved unprecedented scales of reactive atomistic simulations: 0.56 billion-atom P-ReaxFF and 1.4 million-atom (0.12 trillion grid points) EDC-DFT simulations, in addition to 18.9 billion-atom MRMD simulation.

COMP 143 Al nanoparticles: Accurate energetics and structures

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Nanoparticles are intermediate between bulk materials and small molecules or clusters, but it is hard to obtain experimental data for their properties as a function of size or their reactivity as a function of structure. Consequently computations can provide information that is inaccessible experimentally, but computations of nanoparticle properties can be harder than for bulk properties because one cannot apply efficient bulk methods such as periodic boundary conditions to nanoparticles. Furthermore, accurate ab initio methods become intractable for systems larger than a few atoms. This paper will report studies of Al nanoparticles using an approach where we begin with highly accurate ab initio calculations for small systems and use these to validate more approximate methods such as density functional theory (DFT), which can be applied much larger systems. Using DFT with a newly developed effective core potential and valence electron basis set, we can model nanometer-sized systems with highly accurate DFT methods and begin to understand how the energetics, structure, and reactivity of Al particles evolve from the small-molecule limit to the bulk limit. We have found this approach to be useful in testing and parameterizing more approximate methods such as analytic potential energy functions.

COMP 144 Recent progress in large-scale first-principles molecular dynamics simulations

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Since their introduction in 1985, first-principles molecular dynamics (FPMD) simulations have been successfully applied to numerous areas of chemistry. First-principles simulations provide a unified description of electronic and structural properties of matter, and do not rely on empirically adjusted parameters, thus providing a genuinely predictive computational tool. The high computational cost of FPMD has limited its applicability to systems containing only a few hundred atoms. We discuss the current limits of this method and describe recent research aimed at increasing the size of feasible simulations. In particular, the development of “terascale” computers has considerably extended the limits of FPMD. Results obtained on the BlueGene/L supercomputer using up to 32,768 processors will be presented. New linear-scaling algorithms and their implementation on massively parallel computers will also be described. Work performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48

COMP 145 Computational Chemistry at the Terascale

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We have performed large scale simulations on a variety of new advanced architectures. These architectures include the Cray-X1, Cray-redstorm and the Cray XD1. These architectures vary in their hardware design ranging from multistreaming vector processors (X1) to opteron based system (redstorm) and finally field programmable gate array based system (XD1). In our presentation we will highlight the performance of a number of quantum chemistry codes to elucidate their performance and in some cases how to better optimize these codes for obtaining higher computational efficiency. Lastly, we will present scientific results for a number of systems consisting of hundreds of atoms (e.g. TiO2 defect surface, transport calculations, etc.) in order to highlight what large scale systems might be possible to simulate on these advanced architectures.

COMP 146 Implementation Of Self Interaction Corrected DFT And Hybrid Functionals For Pseudopotential Plane-Wave Programs

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One of the more persistent failures of standard DFT methods has been their failure to yield localized charge states such as polarons, excitons and solitons in solid-state and extended systems. It has been suggested that standard DFT functionals which are not self-interaction free tend to favor delocalized electronic states since self-interaction creates a Coulomb barrier to charge localization. Pragmatic approaches in which the exchange correlation functionals are augmented with small amount of exact exchange have shown promise (i.e. B3LYP and PBE0) in localizing charge states. However, a large amount of exact exchange must be added in order for a these methods to yield localized charge states, which results in band-gaps and reaction barriers being overestimated. Self-interaction corrected (SIC) DFT has also shown great promise predicting localized charge states as well as accurate band-gaps and reaction barriers. We have recently developed a framework for implementing SIC-DFT and Hartree-Fock (HF) into pseudopotential plane-wave density functional theory (PSPW). The technique combines two procedures: construction of maximally localized Wannier functions (MLWF, procedure due to Marzari and Vanderbilt and to Silvestrelli) and direct minimization of the SIC-DFT/HF total energy functional. The technique developed can be employed in PSPW methods without adding significant expense. Furthermore, atomic forces and stresses are straightforward to implement, making it applicable to both confined and extended systems, as well as to Car-Parrinello ab initio molecular dynamic simulations. Various aspects of the implementation and computational efficiencies will be discussed. This method has been applied to several systems for which standard DFT methods do not work well, including excitons in quartz and rutile, polarons in hematite and annite, and oxygen vacancy on 110 rutile surface. Using the newly developed SIC-DFT and HF methods we have been able to obtain a significant degree of charge localization.

COMP 147 Building and using an in-house platform for data mining and analysis integrating open source and proprietary software: II. Model building and library analysis

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We have constructed an infrastructure that enables computational chemistry workflows using open source software integrated with closed source applications. In our use, this has proven to be a highly scalable and productive platform. We will describe workflows involving model construction, selection of targeted compounds with lead-like properties and the analysis of the selected compounds. Properties are based on 2D and 3D descriptors calculated with QikProp™, JOELib, and proprietary applications. Molecules are picked based upon strict property cut-offs and sampling both model space and desired distributions in property space. Examples will include the design and selection of a protein family-targeted screening library assembled from internally

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COMP 148 Use of structural keys to classify cytochrome P450 substrates

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The 166 and 324 MDL structural keys were evaluated for their ability to classify correctly substrates in terms of their likelihood to be metabolized by one of five different cytochrome P450 mixed function oxidases. The substrates were in an extensive relational database of 41,000 compounds linked to 65,000 routes of metabolism. Additional data included enzymes, animals and reaction conditions. For this study, only metabolism in humans was included. The five CYP P450 enzymes CYP1A2, CYP2B6, CYP2C9, CYP2D6 and CYP3A4 were considered. Five different classification schemes were used: Bayes-Naïve, Java C45 Decision Tree, Ripper Decision Rule, K-Nearest Neighbor and Support Vector Machine. Stratified cross validation was used with each classifier. This project showed the problem with having a consistent database to test structural keys and classifier algorithms.

COMP 149 Use of multiple-category Bayesian modeling to predict side effects
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The rapid growth of in the amount of biological information available from high-throughput screening studies and drug compendia such as MDL's Drug Data Reports (MDDR) and Derwent's World Drug Index would appear to provide a strong experimental base for the flagging of potential drug side effects. However, current methods, such as rational drug design, virtual docking, and QSAR modeling, do not appear to be easily applied to this task, due to slow computational speed, difficulty in automating, or difficulty in handling large, diverse data sets.

Laplacian-modified Bayesian modeling was developed to rapidly analyze high-throughput screening data using 2D molecule fingerprints. It can be extended so that a single model can predict the absolute probability of thousands of different activity classes. From this prediction, one can not only see what class a particular molecule is most likely active in, but competitive activity classes that may appear later as side-effects. The process is rapid enough to learn all of a drug compendium such as MDDR in minutes, and can then be used to suggest primary effects and side effects of hundreds of molecules per minute.

COMP 150 Property matching of reference datasets for classification models
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Binary classification schemes have found many applications within computational drug discovery. Among the earlier examples were schemas to discriminate between “drugs” and “non-drugs” but the technique is applied to problems such as prediction of toxicity and “frequent hitters” as well as “target class” library design. Virtual screening protocols can be regarded as classification models: the end point is a computational procedure to partition the screening database into binders and non-binders. Commonly, classification models are developed from rather large datasets of actives (such as “in-house and literature compounds acting towards target X”). However there is usually a lack of negative data and one often resorts to a set of randomly selected compounds from a suitable database. Compounds targeting a specific target or protein family commonly have a similar physico-chemical profile and there is a marked risk that any classification scheme will model the difference in physico-chemical properties rather than any specific pharmacophoric features. We have developed a simple procedure to extract reference datasets with physical-chemical properties matching those of the target datasets. The procedure uses the F-test in combination with a genetic algorithm based optimisation to select a reference set with matched distributions. The procedure is broadly applicable in the development of classification models and virtual screening protocols for the common case that there is a scarcity of negative (inactive) reference data. In some example applications of the algorithm we show that this provides an easy means to avoid some common pitfalls of classification models. It is notable that without deteriorating test-set performance one can remove bias from differing physical-chemical distributions for target class models. The procedure also highlights the need to take property differences into account when docking / virtual screening protocols are developed.

COMP 151 Electron paramagnetic resonance and equilibrium atomic configurations studies of binuclear niobium molecules in Li-Nb phosphate glass dielectrics
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