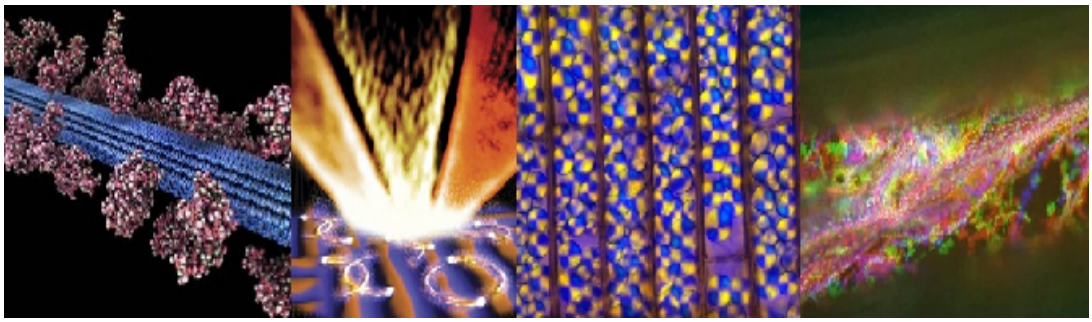
Building an Advanced Center for Data and Computing for ESS

Copenhagen, September 17-18, 2012

Building an Advanced Center for Data and Computing for ESS

Invited Speakers:
Per Christian Hansen
Arno Hiess
Rasmus Larsen
Michael Marek Koza
Sylvia McLain
Abbas Ourmazd
AJ (Timmy) Ramirez-Cuesta
Thomas Holm Rod
Jeremy C. Smith
Ilpo Vattulainen
Brian Vinter



Building an Advanced Center for Data and Computing for ESS

About the workshop:

This workshop brings together experts from different fields with the intent in reviewing and discussing the development of a theoretical and computational modeling infrastructure that is relevant to the diverse scientific community that will use ESS.

Our aim is to use this workshop as an input to our planning so that once the first experiments are made, ESS and its users are prepared to harness the most out of the scientific potential of their data.

The **Building an Advanced Center for Data and Computing for ESS** will take place on September 17 and 18, 2012, in Copenhagen, Denmark.

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SCIENTIFIC PROGRAM

Building the Advanced Center for Data Analysis and Computing for ESS, September 17-18, 2012		
Monday, 1st day		
9:00 – 9:30	Registration and Welcome	
9:30 – 9:45	Arno Hiess (ESS)	Identifying Science Drivers for ESS
9:45 – 10:30	Michael Marek Koza (ILL)	Neutrons and Computational Models: Prospect from a Scientist at the ILL
10:30 - 11:00	Coffee break	
11:00- 11:45	Ilpo Vattulainen (Tampere Univeristy of Tecnology)	Modeling of complex systems using inter-disciplinary approaches
11:45 – 12:30	Brian Vinter (NBI)	Access to giant data sets
12:30 - 14:00	Lunch	
14:00 – 14:45	Jeremy Smith (Tennessee Universiy and ORNL)	Neutron Scattering with Computers
14:45 – 15:15	Per Christian Hansen (DTU)	Old, New, and Future Algorithms for Tomography
15:15-15:30	Materials Innovations Infrastructures Moderator: Heloisa N. Bordallo (NBI)	
15:30-15:45	Dimitri Argyriou (ESS)	User Interface
15:45-16:00	Linda Udby (NBI)	Virtual Instruments & Theory for You
16:00-16:15	Andrew Jackson (NBI)	The role of condensed matter theory in a large scale facility
16:15-16:30	Juergen Eckert (UFS)	High performance computers: For all users or for some?
16:30-17:00	Coffee break	
17:00-19:00	Panel discussion: ESS Science: Opportunities, Ideas & Views Moderator: Robert Feidenhans'l (NBI)	
19:30 -	Dinner at Madklubben – Bistro de Luxe - http://www.bistrobooking.dk/madklubben//	
Tuesday, 2nd day		
9:00 – 9:45	Timmy Ramirez-Cuesta (ISIS)	Neutrons and Computational Models: Prospect from a Scientist at ISIS
9:45 - 10:30	Sylvia McLain (Oxford University)	Neutrons, Modeling and Biochemistry
10:30-11:00	Thomas Rod (NBI)	How I see the actual DMSC developing
11:00 - 11:30	Coffee break	
11:30-11:45	Anders Kæstner (PSI)	Data handling and processing for neutron imaging
11:45 - 12:15	Rasmus Larsen (DTU)	Quantitative Image Analysis
12:15 - 13:00	Abbas Ourmazd (University of Wisconsin Milwaukee)	Structure and Dynamics from Noisy Random Observations: A New Paradigm
13:00- 14:30	Lunch and Good bye	

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INVITED TALKS

Old, New, and Future Algorithms for Tomography

Per Christian Hansen

Technical University of Denmark (DTU)

Lygnby, Denmark

Tomographic reconstruction algorithms come in many variants. Two key issues are: 1) how to handle the computing times and the large amount of data involved in 3D reconstructions, and 2) how to incorporate prior information about the solution in order to stabilize the inverse problem and compute physically meaningful reconstructions.

Algorithms based on analytic expressions for the inversion (such as filtered back-projection and FDK, based on the inverse Radon transform) are fast because they are based on fast transforms such as the FFT – but it is difficult to incorporate priors and constraints. Algorithms based on variational formulations are more computationally demanding, but they allow a broader range of constraints to be incorporated. Algorithms based on sampling methods allow a wide variety of priors to be incorporated, but these methods tend to converge very slowly.

"High-Definition Tomography" is a new research project at DTU Informatics, funded by the European Research Council, whose aim is to develop a new generation of efficient large-scale algorithms that can incorporate many types of priors. This can be done, e.g., by utilizing the concept of "training," by exploiting sparsity and other structures of the underlying mathematical problem, and by utilizing current developments in first-order optimization methods. For more information, see imm.dtu.dk/~pch/Hdtomo.

Identifying Science Drivers for ESS

Arno Hiess

European Spallation Source

Lund, Sweden

Identifying the science drivers for ESS is required to guide the development of the scientific facilities at ESS.

Here I present our current findings based on the present use of neutron facilities and by harvesting input from the neutron user community via ESS science symposia:

* Where is the science going and what are the experimental challenges?

* Which instruments would be needed?

* What alternative techniques and support facilities are relevant for this science are?

A special emphasis will be put on requirements for computational requirements for scientific modeling.

The path to a sustained ESS science strategy will be discussed.

Quantitative Image Analysis

Rasmus Larsen

Technical University of Denmark (DTU)

Lygnby, Denmark

Quantitative image analysis – including image segmentation and extraction of geometrical and textural properties - provides the means for assessing structural material properties from 3D tomographic imaging. Manual segmentation of a 3D image is at best cumbersome. Segmentation of dynamically evolving structures in temporal 3D imaging or segmentation of even moderate sample sizes of 3D images is impossible.

We will illustrate automated image segmentation and quantification methods applied to application examples from material science as well as biomedical imaging. Moreover, we will see how geometry processing allows for simultaneous modelling and evolution of volumetric and surface properties.

Neutrons and Computational Models: Prospect from a Scientist at the ILL

Michael Marek Koza

Institut Laue Langevin

Grenoble, France

Neutrons, Modelling and Biochemistry

Sylvia McLain

Department of Biochemistry, University of Oxford

Oxford, United Kingdom

Natural biological processes, from proteins folding so that they can function to deciphering the DNA code, almost always take place in solution. As humans, around 60% of our body weight is from water and the solutions in our body help to deliver nutrients and oxygen to our many different types of cells. Even though biological solutions are essential to life there is relatively little known about interactions between these molecules in solutions. Neutron scattering techniques, both diffraction and inelastic scattering, provide a unique opportunity to understanding the interactions between biological molecules in physiologically relevant environments at the level where these interactions occur - the atomic and molecular level.

By using a combination of both neutron measurements and computational (Molecular Dynamics and reverse Monte Carlo (EPSR)) techniques to probe the interplay between biological molecules from the angstrom scale (10-10 meters (vÖ)) to the nanoscale (10-9 meters) we are working towards a better understanding of how biological processes occur in nature.

Structure and Dynamics from Noisy Random Observations: A New Paradigm

Abbas Ourmazd

University of Wisconsin Milwaukee

Milwaukee, USA

The best observations are thought to be those obtained with the greatest control over the system trajectory in phase space. But the full potential of major new instruments, such as photon and neutron sources, can be realized only by random observations along unknown system trajectories. Emerging data-analytical techniques are circumventing this apparent limitation, in some cases yielding more information than typically obtained in "well-controlled" experiments. I will describe on-going efforts to extract information on structure and dynamics from heterogeneous datasets consisting of a large number of noisy, random snapshots. Examples will include the structure and conformations of weakly scattering objects, and the dynamics of processes on time scales far below the limit set by timing jitter. The full exploitation of such approaches requires new experimental and data-analytical paradigms.

Neutrons and Computational Models: Prospect from a Scientist from ISIS: Data reduction, analysis and interpretation in neutron scattering

AJ (Timmy) Ramirez-Cuesta

ISIS / STFC

Didcot, United Kingdom

Managing the large amounts of experimental data coming from central facilities is a major computing challenge. The increased neutron fluxes and very large detector areas is already a major driver in the direction that data acquisition and reduction is taking nowadays. An example of a unified approach to data reduction is the Mantid project. Data reduction is the first step in the process of generating information and knowledge out of neutrons scattering.

Neutron scattering is a very powerful tool; neutrons provide a wealth of information; however the interpretation of the data is sometimes far from straightforward. Computer modeling is very ubiquitous and is also becoming a fundamental part in the interpretation of neutron data, but because of the variety of neutron techniques there is no unique way of modeling the experimental data. Certain problems, like neutron powder diffraction, are relatively simple to model and Rietveld refinement is used routinely. Other techniques like quasi-elastic and inelastic neutron scattering, disordered materials, magnetism, neutron reflectrometry etc use a variety of techniques like ab-initio, empirical potentials, molecular dynamics, Monte Carlo and more. There is no silver bullet, since the space and time domains explored by these modeling techniques are very different.

Finally, in order to produce a publication, the data has to be interpreted in the context of the field of science. These different levels of expertise required for the modeling are sometimes a terrifying prospect for new users and a hindrance to the growth of the neutron community.

The EES is a facility that will have DMC in place well before neutrons are going to be produced; this is a unique opportunity to build up the neutron data reduction/modeling setup from scratch. A variety of strategies to optimize the scope and future impact of the DMC should be careful considered.

How I see the actual DMSC developing

Thomas Holm Rod

Niels Bohr Institutet

Copenhagen, Denmark

The Data Management and Software Centre (DMSC) will be in charge of much of the IT that visiting scientists at the European Spallation Source will use, all the way from their first contact with ESS to the publishing of their results: web portals, instrument control, as well as data acquisition, reduction and analysis. Combining all these functions into one department provides a unique opportunity to use a holistic view on how the IT environment can help the visiting scientists to maximize the outcome of their time at ESS. The DMSC will strive to cater to the needs of the scientist from idea to publication by providing a comprehensive and integrated IT solution.

Anchored in the work on the design update for the DSMC and in my experiences with scientific software development and entrepreneurship, I will give my view on how the DMSC can develop into an efficient organisation that focuses on its users and their needs. I will also discuss how a clever choice of software architecture and a software development methodology can help obtain this goal.

One of the challenging tasks for the DMSC will be to define where best to spend resources. Some activities are pivotal to the functioning of the facility, such as instrument control, others are desirable, but not essential, such as support for atomic-scale modelling and simulations. Nonetheless, the latter has the potential to dramatically increase the scientific return-on-investment of the ESS and it is therefore reasonable to consider if time is not well spent in providing some level of support within such fields. Based on the discussions at this workshop I will explore this aspect in more detail. I will discuss what the must-have features are and how the desirable, but nonetheless important, features can be incorporated without jeopardising the core activities of the DMSC.

Neutron scattering with computers

Jeremy C. Smith

University of Tennessee / Oak Ridge National Laboratory

Oak Ridge, USA

Integration with high-performance computer simulation promises to revolutionize the type of information obtainable from experiments on next-generation neutron sources. We discuss the challenges inherent to such an approach, and give examples from protein structure and dynamics. Some relevant recent literature is below:

1. M. LOPEZ, V. KURKAL-SIEBERT, R.V. DUNN, M. TEHEI, J.L. FINNEY, J.C. SMITH and R.M. DANIEL. Activity and dynamics of an enzyme, pig liver esterase, in near-anhydrous conditions. Biophysical Journal 99 (8), L62-L64 (2010)
2. F. NOE, S. DOOSE, I, DAIDONE, M, LOLLMANN, M. SAUER, J.D. CHODERA & J.C. SMITH. Dynamical Fingerprints: Probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences (U.S.A.) 108(12):4822-7 (2011).
3. L. PETRIDIS, S.V. PINGALI, V. URBAN, W. T. HELLER, H. M. O' NEILL, M. FOSTON, A. RAGAUSKAS & J C. SMITH. Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation. PRÉ 83 061911 (2011)
4. E. BALOG, D. PERAHIA, J.C. SMITH & F. MERZEL, Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B. 115(21):6811-7 (2011).
5. S. V. PINGALI, H. M. O'NEILL, J. MCGAUGHEY, V. S. URBAN, C. S. REMPE, L. PETRIDIS, J. C. SMITH, B. R. EVANS and W. T. HELLER. Small-angle neutron scattering reveals pH-dependent conformational changes in Trichoderma reesei cellobiohydrolase I: Implications for enzymatic activity. Journal of Biological Chemistry. 286(37):32801-9 (2011).
6. A. JOHS, I.M. HARWOOD, J.M. PARKS, J.C. SMITH, L. LIANG & S.M. MILLER. Structural characterization of intramolecular Hg2+ transfer between flexibly-linked domains of mercuric ion reductase. Journal of Molecular Biology. 413(3):639-56 (2011).
7. L. HONG, B. LINDNER, N. SMOLIN, A. SOKOLOV & J.C. SMITH. Three classes of motion in the dynamic neutron-scattering susceptibility of a globular protein. Physical Review Letters. 107, 148102 (2011)
8. A. GODEC, J.C. SMITH and F. MERZEL. Increase of both order and disorder in first hydration shell with increasing solute polarity. PRL 107, 267801 (2011)
9. B. LINDNER and J.C. SMITH. Sassena - X-ray and Neutron Scattering Calculations from Molecular Dynamics Trajectories using Massively Parallel Computers. Computer Physics Communications. 183(7) 1491-1501 (2012)
10. N. SMOLIN, R. BIEHL, G.R. KNELLER, D. RICHTER & J.C. SMITH. Functional Domain Motions in Proteins on the ~1-100ns Timescale: Comparison of Neutron Spin Echo Spectroscopy of Phosphoglycerate Kinase with Molecular Dynamics Simulation. Biophysical Journal. 102(5), 1108-1117 (2012).
11. Y. ZHENG, Y. MIAO, J. BAUDRY, N. JAIN and J.C. SMITH Derivation of Mean-Square Displacements for Protein Dynamics from Elastic Incoherent Neutron Scattering. Journal of Physical Chemistry B. In Press.
12. L. HONG, X. CHENG, D. C. GLASS & J.C. SMITH Surface hydration amplifies single-well protein atom diffusion propagating into the macromolecular core. Physical Review Letters. 108 23 238102 (2012)

Modeling of complex systems using inter-disciplinary approaches

Ilpo Vattulainen

Tampere University of Technology

Tampere, Finland

Theory and computer simulations are more than useful to better understand what happens in nature. Yet the most crucial cornerstone of natural sciences is experimental research. Thus, it seems rational to think that one of the main objectives of theoretical natural sciences would be to complement experiments. The most fruitful means to support this objective is to collaborate: to bridge experiments with theoretical and computational considerations, with an aim to unify the resulting insight as joint publications. In some cases this is easy, sometimes less. In this talk, the purpose is to discuss ways to promote collaborations between theoretical/computational groups and experimental teams. In particular we consider circumstances where the science deals with biological phenomena over molecular scales, and where experiments are based on using large-scale facilities. We also discuss means to promote cross/inter/multi-disciplinary collaborations, and challenges to use simulations to determine primary observables which would allow direct comparison of simulation results with experiments, without assumptions often used to interpret experimental data. Examples showing how molecular simulations can provide added value to experimental science are given here, too.

Access to giant data sets

Brian Vinter

Niels Bohr Institutet

Copenhagen, Denmark

An interesting generation gap is currently showing itself; old-school researchers keep their data on their own computer and may perhaps share it through an FTP server, younger researchers on the other hand have grown up in a world where information equals the Internet and ownership is a very diffuse concept. For a facility like ESS a data access model must be devised that makes both kinds of researchers, and everybody in between, feel confortable and, more importantly, work productively. Fortunately this problem is not ESS specific, but in fact a very general problem, and a number of solutions to this challenge is currently maturing and will be ready for the launch of ESS. My talk will describe the problems nature and show the solutions we may be moving towards.

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