Molecular Science Computing Facility

The Molecular Science Computing Facility (MSCF) supports a wide range of computational activities in environmental molecular research, from benchmark calculations on small molecules to reliable calculations on large molecules, from solids to simulations of large biomolecules, and from reactive chemical transport modeling to regional cloud climate modeling. MSCF provides an integrated production computing environment with links to external facilities and laboratories within the U.S. Department of Energy (DOE) system, collaborating universities, and industry.

Capabilities

MSCF provides computational resources for Computational Grand Challenges in environmental molecular science and basic and applied research areas that address the environmental problems and research needs facing DOE and the nation. Computational grand challenge projects typically involve multiple investigators from universities, national laboratories, and industry working collaboratively as teams. These projects are usually granted computer time allocations for three years. MSCF supported 16 three-year grand challenge projects during 2006. The average annual computer time allocation for grand challenge projects in 2006 was 872,929 central processor unit (CPU) hours, down slightly from the previous year. The decrease is attributed to time allocations for EMSL Science Theme projects.

Instrumentation & Capabilities

- **MPP2**. Production cluster of 980 HP rx2600 nodes, 1960 1.5-gigahertz IA64 processors, 450-terabytes local disk, 6.8-terabytes memory, and 11.8-teraflops theoretical peak performance
- **Dtemp**. Shared parallel high-performance filesystem on MPP2, 53 terabytes
- **NWfs**. EMSL long-term data store, 300 terabytes
- **Network**. OC196 (10 GBit/sec) internet connection, 10 Gigabit Ethernet MSCF backbone
- **NWVisus**. Visualization server, SGI Onyx 3400Graphics, 8 processors, 8-GB RAM, two Infinite Reality3 pipes, 144-GB disk, with a PanoramTech 3-screen monitor Digital video editing suite
- **Molecular Science Software Suite**. NWChem, Ecce, GA Tools

MSCF also supports smaller, shorter-term projects called MSCF Pilot Projects. Pilot Projects are limited to a maximum of 75,000 processor hours and a one-year duration, with short extensions occasionally granted for project completion. MSCF supported 35 Pilot Projects during 2006, with an average allocation of 70,914 CPU hours. Pilot Projects are typically directed at developing the capability to submit a Computational Grand Challenge proposal in the future (e.g., a combination of theory/method or code development activities, or calculations that provide the initial scientific basis of a Computational Grand Challenge proposal). Pilot Projects are also awarded for computer support of experimental research taking place within other W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) facilities.

A third category of MSCF computer projects are provided to the Office of Science. In 2006 there were four such projects for a total of 750,000 CPU hours.

A new category of MSCF computer project was initiated in 2006, that of the EMSL Science Themes. These projects center around four science themes and encourage users to allocate time in multiple EMSL facilities. In 2006, there were 10 such projects that were awarded an average allocation of 75,500 CPU hours.

User Computing in MSCF. To optimally address the complex environmental problems facing DOE and the nation and to best use limited staff resources, EMSL follows the recommendation of the EMSL Science Advisory Committee to use a Computational Grand Challenge approach to providing large blocks of resources to the user community. A call for proposals is issued annually, and teams of computational scientists respond with peer-reviewable proposals for system time allocations. Access for the grand challenge teams is granted for periods of one to three years. The following criteria are used when reviewing proposals:

- scientific merit
- appropriateness of the proposed method or approach
- relevance to the environmental problems and research needs of DOE and the nation
- technical competence of the investigators, potential for high visibility journal articles
- reasonableness and appropriateness of the proposed computer resources.

The process used to review proposals and allocate MSCF computing resources is shown in Figure 1. The request for proposals is open to all researchers, regardless of their institution or source of funding. A call for Computational Grand Challenge applications was made April 1, 2006. The facility received 21 letters-of-intent requesting over 20 million CPU hours. Thirty seven external scientific reviewers from leading universities and research institutions from around the world reviewed the 18 full proposals. Each proposal received three reviews on average and was awarded time according to how well they rated and their allocation request. The average time awarded was 547,000 CPU hours.

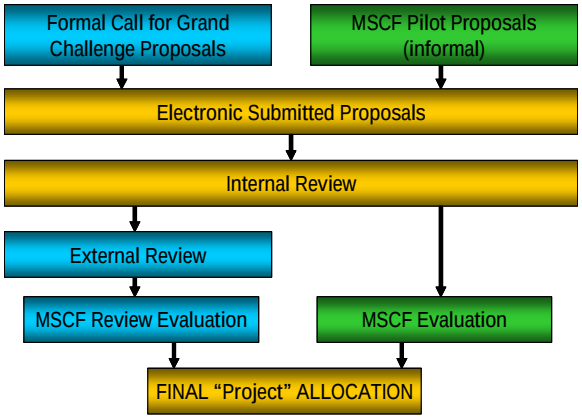

Figure 1. Review process and allocation proposal flow chart.

MSCF Resources

MSCF provides a combination of production computing hardware and software resources and visualization tools to support the scientific research activities of the Computational Grand Challenge and EMSL Pilot Projects. The hardware and visualization resources are the High-Performance Computing System-2 (MPP2), NWfs, the Graphics and Visualization Laboratory (GVL), and the Molecular Science Software Suite (MS^3). These resources are discussed below.

MPP2. MPP2 provides a balanced supercomputer. Since becoming operational in July 2003 with a theoretical peak performance of 11.8 teraflops, 6.8 terabytes of RAM, and 450 terabytes of disk, the Hewlett-Packard supercomputer (Figure 2) has been tailored to meet the operational needs of EMSL users.

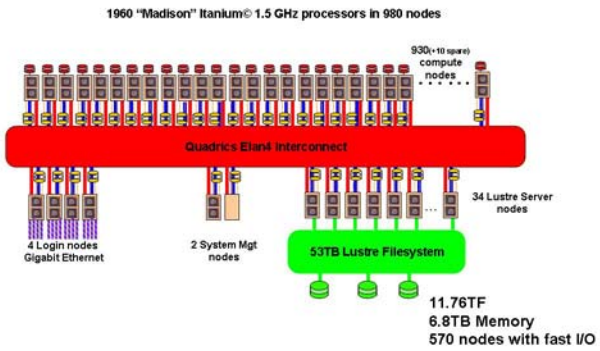

Figure 2. MPP2 Configuration.

NWfs. NWfs, which is the EMSL archive system located in MSCF, uses a groundbreaking approach to disk storage that clusters many low-cost commodity disks to provide fault-tolerant, scalable, long-term storage. Such large-capacity archive systems usually rely on tape for mass storage, but NWfs distinguishes itself by having all its data instantly accessible on disk-based storage. NWfs currently has a capacity of 300 terabytes and the ability to grow as needed to over a petabyte.

GVL. GVL provides production graphics and visualization facilities for the display and analysis of complex datasets from both experiments and simulations. GVL contains four high-performance graphics stations based on Silicon Graphics Incorporated (SGI) technologies with high-speed Gigabit Ethernet connections to the production supercomputers and to NWfs, a digital video system integrated with the workstations to facilitate the display and capture of scientific data, and digital video editing equipment for the preparation of scientific presentations. The video system also is connected to the EMSL auditorium and to the World Wide Web to facilitate internet conferencing. An IBM Scalable Graphics Engine is connected to the MSCF Dell Linux Cluster to provide the highest performance visualization capabilities.

MS^3. Software resources include MS^3, which is a comprehensive, integrated set of tools that enables scientists to understand complex chemical systems at the molecular level. MS^3 couples the power of advanced computational chemistry techniques with existing and rapidly evolving high-performance massively parallel computing systems with extensible problem-solving capabilities. The suite consists of three components: 1) the Northwest Computational Chemistry Software (NWChem), 2) the Extensible Computational Chemistry

Environment (Ecce), and 3) the Global Array Tools (GA Tools). These three components are briefly described below.

- ***NWChem***. Version 5.0 of NWChem was released in September 2006. Documentation and information are available on the NWChem Website (http://www.emsl.pnl.gov/docs/nwchem). NWChem provides many methods for computing the properties of molecular and periodic systems using standard Gaussian and planewave-based quantum mechanical descriptions of the electronic wave function or density. In addition, NWChem can perform classical molecular-dynamics and free-energy simulations. These approaches may be combined to perform mixed quantum-mechanics and molecular-mechanics simulations.

  NWChem is available on almost all high-performance computing platforms, workstations, PCs, and clusters of desktop or workgroup servers. NWChem development provides maximum efficiency on massively parallel processors. Among the new features available in the 5.0 version, the following are worth mentioning:
  - A completely new quantum mechanical/molecular modeling module that interfaces between classical molecular mechanics and quantum mechanical modules
  - Several new response properties of the density functional theory and Hartree-Fock wavefunctions.

- ***Ecce***. Ecce, which is composed of a suite of client/server Unix-based applications, is a domain-encompassing, problem-solving environment for computational chemistry. Applications for setting up, running, and analyzing the results of computational chemistry studies are built on top of a Web-based data management and inter-application messaging server framework. A computational code registration capability supports several underlying chemistry codes and the ability to integrate new ones without reworking core Ecce applications. Running jobs through industry standard remote communications, like secure shell, and a batch queue management system registration capability allows transparent access to high-performance compute resources from users' desktop workstations. A simple installation procedure and extensive online help combine to make Ecce a preeminent user environment for computational chemistry. The current production release of Ecce is version 4.0, released in September 2006. There are six major application components:

  1. Calculation Manager aids in the organization and manipulation of computational chemistry studies. This tool allows an at-a-glance overview of the status of every calculation and easy access to key setup parameters and run statistics.
  2. Molecule Builder is an intuitive point-and-click tool that enables the building, visualization, modification, and manipulation of three-dimensional representations of chemical systems.
  3. Basis Set Tool enables users to select from nearly 300 predefined Gaussian basis sets or the ability to create new ones for use in *ab initio* electronic structure calculations.
  4. Calculation Editor allows the user to choose input options using point-and-click interfaces for different chemistry codes, and then generates the code-specific input.

5. Job Launcher is used for submitting a calculation to a computer for processing. The user may submit a calculation to any computer that has been registered within Ecce and for which the user has an account.
6. Calculation Viewer provides convenient access to current information for a single calculation during execution or after completion. It has many features for viewing and visualizing chemical system properties.

- ***GA Tools***. GA Tools (also known as ParSoft) includes high-performance computing libraries and tools for applied parallel computing focused on inter-processor communications through the aggregate remote memory copy interface, high-performance input/output through the Parallel I/O tools, and programming models for hierarchical memory systems through the Global Arrays and Memory Allocator libraries. The development of these tools is driven by needs of real scientific application codes on the high-end parallel systems. Development of Aggregate Remote Memory Copy has been supported by EMSL operations and by the DOE Center for Programming Models for Scalable Parallel Computing. The most recent version of GA Tools, Version 4.0, was released in April 2006.

MSCF Organization

MSCF is organized into three project groups: 1) the Visualization and User Services Group, 2) the High-Performance Software Development Group, and 3) the Computer Operations Group.

Visualization and User Services Group (VisUS). This group provides an extremely diverse set of services for all users of the MSCF high-performance computers and GVL. Scientists who need access to high-end computing equipment frequently have difficulty getting started. The difficulties encountered range from logging in to getting user codes to run efficiently. VisUS handles user proposal applications, follows user progress during computational projects, manages proposal reviews for both Computational Grand Challenge projects and Pilot Projects, helps with user accounts, provides general consulting support for MSCF software packages, supports and maintains software, manages the GVL, conducts training and user workshops, develops visualization software and high-quality visualizations, and maintains Websites.

The group manages the Computational Grand Challenge and Pilot Project proposal process for the MSCF. This activity includes receiving proposals, providing preliminary review for EMSL missions, assigning external peer reviewers, evaluating peer reviews, granting project allocation, and managing the allocations by using GOLD, a dynamic-reservation-based allocations management system originally developed at PNNL.

Consultants have various roles, including those of administrator, scientific point of contact, tutor, programmer, or research scientist, and field a variety of requests for support. During 2006, five scientific consultants responded to more than 585 e-mail requests, and about 500 additional requests were handled over the telephone or during office visits. Consultants also

work directly with MS³ development teams to give customer feedback and to test functionality.

Information about the use and configuration of the MSCF computational resources is critical to the user base and is provided efficiently to users via the Internet through the MSCF home page. The MSCF Website contains all necessary information about how to establish accounts and get started, and about computer configurations as well as documentation and Web-based tutorials for MS³. Scientists generate enormous amounts of data either from computational resources or from EMSL instruments. These data are usually complex and difficult to understand. The capabilities and expertise available in the GVL, including its high-performance graphics compute servers and state-of-the-art multimedia equipment, help scientists visualize these complex data. The real-time digital video capture capability from the graphics compute servers allows fast, yet high-quality, video production. Users can generate presentation media in any form—from video (including all international video standards) to Web-based animations. The group also provides basic video production services.

High-Performance Software Development Group. This group has the primary responsibility for developing and supporting MS³. This effort includes:

- developing high-performance versions of the software and new high-performance algorithms
- continually refreshing the underlying software architecture to stay current with new hardware and software technology and standards
- responding to user requests for additional features
- supporting and maintaining the software
- diagnosing MS³ problems associated with computer vendor hardware and software
- consulting on specific MS³ problems
- distributing MS³ to remote sites
- porting software to new architectures
- conducting training and user workshops.

The MS³ project group focuses on developing next-generation molecular modeling software for newly evolving computer technologies, especially massively parallel computers. The project group is composed of computational chemists and computer scientists (with external collaborations to mathematicians) who work together to develop the MS³ software. This software is used by many of the MSCF Grand Challenge projects and has been distributed to almost 1600 sites worldwide. In addition to the development activities, this group is also responsible for training software users, conducting tutorial workshops, and providing user support. Several resources have been developed to facilitate user support and training. These resources include MS³ Websites with user and reference manuals, download information, release notes, FAQs, a list of known bugs, tutorials, and benchmark information, Web-based context-sensitive help available from within the software, as well as a mailing list where users can post support-related questions and get answers either from experienced users or from the NWChem developers.

Computer Operations Group. This group operates, maintains, and advances the capabilities of the MSCF scientific computing systems. The group is responsible for the operation and implementation of the various production supercomputers in the MSCF and has developed unique system management, monitoring, allocation management, and scheduling capabilities. The primary focus is on providing high-quality, reliable production computing cycles and storage capabilities in the MSCF to support very large parallel calculations for Computational Grand Challenge projects.

Upgrades

In Fiscal Year 2006, the following capability development occurred in the MSCF:

- **NWChem, Version 5.0.** NWChem, Version 5.0 was released in September 2006. Some of the important new capabilities in this release include new and improved high-accuracy methods; a new quantum mechanical/molecular mechanical module with functionality essential for studies of large biological systems and for understanding reaction pathways, kinetics, and equilibriums in complex chemical systems; improved parallelization of plane wave code; and improvements to the molecular dynamics module.

- **Ecce, Version 4.0.** Ecce, Version 4.0 was released in September 2006. In addition to the version 4.0 release, Ecce also had two minor 3.2.x production releases. The minor releases (Ecce 3.2.4 and Ecce 3.2.5) contained updated basis sets, enhancements to molecular orbital visualization and POV-Ray publication quality output, GAMESS-UK (see http://cfs.dl.ac.uk) code registration developed in collaboration with Daresbury Laboratory, and fixes resulting from user feedback. The major new capability in Ecce 4.0 is the end-to-end support for the NWChem molecular dynamics module. User interfaces were developed in tight collaboration with the NWChem developers and represent very close to a full mapping of the options available to NWChem molecular dynamics users who manually create input files.

- **Global Arrays, Version 4.0.** Global Arrays, Version 4.0 was released in April 2006. New features include processor group awareness and support for multilevel parallelism, support for very large arrays, optimized nonblocking one-sided operations and matrix multiply with SRUMMA, and port to the Cray X1 and SGI Altix. The first three features directly affect the capability of NWChem to perform cutting-edge scientific computations, enabling scalability to thousands and possibly tens of thousands of processors, and studies on problem sizes with correlated methods larger than for any other software suite.

- **Gaussian Basis Set Library.** EMSL's Gaussian Basis Set Library was released in September 2006. One of the most widely used databases associated with EMSL (http://www.emsl.pnl.gov/forms/basisform.html), the Gaussian Basis Set Library is a very important chemistry community resource reaching nearly 3000 unique visitors each month, but for the last two years, this database has received very little attention. Through SciDAC-I funding, a much improved version now enables efficient management of the database and underlying programs, provides a greatly improved web interface for browsing and downloading data, and allows basis set developers to directly contribute new data sets to the database. Some EMSL Operations funding was used to make this new resource production ready. This improved capability provides new basis sets for NWChem.

- **2-petabyte tape library**. A new 2-petabyte tape library will be used to make backup copies of MSCF data, particularly those from NWfs and MPP2. The library is expected to have a useful lifetime of at least five years.

- **Raised floor.** Nearly 4,000 square feet of raised floor was added in EMSL's supercomputing operations center, where the next-generation supercomputer will be housed.

- **Data storage capability.** A new method was developed for performing backups of NWfs data. This new capability will substantially decrease recovery time in the event of catastrophic failure of one or more NWfs nodes.

- **Development of a shared spreadsheet for tracking foreign national.** Many limits exist as to how long foreign national accounts can be active. When passports, visas, or work permits expire, so do their holders' computer accounts. Renewing an account requires the same amount of work as the original account. Multiple email messages arrive over the weeks alerting the facility host and Scientific Facility Lead of accounts nearing termination. This new spreadsheet allows the Visualization and User Services Group to track whether to extend an account or allow it to expire and has saved much time by avoiding double, triple and quadruple checking each time an email message arrives.

- **Improvement of scalability and efficiency of several codes.** Visualization and User Services consultants working with software developers, using EMSL's supercomputer, to suggest modifications to their code in order to improve efficiency and scalability.

- **A new script for gleaning CPU time used per project for the GOLD Allocation manager** saves two to four hours per month with increased accuracy. This script creates a file that is used to populate a master spreadsheet developed last fiscal year for monitoring computer use by each of the projects that have time allocated.

- **Video editing and computer visualization upgrade.** Equipment in the GVL has passed useful life and must be replaced to meet current and future needs of EMSL users. This equipment has been delivered and is being set up, with the old equipment excessed.

Future Directions

In Fiscal Year 2007, the MSCF will continue to support researchers by providing state-of-the-art computational resources. All advanced computing systems require continued effort in maintaining the system at peak performance as well as implementing the appropriate software and science knowledge base to effectively and efficiently use the technology. To address these needs, MSCF Operations will continue to operate facility systems, including MPP2 and NWfs. The facility will continue to provide support for computing installations and upgrades, operating systems support, improvements to the quality of the system software to improve the user environment, allocation tracking, direct interfacing with the vendor, system security, and system-level support to users.

The HPCS-3 project to procure and implement the next generation of computational resources will be a primary focus for the Operations team. The project will be compliant with DOE O413.3 (the DOE Critical Decision process).

Planned activities under Molecular Science Computing Facility Operations for Fiscal Year 2007 include:

- **Procurement of HPCS-3**, the next-generation marquee supercomputer for EMSL.
- **Continued operation of facility systems**, especially of MPP2 and NWfs.
- **Expansion of NWfs** disk storage capacity (currently estimated to be 450 additional terabytes).
- **Benchmarking of facility power consumption and efficiency** in order to gain a better understanding of how power is consumed in the facility. This will help facility staff learn to reduce the quantity of power consumed by power distribution and cooling, and to supply more power to systems within existing facility constraints.

In Fiscal Year 2007, MSCF High-Performance Software Development will continue to support users by providing state-of-the-art computational chemistry software. By providing cutting-edge capabilities and a fast time-to-solution, the goal is to increase the number of publications citing NWChem and Ecce to more than 110, with 70 in top-10 journals and 50 in top-5 journals.

Most of the EMSL user proposals using resources of this facility require NWChem. Proposed performance improvements, developments, and support are aligned with the needs of those proposals. Development of new methods and capabilities is essential for the long-term success of NWChem. Without the new methods and software development, NWChem will fall behind in providing solutions to scientists' challenges.

In Fiscal Year 2007, a NWChem Developers Meeting, "NWChem – Future Developments, Science Driven Petascale Computing and Capability Development," will be held. This meeting, featuring leading computational chemists, will lead to a report on the science needs within the DOE Office of Biological and Environmental Research and within the computational chemistry community that will drive new capability and petascale development in NWChem.

- **NWChem core and user support.** Improvements that will be made in Fiscal Year 2007 include:
  - Further improvements in time-to-solution, memory and disk needs, and the handling of even larger problem sizes for high-accuracy methods.
  - Further developments in efficiency and functionality of quantum mechanics/molecular mechanics methodologies to enable more realistic descriptions of dynamical (reaction) processes.

- Extension of the Molecular Dynamics module to include general task-level parallelism using the Global Arrays processor group functionality. This will allow methods such as Replica Exchange to be easily implemented and will provide enhanced sampling for Free Energy calculations,

- A major rewrite of the Molecular Dynamics module documentation. This documentation has not been updated for several years and requires major revisions. As molecular dynamics codes in general are hard to use, and to increase the ease-of-use for the users of the Molecular Science Computing Facility computing resources a new tutorial will be developed.

- Further improvements in parallelization and efficiency of the plane wave and band structure code, with a focus on large numbers of processors to enable users to study larger systems at longer time-scales

- **Global Arrays Toolkit.** The Global Array Toolkit provides a high-performance programming interface for the scientific programmer by exploiting low-level network protocols and operating system-dependent interfaces. A significant component is maintenance and optimizations of software to keep it robust given the ongoing evolution of the compiler and operating systems. In Fiscal Year 2007, a new release (version 4.1) is planned that will include support for block cyclic distribution to allow better integration with Scalapack. In addition, this release will provide improved support for the Infiniband OpenIB standard, IBM LAPI and BlueGene/L, and Cray XT3 architectures. Each new capability was developed using other funding sources and EMSL core funding is used to make them production ready. These new architectures prepare the Global Arrays Toolkit and NWChem for EMSL's next-generation supercomputer and allow NWChem to run on the first-generation petascale platforms.

- **Ecce core and user support.** Improvements that will be made in Fiscal Year 2007 include:

  - Support for EMSL one-time login policy for MPP2 access to enable external users of the facility to use Ecce as a front end to submit calculations and to analyze results.

  - Enhancements to create full end-to-end NWChem Molecular Dynamics support, such as supporting the free energy task, essential dynamics in the analysis module, extended trajectory analysis/visualization.

  - Ecce user support, outreach, and education for the new molecular dynamics capability, which gives users an easy way to set up, run, and analyze calculations.

  - NWfs archival file support for large output files. This development is critical given the huge size of trajectory files for molecular dynamics, and the need to store this data in an archive.

  - Improving support for minor new NWChem features in Ecce.

- Continued porting of Ecce Basis Set Tool and Builder modules to the wxWidgets cross-platform user interface to allow users to run Ecce from any of their home platforms, including Windows machines.

- **NWChem and Ecce user support for user agreements.** In Fiscal Year 2007, approximately $100K will be spent on administering the user agreements for NWChem and Ecce. The distribution of NWChem and Ecce is getting more difficult every year due to addition distribution constraints and an ever-increasing number of new and returning sites. In Fiscal Year 2007, an additional 10% full-time equivalent has been allocated to develop a strategy, and to switch to an Open Source distribution model. There are three reasons to pursue the Open Source model:

  1. The approximately $100K can be used for the development of new science capabilities requested by the users of NWChem and the Molecular Science Computing Facility.

  2. Many developers interested in improving NWChem and Ecce, or adding new functionality, are reluctant to do so because of the user agreement restrictions. Moving NWChem and Ecce to Open Source will increase participation of external developers, and can lead to a reduction of core costs.

  3. One major target for NWChem development is the ability to run efficiently on petaflop platforms. The appropriate funding agency, DOE Office of Advanced Scientific Computing Resources, is mainly interested in supporting Open Source software.

- **EMSL Basis Set Support.** Funding is required to maintain the servers.

Molecular Science Computing Facility's VisUS will work with the rest of the facility and EMSL to provide the necessary services in computer operations, software development, and scientific consulting.

One of the goals is to focus research on challenging scientific problems in the environmental molecular sciences in support of the needs of DOE and the nation by providing unique computational capabilities that are likely to result in or contribute to a Nobel Prize, major articles in *Science*, *Nature*, or the *Proceedings of the National Academy of Science*, or Hot Papers as defined by ISI, or covers in ISI top-5 journals. With two-thirds of the Computational Grand Challenge projects (10) ending and 18 Computational Grand Challenge Applications accepted, the group expects a large turnover in user accounts. Some of the projects will be continuations of previous projects but even so, twice as many computer accounts are expected to be processed. Twice as much user support work is also expected this next fiscal year, which requires either additional personnel or decreased user support.

- **Increased publications.** With so many Grand Challenge projects coming to an end, the group expects to have an increased number of publications, with more of them in top-10 journals.

- **Support selection of computing resources.** The VisUS group will work with the Molecular Science Computing Facility team on the Request for Proposal and vendor selection for major computing resources. The group also expects to spend time testing the Phase I version of HPCS-3.

- **Provide consulting and other services.** The VisUS group will continue to provide users with access to consulting services, visualization, advanced data analysis and tutorials. The group will need to have at least one individual knowledgeable in each of the EMSL science themes and be able to provide the expertise necessary for all users to effectively use the facility's computational resources. With additional compute power available in the near future, the group needs to start training new scientific consultants so they are ready when the number of users increases dramatically.

- **Obtain additional staff.** Additional trained personnel are needed to provide visualization and advanced data analysis support as well as outreach efforts to expand the number of first-time users of the facility. Animations and user highlights can be produced to emphasize the computational science accomplished in EMSL as well as presentations given at conferences and workshops that display both exceptional science and eye-catching, content rich graphics, and animations.

- **Encouraging multi-facility use.** Annual calls for participation will be modified so that EMSL science theme calls that encourage multi-facility utilization will have increased priority. Separate Computational Grand Challenge calls will be issued later in the year as computer time is available. There will be continued support for the EMSL Scientific Grand Challenge Projects.

Estimated IR and Phosphorescence Emission Fluxes for Specific Polycyclic Aromatic Hydrocarbons in the Red Rectangle

G Mulas,[a] G Malloci,[a] C Joblin, [b] and D Toublanc[b]

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(b) Centre d'Étude Spatiale des Rayonnements, CNRS and University Paul Sabatier, Toulouse, France

Calculated infrared spectra of polycyclic aromatic hydrocarbons were compared with available experimental infrared data to correctly identify spectroscopic components of the Red Rectangle Nebula (considered to be a Rosetta Stone for astrophysical processes).

Following tentative identification of the blue luminescence in the Red Rectangle Nebula by Vijh et al. 2004, Mulas and collaborators used EMSL's computational chemistry software, NWChem, to compute absolute fluxes for the vibrational infrared emission of three small polycyclic aromatic hydrocarbons (Vijh et al. 2005). The calculated infrared spectra were compared with available observational data from the Infrared Space Observatory (see Figure 1 for spatial distribution). A subset of the emission bands are predicted to be observable using presently available facilities and can be used for an immediate, independent, discriminating test of their alleged presence in this well-known astronomical object.

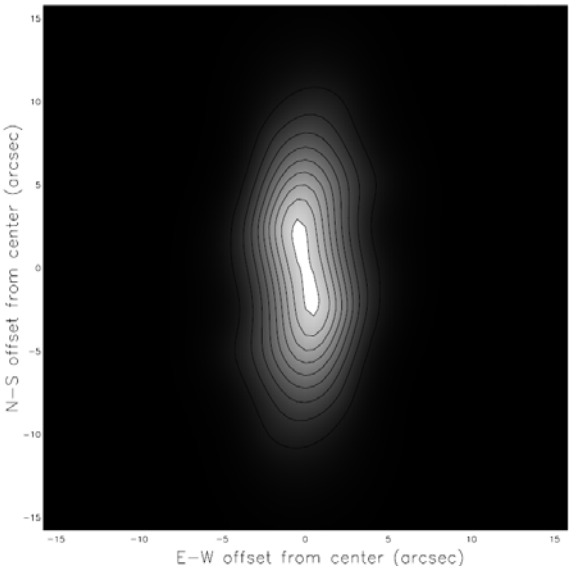

Figure 1. Spatial distribution of the blue luminescence surface brightness of the Red Rectangle Nebula, interpolated from the values given by Vijh et al. 2005. East is left, north is up, and contour lines are in 5% intervals.

Simulations of the photophysics of the candidate molecules were carried out using a Monte Carlo code, together with quantum-chemical calculations (NWChem and Octopus computer codes) for the relevant molecular parameters, and available laboratory measurements for the photoabsorption spectra and for the visible and infrared fluorescence quantum yields. This produced a quantitative prediction of the infrared and phosphorescence emission spectra for each given molecule, which must be related to the integrated blue luminescence attributed to this same molecule.

Citations

Mulas G, G Malloci, C Joblin, and D Toublanc. 2006. "Estimated IR and Phosphorescence Emission Fluxes for Specific Polycyclic Aromatic Hydrocarbons in the Red Rectangle." *Astronomy & Astrophysics* 446(2):537-549.

Vijh UP, AN Witt, and KD Gordon. 2004. "Discovery of Blue Luminescence in the Red Rectangle: Possible Fluorescence from Neutral Polycyclic Aromatic Hydrocarbon Molecules." *The Astrophysical Journal* 606:L65-L68.

Vijh UP, and AN Witt. 2005. "Small Polycyclic Aromatic Hydrocarbons in the Red Rectangle." *The Astrophysical Journal* 619:368-378.

Effect of Pore Scale Heterogeneity in Transport

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While there is general agreement that pore-scale heterogeneity plays an important role in subsurface reaction and flow/transport processes, characterization efforts have typically focused on sediment properties on the scale of architectural elements while essentially neglecting fine-scale heterogeneity. Consequently, there is a lack of consensus on which microscopic geometrical properties are needed to predict the macroscopic transport properties required for field-scale model predictions.

This project has been focused on 1) identifying which microscopic geometrical properties are needed to predict direction-dependent macroscopic properties, 2) quantifying the effects of pore-scale heterogeneity on macroscopic transport properties, and 3) comparing the relative contributions of physical and geochemical heterogeneities to field-scale reactive transport. Resolution of the effects of multiscale heterogeneity on subsurface transport requires large simulations, typically ~10^5-10^7 grid cells. Progress in this research is dependent on a variety of computer simulation tools, most of which have been developed for use on massively parallel computers, such as EMSL's supercomputer.

Ward and coworkers made use of a Lattice-Boltzmann model (Stewart et al. 2006, in press) and digital representations of porous media with different degrees of heterogeneity and particle aspect ratios (see Figure 1). The Lattice-Boltzmann flow simulation method can efficiently use massively parallel computers to resolve the effects of complex boundaries.

This work has led to the development of new constitutive theory for describing saturation-dependent anisotropy for porous media (Ward et al. 2006). The new theory has been incorporated into the PNNL STOMP (Subsurface Transport Over Multiple Phases) computer model and is already being used for the evaluation of remedial options for a variety of waste management areas at the Hanford Site and within the DOE complex.

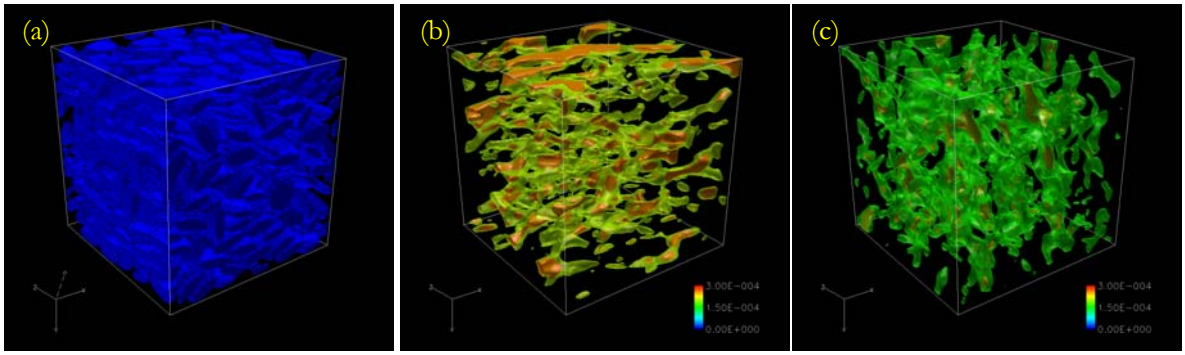

Figure 1. (a) Random particle pack with 3:1 aspect ratio and 0.58 porosity, (b) velocity distribution imposed by horizontal gradient, and (c) velocity distribution imposed by vertical gradient. Note the higher velocities in the horizontal flow case, indicated by yellow and red versus the green in the vertical flow case.

Citations

Stewart ML, AL Ward, and DR Rector. "A Study of Pore Geometry Effects on Anisotropy in Hydraulic Permeability Using the Lattice-Boltzmann Method." *Advances in Water Resources*, 29 (In Press).

Ward AL., ZF. Zhang, and GW Gee. 2006. "Upscaling Unsaturated Hydraulic Parameters for Flow Through Heterogeneous Anisotropic Sediments." *Advances in Water Resources* 29(2):268-280.

MSCF Users Leading the Way to Zero Emission Transportation

J Li[a] and MS Gutowski[b]

(a) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

(b) Pacific Northwest National Laboratory, Richland Washington

Hydrogen fuel cells are an environmentally friendly way to power vehicles. Recent years have seen increasing interest for research on efficient hydrogen fuel cells from the federal government and the transportation industry. The main challenge today for energy industries is how to make hydrogen fuel cells economically competitive with their conventional fuel counterparts. A key issue that must be addressed is the efficient storage of hydrogen, which would allow hydrogen-powered cars to cover longer distances on a single "tank" and fuel distributors to efficiently deliver hydrogen to consumers.

The idea of "zero-emission" transportation has long been a dream for protecting the environment. Hydrogen-powered cars would bring that dream a step closer to becoming an economically viable alternative to conventional transportation fuels. Many research efforts focus on hydrogen fuel cells; however, hydrogen storage is a key bottleneck to implementing this approach. While highly compressed hydrogen gas and liquefied hydrogen are unlikely to be of sufficient volumetric density, the use of chemical hydrogen storage materials based on light elements is possibly a feasible approach. Recently a joint computational and experimental research project, led by PNNL scientists M Gutowski and T Autrey, has made important progress on ammonia borane (BH_3NH_3)-based materials, which hold great promise for hydrogen storage (Gutowski and Autrey 2006). The computational research of this project is part of the Molecular Science Computing Facility Computational Grand-Challenge 9601 (Computational Design of Materials for Hydrogen Storage, PI: Jonnson), which is one of the computational projects supported by the EMSL.

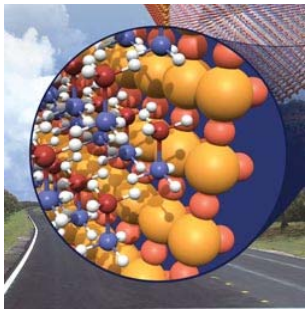

Figure 1. Ammonia borane materials consist of interlocking networks of ammonia and borane units, which form a structural and electrical scaffolding that can hold hydrogen.

The main challenges for making hydrogen fuel cells competitive with conventional fuel involve scale. A viable hydrogen storage medium would have to optimize the density of hydrogen while maintaining favorable electrical and thermodynamic properties. For ammonia borane compounds, the density of hydrogen storage is between 19% and 24%, which make these materials excellent study candidates for hydrogen storage. The computational simulation work has demonstrated that for a variety of ammonia borane materials, the release of hydrogen is for the most part thermodynamically neutral (i.e., the release and uptake of hydrogen from the material is nearly reversible at equilibrium). Currently, removing hydrogen from ammonia borane materials has been shown to be feasible at relatively low temperatures, which is an important characteristic for making

hydrogen fuel cells practical in vehicles. However, a significant challenge still exists in that there is a large energy barrier associated with "filling" ammonia borane materials with hydrogen. This energy barrier represents a practical limitation in that to be competitive, distribution of alternative fuels to consumers must be easy. Future work from this Grand Challenge will focus, in part, on searching for a solution to this limitation for ammonia borane materials. If successful, this project could help pave the way to zero-emission transportation fuels that would revolutionize the automobile industry and have a significant impact on providing a solution for achieving and sustaining a clean environment.

Citation

Gutowski MS and T Autrey. 2006. "Hydrogen Gets Onboard." *Chemistry World* 3(3):44-48.

Using Advanced Statistical Models to Improve High-Throughput Proteomics

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Genes are DNA segments that when "turned on" provide living cells with instructions on how to build proteins, which are molecules that can be used as the cellular "skeleton," allow some cells to move, process energy and waste products, and participate in virtually every function required for cells to live. Understanding how organisms work requires us to get a detailed picture of the proteins inside them. High-throughput proteomics is a rapid way to measure the protein content of biological samples, but the veracity of those measurements is, in part, determined by the rate of correctly identifying proteins or protein pieces.

Detecting bioterrorism threats, ensuring a safe food supply, and using microbes to clean up the environment or as a "clean" energy source are just some of the areas of biology where rapidly analyzing very large collections of proteins, or working molecules is a key technology. High-throughput proteomics is a signature capability at PNNL, where the capability is made available to a worldwide community of users to rapidly identify all the proteins in a biological sample. Reliably identifying the protein content of a cell gives important information about its function, making it possible to develop new ways in which cells can easily be identified, which is important in detecting bio-threats.

The main computational challenge associated with high-throughput proteomics is the task of identifying protein fragments (peptides) from measurements of the mass-to-charge ratio (m/z) of small pieces of the peptides. In a high-throughput method known as tandem mass spectrometry (MS/MS), this collection of m/z values can be used as a mass fingerprint to identify the correct peptide sequence from a large list of candidate peptides. *Polygraph*, a high-performance application designed to perform this peptide identification task, has been demonstrated to improve the identification rate of peptides measured by MS/MS. This performance improvement is achieved, in part, by using an advanced statistical model to better understand and identify the fingerprint associated with each peptide. Previous

methods generally worked under the assumption that peptides are equally likely to fragment anywhere along their length. However, measurements of the probability of fragmentation along the peptide have shown that there is a strong position-dependence to the likelihood of fragmentation (Figure 1). Including this additional information into *Polygraph* has resulted in a substantial improvement in the ability to correctly identify peptides.

Future directions of this Computational Grand-Challenge 9603 research include development of a data-intensive version of *Polygraph* that would reduce by a factor of one-third the time required to accurately identify peptides from MS/MS data.

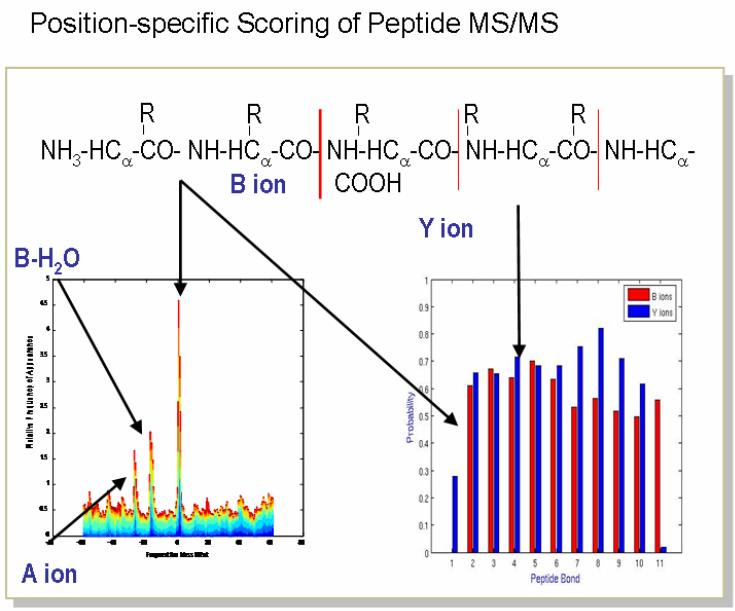

Figure 1. Using a position-dependent description of likelihood of peptide fragmentation has resulted in a fourfold reduction in the false positive identification rate.

Publications Resulting From This Grand Challenge and Pilot Project

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Cannon WR, KH Jarman, BM Webb-Robertson, DJ Baxter, CS Oehmen, KD Jarman, A Heredia-Langner, KJ Auberry, and GA Anderson. 2005. "A Comparison of Probability and Likelihood Models for Peptide Identification from Tandem Mass Spectrometry Data." *Journal of Proteome Research* 4(5):1687-1698.

Heredia-Langner A, WR Cannon, KD Jarman, and KH Jarman. 2004. "Sequence Optimization as an Alternative to *De Novo* Analysis of Tandem Mass Spectrometry Data." *Bioinformatics*. 20(14):2296-2304.

Jarman KD, WR Cannon, KH Jarman, and A Heredia-Langner. 2003. "A Model of Random Sequences for *De Novo* Peptide Sequencing." In *Proceedings of the 3rd IEEE International Symposium on Bioinformatics and Bioengineering*, pp. 206-213, IEEE Computer Society, Los Alamitos, California.

Malard JM, A Heredia-Langner, DJ Baxter, KH Jarman, and WR Cannon. 2004. "Constrained *De Novo* Peptide Identification via Multi-Objective Optimization." In *Proceedings of the 18th International Parallel and Distributed Processing Symposium*, pp. 191-199, IEEE Computer Society, Los Alamitos, California.

Malard JM., A Heredia-Langner, WR Cannon, RW Mooney, and DJ Baxter. 2005. "Peptide Identification via Constrained Multi-Objective Optimization: Pareto-Based Genetic Algorithms." *Concurrency and Computation: Practice and Experience* 17(14)1687-1704.

Full Collection of More Than 1.6 Million Proteins Analyzed Using ScalaBLAST

CS Oehmen[a] and P Hugenholtz[b]

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(b) Lawrence Berkeley National Laboratory, Berkeley, California

ScalaBLAST is a high-throughput sequence analysis engine based on the National Center for Biotechnology Information BLAST distribution. It allows users to harness the power of supercomputers or commodity clusters to accelerate the rate of performing normal BLAST searches against a target database.

One of the key limitations in any sequence analysis pipeline is the need to compare a large collection of proteins from many organisms against itself to detect commonalities between the proteins of different species and within a species. In conjunction with the Joint Genome Institute, current steward of a large collection of microbial genomes, CS Oehmen of Pacific Northwest National Laboratory and P Hugenholtz of Lawrence Berkeley National Laboratory used ScalaBLAST to analyze the full collection of more than 1.6 million proteins against itself in less than 13 hours using 1000 processors of the MPP2 supercomputer in the EMSL Molecular Science Computing Facility (MSCF).

An additional large search was performed in which each of the 1.6 million microbial protein sequences was compared to the nonredundant list of more than 3 million proteins distributed by the National Center for Biotechnology Information. This step is often performed on genomes as part of a quality control process. For a dataset of this size, it is not possible for most BLAST users to analyze the full dataset in a tractible time, because for most standalone BLAST installations, a single genome of a few thousand proteins takes many days to process.

Oehmen and Hugenholtz were able to use ScalaBLAST on MPP2 to process the entire list of 1.6 million proteins against the nonredundant database using 1500 processors in fewer than 20 hours. This collection of results will be shared with the Joint Genome Institute to

be used in conjunction with the microbial genome data as a significant information resource for the worldwide community of biological researchers.

Full Stannaspherene: A Highly Symmetric Cage of Sn_{12}^{2-} Dianion

L-F Cui,[a,b] X Huang,[a,b] LM Wang,[a,b] DY Zubarev,[d] AI Boldyrev,[d] J Li,[c] and LS Wang[a,b]

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(c) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

(d) Utah State University, Logan, Utah

In an effort to understand the semiconductor-to-metal transition in main-group elemental clusters, photoelectron spectroscopy (PES) was used to observe a remarkably stable tin cluster. The spectrum of Sn_{12}^- is remarkably simple and totally different from the corresponding Ge_{12}^- cluster, suggesting that Sn_{12}^- is a unique and highly symmetric cluster.

Theoretical analysis and computational calculations show that the neutral Sn_{12}^- monoanion cluster has a slightly distorted icosahedral cage with C_{5v} symmetry (Figure 1). Adding an electron to Sn_{12}^- results in a stable closed-shell icosahedral I_h-Sn_{12}^{2-} cluster, which was synthesized in the form of KSn_{12} ($K^+[Sn_{12}^{2-}]$) with a similar PES spectrum as Sn_{12}^-. The calculated energy gap between the highest occupied and lowest unoccupied orbitals in the I_h-Sn_{12}^{2-} is 1.9 eV, which is even larger than that in C_{60} (1.62 eV), providing further evidence for its high stability. The theoretically calculated energy levels, including spin-orbit coupling effects, are in good agreement with the experimentally observed spectra. The I_h-Sn_{12}^{2-} cage is shown to be bonded by four delocalized radial π bonds and nine delocalized on-sphere tangential σ bonds from the 5p orbitals of the tin atoms, whereas the $5s^2$ electrons remain largely localized and nonbonding. The bonding pattern in Sn_{12}^{2-} is similar to the well-known aromatic $B_{12}H_{12}^{2-}$ cage, with the 12 $5s^2$ localized electron pairs replacing the 12 B-H bonds. Because of the delocalized π bonding in Sn_{12}^{2-} and its spherical symmetry, the name "stannaspherene" is suggested for this highly stable species.

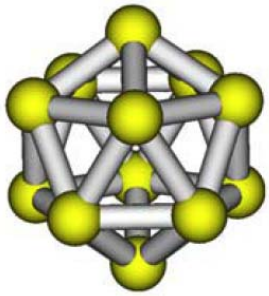

Figure 1. Computationally optimized structures of icosahedral Sn_{12}^- cluster.

While cage structures involving tin were known in inorganic complexes and the Zintl phases, the I_h-Sn_{12}^{2-} cage was unknown. The high stability of this cluster suggests that it may be synthesized in the solid state using suitable ligands or counter ions. More interestingly, the Sn_{12}^{2-} cage has a diameter of ~6.1 Å, which is only slightly smaller than that of C_{60}, and it can host an atom inside much like the endohedral fullerenes. Preliminary experimental and

theoretical results suggest that most transition metal atoms can be hosted inside the Sn_{12}^{2-} cage, yielding a large class of novel endohedral stannaspherene. These metal-encapsulated stannaspherene clusters give rise to a large family of endohedral chemical building blocks for cluster-assembled nanomaterials. This work is published in the Journal *of the American Chemical Society* (Cui et al. 2006).

Citation

Cui L-F, X Huang, LM Wang, DY Zubarev, AI Boldyrev, J Li, and LS Wang. 2006. "Sn_{12}^{2-}: Stannaspherene." *Journal of the American Chemical Society* 128(26):8390-8391.

Computer Simulation of Radiation Effects in Zircon

R Devanathan,[(a)] LR Corrales,[(a)] WJ Weber,[(a)] A Chartier,[(b)] and C Meis [(b)]
(a) Pacific Northwest National Laboratory, Richland, Washington
(b) INSTN/UEPEM CEA-Saclay, Gif-Sur-Yvette, France

Using the computational resources of the MSCF MPP2 supercomputer and the NWfs (Northwest file system), massively parallel molecular dynamics simulations of uranium recoil damage in zircon were performed. Zircon is a durable ceramic that is a promising candidate for the safe immobilization of excess weapons-grade plutonium and high-level nuclear waste.

When doped with actinides, zircon undergoes α-decay that produces 70- to 100-keV heavy ion recoil. The recoil dissipates its energy by a cascade of atomic collisions, leading to defect production at the atomic-level, loss of crystalline structure, significant increase in leach rate of actinides, and degradation of mechanical properties. Because of the short time (ps) and length (nm) scales over which these processes take place, they are not easily accessed by experiments. To understand the fundamentals of radiation damage in ceramics and to design better nuclear waste forms, realistic computer simulations are needed in conjunction with experiments to shed light on the dynamics of collision cascades.

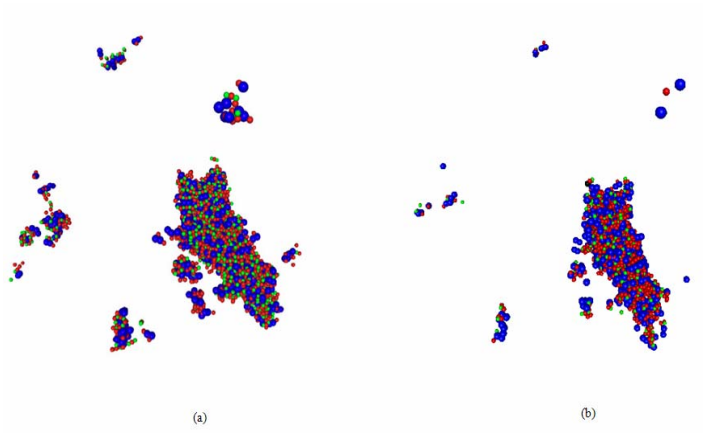

Figure 1. 30-keV uranium cascade in zircon showing (a) defects and (b) amorphous regions. The elements zirconium, silicon, and oxygen are represented by green, blue, and red, respectively.

In this project, the researchers simulated 10- and 30-keV uranium recoils in zircon, and developed new algorithms to distinguish between perfect crystalline, defective crystalline, and amorphous regions in the resulting collision cascade. The simulation cell contained more than one million atoms, which is remarkable in view of the long range of the Coulombic potential. Figure 1 shows the defects (a) and the amorphous regions produced by a 30-keV uranium recoil in zircon (b). The figure shows the formation of small amorphous clusters around the central amorphous core and nanoscale phase separation into zirconium- and silicon-rich regions. The observation of small nanosized amorphous clusters and segregation at the nanoscale enhances our under-standing of defect production in collision cascades in ceramics and provides useful information to guide the design of ceramic waste forms for nuclear waste disposal.

ScalaBLAST: A Scalable Implementation of BLAST for High-Performance, Data-Intensive Bioinformatics Analysis

CS Oehmen[a] and J Nieplocha[a]

(a) Pacific Northwest National Laboratory, Richland, Washington

Developers at PNNL have developed ScalaBLAST, a high-performance, sequence-alignment application that accommodates very large databases and scales linearly to hundreds of processors on both distributed memory and shared memory architectures. This new software represents a substantial improvement over the current state of the art in high-performance sequence alignment with scaling and portability and should have wide-ranging application to other informatics-driven sciences.

Genes in an organism's DNA (genome) have embedded in them information about proteins, which are the molecules that do most of a cell's work. A typical bacterial genome contains on the order of 5000 genes. Mammalian genomes can contain hundreds of thousands of genes. For each genome sequenced, the challenge is to identify protein components (i.e., proteomes) being actively used for a given set of conditions. Fundamentally, sequence alignment is a sequence-matching problem that focuses on unlocking protein information embedded in the genetic code, making it possible to assemble a "tree of life" by comparing new sequences against all sequences from known organisms. However, the memory footprint of sequence data is growing more rapidly than per-node core memory. Despite years of research and development, high- performance, sequence-alignment

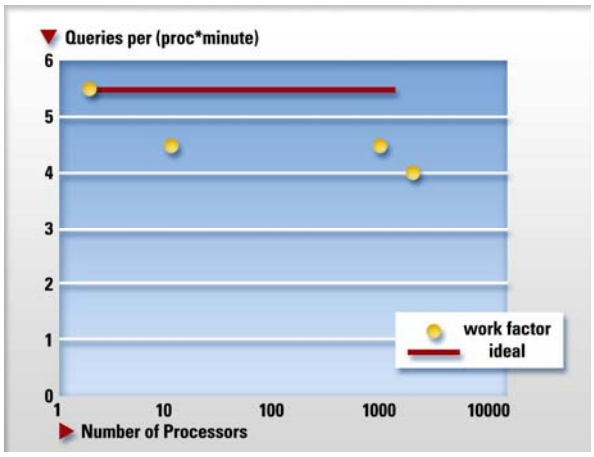

Figure 1. ScalaBLAST scalability

applications do not scale well, cannot accommodate very large databases, or require special hardware. To solve these propblems PNNL researchers developed ScalaBLAST, a high-performance, sequence-alignment application that accommodates very large databases and scales linearly to hundreds of processors on both distributed memory and shared memory architectures (see Figure 1). ScalaBlast represents a substantial improvement over the current state of the art in high-performance sequence alignment with scaling and portability. It relies on a collection of innovative techniques (e.g., target database distribution over available memory, multi-level parallelism to exploit concurrency, parallel input/output, and latency hiding through data pre-fetching) to achieve high performance and scalability. This demonstrated approach of database sharing combined with effective task scheduling should have wide-ranging application to other informatics-driven sciences.

Citation

Oehmen CS and J Nieplocha. 2006. "ScalaBLAST: A Scalable Implementation of BLAST for High-Performance, Data-Intensive Bioinformatics Analysis." *IEEE Transactions on Parallel and Distributed Systems* 17(8):740-749.

High-Throughput Visual Analytics for Biological Sciences: Turning Data into Knowledge

CS Oehmen,[a] LA McCue,[a] JN Adkins,[a] KM Waters,[a] T Carlson,[b] WR Cannon,[a] BJ Webb-Robertson,[a] DJ Baxter,[b] ES Peterson,[a] M Singhal,[a] A Shah,[a] and KR Klicker [a]

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

A diverse team of researchers collaborated on an entry for the International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC 06) Analytics Challenge and was named one of the top three finalists. The final competition will take place in November at the SC 06 meeting in Tampa, Florida.

For the SC 06 Analytics Challenge, we have demonstrated an end-to-end solution for processing data produced by high-throughput, mass spectrometry (MS)-based proteomics. This approach, which allows biological hypotheses to be explored, is based on a tool called the Bioinformatics Resource Manager (BRM). BRM will interact with high-performance architectures and experimental data sources to provide high-throughput analytics to specific experimental datasets. Peptide identification is achieved by a specially developed, data-intensive version of Polygraph, which has been shown to scale well beyond 1000 processors. Visual analytics applications, such as PQuad or Cytoscape, may be used to visualize protein identities in the context of pathways using data from public repositories such as the Kyoto Encyclopedia of Genes and Genomes. The end result is that a user can go from experimental spectra to pathway data in a single workflow, thereby reducing the time-to-solution for analyzing biological data from weeks to minutes. To view the video included with the PNNL/EMSL entry go to mms://ims4.pnl.gov/winmedia/2006/BRM/brm.wmv.

User Projects

Collaborative Development of Software for Electronic Structure Calculations

MF Guest, CCLRC Daresbury Laboratory, Warrington, United Kingdom

Calculated Rates of Water-Exchange on Large Aqueous Aluminum Nanoclusters

AG Stack, WH Casey, University of California, Davis, Davis, California

Coupled Quantum Simulation Techniques for Studying Nanostructured Materials

AJ Williamson, F Gygi, Lawrence Livermore - National Laboratory, Livermore, California

Correlation of Structure and Function of Zinc Metalloproteins Via Solid-state NMR Methods

G Parkin, Columbia University, New York, New York

ER Kantrowitz, Boston College, Chestnut Hill, Massachusetts

AS Lipton, PD Ellis, R Heck, Pacific Northwest National Laboratory, Richland, Washington

Single Enzyme Nanoparticle Crosslinking Polymerzation

MC Perkins, Pacific Northwest National Laboratory, Richland, Washington

Sub-Grid Modeling of Diesel Particulate Filtration Using the Lattice-Boltzmann Method

ML Stewart, Pacific Northwest National Laboratory, Richland, Washington

Computer Simulation of Optical Spectroscopy

D Pan, Pacific Northwest National Laboratory, Richland, Washington

HP Lu, Bowling Green State University, Bowling Green, Ohio

Integrated Multiscale Modeling of Molecular Computing Devices

L Tsetseris, Vanderbilt University, Nashville, Tennessee

RJ Harrison, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Molecular Modeling

NU Mayer-Cumblidge, P Yan, H Cao, Pacific Northwest National Laboratory, Richland, Washington

Animation for Morphing Catalysis

MC Perkins, Pacific Northwest National Laboratory, Richland, Washington

MP2/CBS Pair Corrrelation Function of Liquid Water

RH Wood, University of Delaware, Newark, Delaware

HPC Challenge Benchmark

KM Fox, Environmental Molecular Sciences Laboratory, Richland, Washington

Simulation of HVDC Converter Valve Control and Protection Algorithms

JM Johnson, Pacific Northwest National Laboratory, Richland, Washington

Quantification of the Ligand Effects in Transition Metal Coordination Compounds using Electronic Structure Calculation Methods

CA Tsipis, C Kefalidis, Aristotle University of Thessaloniki, Greece, Thessaloniki, Greece

Establishing Benchmarks for Stability Testing of Future Intermediate Range Compute Server

V Glezakou, Pacific Northwest National Laboratory, Richland, Washington

LR Corrales, University of Arizona, Tucson, Arizona

Fluorescent Labeling of Proteins Based on Known Crystal Structures

L Rodriguez, Pacific Northwest National Laboratory, Richland, Washington

First-Principles Catalyst Design for Environmentally Benign Energy Production

E Mavrikakis, PA Ferrin, LC Grabow, S Kandoi, AA Gokhale, AU Nilekar, RP Nabar, University of Wisconsin-Madison, Madison, Wisconsin

Real-Time Atomistic Simulation Studies of Light Harvesting and Charge Transport for Hydrogen Production in Solar Cells

EJ Bylaska, Pacific Northwest National Laboratory, Richland, Washington

DS Kilin, SV Kilina, K Tsemekhman, O Prezhdo, WR Duncan, BF Habenicht, University of Washington, Seattle, Washington

Comparative Protein Structure Modeling: From Protein Sequence to High-accuracy Protein Structure

Y Xu, Jn Guo, University of Georgia, Athens, Georgia

TP Straatsma, Pacific Northwest National Laboratory, Richland, Washington

Comparative Molecular Trajectory Analysis

SK Wurstner, TP Straatsma, M Singhal, Pacific Northwest National Laboratory, Richland, Washington

DOE Matrix

KJ Roche, Oak Ridge National Laboratory, Oak Ridge, Tennessee

High-Fidelity Direct Numerical Simulations of Turbulent Combustion - Compression Ignition under HCCI Conditions and NOx Formation in Turbulent Jet Flames

JH Chen, Sandia National Laboratory, Livermore, California

HG Im, Cn Yoo, University of Michigan, Ann Arbor, Michigan

Y Wang, University of Wisconsin-Madison, Madison, Wisconsin

Y Wang, AC Trouve, University of Maryland, College Park, Maryland

Wet Electrons at Metal Oxide Surfaces

H Petek, J Zhao, University of Pittsburgh, Pittsburgh, Pennsylvania

Snow Pack Predictions for Next 50 Years in the Pacific Northwest

MC Perkins, Pacific Northwest National Laboratory, Richland, Washington

Thrust Area #2: Molecular Modeling of Electron Transfer in Fe(III) Oxides

KM Rosso, SN Kerisit, X Wang, Pacific Northwest National Laboratory, Richland, Washington

FN Skomurski, University of Michigan, Ann Arbor, Michigan

M Valiev, Environmental Molecular Sciences Laboratory, Richland, Washington

MC Wander, State University of New York at Stony Brook, Stony Brook, New York

JD Kubicki, Pennsylvania State University, University Park, Pennsylvania

Joint Application of Theory and Experiment to the Chemistry of Environmentally Important Organic Peroxides

GB Ellison, University of Colorado, Boulder, Colorado

BK Carpenter, A Litovitz, Cornell University, Ithaca, New York

JF Stanton, University of Texas at Austin, Austin, Texas

High Performance Sequence Analysis for Data-intensive Bioinformatics

CS Oehmen, L Mccue, HJ Sofia, Pacific Northwest National Laboratory, Richland, Washington

EA Welsh, Washington University in St. Louis, St. Louis, Missouri

DJ Baxter, Environmental Molecular Sciences Laboratory, Richland, Washington

Megaports Training Video Development

RA Pappas, BA Mcquerry, Pacific Northwest National Laboratory, Richland, Washington

Proton Transport in Polymer Electrolyte Membranes

R Devanathan, M Dupuis, A Venkatnathan, Pacific Northwest National Laboratory, Richland, Washington

***De Novo* Structure-Based Molecular Design**

V Bryantsev, California Institute of Technology, Pasadena, California

BP Hay, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Compare Thermal Signature of Air-cooled RX2600 Node with SprayCool FX2600 Node

KM Regimbal, RW Mooney, Environmental Molecular Sciences Laboratory, Richland, Washington

Nanostructured Catalysts for Fuel Cells

CH Turner, CK Acharya, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

DFT Studies of Size and Structure Effects of Ir Nanoparticles on Their Catalytic Activities for Methane Dissociation

L Wang, Southern Illinois University, Carbondale, Illinois

Computational Study of Oxygen Reduction on SOFC Cathode Surfaces

M Liu, J Wang, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia

Architectural Rendering of EMSL Office Expansion

MC Perkins, Pacific Northwest National Laboratory, Richland, Washington

Defect Processes, Phase Transformations, and Nanoscale Phenomena in Complex Ceramics

R Devanathan, F Gao, WJ Weber, Pacific Northwest National Laboratory, Richland, Washington

Cover Graphic for Nanoscience and Nanotechnology Trade Journal

MC Perkins, Pacific Northwest National Laboratory, Richland, Washington

Energy and Entropy Effects in Dissociation of Non-Covalent Complexes: Experimental and Theoretical Investigation of the Structures and Interactions of Glycopeptide Antibiotics-Cell Wall

Z Yang, J Laskin, Pacific Northwest National Laboratory, Richland, Washington

Investigation of DNA Structural Perturbations Induced by the Guanine Oxidation Products Spiroiminohydantoin and Guanidinohydantoin

ND Priestley, KD Sugden, University of Montana, Missoula, Montana

Asynchronous File System Experiments

MI Seltzer, CA Stein, Harvard University, Cambridge, Massachusetts

Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences, and Fusion Energy Sciences

JP Colgan, Los Alamos National Laboratory, Los Alamos, New Mexico

Pn Krstic, T Minami, CO Reinhold, Oak Ridge National Laboratory, Oak Ridge, Tennessee

MS Pindzola, SD Loch, FJ Robicheaux, Auburn University, Auburn, Alabama

NR Badnell, University of Strathclyde, Glasgow, Scotland, United Kingdom

DC Griffin, CP Balance, Rollins College, Winter Park, Florida

Theoretical Investigations of Chiral Self-Assembly at Solid Surfaces

I Paci, M Ratner, Northwestern University, Evanston, Illinois

Virtual Tools for Cardiac Remodeling

JM Guccione, University of California, San Francisco, San Francisco, California

DR Einstein, Pacific Northwest National Laboratory, Richland, Washington

Molecular Dynamics of Aqueous $NaNO_3$ and NaCl Solutions: The Surface Propensity and Thermodynamic Properties of Aqueous Anions

JL Thomas, BJ Finlayson-pitts, DJ Tobias, University of California, Irvine, Irvine, California

LX Dang, Pacific Northwest National Laboratory, Richland, Washington

First-Principles Calculations of $La(1-x)Sr(x)Fe(1-y)Co(y)O_3$ Solids and Surfaces

C Lee, SB Sinnott, University of Florida, Gainesville, Florida

R Devanathan, Pacific Northwest National Laboratory, Richland, Washington

Theoretical Characterization of H_3O^+ on the Water - Vapor Interface

LX Dang, Pacific Northwest National Laboratory, Richland, Washington

J Cui, KD Jordan, University of Pittsburgh, Pittsburgh, Pennsylvania

Molecular Recognition at the Electronic Level

JJ Stezowski, University of Nebraska, Lincoln, Nebraska

PA Karr, Wayne State College, Wayne, Nebraska

High Performance Sequence Alignment: OMB Software Effectiveness Metric Studies for FY06

CS Oehmen, Pacific Northwest National Laboratory, Richland, Washington

KJ Roche, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Investigations into Sulfur Poisoning Mechanisms in Solid-State Oxide Fuel Cells Using Quantum-Chemical Computations

M Liu, Jn Wang, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia

Molecular Dynamics Study of an Actin Septamer: Testing the Holmes Model and the Hydrophobic Plug Loop Hypothesis

GC Schatz, KM Barrett, MJ McCullagh, JT Paci, Northwestern University, Evanston, Illinois

KC Holmes, Max Planck Institut fur medizinische Forschung, Heidelberg, Germany

Exploratory High-throughput Sequence Analysis on Microbial Genomes

CS Oehmen, Pacific Northwest National Laboratory, Richland, Washington

E Szeto, Lawrence Berkeley National Laboratory, Berkeley, California

P Hugenholtz, Joint Genome Institute, Walnut Creek, California

Design Criteria for Organic Charge Transporting Materials through Computational Modeling

LS Sapochak, AB Padmaperuma, PE Burrows, Pacific Northwest National Laboratory, Richland, Washington

M Valiev, Environmental Molecular Sciences Laboratory, Richland, Washington

Oxide Surface Structure and Acidity

KM Rosso, SN Kerisit, Pacific Northwest National Laboratory, Richland, Washington

BR Bickmore, Brigham Young University, Provo, Utah

Lustre Scalability Research

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SGI Altix Allocation for Advanced Computing Technology Lab

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NMR Chemical Shift Calculations for Novel Bioactive Metabolites from an Acid Mine Waste Organism

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Computed Frequencies to Support Experimental Quests for Novel Molecules

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***Ab initio* Calculations on a Proposed Gating Mechanism for the KcsA Channel**

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Computational Study of Protein-protein Interaction Dynamics

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Multi-Region Reactive Transport Due to Strong Anisotropy in Unsaturated Soils with Evolving Scales of Heterogeneity

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***Ab-initio* Simulations of the Catalytic Mechanism in Protein Kinases**

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Defects, Defect Processes and Ion-Solid Interactions in Ceramics

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Computational Chemical and Materials Science to Study Nanoscale Surface Reactivity and Radiation Resistance of Metal Oxides

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Direct Numerical Simulations of Turbulent Combustion- Temperature Inhomogeneity Effects on the Autoignition of H_2/Air Mixtures in the Sponteneous Ignition Regime

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Quantum and Classical Simulations of Clusters, Self-assembly, Nano-scale Manipulations, Nanotribology, and Biological Processes

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