Workshop on the Monte Carlo simulation of neutron scattering instruments (MCNSI7)

Prague, 23-24 July 2011
Satellite meeting of the 5th European Conference on Neutron Scattering (ECNS 2011).

You may visit the workshop web page for updated on-line information.

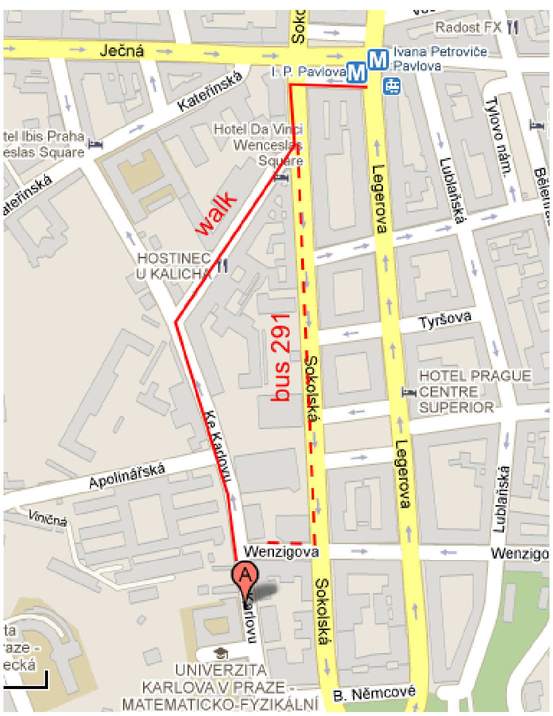
Program

The workshop program begins on Saturday at 14:15, so that participants of the preceding ESS&S meeting have sufficient time to join us at the workshop venue, and continues on Sunday morning. It starts with overviews of recent MC simulation software developments, followed by talks on instrumentation and simulation techniques. Average time provided for each oral contribution is 20-25 min. including discussion. In addition, long coffee breaks are planned each day with the intention to provide sufficient time for poster presentations and further discussions.

The **program time table** is attached.

Travel information

The workshop takes place at the Charles University, Faculty of Mathematics and Physics, Ke Karlovu 5, in the lecture room F2 (1st floor).



From the Clarion Congress Center (ECNS venue)
Use metro line **B** from "Vysocanska" (station at the hotel) to Florenc. Change for metro line **C** and exit at the station "I.P. Pavlova". Cross to the opposite side of the I.P. Pavlova square and follow the streets "Na Bojisti" and "Ke Karlovu". Alternatively, you may go one stop by the bus No. 291 (see the attached map).

From Karolinum (ESS&S venue)
Walk to the metro line **A** Mustek through the streets "Zelezna", "Rytirska", "Na mustku" (see the map), take one stop to "Muzeum" and change for metro line **C**, one stop to the station "I.P. Pavlova" and further follow the walk route described above. There should be a person to guide you from Karolinum to the workshop place on Saturday (expected departure at 13:40).

In both cases, you need a single short-term ticket (24 CZK), which permits for all kinds of transfer within the 30 min. of ticket validity. For more information, you may visit the DPP web pages.

For authors

A computer (Windows) and data projector will be available for **oral contributions**. The time is limited to 20-25 min. per contribution, including discussion. If possible, please prepare your talks in PowerPoint (ppt), OpenOffice (odp) or PDF formats and provide a copy well before your talk so that we can avoid time losses due to laptops reconnection etc.

Poster boards will be available for the standard A0 portrait format. They can be hanged on throughout the duration of the workshop till Sunday noon. There are currently 4 poster presentation registered, but you are encouraged to *bring also your posters from ECNS* to enlarge the basis for discussions. Please *let us know if you intend to do so*, so that we can ensure sufficient space for your posters.

Proceedings

Proceedings from the workshop will be published in the Journal of Neutron Research. The deadline for manuscript submission is on the **1st of September**. The paper length limit is 8 printed pages. You may refer to the journal documents for authors concerning manuscript style. Details of submission procedure will be available at the meeting website later.

Contact:

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Time table

MCNSI7, Prague, 23-24 July 2011

Saturday 23 July 2011			
14:15	14:30	J. Šaroun, K. Lefmann	*Welcome*
14:30	14:55	Peter Willendrup	*New developments in the McStas simulation package*
14:55	15:20	Klaus Lieutenant	*VITESS 2.10*
15:20	15:45	Jan Šaroun	*Optimization of crystal and TOF powder diffractometers with RESTRAX*
15:45	16:45		*COFFEE BREAK + POSTERS*
16:45	17:05	Kim Lefmann	*Propagation of neutron polarization in McStas*
17:05	17:25	Linda Udby	*McStas-model of the Delft SE-SANS*
17:25	17:45	Alexander Ioffe	*Neutron polarization in VITESS: simulations of spin handling components and spin-echo based instruments*
17:45	18:05	Geza Zsigmond	*Technical aspects of simulation of storable neutrons in inhomogeneous and RF magnetic fields*
Sunday 24 July 2011			
09:00	09:20	Emmanuel Farhi	*Optimizing MC simulations*
09:20	09:40	Morten Sales	*Thermal Powder Diffractometers at long pulse sources*
09:40	10:00	Tilo Seydel	*Neutron optics simulations for the new backscattering spectrometer IN16B*
10:00	11:00		*COFFEE BREAK+ POSTERS*
11:00	11:20	Kaspar Hewitt Klenø	*Systematic Performance Study of Common Neutron Guide Geometries*
11:20	11:40	Nikolaos Tsapatsaris	*Chopper optimisation and fault detection in the future Time Of Flight NEAT instrument using MC. What the analytics cant see ...*
11:40	12:00	Mancinelli Rosaria	*Multiple scattering corrections. Some general equations to do fast evaluations.*
12:00	12:20		*Closing discussions*
POSTERS			
P1		Andreas Houben	*Elliptic Neutron Guides with Octagonal Cross Section - Concept and Simulation Results for the POWTEX Instrument*
P2		Raul Victor Erhan	*Monte Carlo simulations of neutron optical elements for a SANS spectrometer at the IBR-2M pulsed reactor*
P3		Britt Rosendahl Hansen	*Determination of neutronic performance from cold and thermal moderators from MC simulations*
P4		Jonas Okkels Birk	*Realistic simulations of absolute intensities for all neutron guides at PSI*

Abstracts

MCNSI7, Prague, 23-24 July 2011

Contents

The VITESS Monte Carlo simulation package

K. Lieutenant, M. Fromme, S. Manoshin, A. Houben, D. Nekrassov, C. Zendler
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The Vitess simulation package is a program to simulate virtual neutron scattering experiments. After the release of the first version in 1999, it has been continuously improved; in June 2011 version 2.10 was released. It has been used to simulate instruments at ESS, HZB, JCNS, IFE and other sources. The staff in Berlin has recently been significantly increased to boost the development in order to meet the demands of the ESS project.

The package allows simulating practically all kinds of neutron scattering instruments both on continuous and pulsed sources. Nearly all components existing in instruments today can be simulated, especially all usual components used for polarised neutrons. An important feature is its easy to use graphical user interface that enables the user to perform simulations without writing any code or script.

Here we present the concept of VITESS and its use, the new modules and features in version 2.10, a few recent applications and plans for the future.

Optimization of crystal and TOF powder diffractometers with RESTRAX

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The program package RESTRAX, namely the SIMRES program [1], provides fast ray-tracing code for modelling neutron beamlines mainly at steady-state sources. Recent development has been aimed to the *extensions allowing for simulations of time-of-flight instruments*. Adding new components, such as disc chopper, pulsed source and time resolution area detector, together with appropriate TOF data handling functions permitted us to carry out *comparative simulations for powder diffractometers* in TOF and crystal-monochromator configurations, placed at the envisaged *long pulse source* of the ESS. The new TOF components, as well as all other SIMRES components, make use of the *automatic sampling optimization* procedure [2], which makes the simulations very fast without the need of any special attention from the users side. With the speed of the order of 10^3 successful events per second, optimization of a whole instrument in many-dimensional parameter space becomes feasible. For this purpose, new *optimization* module using *swarm algorithm* [3] has been implemented. We could thus optimize our models of powder diffractometers and compare the best performances of various configuration types in terms of the chosen figure of merit (intensity/resolution^2). As expected, the TOF configuration outperforms the crystal-monochromator option provided that sufficient flight path is allowed. However, the simulation results express this difference quantitatively, which may help in considerations involving other aspects like cost, flexibility and possibilities for sample environment.

[1] http//neutron.ujf.cas.cz/restrax
[2] J. Šaroun, J. Kulda, "Raytrace of Neutron Optical Systems with RESTRAX", in Modern Developments in X-Ray and Neutron Optics, eds. A. Erko, M. Idir, T. Krist, A.G. Michette, Springer Berlin 2008, p. 57-68.
[3] P. M. Bentley and K. H. Andersen, J. Appl. Cryst. (2009). 42, 217-224

Propagation of neutron polarization in McStas

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[5] *ESS, Lund, Sweden*

Ray-tracing simulation of polarized neutrons faces a challenge when the neutron propagates through an inhomogeneous magnetic field. This is in particular important for novel instruments using encoding of energy or angle into the neutron spin. The direct solution of the Bloch equations in time steps smaller than the inverse Larmor frequency is computationally too expensive, and other solutions must be found. In McStas, we have adopted a modification of the method by Seeger and Daemen. We present the implementation and it limitations, and we show a few recent examples, including simulation of a classical spin echo instrument. In addition, we present how simulation of polarized neutrons are carried out within McStas.

McStas-model of the Delft SE-SANS

Linda Udby[2], Erik B. Knudsen[1], Peter K. Willendrup[1], Kim Lefmann[2,3], Wim Bouwman[4]
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[2]*e-Science and Nanoscience Centers, Niels Bohr Institute, University of Copenhagen, Denmark*
[3]*ESS, University of Lund, Sweden*
[4]*TU-Delft, The Netherlands*

We present simulation results taking first virtual data from a model of the Delft, Spin-Echo Small Angle Scattering (SESANS) instrument[1] in the framework of the McStas[2] Monte Carlo software package. Polarisation instrumentation is now included natively in the McStas kernel, including options for Magnetic fields and a number of utility components. The development has now brought us to a point where realistic models of polarisation-enabled instrumentation can be built. One focus has been on making a model of the Delft SE-SANS instrument including the special foil-flippers which can be used for e.g. investigation of micro-metre structures. We here present the first virtual data from the model and compare it to measured data. using a refracting prism sample[3].

[1] M. T. Rekveldt, J. Plomp, W. G. Bouwman, W. H. Kraan, S. Grigoriev, and M. Blaauw, "Spin-echo small angle neutron scattering in Delft", Review of Scientific Instruments 76, 033901 (2005).
[2] http://www.mcstas.org
[3] E. B. Knudsen, L. Udby, P.K. Willendrup, K. Lefmann and W.G. Bouwman, "McStas-model of the Delft SESANS",Physica B 406, 2361 (2011)

Technical aspects of simulation of storable neutrons in inhomogeneous and RF magnetic fields

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Ultracold neutrons (UCN) can be stored due to their very low kinetic energy (E_kin < 300 neV) since they are totally reflected at any angle of incidence from certain materials. This makes them a useful probe in addressing important questions of particle physics and cosmology. The search for a permanent neutron electric dipole moment with UCN is one of the prominent experiments to test violation of fundamental symmetries at this low-energy precision frontier. This measurement is based on the

Ramsey method of separated RF magnetic fields, precisely determining shifts in the Larmor frequency. Monte Carlo simulations play an important role in helping the determination of systematic errors on the

frequencies. Several technical features of the simulation could also be transferred to high precision computation of neutron spin echo (NSE). In this presentation we focus on what simulated ultracold and cold neutrons can have in common.

Optimizing MC simulations

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You may have a dream: find automatically the best instrument configuration that optimizes some measurement criteria. This is now within reach: first design an instrument simulation model with McStas, then use iFit to do the work.

iFit <ifit.mccode.org> is a new Matlab-based software that can import seamlessly any data set (text, binary, 1D, 2D, 3D, ...), arrange and manipulate, visualize, perform any mathematical operations, export, and fit to models. The fit procedure makes use of advanced optimization methods that can also be used to optimize McStas simulations <mcstas.org>.

We shall demonstrate the use of this package on a set of neutron instruments, as well as on a full guide system model at the ILL.

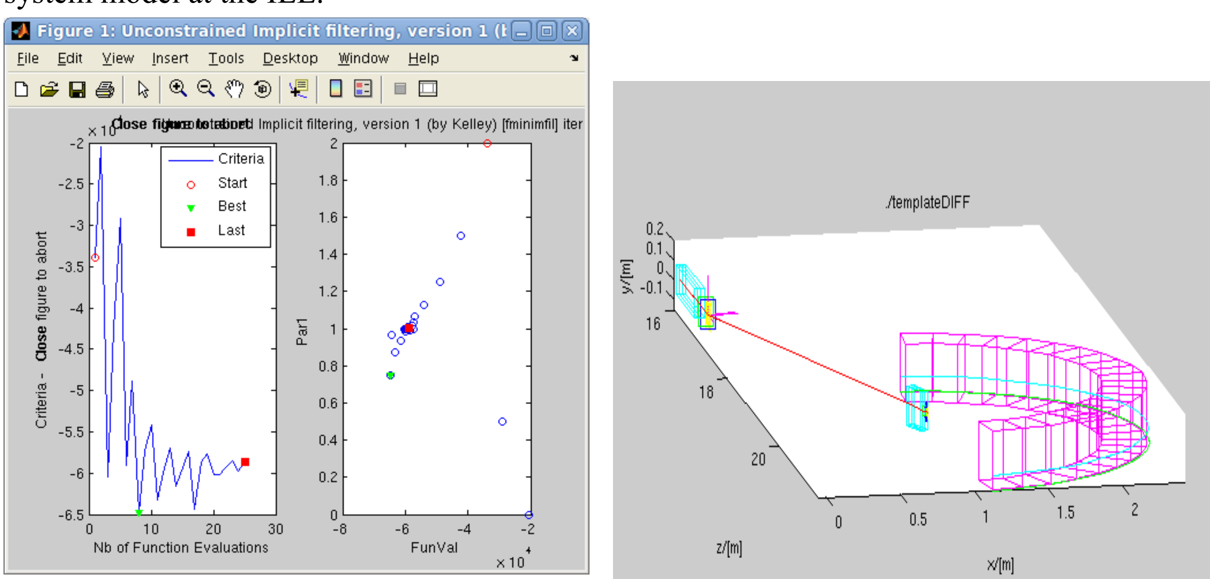

Figure 1: optimizing the monochromator curvature of a diffractometer with iFit/McStas.

Powder diffractometers at long-pulsed sources

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We have investigated the performance of a cold and a thermal neutron powder diffractometer installed at a long-pulsed source with the use of Monte Carlo ray tracing simulations. We show that the cold powder diffractometer will be a very powerful instrument when a relaxed resolution can be accepted - e.g. for magnetic studies. A comparison between a high resolution thermal powder diffractometer with and without Wavelength Frame Multiplication (WFM) [1] show that the WFM technique can be used to achieve shorter instrument length without losing flux. The thermal powder diffractometer will be competitive with the existing high resolution powder diffractometers. The flux at the sample position has been simulated for different time structures of the source, and an investigation of the effect of a moderator hot spot has been done.

[1] K. Lieutenant and F. Mezei, Journal of Neutron Research, 14(2):177–191, June2006.

Neutron optics simulations for the new backscattering spectrometer IN16B

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Backscattering spectrometers are designed for inelastic neutron scattering experiments at a high energy resolution, where 0.5 μeV FWHM can routinely be achieved at an incident wavelength $\lambda \approx 6.3$˚ A. The high energy resolution comes at the cost a low flux, and the typically weak scattering signals mostly require large detection solid angles. These large solid angles render an increased beam divergence at future spectrometers acceptable and motivate new instrument designs. The future new cold neutron backscattering spectrometer IN16B [1-3] will profit from an enhancement of the flux at the sample position by the Phase Space Transformation (PST) technique [4]. The PST ”compresses” a relatively large energy bandwidth out of an adequate neutron beam arriving at the primary spectrometer into a narrower energy band at the expense of an acceptably increased beam divergence. To optimize the PST, the instrument has to be located at a guide end position, and optical components such as a ballistic neutron guide, a velocity selector, a focus guide, and a PST chopper disk with mosaic deflecting crystals have been designed and optimized. We present new insights gained from the neutron optics simulations for the N16B instrument, including the optimum velocity of the PST [4].

[1] B. Frick, H.N. Bordallo, T. Seydel, J.-F. Barthelemy, M. Thomas, D. Bazzoli, H. Schober, Physica B Condens. Matter, 385-386, 1101 (2006).
[2] H.N. Bordallo, B. Frick, H.Schober, T. Seydel; J. Neutron. Res. 16, 39 (2008).
[3] B. Frick, E. Mamontov, L. van Eijck, T. Seydel; Z. Phys. Chem. 224, 33 (2010).
[4] M. Hennig, B. Frick, T. Seydel; J. Appl. Cryst. 44, 467 (2011).

Chopper optimisation and fault detection in the future Time Of Flight NEAT instrument using MC. What the analytics cannot see ...

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The NEAT upgrade project is heavily underway with the finalisation and optimisation stages of its new design. The expected 40+ gain of the instrument if one accounts for the new cold neutron source yield, neutron optics improvements, increase in the overall solid angle coverage and optimization of the entire instrument setup is going to bring the instrument again in the forefront of neutron TOF instruments worldwide.

An important part of the design is the optimization of its final double chopper double slit configuration and their shape in accord with the new guide design which will include exchangeable guide focusing sections for a truly user oriented and sample tuned instrument performance.

Verification of expected improvements and optimization of chopper components were performed using entire NEAT instrument simulations with the help of the VITESS software package. We have simulated and fine-tuned different scenarios of chopper configuration in comparison to the OLD NEAT instrument. The validity of the calculations and our intensity claims have been verified with simulations of the old NEAT instrument and benchmarking with real experimental data recorded at different chopper configurations.

MC simulations have proved indispensable at locating possible faults and revealing the limitations of purely analytical solutions at the preliminary instrument design and predicting spurions at complicated parts of the instrument that cannot be analytically approximated easily.

Tomographic reconstruction of a virtual sample based on Monte Carlo simulations

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The new instrument IMAT at ISIS (Target Station-II) will be the first instrument developed on a pulsed source combining a cold-neutron radiography and diffraction facility for applications including materials science, engineering and cultural heritage studies. A primary guide transporting the neutrons from the moderator to the sample is required to combine imaging and diffraction modes and to achieve a good energy-resolution and energy-dependent radiography.

One of features of IMAT we are particularly interested in is the application of a new bridge technique, Tomography Driven Diffraction (TDD), developed at The Open University and used for studying structurally and geometrically complex samples.

To investigate the viability, efficiency and future potential of the TDD to the IMAT and also the image quality we can expect from this instrument, we created a sample in McStas (e.g., a cylinder) and then radiographies of this sample (using fast computer clusters) were produced using the virtual IMAT instrument. The reconstruction of the neutron data was achieved with the Octopus software and the tomography was subsequently segmented and meshed using the commercial VGStudio software package.

Elliptic neutron guides with octagonal cross section – concept and simulation results for the powtex instrument

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In order to provide the chemistry and geo-science communities with a very powerful tool for rapid neutron-data acquisition, the new TOF diffractometer POWTEX will be installed at the FRM II reactor. The instrument is being designed and built by the RWTH Aachen University and the Forschungszentrum Jülich. The University of Göttingen will provide sample environments for geo-science applications. Both projects are funded by the German Federal Ministry of Education and Research (BMBF). Once finished, POWTEX will be part of the JCNS instrumentation pool. POWTEX is an abbreviation for POWder and TEXture. It will fulfill the needs of the solid-state chemistry, the geo- and partly the materials science communities with regard to powder and texture diffraction. We expect to outperform comparable monochromator instruments by one order of magnitude in intensity (> 10^7 n/cm^{2}s) for samples of less than a cubic centimeter. This extraordinary performance will be achieved by combining several new concepts. These are, namely, the double-elliptic neutron-guide with an octagonal cross section, the four-unit disk-chopper system, including the pulse double chopper and the access of full Debye-Scherrer cones by a huge solid angle (≈10 sr). The high intensity will allow us, to perform in situ powder diffraction experiments on chemical reactions and to characterize phase transitions as a function of T, p and B0 (or others) by parametric studies in comparatively short measurement times. Geo- and materials sciences applications at this instrument are mainly related to texture measurements on series of natural samples, in situ deformation and recrystallization/annealing experiments and simultaneous stress/texture measurements. While POWTEX is under construction at the very moment, we expect to conduct the first measurements in the year 2012. The current project status and conceptual evolutions, including new concepts in instrument simulations and the status of our 3He-free detector prototypes, are shown.

Monte Carlo simulations of neutron optical elements for a SANS spectrometer at the IBR-2M pulsed reactor

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We proposed a configuration for a small angle neutron scattering instrument at the IBR-2M pulsed reactor using a combined (thermal + cold) moderator system. This system provides added-up spectra from the cold and thermal parts of the moderator [1]. Our efforts have the purpose to obtain a better resolution (especially for significant sample sizes) and an increased neutron flux, as well as decreasing the neutron and gamma background for the small-angle neutron scattering instrument.

We suggest a combined collimation system composed of neutron optics elements (divergent or elliptical neutron guides) and further different configurations of multiple pinhole collimation system. Also, a stack of neutron lenses will be considered as an alternative option for improvement of the spectrometer in the pinhole configurations. The performance of the final collimation system has been evaluated. The results proposed for the neutron optical devices and the extraction system for the SANS spectrometer were obtained using VITESS software package.

[1] R.V. Erhan, S. Manoshin, G. Pepy, A.I. Kuklin, A.V. Belushkin and N.V. Zamfir, A concept for the modernization of a SANS instrument at the IBR-2M pulsed reactor, Nucl. Instr. Meth. A, Volume 634, Issue 1, Supplement 1, 1 April 2011, Pages S161-S164.

Realistic simulations of absolute intensities for all neutron guides at PSI

Jonas Okkels Birk

University of Copenhagen

Monte Carlo simulations of neutron scattering have found many uses by expert users, including testing and optimizing new instrument designs[3]. In general line width and shape are well represented while abs intensities are more difficult [2]. With ever better computers and wider simulation packages the users and applications has increased. It is thus hoped to make neutron scattering simulations accessible to all users [4] - before after and during measurements. This will open the possibilities to: Investigate whether a measurement is possible and realistic prior to measurements. Investigate unexpected features during the measurements. And find the exact resolution functions during data analysis [5]. Before this can be achieved thorough simulations of neutron instruments should be available so the common user only brings the knowledge of their specific sample while the rest is done by people with knowledge of the instrument outlay and simulations. Here we summarize a step towards this goal: Systematic simulations of all neutron guides at SINQ, Paul Scherrer Intitute, Switzerland with the McStas [1] neutron simulation package. The simulations concentrate on source description, better mirror models and thorough modeling of the guides, paving the way for later the instrument simulation with correct absolute neutron intensities.

[1] Mcstas website, http://www.mcstas.org.

[2] S. Klausen et al. Simulations and experiments on rita-2 at psi. Applied Physics A., pages s1508–s1510, 2002.

[3] K. H. Klenø, K. Lefmann, P. K. Willendrup, P. Christiansen, and R. Bewley. Simulations of chopper jitter at the let neutron spectrometer at the isis ts2. Pending rewiev.

[4] K. Lefmann et al. Virtual experiments: the ultimate aim of neutron ray-tracing simulations. Journal of neutron Research, Volume 16, Number 3-4 / 2008, pages 97-111.

[5] L. Udby. Superoxygenated (La,Sr)2CuO(4+y) - virtual and physical experiments. PhD thesis, Copenhagen University, 2009.

Neutron polarization in VITESS: simulations of spin handling components and spin-echo based instruments

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[2]*Joint Institute of Nuclear Research, Frank Laboratory of Neutron Physics, 141980 Moscow region, Russia*

As neutron simulations packages are used for analysis of the expected performance for practically all new built neutron instruments, possibilities for simulations with polarized neutrons have been relatively underdeveloped.

During last years we developed a new approach for the representation of time-dependent magnetic fields (both in magnitude and direction) for the VITESS simulation package. This allowed us to simulate the neutron spin dynamics in practically all polarized neutron devices (RF neutron flipper, adiabatic gradient RF flipper, the Drabkin resonator, etc.). In this presentation the above-mentioned VITESS instrument components (modules) we will be presented and the simulated performance of a number of polarized neutron scattering instruments (NRSE, MIEZE, SESANS, etc.) will be demonstrated.

Thus, we practically completed the polarized neutron suite of the VITESS that seems sufficient for the simulation of performance of any existing polarized neutron scattering instrument. Future work will be concentrated on developments of dedicated sample modules (kernels) to allow for virtual experiments with VITESS.