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Virtual experiments: the ultimate aim of neutron ray-tracing simulations

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Virtual experiments: the ultimate aim of neutron ray-tracing simulations

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We define a virtual neutron experiment as a complete simulation of an experiment, from source over sample to detector. The virtual experiment (VE) will ideally interface with the instrument control software for the input and with standard data analysis packages for the virtual data output. Virtual experiments are beginning to make their way into neutron scattering science with applications as diverse as instrument design/upgrade, experiment planning, data analysis, test of analysis software, teaching, and outreach. In this paper, we summarize the recent developments in this field and make suggestions for future developments and use of VEs.

Keywords: Monte Carlo simulations; Neutron scattering; Neutron instrumentation; Data analysis

Introduction

The field of neutron ray-tracing simulations for scattering purposes has exploded during the last decade. This has primarily been caused by the increase in detailing level and user friendliness of the available software packages. The topic was pioneered by the legendary

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neutron transport code MCNP (MCNP home page, mcnp-green.lanl.gov) and for scatteringpurposes by the NISP package (NISP home page, paseeger.com). In the late 90s, a new generation of freeware simulation packages were initialized, the most prominent being McStas [1], VITESS [2], RESTRAX [3], and IDEAS [4]. These packages have been developed concurrently since, in an atmosphere of friendly competition and have actively compared results and shared ideas for common benefit. At present, the packages have reached a level where actual 'virtual experiments' (VEs) can be performed. In this paper, we will make a proper definition of VEs and give recent examples of their broad usefulness.

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Definition of VEs

The term VE is being widely used within the neutron simulation community, but has never been clearly defined. We will here establish the term VE by the definitions:

- The neutrons rays must have absolute intensity units and should be traced through the whole instrument, from source to detector [5]. (This can be done either by simulating each ray through the instrument or by breaking the simulation up into several bits.)
- The description of the instrument should be as close as possible to the reality. This is in particular the case for the sample.
- The virtual instrument is controlled like the real instrument, and the resulting data are analyzed like real data.

The input to a VE is the complete state and setting of the instrument: angles and collimation for a steady-state instrument, and chopper phases, etc. for a time-of-flight instrument. In addition, the state of the sample (*e.g.* orientation and temperature) must be specified. Preferably, the input to the VE should come from the instrument control software itself.

The outcome of VE are virtual data sets, which can be handled by standard analysis programs. The virtual data are used to obtain knowledge of the response of the neutron instrument to a particular sample.

One thing that cannot be deduced from the virtual data is, of course, the properties of the sample itself. In all simulation packages, this is specified by the user. However, it is very useful to simulate a sample with certain characteristic scattering features, in order to test whether a particular instrument is able to resolve these features. Examples of this are shown in the following.

Instrument upgrade and design

The most frequent application of VE – and of neutron ray-tracing simulations as such – is design of novel instruments. Initially, the most frequent use was for design of primary spectrometers (in particular guide systems), but with the advent of realistic sample components, also features of the secondary spectrometer have been simulated. This is in particular the case for the new and emerging sources FRM-II, OPAL, SNS, J-PARC, and ESS, but also for major existing source upgrades like the ILL millennium program and ISIS second target station.

The use of VE in instrument design is straightforward. By performing a VE on the instrument under design, one can obtain an idea of typical data, with respect to signal quality (*e.g.* peak shape), intensity, and possibly sample background. Simulation of room background from *e.g.* fast neutrons is, however, usually out of reach for ray-tracing simulations, and more exact neutron transport codes must be employed, *e.g.* MCNP.

To estimate the value of the improvement by new instrument design – or instrument upgrade – it is usual to compare VE data from the new instrument and a baseline instrument. In principle, a comparison can be also performed between VE data and data measured on an existing instrument. One should, however, bear in mind that non-ideal properties of the instrument, not considered in the simulations, may lead to over- or underestimation of the simulated instrument performance, typically in the absolute intensities. Hence, a comparison between two simulations is usually the preferred procedure.

The IN20 flat-cone multianalyzer (ILL)

One of the first examples of VE in instrument design was the flat-cone upgrade of IN20, ILL. Here, the upgrade consists of replacing the standard triple-axis analyzer with a bank of 31 analyzers, 2.5° apart, which scatter out of the horizontal plane. All analyzers are fixed to accept the same energy [6]. This mode of running a triple-axis instrument compares with the monochromatic imaging mode of the 7 blade analyzer at RITA-2, PSI [7]. However, the flat-cone design has a much larger angular coverage.

The IN20 VE was performed using a sample with phonon dispersion in Si. In the VE, the sample rotation was scanned. This effectively produced a cut of constant energy transfer, obtaining a two-dimensional monochromatic cut in reciprocal space. Figure 1 shows the cut through the phonon dispersion ifself and the comparable outcome of the VE. All phonon features are clearly reproduced. This was a strong support for the decision of actually performing the flat-cone upgrade.

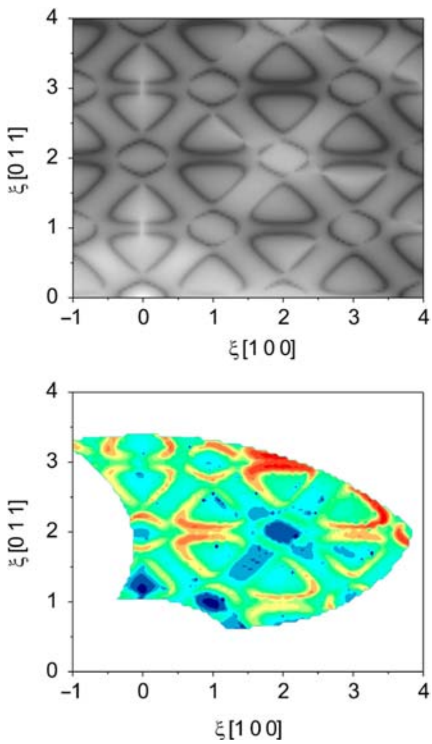

Figure 1. Inelastic (20 meV) 2-dimensional cut through the phonon dispersion of Si. Top panel shows the phonon dispersion model, bottom panel shows virtual data, obtained from a RESTRAX VE on IN20 (ILL).

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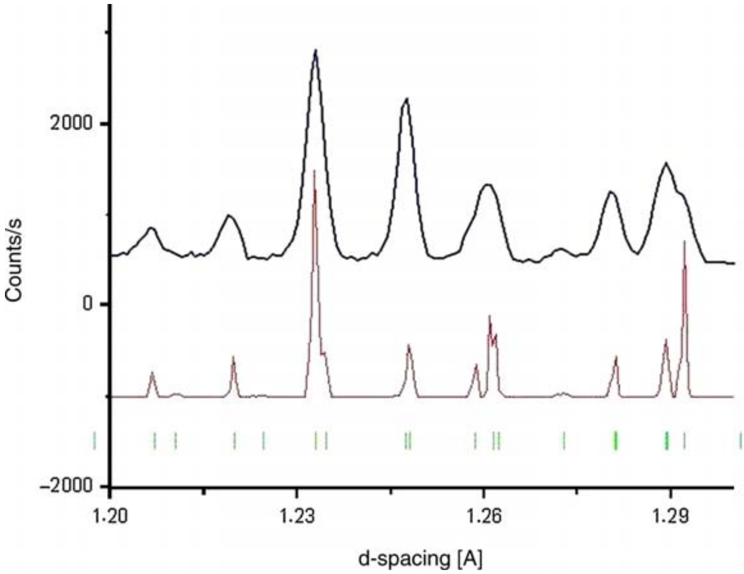

Figure 2. Powder diffraction pattern of $TbMnO_3$. Data from a VITESS VE at the planned HMI diffractometer EXED (middle, red), measured data at E9, HMI (top, blue), and the nominal peak positions for $TbMnO_3$ (bottom, green) (colour online).

Design of EXED (HMI)

VE has been used to evaluate the performance of the extreme environment diffractometer (EXED), under construction at the new guide hall at HMI. This instrument is special in the sense that is contains a set of unsplit solenoid coils for very high magnetic fields in the direction of the incident beam. Hence, scattering can be observed only in small angles and close to backscattering. Using the time-of-flight technique, the incoming wavelength can be scanned so that one has access to a large range of q-values. The backscattering condition gives a very high resolution in powder diffraction. This is illustrated in figure 2, where part of the virtual data are presented, together with the nominal peak positions. The data is compared with (scaled) real diffraction data from $TbMnO_3$, recorded at E9 (HMI). For this example, the resolution of EXED is clearly superior to E9. For more details about EXED, we refer to Ref. [8].

Instruments for ESS long-pulse target station (LPTS)

As the last examples of VE for design of new instruments, we show simulations of two instruments for the ESS long-pulse target station. A powder diffractometer on a long-pulsed source nominally suffers from lack of resolution. However, a clever use of pulse-shaping choppers close to the source makes the instrument strongly competitive to a diffractometer on a similar short-pulsed target [9]. Figure 3 shows a comparison between VE data on these two instruments. The LPTS instrument has both better intensity and a superior peak shape.

ESS LPTS instruments in general take advantage of the high integrated intensity of the 2 ms long pulse. The simulated cold-neutron chopper spectrometer further utilizes the low repetition rate (16 2/3 Hz), to select a number of pulses from each frame with different wavelengths. As an example, if the pulses are taken 5 ms apart (at the sample position), one can record up to 11 data sets for each pulse, with a wavelength difference of 2 Å between the first and the last pulse [10]. The data from the VE is shown in figure 4. As anticipated, the energy resolution and overall intensity vary significantly with wavelength. From the data, it is clear that the intensities of the different wavelengths are useful but cannot be directly added to obtain the overall performance

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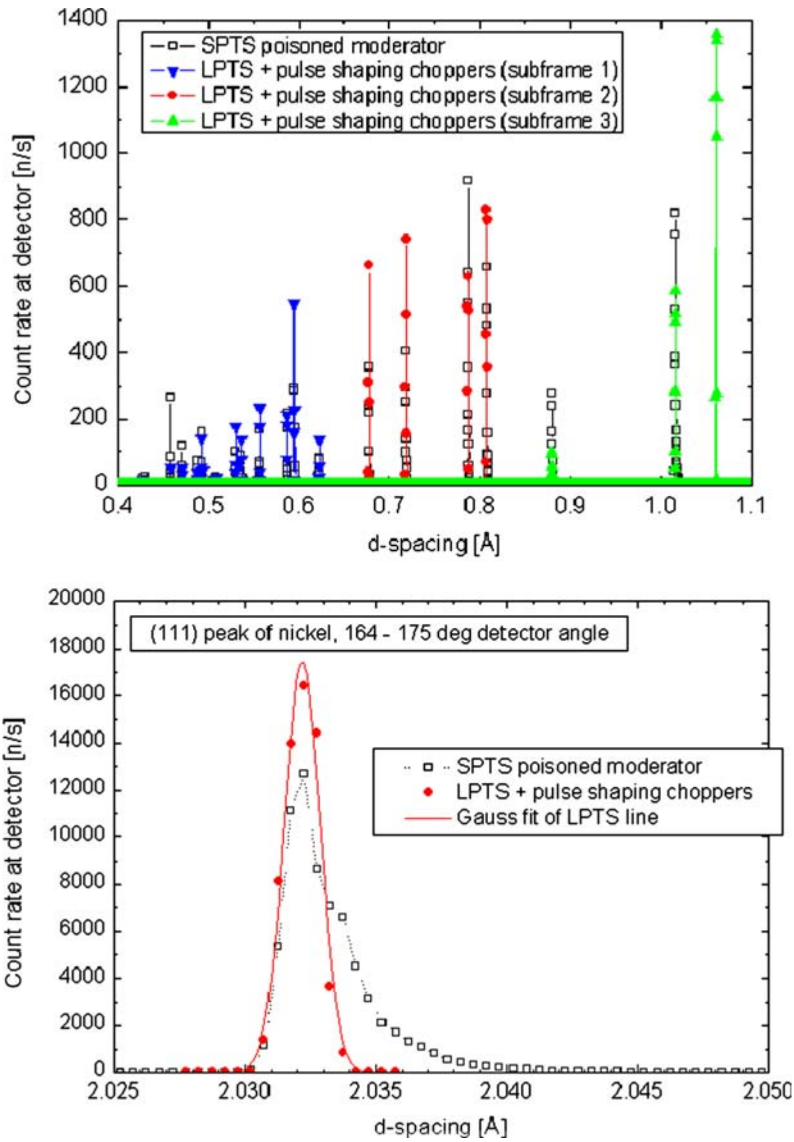

Figure 3. ESS long pulse powder lines, simulated by VITESS. Top panel shows a number of small-d diffraction peaks. Bottom panel shows a zoom on a single large d-peak. From [9].

of the spectrometer. This presents challenges for the optimization of the instrument and for the subsequent data analysis packages. This spectrometer and other instruments were simulated at a workshop in Rencurel (F), September 2006, later at the island of Ven (S), October 2008 (homepage of the Rencurel 2006 meeting, wwwold.ill.fr/Computing/links/meetings/ESS-LP/).

Experiment planning and optimization

In principle, a VE on a detailed model of an existing instrument can help users and instrument responsibles to estimate the feasibility of a planned project and help selecting the mode of running the instrument. This task is non-trivial, since it requires detailed models of the (expected behaviour of the) sample. Furthermore, a useful optimization tool for the

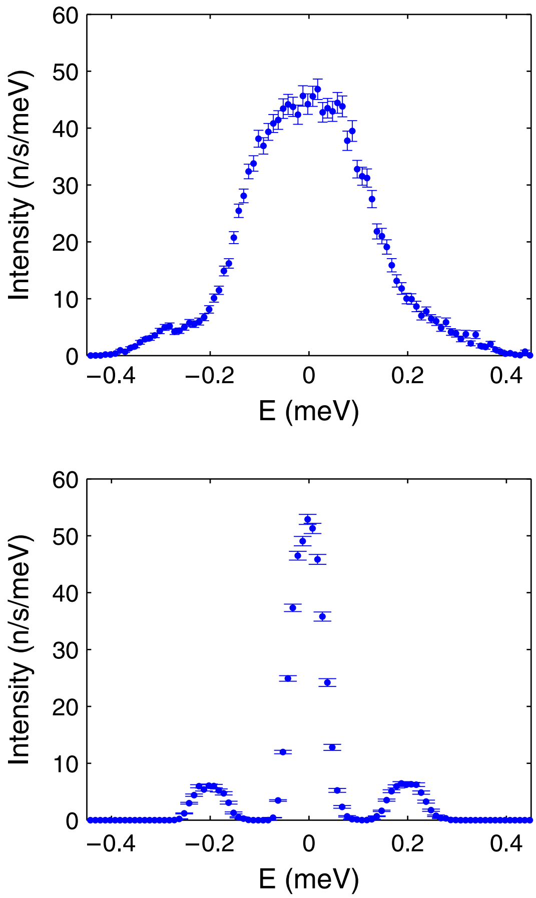

Figure 4. Inelastic scans on the cold-neutron chopper spectrometer for ESS long pulse target station. The data shows inelastic cuts through scattering data for a generic sample with an elastic line and 'tunnel peaks' at ±0.2 meV. Top and bottom figure shows McStas virtual data for the same pulse with incoming wavelengths of 4 and 6 Å, respectively.

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experimental mode must be easily available for non-specialist users. This is in sharp contrast to present-day optimization, which requires much expert knowledge and detailed analysis of simulated data, *e.g.* due to strong correlation between parameters.

Web simulation tools for neutron users

As the first prototype towards this goal, a simple user simulation tool has been constructed for the cold-neutron powder diffractometer DMC, PSI. The McStas simulation is controlled via the PSI instrument control program, SICS, which is in turn run from the instrument home page (DMC home page sinq.web.psi.ch/sinq/instr/dmc) [11]. Only the few most used settings of the instrument can be selected. The user will upload a standard crystallographic definition file, which is used together with geometrical information to define the sample. An illustration of this home page is shown in figure 5.

Scaling to absolute measurement times

One of the foreseen uses of VE is experiment planning. One aspect of this is the optimal configuration of the instrument, which will be considered below. Here, we will consider the determination of the total measurement time, relevant *e.g.* in connection with beamtime

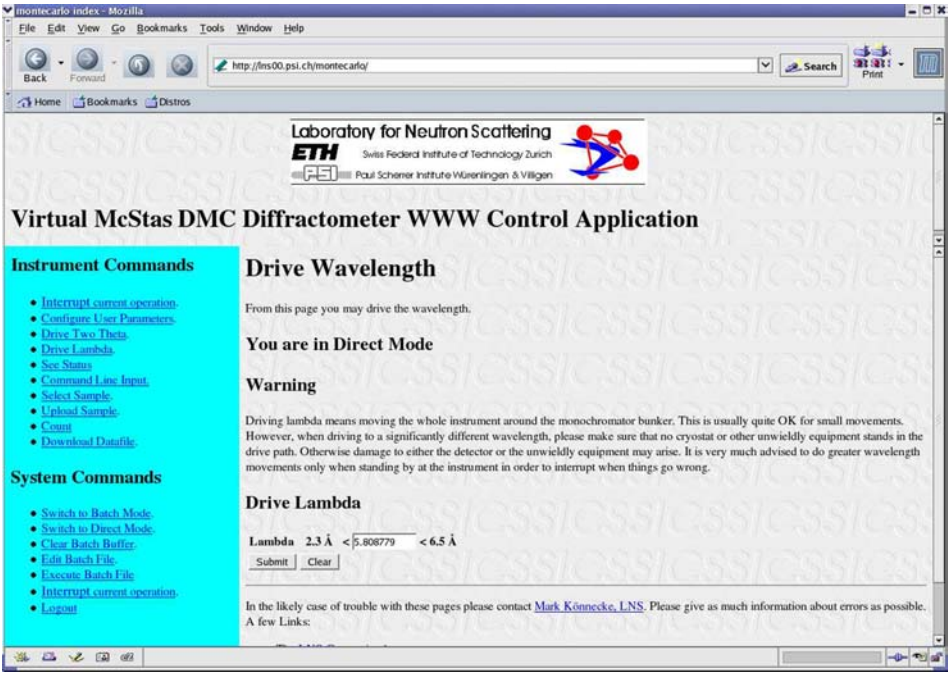

Figure 5. Front screen of the SICS–McStas web interface for the DMC powder diffractometer af PSI. The user can change the most standard settings of the VE through this portal.

proposals. It is thus essential for the simulations to give reliable estimates of the actual detector counts.

The ray-tracing simulation packages deal with intensities and error bars in very similar ways. The primary simulation unit is intensity (counts per second), so the assumed measurement time (the 'virtual time') is used to scale the virtual data to obtain integrated detector counts. In order to estimate total measurement time, realistic counting statistics must be imposed on the simulation counts, C, to reach the counts of the VE, C_{VE}. Since this has not been discussed in the litterature, let us describe it more thoroughly here.

Let n be the number of neutron rays reaching the detector, and let the rays have (different) weights, w_i. The simulated intensity is then given by

$$I = \sum_{i=1}^{n} w_i. \tag{1}$$

The estimate of the error on this number is calculated in the McStas manual [1], and the standard deviation is approximated by

$$\sigma^2(I) = \sum_{i=1}^{n} w_i^2. \tag{2}$$

In real experiments, $w_i = 1$, whence we reach $I = n$ and $\sigma(I) = \sqrt{I}$ as expected (for counts exceeding 10). Let the virtual time be denoted by t. The simulated counts during this time becomes

$$C = tI, \tag{3}$$

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and its error bar estimate is

$$\sigma^2(C) = t^2\sigma^2(I). \tag{4}$$

However, to simulate a realistic counting statistics, we must fulfill

$$\sigma_{\mathrm{VE}}(C_{\mathrm{VE}}) = \sqrt{C_{\mathrm{VE}}}. \tag{5}$$

This is obtained by adding to (3) a Gaussian noise $E(\Sigma)$ of mean value zero and standard deviation Σ:

$$C_{\mathrm{VE}} = tI + E(\Sigma). \tag{6}$$

The standard deviation for the VE becomes

$$\sigma^2_{\mathrm{VE}}(C) = t^2\sigma^2(I) + \Sigma^2. \tag{7}$$

Now, the requirement (5) allows us to determine Σ:

$$\Sigma^2 = tI - t^2\sigma^2(I). \tag{8}$$

Since Σ^2 must remain positive, we reach an upper limit on t

$$t_{\max} = \frac{I}{\sigma^2(I)}. \tag{9}$$

Above this virtual time, it is not possible to obtain realistic error bars in the VE. This rule applies to each bin in a detector array, so the effective value of $t_{\max}$ is the smallest of the values in the individual bins.

One sentence of caution should be added: to avoid bins with zero (or very low) count rates, it may be necessary to apply a suitable rebinning and/or including an overall background (representing fast neutrons and/or electronic noise) before adding counting statistics.

Generic optimization

As a step towards easing optimization of instruments and experimental set-ups, we have been developing the use of evolutionary algorithms, widely used in machine-learning, engineering, and finance applications [12]. Through series of VE, these methods are able to evolve the design of instruments to arrive at the best possible configuration, *e.g*. for a given experiment.

In the first instance, it was demonstrated that genetic algorithms are able to adapt an existing spectrometer to accommodate new hardware at the maximum possible resolution, and find an operating configuration at the physical tolerance limits of components [13]. Figure 6 shows the convergence of a genetic algorithm upon a set of operating currents of a neutron spin-echo spectrometer, which are strongly dependent on the position of the 1 m diameter coils (also adjusted by the algorithm but not shown in the figure). In this figure, the vertical bars indicate the standard deviation of the parameters across the whole population of solutions, (but the deviations are not normally distributed around the mean value). Clearly seen are frequent fluctuations in parameter values, leading to a large change in the standard deviations, caused by the pseudo-random nature of the evolution process. The use of such algorithms allows scientific instruments to be quickly adapted for new experiments that were not considered in the original design.

Another application of these ideas was to evolve the design of an entire neutron spin-echo spectrometer. It was shown that a genetic algorithm was capable of arriving at a superior design to that obtained by traditional, manual means [14]. Furthermore, whereas the human

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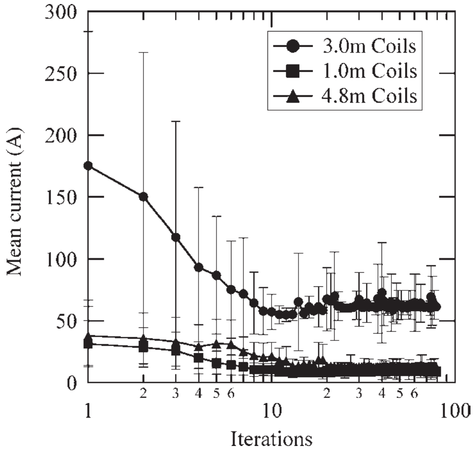

Figure 6. Evolving adjustment of the precession coils' and correction coils' currents on the spin-echo spectrometer SPAN, taken from [13], as described in the text.

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design typically takes several weeks, the total calculation time for a genetic algorithm was less than 24 h. It is this ability, to change the criteria of the instrument design and find a new optimum at such short notice, which makes such artificial-intelligence based solutions such an attractive and powerful tool. The total programming time required is approximately equal to the manual design of an instrument, but thereafter the design can be modified at will, based upon new engineering constraints, adjacent experiments, and so forth. Clearly, this method is attractive for the optimization of any type of scientific instruments, with the figure-of-merit being the quality of the virtual data, evaluated by automated data analysis.

VEs play a crucial role in assessing the quality of the instrument for any given set of configuration parameters, since a figure of merit is used as a quantitative comparison of the quality of competing designs. The more accurate the results of the simulation, the better optimized the design will be for a given experiment. This makes such evolutionary algorithms very attractive for optimizing experiment with a given instrument and sample, and for a given region of interest of data. It has been demonstrated, albeit at an early stage [13,15], that genetic algorithms are also well suited for the tuning of resolution ellipsoids to a given dispersion curve in triple axis spectrometers. With further developments, we are confident that this will become a routine method of optimizing neutron instruments to a given experimental configuration. For example, the user can enter the desired resolution and the position in reciprocal space, and the artificial intelligence algorithm is able to select the optimum configuration to make the best use of experimental time, taking into consideration external factors such as background, multiple scattering, etc., and an accurate simulation of the behaviour at the sample. Such a tool would be invaluable for making the best use of experimental time for many scientific instruments.

Data analysis

To analyze data from VE, it is strongly preferable to use existing data analysis programs. This avoids discrepancies in analysis schemes and saves the simulator from developing new tools, at the expense of developing interfaces to suitable data format One emerging, site-independent format, sufficiently general to contain all types of neutron data, is NeXus (NeXus home page www.nexus.anl.gov). The packages VITESS, RESTRAX, and McStas all support NeXus.

An important use of VE is to obtain additional knowledge of the interplay between instrument and sample, allowing for high accuracy in the data treatment. This is detailed below.

Resolution effects

An obvious example of VE taking non-idealities into account is that the instrument resolution is automatically included in simulations. Furthermore, VE have the capabilities of determining the resolution to a higher precision than analytical calculations (for most instruments).

This effect was recently used to analyze data from an experiment at RITA-2, PSI. Here it was of high importance to conclude whether finite-size broadenings could be detected in certain diffraction signals [16]. To obtain maximal accuracy in determining the intrinsic instrument resolution, an 'alignment' was performed on parameters of the simulated instrument. This lead to a very good (within 1%) agreement in widths between a series of experimental and simulated scans (standard powder, vanadium, and sample rocking curve) [17]. Figure 7 compares the simulated resolution to the experimental results. It is seen that while the left and right peaks are broadened, the central signal appears to be resolution limited.

Multiple scattering

One feature that is inherently present in neutron scattering data is the unwanted scattering from the sample environment, multiple scattering in the sample, or multiples between sample and sample environment. Analysis of these effects is very well suited for ray-tracing simulations, and the first analyses of multiple scattering was performed long ago by the sample-scattering package MSCAT [18].

Recent advances in full-fletched VE have incorporated this functionality, and it is now possible not only to simulate sample environment background but also to distinguish different contributions. This very powerful capability is illustrated by a virtual inelastic time-of-flight experiment as shown in figure 8. This is a part of a larger effort, to be presented elsewhere [19].

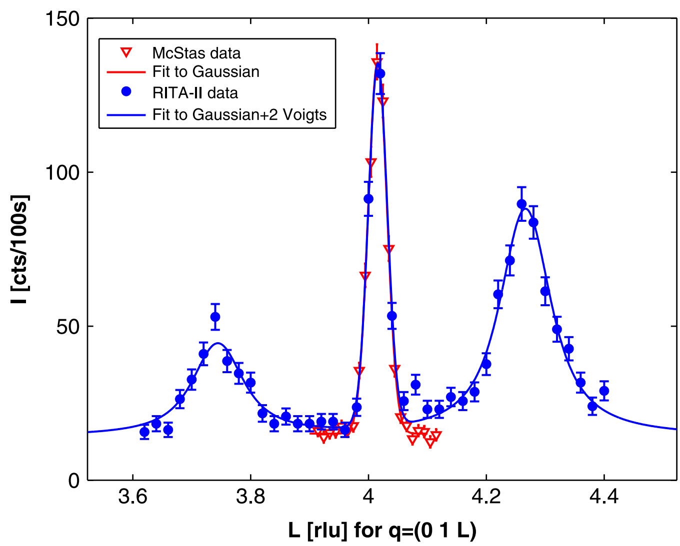

Figure 7. Real (circles) and VE (triangles) diffraction data on a single crystal, performed at RITA-2, PSI. The McStas model has been adjusted with respect to mosaics of the monochromator, analyzer, and sample to obtain agreement between virtual and real line-up scans. The central peak is clearly seen to be resolution limited [16].

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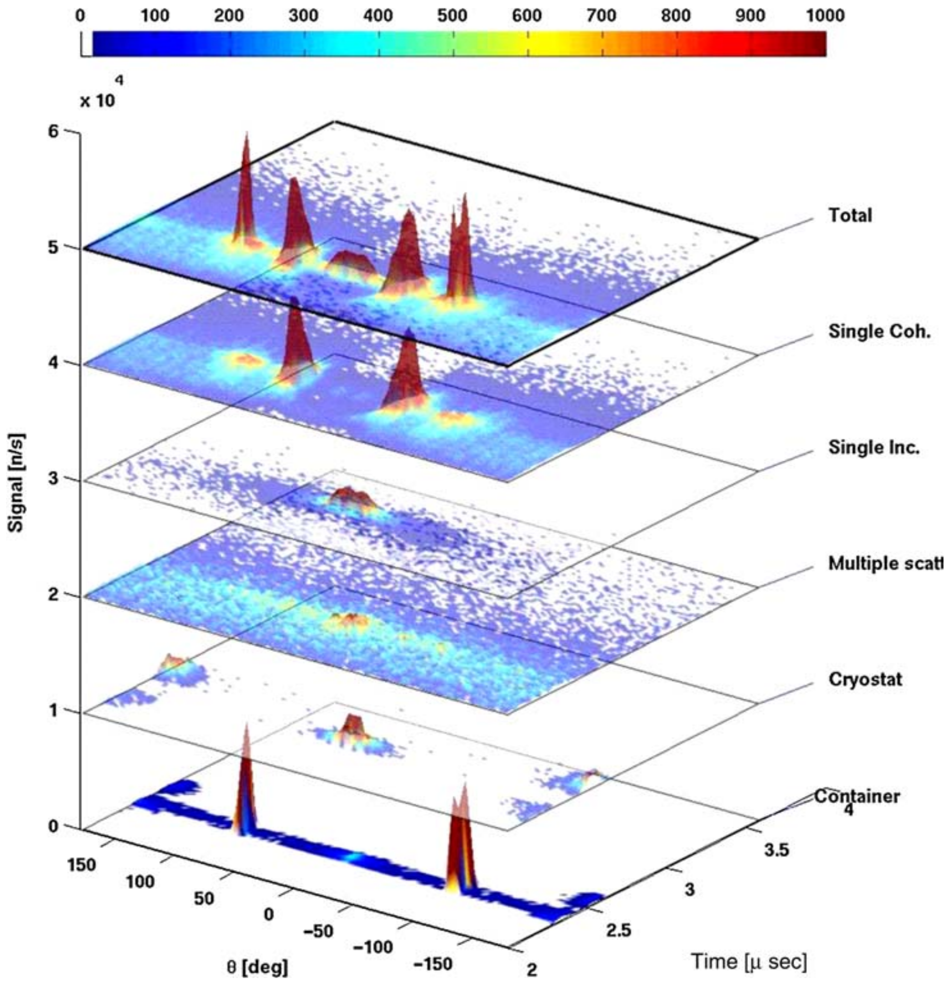

Figure 8. Data from a virtual inelastic time-of-flight experiment on a liquid metal sample, performed by McStas at a model of IN6, ILL. The scattering is presented horizontally and color coded, as a function of time-of-flight (depth) and scattering angle (vertical). The different layers in the figure represent different, clearly recognizable contributions to the total observed scattering (top layer). From [19] (colour online).

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Testing analysis programs

By combining analysis programs and VE, the possibility opens to perform detailed, quantitative tests of the analysis programs themselves. The essential advantage of this test procedure is that the scattering cross section producing the virtual data is known.

Detailed VE data have been used to test the analysis program for the new time-of-flight backscattering instrument MARS, PSI. This was performed prior to the commissioning of the instrument [20]. A detailed analysis of a virtual quasielastic spectrum with the MARS analysis software, using a VE on a prototype instrument, resembling OSIRIS (ISIS) is shown in figure 9.

Analysis of non-standard experiments

The last example of data analysis deals with an individual experiment of non-trivial and non-standard character. Instead of writing a stand-alone analysis program for this single purpose, the VE scheme for data analysis may in fact be the most effective and fruitful way.

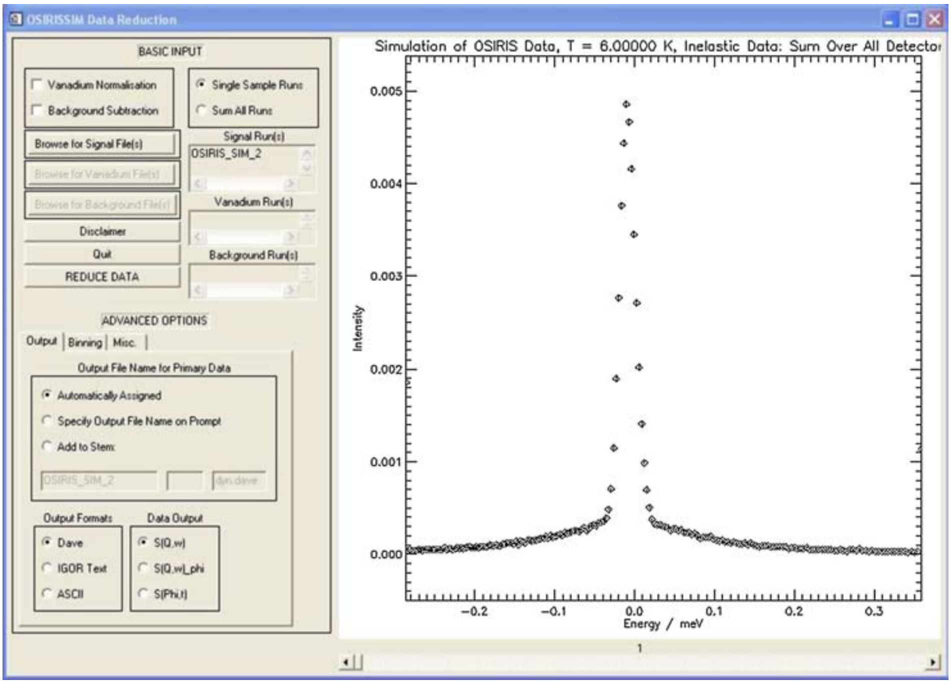

Figure 9. Data from a VE on a backscattering time-of-flight spectrometer, resembling OSIRIS (ISIS). The virtual sample has an incoherent elastic line and a quasielatic component. The data points show the data produced by a McStas VE, processed through the data analysis program [20].

One example in this direction is the determination of Fermi potential parameters of diamond-like carbon. This was determined through transmission measurements and concurrent VE of the experimental set-up [21,22]. The data are shown in figure 10.

Teaching and outreach

As an additional benefit to their intended scientific use, simulations have proved to be of very high value for illustration and teaching purposes, both at the university and the general public level. A few recent examples are shown below.

University teaching

Since 2005, simulations have been employed as a teaching tool for a course in neutron scattering for 4th year undergraduates and 1st year graduates at University of Copenhagen. The students are taught the simulations tools alongside the usual theory, and perform VE on guide construction, small-angle scattering, powder diffraction, and triple-axis spectroscopy. The data from VE are analyzed using standard packages, like MFIT (MFIT home page, www.ill.fr/tas/matlab/doc/mfit4/mfit.html) and FULLPROF (FULLPROF home page, www.ill.fr/dif/Soft/fp), see figure 11. The course ends by real experiments at RITA-2 and SANS-2, PSI.

The effect of including VE in the teaching has been surprisingly strong. The students learn the theoretical material faster than usual, maintaining a high level of motivation. In addition, the students obtain a genuine ‘hands on’ experience with neutron scattering, including data analysis and instrumention, before the arrival at the facility. This use of VE can be of great

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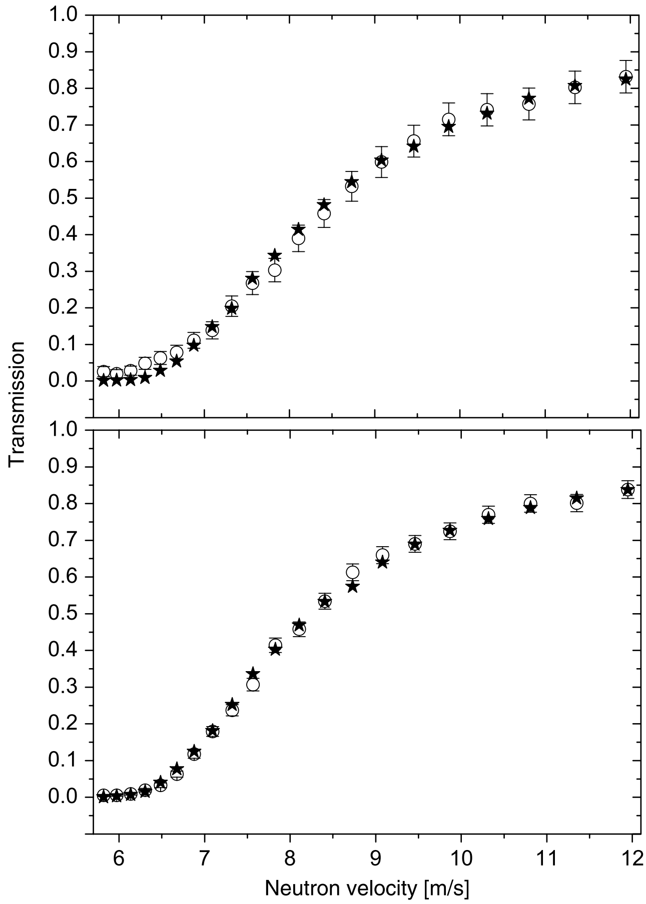

Figure 10. Measured reflectivity data (open circles) and data from the corresponding VE (stars) for the transmission of ultracold neutrons through material foils. Top: 150 nm diamond-like carbon (DLC) on 180 μm aluminium. Bottom: 200 nm beryllium on a 525 μm silicon wafer. The neutron Fermi pseudo-potential parameters for DLC and beryllium were extracted by fitting the measured data with the simulated ones via scanning the model parameters using VITESS. From Refs. [21,22].

importance for training of new users at the emerging powerful facilities, where real beam time may become too valuable (and too short) to use for training purposes.

Public outreach

Another use of VE is for the purpose of addressing the general public. Figure 12 shows a snapshot from a Danish home page, targeted at the educated public (high school level). Here, the basics of neutron scattering is presented, and much of the home page functionality is supported by ray-tracing simulations. The users can 'control' a selected set of easy VE and use them to rediscover important historical moments in neutron scattering, *e.g.* the discovery of antiferromagnetism and the first phonon dispersion curves.

Summary and outlook

As we have shown with a series of examples, VEs have large potential benefits for neutron scattering community as a whole, some of which unfold as we write. VE are already in use

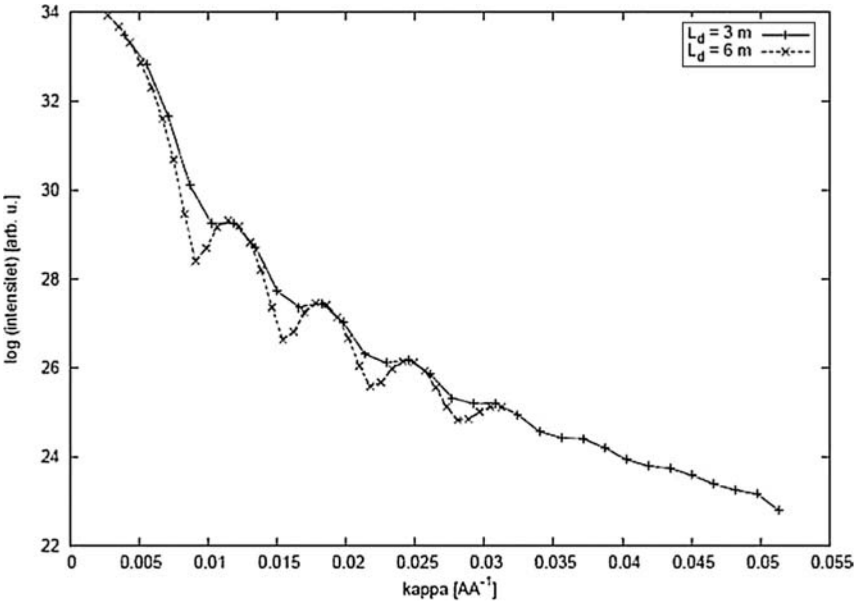

Figure 11. Virtual SANS data from a course in neutron scattering at University of Copenhagen, 2006. The McStas VE was performed on a model of SANS-2 (PSI), using a sample of dilute, hard spheres. The VE is performed for two settings of the instrument: collimator/detector lengths of 3 and 6 m.

for the design of new instruments and instrument upgrade at all major facilities. It is likely that VE will soon be a common tool for experiment preparation and in analysis of subtle effects of non-idealities in the obtained data.

VE is found to be very demonstrative for educational purposes at different levels. Furthermore, we can foresee that VE will be used as on-the-fly diagnostics tool for spotting problems during experiments.

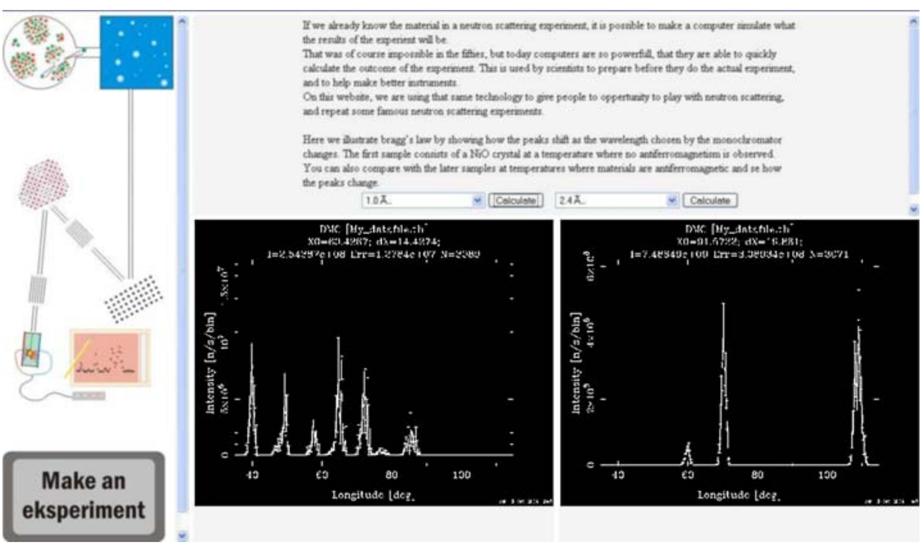

Figure 12. Simulations are used to illustrate the process of neutron scattering in an interactive home page for the broader public. The figure shows virtual diffraction patterns from NiO, at two different wavelengths, below the antiferromagnetic transition temperature.

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It should be made clear, however, that each of the examples shown have required significant preparation time. Thus, development of VE on most neutron instruments worldwide will be a major, although potentially very rewarding task, involving users, instrument responsibles, and dedicated simulators alike.

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