E-learning neutron scattering

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Introduction to the VNT project

Since experimental neutron scattering is mostly restricted to large-scale facilities, not all students have access to learning the technique at their home institution. Providing a freely accessible e-learning portal for neutron scattering is therefore an important outreach task in order to secure and educate the future users and scientists at neutron scattering facilities. This task and challenge has been taken up by the Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (NMI3).

In 2010, we initiated investigations into the possibilities for e-learning neutron scattering. Subsequently, a pilot project started in 2011, through co-funding from the University of Copenhagen, that is now (2012) growing to a full-scale 4-year international e-learning project called Virtual Neutrons for Teaching (VNT) [1] with support from NMI3-II via the "E-learning neutron scattering" work package. The collaborators in the project are based at the University of Copenhagen and the research reactors FRM-II (Technical University of Munich) and ILL in Grenoble.

The people involved in the collaboration span a broad range of competences from didactics and teaching in physics, through neutron scattering in theory, simulation and experiment to programming and web-design. We aim

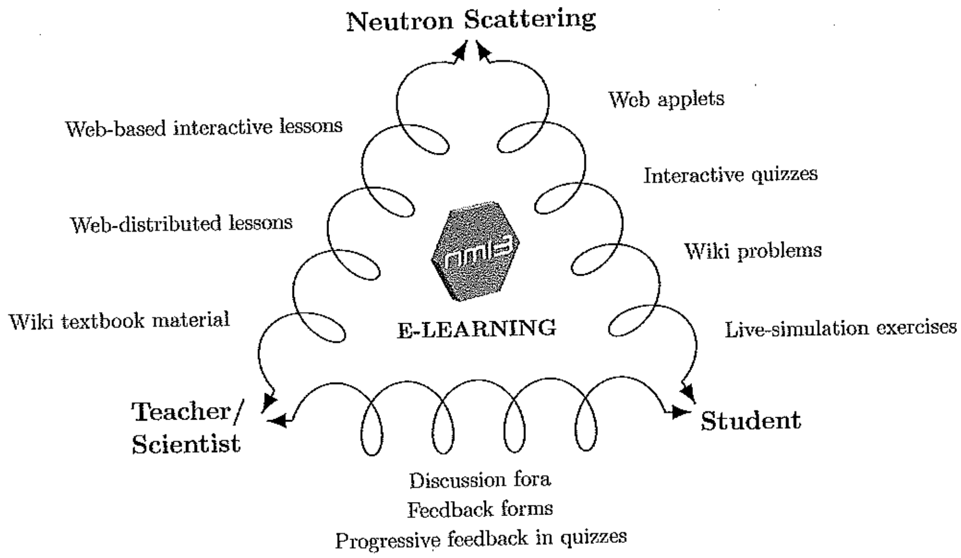


Figure 1. The tools of interaction between the teacher, student and material in the VNT e-learning project.

to offer online teaching material to university students and their teachers as well as scientists from other fields wanting to learn about neutron scattering techniques.

The didactic triangle for e-learning

Any learning situation can be schematically described in general terms by the interactions between three parts (topic, teacher and student) in the so-called didactic triangle. In a pure e-learning situation the means of interaction are not the same as in a face-to-face class-room situation; some tools are missing while others are gained. The challenge in any learning situation is to balance the interactions on the sides of the triangle in order to optimise the outcome for every student. In Figure 1, we have shown schematically some of the neutron e-learning tools we are developing for VNT and how they fit into the didactic triangle.

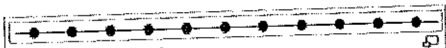
The three legs of VNT

The VNT project is moving on three legs:

- A neutron scattering wiki textbook (VNT-wiki)
- Invited and contributed specialised interactive lessons (VNT-lessons)
- A live simulation web portal (VNT-livesim)

A wiki is an online encyclopaedia which allows users to add, modify or delete its content via a web-browser. The VNT-wiki is structured like an introductory textbook and is primarily built on our own notes which are used in the class-room neutron scattering course at the University of Copenhagen called 'Neutron Scattering in Theory, Simulation and Experiment' (NSTSE). Some sections are contributed by invited scientists and moderated in terms of syntax and seamless integration into the wiki by the VNT team. Besides text and web-applets/animations the wiki contains exercises with hints and solutions embedded by a show/hide functionality that enables student controlled differentiated teaching. One example of the show/hide function is shown in Figure 2. The wiki also contains a series of Monte Carlo (MC) simulation projects intended for the students to learn how to use MC simulation to build a virtual instrument in order to investigate properties of existing or generic neutron scattering instruments. In the NSTSE course the students build virtual copies of three different neutron scattering instruments located at the Paul Scherrer Institute (PSI) in Switzerland, and are thus well equipped to participate directly in scientific projects when they go for practicals at PSI in the last week of the course.

Problem:Fourier transform



One-dimensional crystal.

Mathematically the scattering amplitude is the Fourier transform of the distribution of scattering centers (nuclei, electrons, spins) within the material. The scattered intensity (the scattering function) is the square of the scattering amplitude.

The Fourier transform of a function $\rho(r)$ is written as

$$F(q) = \int \rho(r) \exp(iqr) dr,$$

where $\rho(r)$ is the function in real space given by positions r, and q is a coordinate in Fourier space (which in scattering terms usually is called "reciprocal space"). $\rho(r)$ is in case of scattering theory the position sensitive scattering length density within the sample.

We will consider a one-dimensional space, *i.e.* all particles (scattering centers) are positioned on a line, and correspondingly only calculate the one-dimensional Fourier transform. We assume further that all particles are points (size = 0).

Contents [show]

Question 1

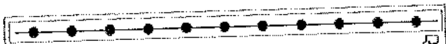
Calculate the Fourier transform and the scattering intensity of a sample with only one particle, and plot the normalized scattered intensity $I(q) = |F(q)|^2/N^2$ versus qR [show]

Hint [show]

Hint [show]

Solution

Problem:Fourier transform



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Calculate the Fourier transform and the scattering intensity of a sample with only one particle, and plot the normalized scattered intensity $I(q) = |F(q)|^2/N^2$ versus qR [hide]

Hint

A point-particle may mathematically be described as a Dirac δ-function with the property

$$\int \delta(r_0) f(r) dr = f(r_0).$$

[hide]

Hint

Place the particle in origo $(0, 0)$. [hide]

Solution

Fourier transform:

$$F(q) = \int \delta(0) \exp(iqr) dr = \exp(0) = 1.$$

Scattering intensity:

$$I(q) = F^2(q) = 1^2 = 1.$$

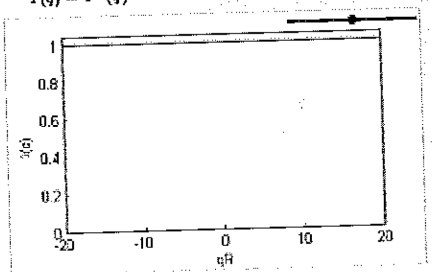

Figure 2. Example of a wiki-problem with hints and solution hidden (top) and shown (bottom).

For those who are not interested in learning how to program MC simulations in terms of building their own virtual instruments on their personal computer, but still would like to learn by visualisation of virtual experiments [2–5], we provide some pre-defined, but tuneable virtual instruments via a live-simulation web-portal which is accessible by browser. The web-portal is connected to a small cluster-grid that runs the MC ray-tracing software McStas [6–8] behind the user-interface. The user can log in and run a live-simulation of an experiment, visualise the ray-tracing in the instrument from any angle, download the synthetic data and plots from the 'detector' or share them via a static link, see Figure 3.

Furthermore, interactive special topical quiz-lessons will be prepared in collaboration between contributing scientists and the didactics researcher in the VNT team, see Figure 4. The responses from the students can be, e.g., clicking on pictures or typing in numbers, formulae or essays. Feedback is given automatically for every student answer and can be adapted to the nature, content and quality of the particular answer.

We are planning to collect these and more features, such as classical neutron scattering books, notes and material from, e.g., summer-schools in a common learning management system (LMS). Although entry assessment and grading of students' work for certificates is possible to make within the LMS frame it is not the scope of the current project. We do, however, intend the portal to be valuable and educational to students from different backgrounds such as bio-physics, chemistry, physics and engineering, either as stand-alone or complementary material for neutron scattering courses. It will address students starting from bachelor level and a well-chosen structure will guide more experienced students with a

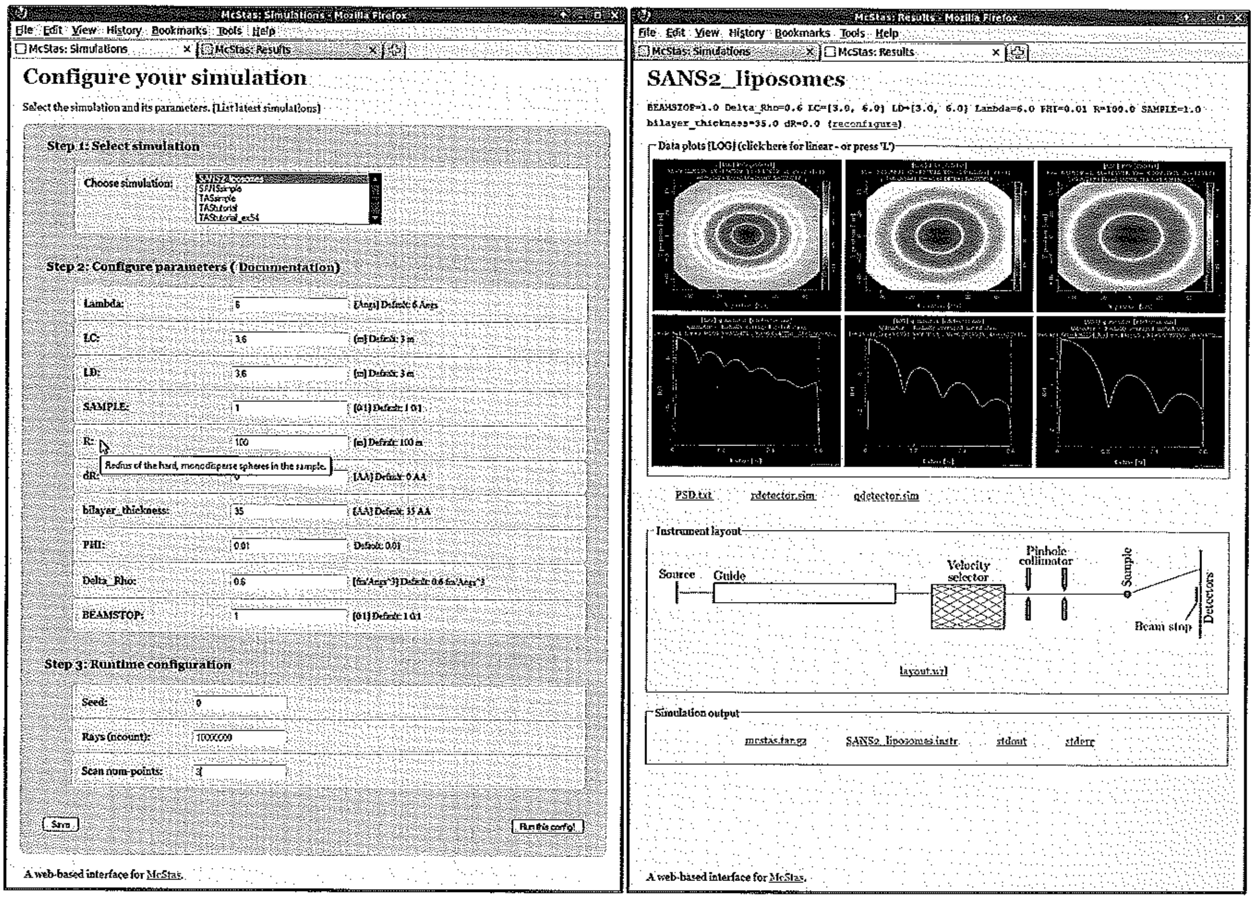

Figure 3. Example screenshot of a web-based live-simulation which shows the scattering data from a sample with monodisperse hard spheres in three different matching collimator- and detector length configurations of a SANS instrument. The configuration of the instrument is set in the first window (left) and the results of the simulation are then spawned in a new window (right) with a permanent link for sharing or revisiting the data.

Scientific Reviews

Information

Flag question

Edit question

The scattering intensity from diluted monodisperse liposomes is given by

$$I(q) = \phi V(\Delta\rho)^2 F^2(q)$$

where

- ϕ is the volume fraction of liposomes,
- $V = V_{\text{out}} - V_{\text{in}}$ is the volume of the liposome,
- $\Delta\rho$ is the excess scattering length density in the shell, and
- $F(q)$ is the form factor amplitude.

In the following we are going to work with the different parts of this equation.

Please press "submit" when you have answered all the subquestions of a question. Please press "submit all and finish", when you reach the end of the lesson. Also, for some of the questions, pressing "submit" will reveal additional information!

Question 1

Correct

Mark 1.00 out of 1.00

Flag question

Edit question

Neutron scattering techniques can be used to discern different features of particles in a sample. In these problems we look at a class of particles which can be described as thin spherical shells.

The shell itself has structure, since it is composed of two layers. This double layer is called a bilayer.

The layer consists of molecules, which themselves have structure. They consist of a headgroup and a double chain. The headgroup is usually pictured as a circle, while the chains are pictured as wiggly lines. Here, we deal with a class of these molecules called phospholipids, and the specific molecule you are going to work with is called Di-Myristyl Phospatidyl Choline (DMPC).

In an aqueous environment, the phospolipids can assemble to the thin spherical shells called liposomes. The figure shows the bilayer from a small part of the shell.

(PC) and the chains (DM). Use the figure to locate the *hydrophilic*

Master of Science or PhD degree to find the appropriate level to start the training.

Perspectives

E-learning offers a wide range of possibilities for evaluation and directly measuring how the students use the material and learn. This is made possible since all clicks and replies in quizzes etc. are stored in a database on which web analytics tools can be applied.

The VNT features are tested by integrating them into the NSTSE course at the University of Copenhagen as they are developed and we observe, evaluate and analyse them through the students' use online and in the classroom taking account of the students' varied backgrounds from a palette of physics, chemistry, bio-physics, nanoscience, engineering and even computer science.

We are currently developing a method to identify student roles through their online behaviour in each session based on network and clustering analysis [3]. We hope through our didactical research to be able to identify parameters which can enable targeted e-learning in neutron scattering for a wide range of students', teachers' and scientists' backgrounds. Furthermore we intend to use the web analytics tools, feedback from interactive lessons, discussion fora and feedback forms for continuous improvement of the VNT.

Invitation to collaborate

Our goal is to improve existing tools for educating students and new neutron users by employing state-of-the-art e-learning methods and by drawing upon existing expertise. We aim the efforts to be of value for universities and facilities alike, and we invite everyone to contribute material or join in the development and usage of the new e-learning portal.

References

1. Virtual Neutrons for Teaching: http://vnt.nmi3.org
2. K. Lefmann, P. K. Willendrup, L. Udby, B. Lebech, K. Mortensen, J. O. Birk, K. Klenøe, Knudsen, P. Christiansen, J. Saroun, J. Kulda, U. Filges, M. Konnecke, P. Tregenna-Piggott, Peters, K. Lieutenant, G. Zsigmond, P. Bentley, E. Farhi, Virtual experiments: the ultimate aim of neutron ray-tracing simulations, *J. Neutron Res.* **16**, 97–111 (2008).
3. L. Udby, P.K. Willendrup, E. Knudsen, Ch. Niedermayer, U. Filges, N.B. Christensen, E. Farhi, B.O. Wells, K. Lefmann, Analysing neutron scattering data using McStas virtual experiments, *Nuclear Instruments and Methods in Physics Research A*, S138–S143 (2011).
4. P. Willendrup, U. Filges, L. Keller, E. Farhi, K. Lefmann, Validation of a realistic powder sample using data from DMC at PSI, Physica B, **386**, pp. 1032 (2006).
5. E. Farhi, V. Hugouvieux, M.R. Johnson, W. Kob, Virtual experiments: Combining realistic neutron scattering instrument and sample simulations, *J. Computational Physics*, 5251–5261 (2009).
6. http://www.mcstas.org/
7. K. Lefmann and K. Nielsen, McStas, *a General Software Package for Neutron Ray-tracing Simulations*, Neutron News 10 (1999).
8. J. Bruun and L. Udby. *Student use of hints and solutions in an online learning environment*, 10 pages, last revised September 21, 2012.