SNS-NSTG Collaborative Software Development

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The Spallation Neutron Source (SNS) and the Neutron Science TeraGrid Gateway (NSTG) are collaborating on software development. SNS at Oak Ridge National Laboratory is a world center for materials research with neutron scattering. NSTG connects large neutron science instrument facilities with the cyberinfrastructure of the TeraGrid. The TeraGrid is a network of high performance computers supported by the US National Science Foundation. There are eleven partner facilities with over a petaflop of peak computing performance, 136,740 CPU-cores, and sixty petabytes of long-term storage.

I.INTRODUCTION

The Neutron Science TeraGrid Gateway [1] connects large neutron science instrument facilities with the cyberinfrastructure resources of the TeraGrid [2]. Neutron science research enables developments in areas of materials research such as chemistry, complex fluids, crystalline materials, disordered materials, engineering, magnetism and superconductivity, polymers, and structural biology. Neutron scattering is a tool for researching the structure and dynamics of materials at the molecular level. The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory and The Institut Laue-Langevin (ILL) in France are two of the world centers for research in neutrons. They both have new capability for materials research with neutron scattering and need new cyberinfrastructure resources.

As SNS continues to ramp up, we expect ramp up not only from successful outreach to the community but increases as the numbers of SNS users increase. With many proposals expected for the eighteen instruments (Figure 1) of the SNS, the need for data reduction, data analysis, and simulations is expected to soon significantly exceed local computing resources. Access to the resources of the TeraGrid is critical for these needs.

The success of the collaborative software development efforts for the SNS is due to several groups working together effectively. The NSTG staff, SNS Scientific Computing group, SNS scientists, and McStas software developers attend group meetings together, meet at scientific conferences, and develop software working with all the partners in the collaboration.

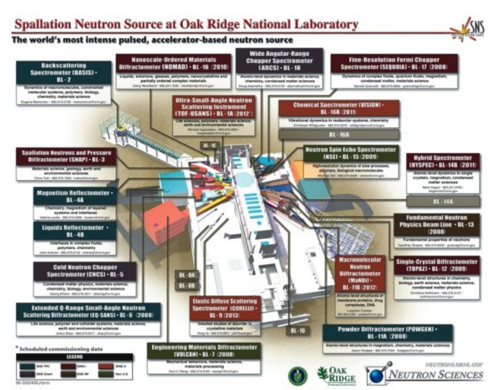

Figure 1 – Instruments at the Spallation Neutron Source.

Closer integration of the SNS and the TeraGrid is the goal of this work. In the future, we plan for the NSTG to flow streaming data from SNS for data reduction workflows on the TeraGrid and move data from the SNS data repository for further processing and analysis on the TeraGrid. Also universities with SNS proposals will use the high bandwidth interconnect of the TeraGrid to support data movement between SNS and their institution. Real-time simulations of experiments can use TeraGrid resources to predict experimental results as they are running or between experiments.

II.VIRTUAL EXPERIMENTS

One such collaboration is virtual experiments [3]. Virtual neutron scattering experiments are possible for many materials using the parallel computing resources of the TeraGrid and agree well with experimental results (Figure 2). The use of Monte Carlo simulations such as McStas [4] is now well established as a tool in the design of neutron scattering beamlines. It has been extensively used for the design of beamlines, e.g. the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, USA, and the Japanese Spallation Neutron Source, Tokai, Japan and the ISIS Spallation Neutron Source Target Station 2, Oxford, UK. As these large new facilities move from construction to operation there is now a desire to use simulation for data analysis by performing virtual experiments that include the sample scattering kernels as well as the beamline in the simulation. In order to do this effectively parallel computing resources are required. Virtual neutron scattering experiments require several steps. The VASP package is used for the time-consuming ab initio molecular dynamics calculations [5] and the trajectory converter is the nMoldyn package [6]. The virtual experiments are completed using the McStas package with nMoldyn input. The McStas calculations are done in parallel on the TeraGrid using MPI. Scaling studies out to 1000 cores show excellent parallel computing scalability (Figure 3). One possible McStas output format is NeXus [7]. The NeXus files can be viewed using the same graphics software based on ISAW [8] available in the Neutron Science Portal for the SNS experimental data.

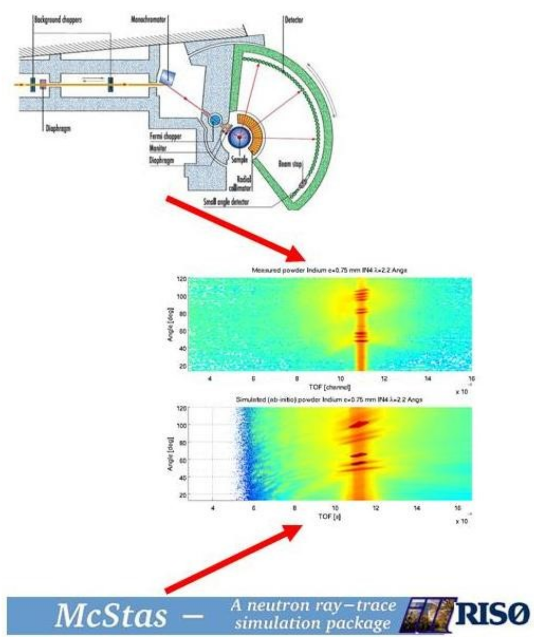

Figure 2 – Results of McStas virtual experiment with powdered Indium sample in the IN4 instrument at ILL agree with experimental results. (Image Courtesy E. Farhi)

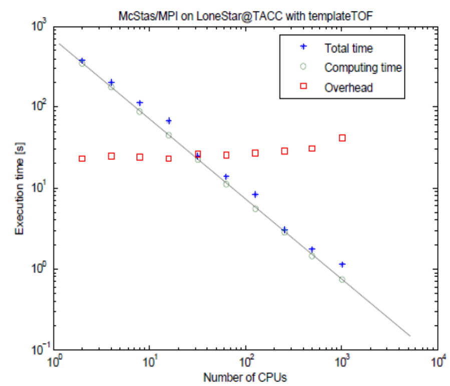

Figure 3 – McStas scales linearly to 1024 cores of the Lonestar TeraGrid computer. (Courtesy E. Farhi)

III.FITTING

The SNS and NSTG are also collaborating on data analysis including a fitting service. The fitting service does a fit of theoretical models to the NeXus data files from the experiments. The user decides which model to use, which fitting algorithm to use, which parameters to vary, and gives initial guesses to the fitting parameters (Figure 4). An adaptive nonlinear least squares algorithm is implemented in parallel on the TeraGrid and shows linear scaling at least up to 32 processors (Figure 5). It minimizes a nonlinear sum of squares using an analytic or numerical Jacobian matrix. The fitting service uses the NL2SOL [9] or Dakota [10] software packages. A Graphical User Input is created from an XML file for access to the fitting service from the neutron Science Portal.

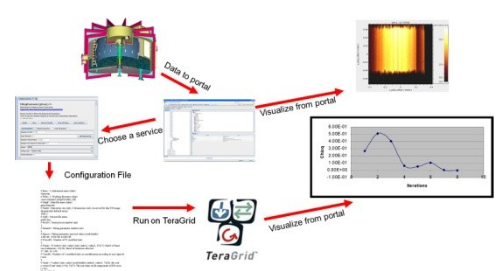

Figure 4 – Job submission of the fitting service.

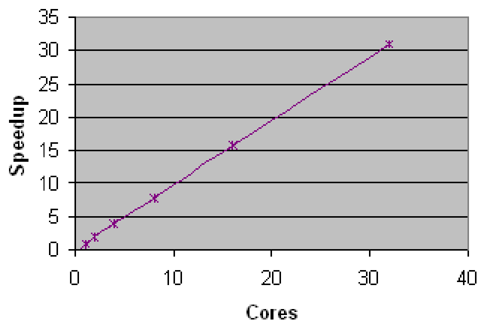

Figure 5 – Fitting service scales linearly to 32 cores.

IV.REDUCTION

Another area of collaboration is amorphous material reduction for the Backscattering and Reflectometry SNS instruments (Figure 6). An attempt has been made to parallelize this calculation by distributing regions of the time-of-flight to each processor. This is accomplished by having each processor read only its region of the NeXus input data file and write a new file containing only that region. Then each processor performs the data reduction on its NeXus file. The S(Q,E) results are merged at the end of the calculation. This is an area of continuing research for the collaboration.

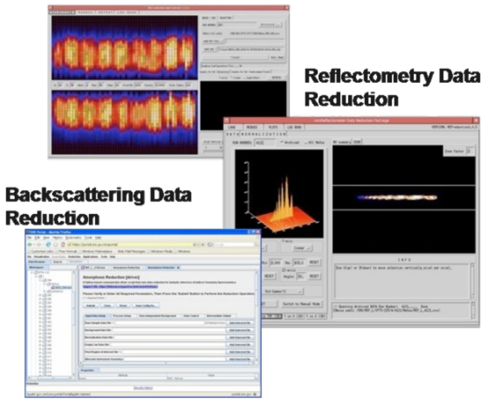

Figure 6 – View of the portal showing reduction services.

CONCLUSIONS

Software development collaborations are valuable for neutron science facilities. The TeraGrid has been a good resource for this work. Virtual experiments have produced structure dynamic factors for common powders found in neutron scattering. These were simulated using *VASP,* then *nMoldyn* and *McStas,* and finally compared (whenever possible) to measurements. This justifies even more large computing power, for an always more complex and detailed description of real neutron scattering beam lines and experiments. Collaborations for fitting and reduction are also in progress and will need TeraGrid resources.

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REFERENCES

1) *J.W. Cobb, A. Geist, J.A. Kohl, S.D. Miller, P.F. Peterson, G.G. Pike, M.A. Reuter, T. Swain, S.S. Vazhkudai, N.N. Vijayakumar, "The Neutron Science TeraGrid Gateway, a TeraGrid Science Gateway to Support the Spallation Neutron Source", in the Journal of Concurrency and Computation: Practice and Experience, Vol. 19, pp. 809-826, 2007.*
2) *C. Catlett et al., "TeraGrid: Analysis of Organization, System Architecture, and Middleware Enabling New Types of Applications", HPC and Grids in Action, L. Grandinetti, ed., 'Advances in Parallel Computing' series, IOS Press, Amsterdam, 2007.*
3) *V. E. Lynch, J. W. Cobb, E. Farhi, S. D. Miller, and M. Taylor, "Virtual Experiments on the Neutron Science TeraGrid Gateway," Proceedings of TeraGrid '08, June 10-12, 2008, Las Vegas, NV* [*http://teragrid.org/events/teragrid08/Papers/papers/5.pdf*](http://teragrid.org/events/teragrid08/Papers/papers/5.pdf)
4) *P. Willendrup, E. Farhi and K. Lefmann, "McStas 1.7 a new version of the flexible Monte Carlo neutron scattering package" Physica B, 350 (2004) 735.*
5) *G. Kresse and J. Hafner, Phys. Rev. B **47,** 558 (1993); ibid. **49,** 14251 (1994).*
6) *nMOLDYN: A Program Package for a Neutron Scattering Oriented Analysis of Molecular Dynamics Simulations, Comp. Phys. Comm. **91**, 191-214 (1995).*
7) *Website for NeXus information.* [*http://www.nexusforum.org*](http://www.nexusforum.org)
8) *Mikkelson, D. J. R. L. Mikkelson, T.G. Worlton, A. Chatterjee, J.P. Hammonds, P.F. Peterson, A.J. Schultz. "Coordinated, Interactive Data Visualization for Neutron Scattering Data", Talk at NOBUGS 2002 Conference, NIST, Gaithersburg MD.*
9) *John E. Dennis, Jr. , David M. Gay , Roy E. Welsch, Algorithm 573: NL2SOL —An Adaptive Nonlinear Least-Squares Algorithm [E4], ACM Transactions on Mathematical Software (TOMS), v.7 n.3, p.369-383, Sept. 1981*
10) *Eldred, M.~S., Adams, B.~M., Haskell, K., Bohnhoff, W.~J., Eddy, J.~P., Gay, D.~M., Griffin, J.~D., Hart, W.~E., Hough, P.~D., Kolda, T.~G., Martinez-Canales, M.~L., Swiler, L.~P., Watson, J.-P., and Williams, P.~J., 2007. "DAKOTA: A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis. Version 4.1 Users Manual," Sandia Technical Report SAND2006-6337, Updated September 2007.*