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A Report of the
Neutron Science Software
Initiative (NESSI) Workshop

October 13-15, 2003
Oak Ridge, Tennessee

Documented by

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A U.S. Department of Energy Multilaboratory Project

SPALLATION NEUTRON SOURCE

Argonne National Laboratory • Brookhaven National Laboratory • Thomas Jefferson National Accelerator Facility • Lawrence Berkeley National Laboratory • Los Alamos National Laboratory • Oak Ridge National Laboratory

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A REPORT OF THE
NEUTRON SCIENCE SOFTWARE INITIATIVE (NESSI) WORKSHOP
OCTOBER 13-15, 2003
SPALLATION NEUTRON SOURCE, 701 SCARBORO ROAD
OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831

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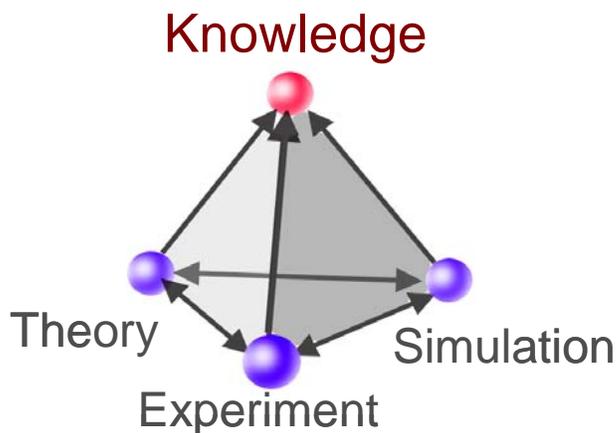
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EXECUTIVE SUMMARY

Neutron scattering as a technique was established more than half a century ago by C. Shull and B. Brockhouse, for which they were awarded the Noble Prize in Physics in 1994. The Spallation Neutron Source (SNS), a \$1.4 billion project under construction in Oak Ridge, Tennessee, is designed to provide the most intense pulsed neutron beams in the world for scientific research and industrial development. Having made such a large investment in SNS, the U.S. government and the general public will demand immediate return, in the form of new scientific knowledge, after the SNS becomes operational in 2006. However, hardware alone produces data, not insights. A modest investment in data analysis will dramatically improve our ability to transform neutron-scattering data into scientific knowledge.

With a few exceptions, today's software for analysis of neutron scattering data is a patchwork of independent programs that are written by nonprofessionals and run on specialized platforms. This workshop was intended to begin a process of defining the requirements for a new, comprehensive set of software for data analysis. Although the focus of the proposed software is on the needs of the SNS instruments, other neutron sources in the United States and around the world will also benefit. SNS will take the lead and work with the user community and other facilities to co-develop this software. Powered by state-of-the-art computing technologies, the new software is expected to inspire a sociological change and revolutionize the ways neutron-scattering experiments are done. Specifically, SNS will provide an integrated environment where all the tools and capabilities can be brought together to solve the problem at hand. Through remote visualization and collaboration, the new software will take neutron-scattering facilities to users, letting the broader scientific community benefit from the use of neutrons.



The new data analysis software will combine experiment, theory, and high-performance computer simulations to rapidly produce scientific knowledge, giving neutron scattering users a brand new total experience.

1. INTRODUCTION

The Spallation Neutron Source (SNS) [1], under construction at Oak Ridge, Tennessee, is currently the largest civilian project (\$1.4 billion) undertaken by the U.S. government. Funded by the Office of Basic Energy Sciences, U.S. Department of Energy (DOE), and being built by six DOE national laboratories (Argonne, Brookhaven, Jefferson, Lawrence Berkeley, Los Alamos, and Oak Ridge), the SNS will provide the most intense pulsed neutron beams in the world for scientific research and industrial development. SNS will have 18 beam lines, which can accommodate a total of 24 instruments. Funding has been secured for the construction of an initial suite of 14 instruments (see Fig. 1), three of which will be commissioned on day 1 when SNS becomes operational in summer 2006. Separately, the High Flux Isotope Reactor (HFIR) [2] at Oak Ridge National Laboratory is undergoing a major upgrade, which includes the construction of a cold-guide hall and upgrade of instruments in the reactor hall. When the upgrade is complete, HFIR will have 15 state-of-the-art neutron scattering instruments (see Fig. 2) that will be among the world's best. Together with other neutron facilities in the United States, SNS and HFIR will offer U.S. and international users unprecedented opportunities in neutron scattering research, breaking new ground in science and technology.

While major investments have been committed to the instrument hardware, the development of data analysis software for these new and upgraded instruments is just beginning. With a few exceptions, today's software for analysis of neutron-scattering data is a patchwork of independent programs that are written by nonprofessionals and run on specialized platforms. Individual neutron facilities do not have adequate budgets to develop complete solutions for data analysis. Although some of the existing programs can be adapted to instruments at SNS, many will have to be substantially modified or rewritten to accommodate the fast data rate that will be realized with the new instruments. The SNS instruments will typically see an increase in data rate on the order of 10 to 100. The benefit of this increased data rate vanishes, however, without compatible software to take advantage of the advanced computing technologies with which the new data are produced, managed, and analyzed. Additionally, modern neutron-scattering instruments at SNS demand new analysis software to permit new types of scientific studies. New scientific insights are possible only with the aide of enabling software.

The United States has had an outstanding tradition in neutron sciences. However, the neutron scattering community in the United States is relatively small compared to Europe, where most of the recent innovations in instrumentation were made. With the construction of SNS, neutron scattering in the United States is poised for a spectacular leap that will bring the U. S. into a leadership position in the use of neutrons for science, medicine, and national defense. To realize the full potential of SNS, there is now a pressing need to broaden the neutron scattering community in the United States to a wide-range of scientific research. Comprehensive, user-friendly software for instrument control, setup, and data analysis is necessary for bringing in and retaining users.

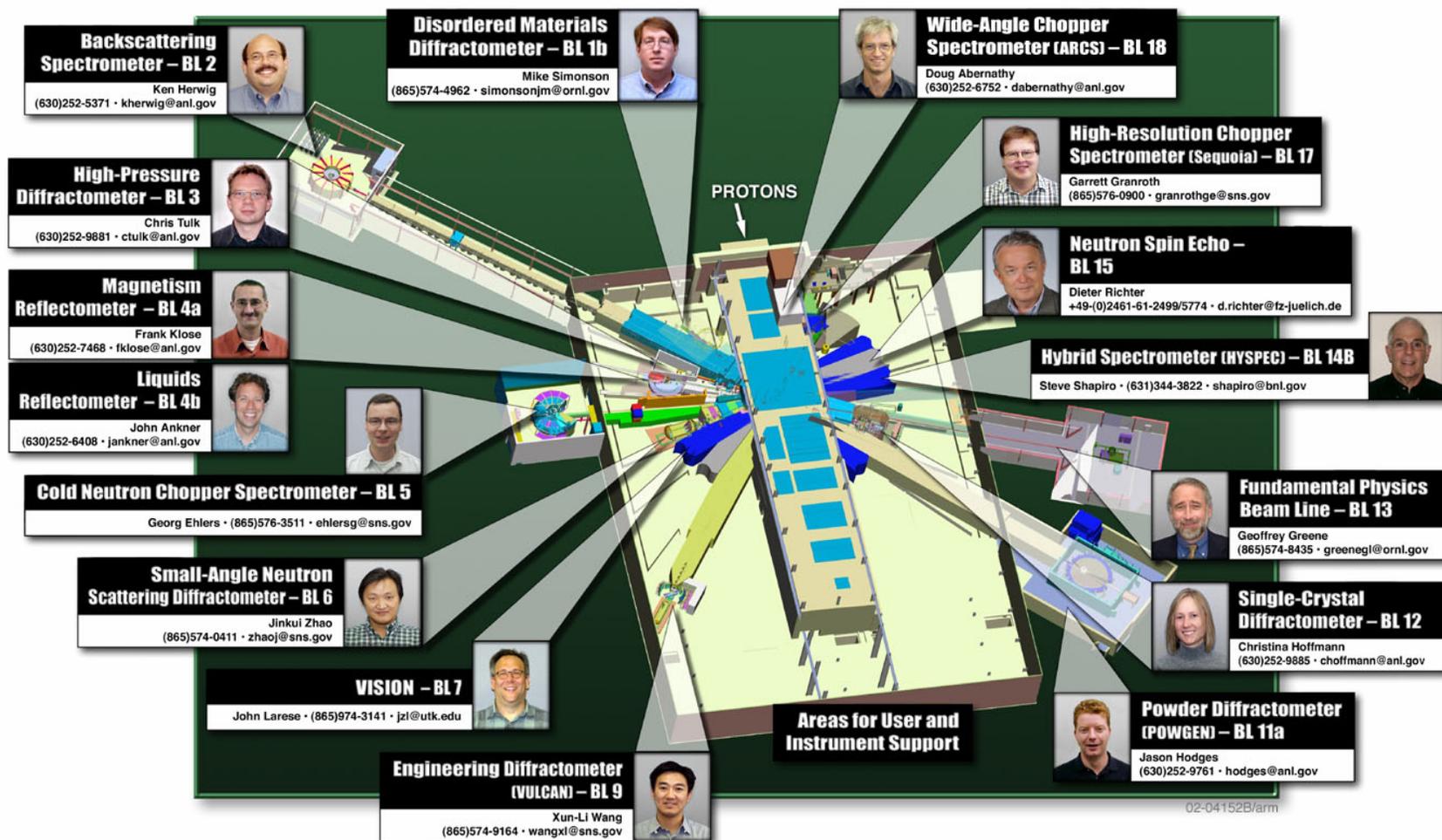


Fig. 1. The initial suite of instruments that have been allocated beam lines at the Spallation Neutron Source. Funding has been secured for all but the Vision and Neutron Spin Echo instruments, bringing the total number of instruments under construction to 14.

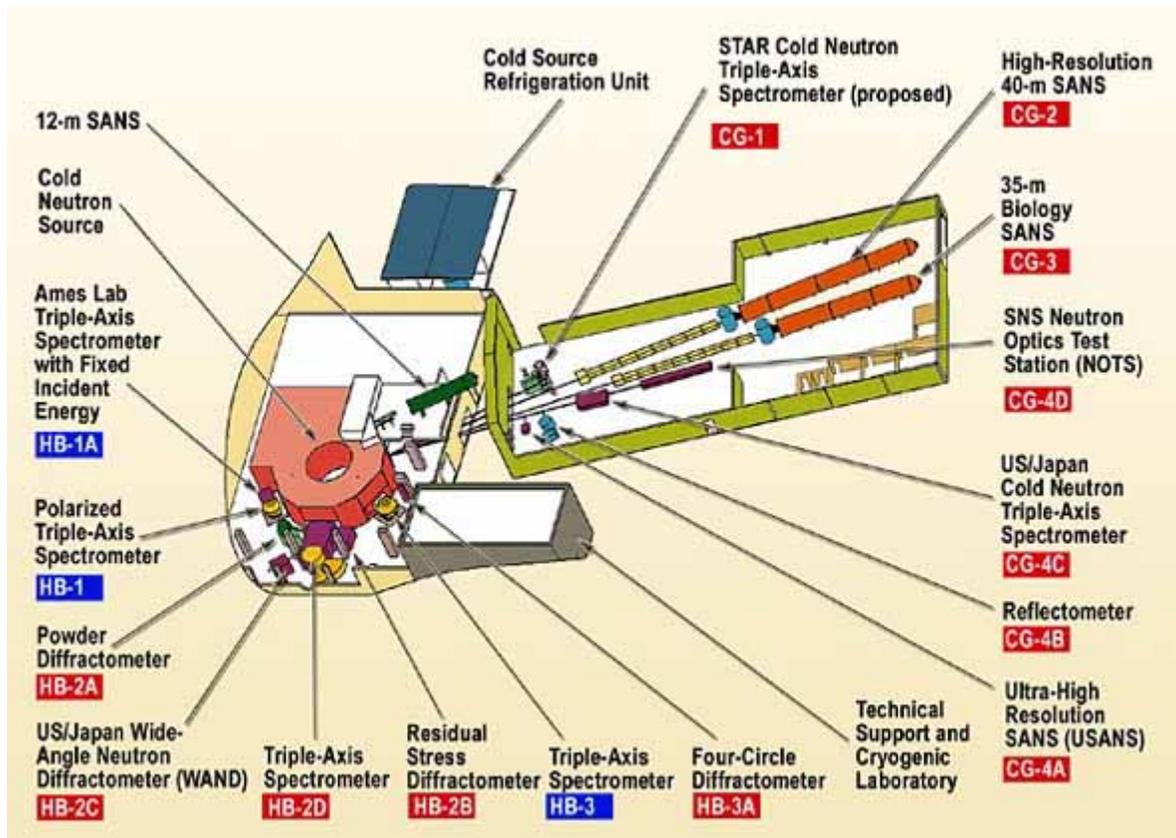


Fig. 2. Instrument layout at the upgraded High Flux Isotope Reactor.

2. WORKSHOP GOALS

The Neutron Science Software Initiative (NESSI) Workshop was intended to begin a process of defining the requirements for the new data analysis software. Although the focus of the proposed software is on the needs of SNS instruments, other neutron sources in the United States and around the world will also benefit. The new software will be designed to achieve the following goals:

- make neutrons a simple tool for both casual and professional users,
- enable new sciences by exploring new analysis methods,
- make efficient use of neutrons by providing tools for experiment planning and optimization,
- bring together all tools and expertise to solve the problem at hand, proving a brand new total experience for users,
- provide tools for archiving and easy access of experimental parameters, data, and analysis results, and
- take advantage of state-of-the-art computing technologies.

Discussions at the workshop centered on the requirements to meet those goals. The consensus of workshop participants is captured below.

3. USERS NEEDS

Understanding users' needs is a prerequisite for any software project. Neutron scattering users come from a diverse field of science and technology, and in general they range in neutron scattering skills

between two categories: casual and professional. The casual users consider neutrons as only one tool in their research arsenal. They are not experts in neutron scattering techniques and come to neutron sources only when needed. However, casual users are expected to comprise the bulk of new users at SNS, due to their broad base, and therefore will have a huge influence on the future of neutron scattering in the United States. The professional users are researchers who use neutron scattering as their primary research tool. They typically are very familiar with scattering techniques and are often involved in the development of new instruments at neutron scattering facilities. Although casual and professional users have a common desire for a basic suite of software for instrument control and data reduction, their needs differ in the advanced stage of data analysis and, for that matter, the use of the instruments.

The consensus of workshop participants is that the basic data reduction software must be available on day 1, when the instrument of interest is commissioned. An essential requirement for the basic data reduction software is

$$t_{analysis} \leq t_{experiment}$$

i.e., the time spent on data analysis should be comparable with that for data collection. Features of this basic software include the following:

- rapid display of raw data in physical units (meV, Å⁻¹) with appropriate 3-D cuts,
- a complete and fully documented set of necessary basic codes to reduce raw data to scattering functions, $S(\mathbf{Q})$ or $S(\mathbf{Q},\omega)$, for all instruments,
- effective push button operation but with access to details if required,
- linkage of appropriate metadata to raw data files for use in basic analysis codes,
- an electronic notebook linked to metadata,
- an extensible software architecture,
- multiple data format output modules to link to existing software (e.g., crystallography analysis codes), and
- intuitively obvious interface and common look and feel for all instruments (fully documented).

When their basic needs for data reduction are met, casual users would like to see further development of an expert system, which contains “model” data and incorporates the experience of instrument scientists. They will also prefer a “black-box” analysis, possibly leading to direct visualization of “end products” (e.g., a stress map or an instantaneous crystal structure) rather than the raw data. This request is much more like what doctors want out of magnetic resonance imaging. Although nuclear magnetic resonance (NMR) is the underlying technology, it is the map of a scanned body that is of interest to the doctors rather than individual NMR signals. A collection of these black-box analysis routines forms a Problem Solving Environment, which allows users to focus on science, rather than details of the experiments, and makes neutron scattering a simple tool to use. Pacific Northwest National Laboratory (PNNL) has an active program developing the tools for Collaborative Problem Solving Environments [3]. Deborah Gracio gave an overview of the development efforts at PNNL, followed by a demonstration of the Extensible Computational Chemistry Environment for theoretical chemistry users.

On the other hand, professional or experienced users would like to have greater control of their analysis. They would like to be able to simulate the experiment and compare simulation results with experimental data. Real-time data analysis and an intelligent system for a quick feedback of on-going experiments are also highly desirable. These features would allow the experienced users to quickly adjust their experiment plan accordingly. Many professional users are familiar with legacy data analysis codes at existing facilities and would like to continue using those codes in some of their analysis.

Further into the future, both groups of users would like to carry out complete simulation of neutron scattering experiments. The simulation discussed here encompasses both instrument and materials simulations. The former calculates neutron scattering intensities at the detectors for a given instrument with a “standard” sample. The latter is computer prediction of the structure and dynamics of materials. Instrument simulation with different instrument configurations will help users to optimize their measurement strategies, thereby substantially improving the possibility of a successful outcome. Linking instrument simulation with materials simulation adds more power and could potentially revolutionize the ways in which neutron scattering data are analyzed. The traditional approach for data analysis treats individual data sets one at a time. Having the ability to simulate the experimental data for real samples under real sample environments allows analysis of multiple data sets all at once. Such a feature will prove indispensable in the future, as several instruments at SNS cover a broad range of (\mathbf{Q}, ω) space, simultaneously probing the structure and dynamics at multiple length and energy scales. It is conceivable, therefore, that in the future, multiple data sets collected by wide angle and small angle detectors through a phase transformation could be analyzed together (e.g., via global fitting with a unique materials model). Data sets by other experimental means (e.g., transmission electron microscopy) could be included in the analysis, imposing additional constraints for deriving a unique solution for structure and dynamics of the material.

For the development of both basic and advanced software, a highly standardized process is desired. Standard numerical libraries, code standards, and graphical user-interface standards should be provided or specified as part of the software architecture. There should also be support for both stand-alone and remote access leading to on-line or off-line analysis. Both graphic as well as script command interfaces are desirable. It was proposed that SNS serve as a central repository for all software tools and packages.

4. SOFTWARE ARCHITECTURE

A component-based architecture ensures extensibility and long-term success of the data analysis software. The Caltech group led by Brent Fultz demonstrated a prototype data analysis software package based on distributed computing [4]. Their approach, named DANSE (Distributed Data Analysis for Neutron Scattering Experiments), is based on the data flow paradigm. Analysis would be performed with reusable computational components that are connected to each other with standardized data streams. Components would be integrated into a coherent interpretive framework using the open source language Python, which permits custom analysis procedures to be constructed easily. Thus designed, the DANSE architecture has the promise to take advantage of the future cyber infrastructure of grid-based computing (see below), while accepting legacy codes through the use of Python wrappers. DANSE has been proposed as a design project for funding by the U.S. National Science Foundation. Separately, Jeremy Walton of Numerical Algorithms Group (a commercial software company in the UK) gave a demonstration of IRIS Explorer [5], a Microsoft Windows-based modular software for data visualization and analysis. While these approaches are being evaluated, the workshop participants would like to see a decision made as soon as possible on the architecture. The architecture for data archive and access is discussed in a separate section below.

5. EXISTING CODES

To avoid duplicating previous efforts, a survey should be conducted of existing analysis codes that could be usefully incorporated. In this regard, it may be desirable to establish a central software repository, where a library of common as well as instrument-specific modules could be stored for reuse. Several newly developed data analysis packages were highlighted at the workshop: ISAW [6] by IPNS for data visualization and some analysis, DAVE [7] by the NIST group for analysis of inelastic neutron scattering data, and SScannSS software by Open University/ISIS (UK) for stress mapping experiments. ISAW is based on JAVA, whereas DAVE and SScannSS were developed in the commercial IDL (The Interactive Data Language, distributed by Research Systems, Inc.) programming environment. All three packages offered many useful features that meet the demands of existing data and are gaining popularity beyond their place of origin.

6. VISUALIZATION

Scientific visualization is the process of exploring data to gain insights and understanding. Workshop participants felt strongly that the ability for users to visualize raw and processed data easily is the key to the success of SNS. A flexible infrastructure (evolving with computer technologies) will be needed for better 3D visualization. A virtual reality 3D CAVE visualization environment was mentioned as a possibility in the future.

Ultimately, scientific communities of various subfields will set the needs for their respective experiments. Regardless of their individual subfields, however, users will want to visualize their data on the timescale of the experiment. Additionally, users and instrument scientists will want to have the flexibility to change tools at the instrument/experiment level without going to a programmer.

Many visualization tools currently exist (see section 5, Existing Codes) that could be adapted at existing neutron scattering centers to serve their data analysis needs and as a test ground for SNS. However, resources will be needed to extend some of the current tools to time-of-flight data. Common problems for pulsed sources include sparse data, cuts through (\mathbf{Q} , ω) space, and non-linear transformations, to name a few. A concerted effort should be organized to deal with these problems up front.

7. REMOTE COLLABORATION

Remote collaboration represents a new way of doing neutron scattering experiments. There are many advantages that remote collaboration will provide to users, to SNS, and to the scientific community at large.

- Remote collaboration allows complementary expertise to be used to plan, execute, and analyze experiments. With the Internet, remote collaboration has world-wide reach, to both theorists and experimenters. It will enable better experiment planning and permit off-site users (e.g., professors or students) to participate during experiments. The synergies generated through remote collaboration will ultimately reduce the time to publication.
- Remote collaboration is also an educational tool. Live or archived distance classes and demonstrations will be offered, allowing new users to consult others who have worked on similar problems and share expertise. This will broaden the “user base” of SNS, as well as the impact of the facility.
- Users and instrument scientists will be able to monitor the progress of an experiment without continuous presence.

The requirements for remote collaboration can be met to a large extent with existing tools. **CUMULVS** (Collaborative, User Migration, User Library for Visualization and Steering) [8], for example, provides run-time visualization for multiple, geographically distributed users of large-scale computation projects (see Fig. 3). The Extensible Computational Chemistry Environment mentioned previously is another example. None of the existing tools is natural to the neutron scattering data analysis environment; therefore, some development efforts will be required to adapt these tools for neutron scattering users. There are also acute security issues that will need to be carefully addressed. Some of the desirable features for remote collaboration include the following:

- desktop availability (perhaps with enhanced capability in specific locations, e.g., special labs at universities),
- Web cam and voice,
- on-line data manipulation and sharing with remote viewing and control,
- replicate data rooms (for teaching at off-site locations),
- an electronic notebook to record interaction sessions, and
- training sessions provided by the facility in the use of the technology.

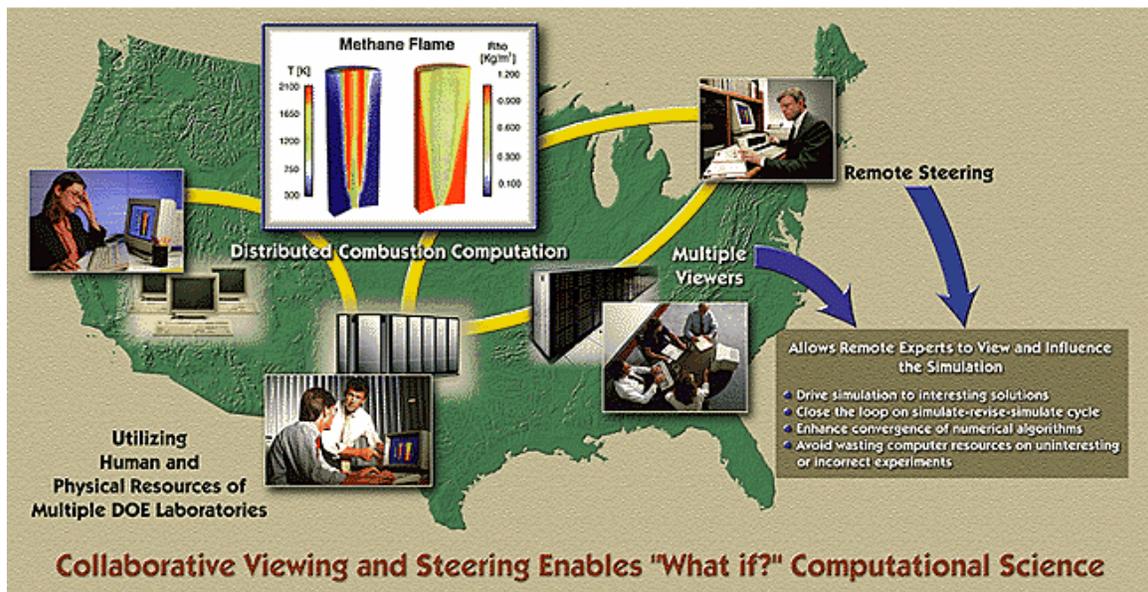


Fig. 3 CUMULVS demonstration of remote collaboration in the Distributed Combustion Computation project.

8. PRE-EXPERIMENT SIMULATION AND PLANNING

For successful planning of an experiment, the user must be able to estimate at the proposal stage the cross sections and hence the time to collect the data. Careful calibrations with standard samples will be needed to yield reliable estimates of count time. These calculations will also need to take into account all relevant sample characteristics, such as the scattering volume, element cross sections, and texture. It is believed that codes for such calculations exist, but they have to be integrated, packaged, and documented. A database containing “model” data would be helpful, especially for new users. To maximize the output of an experiment, tools to optimize measurement strategies will be needed.

Complete computer simulation, incorporating both instrument and materials simulations for real sample under real sample environments, will provide the ultimate solution for pre-experiment planning. For this reason, computing simulation should be regarded as an integral part of the data analysis package. Several popular packages for instrument simulations (e.g., IDEAS [9], McStas [10], and VITESS [11]) have been extensively used in the design of SNS instruments. A variety of materials simulations tools also exist, ranging from first-principle calculations to molecular dynamics simulations to finite element modeling. Some of these are freely available, while others require commercial license. To allow SNS users to make use of commercial programs, a licensing agreement must be arranged with the vendors.

Most materials simulations are computationally intensive, and access to high-performance computing resources is essential. Typical two-dimensional, finite element calculations for thermal-mechanical analysis take 10-100 hours on a single processor node. Three-dimensional calculations of polycrystalline materials can be performed only with the use of massive parallel computing. Some of the popular materials simulation codes, such as ABAQUS, have already been parallelized and are ready to take advantage of parallel computing.

With high-speed data networks, grid computing is becoming a centerpiece of high-performance computing for large-scale simulation projects. Several talks touched on this technology. Marty Humphrey of the University of Virginia introduced the concept of grid computing, as illustrated in Fig. 4, to workshop participants. Here, computing resources of various platforms at various locations are coordinated using standard, open, general-purpose protocols and interfaces. Remote execution is transparent, where a user initiates the “run,” and the rest (selecting resources, coping files, collecting results) is done mostly by the grid operating system. Grid computing also plays an important role in remote collaboration. David Bernholdt of Oak Ridge National Laboratory showed a good example using the Earth System Grid, where the simulated weather data were generated at a few sites but were accessed by dozens to hundreds users across the United States at various levels. He also demonstrated how Common Component Architecture (CCA) helped scientists to build high-performance simulations. CCA specifies component standards and their interactions so that scientists can easily build large applications from diverse pieces.

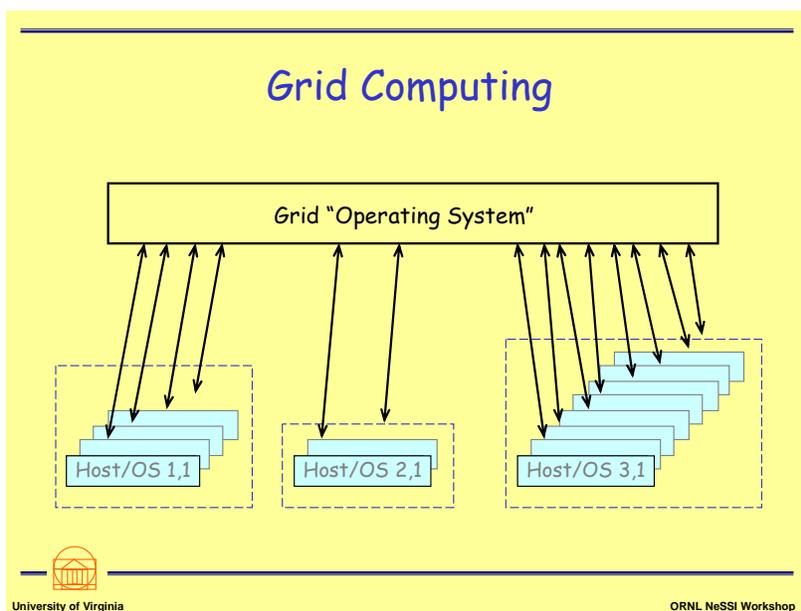


Fig. 4. The concept of grid computing. Hosts of various platforms are linked together through grid operating system [12].

9. ARCHIVING EXPERIMENTS AND DATA ACCESS

It is estimated that SNS instruments will generate 26 Terabytes of data each year. There are many issues associated with storing, access, and computing of those data. Both local and remote users will be involved. It is generally agreed that the SNS data architecture should be designed to meet needs of all users and instruments. It is recognized that SNS data may be stored indefinitely, perhaps even beyond the lifetime of the SNS facility. Depending on the evolving user needs and computing technologies, the data architecture will be allowed to change with time while accepting legacy codes.

To enable remote collaboration, multiple distributed data bases will be set up. All data will adopt standard formats, including one that is specified by NeXus [13]. Common data transfer protocols will be employed to allow users to easily find, backup, and move their data to analysis.

Ownership and open access of data were also discussed. One assessment is that, except for proprietary research, data be owned by SNS. The experiment team would have exclusive access to the data for a certain period time, after which the data would be open to the public. More often than not, the original experiment team publishes only a fraction of the data. This proposed data management scheme would allow the user community at large to make the most use of these data, by encouraging the original experiment team to publish their results as soon as possible and collaborate with others in using the rest of the data later. It would be a facility's decision as to how long the data would be kept private to the original experiment team.

10. METADATA

Robert McGreevy of ISIS brought workshop participants' attention to metadata—scientific annotations explaining what the data are and what has been done to them. Although not a brand new concept, metadata have been underutilized and sometimes were not recorded at all. The exact content or format of the metadata is yet to be determined and may vary from one instrument to another. However, it is generally agreed that accurate and complete metadata should be included as part of the complete data set. Some of the metadata can be loaded directly from the user proposal. Therefore, the facilities will need to set a policy that requires users to enter as much as possible the metadata (e.g., crystal structure of the material) in the proposal stage.

11. REQUIRED RESOURCES

It is difficult to estimate the amount of resources required to develop such a comprehensive software package. Robert McGreevy introduced a rule-of-thumb at ISIS, which essentially amounts to three programmer years per instrument. Given the complexity of the newer generation of instruments at SNS, this figure is likely to be larger. Including the efforts to develop central resources, the total funds needed will likely fall in the range of \$15-20 million. Jennifer White of CPS Imaging, a manufacturer of PET scanners for medical diagnosis, gave a perspective for the medical industry, where the investment in software approximately equals that in hardware. International collaboration will certainly leverage the development efforts. Representatives from ISIS and J-PARC (Japanese Spallation Neutron Source) both indicated their desire to form a coalition to co-develop the software.

12. CONCLUDING REMARKS

Just days before the workshop, the Royal Swedish Academy of Sciences awarded the Nobel Prize in Medicine to P. C. Lauterbur and P. Mansfield for their discoveries concerning “magnetic resonance imaging.” Although the underlying technology, nuclear magnetic resonance or NMR, was discovered decades ago (for which F. Bloch and E. M. Purcell were awarded Nobel Prize in Physics in 1952), it was Lauterbur and P. Mansfield's works that have led to the development of modern magnetic resonance

imaging, a breakthrough in medical diagnostics and research. Visualization and analysis software played an essential role in enabling this modern medical technology. Only history will tell how NESSI will contribute to the advancement of science and technology through neutron scattering research. For more information, visit the NESSI web site at <http://www.sns.gov/workshops/nessi/nessi.htm>

13. REFERENCES

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APPENDIX A. WORKSHOP AGENDA

Neutron Science Software Initiative (NESSI) Workshop
 October 13-15, 2003
 Spallation Neutron Source, 701 Scarboro Road
 Oak Ridge National Laboratory, Oak Ridge, TN 37831

Monday, October 13	Talks and Presentations
8:00	Continental Breakfast
8:30 – 8:45	Opening Remarks
8:45 – 9:00	Ian Anderson (Oak Ridge National Laboratory) Workshop Charge
9:00 – 9:30	Robert McGreevy (ISIS Facilities) Neutron Science Users' Perspective
9:30 – 10:00	Brent Fultz (Caltech) Neutron Science Users' Perspective
10:00 – 10:30	Break
10:30 – 11:00	Xun-Li Wang (Oak Ridge National Laboratory) Instrument Scientist's Perspective
11:00 – 13:00	Demonstrations and Lunch (Moderator: Paul Butler)
	Thomas Worlton (Argonne National Laboratory) Integrated Spectral Analysis Workbench (ISAW)
	Rob Dimeo (NIST) DAVE: Cooperative Development of Data Visualization and Analysis Software
	Joseph Curtis (NIST) Towards Real Time Molecular Dynamics: Applications to Neutron Scattering
	Michael Aivazis and Mike McKerns (Cal Tech) DANSE - Distributed Data Analysis for Neutron Scattering Experiments
13:30 – 14:00	Marty Humphrey (University of Virginia) Computational Infrastructures for Science
14:00 – 14:30	Deborah Gracio (Pacific Northwest National Laboratory) Problem Solving Environments
14:30 – 15:00	David Bernholdt (Oak Ridge National Laboratory) The Earth System Grid and other Initiatives from the SciDAC Program
15:00 – 15:15	Richard Riedel (Oak Ridge National Laboratory) Data Acquisition Systems
15:15 – 15:30	Break
15:30 – 17:30	Demonstrations (Moderator: Greg Smith)
	Robert McGreevy (ISIS Facilities) Spectra to Structure
	Marlon Pierce (Indiana University) Portals and Grids
	Karen Schuchardt (Pacific Northwest National Laboratory) Ecce & CMCS

	Jennifer White (CPS Innovations) Coincidence to Image: PET imaging
18:00 – 20:00	Dinner (Doubletree Hotel)
20:00 – 22:00	Program Planning: Moderators Preparation (at Doubletree Hotel)

Tuesday, October 14	Guided Discussions
8:00	Continental Breakfast
8:30 – 10:30	Session I – User Needs (casual and experienced) and how to meet them Moderator – Shenda Baker, Scribe – Al Ekkebus Moderator – Robert McGreevy, Scribe – Garret Granroth
10:30 – 11:00	Break
11:00 – 12:00	Session II – Collaborative Visualization and Analysis Moderator – Roger Pynn, Scribe – Doug Abernathy
12:00 – 12:30	Lunch
12:30 – 13:30	Demonstrations
	John James (Open University, UK) ENGIN-X Software
	Jim Kohl (Oak Ridge National Laboratory) CUMULVS: Interactive Visualization and Computational Steering of Scientific Software Simulations
13:30 – 14:30	Session III – Pre-Experiment Simulations and planning Moderator – Tom Holden, Scribe – Xun-Li Wang
14:30 – 15:00	Break
15:00 – 16:00	Session IV – Archiving Experiments & Data access Moderator – Al Giest, Scribe – John Cobb
16:00 – 16:15	Writing Assignments and other Homework
16:15 – 16:30	Toshiya Otomo (KEK, Japan) Software Development at JPARC

Wednesday, October 15	Reporting and Summary
8:00	Continental Breakfast
8:30 – 10:00	Presentations of Summaries
10:00 – 10:30	Break and Demonstrations Jeremy Walton (Numerical Algorithms Group, UK) Visualization and Analysis Using IRIS Explorer – An Overview
10:30 – 12:00	Discussions – Ian Anderson What else is needed for an effective Requirements Report?
12:00 – 13:00	Lunch
13:00	Adjourn
13:00 – 15:00	Tour of SNS Site for interested attendees

APPENDIX B. LIST OF ORGANIZERS

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