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Extension of the VITESS polarized neutron suite towards the use of imported magnetic field distributions

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Abstract. Latest developments of the polarized neutron suite in the VITESS simulation package allowed for simulations of time-dependent spin handling devices (e.g. radio-frequency (RF) flippers, adiabatic gradient RF-flippers) and the instrumentation built upon them (NRSE, SESANS, MIEZE, etc.). However, till now the magnetic field distribution in such devices have been considered as "ideal" (sinusoidal, triangular or rectangular), when the main practical interest is in the use of arbitrary magnetic field distributions (either obtained by the field mapping or by FEM calculations) that may significantly influence the performance of real polarized neutron instruments and is the key issue in the practical use of the simulation packages. Here we describe modified VITESS modules opening the possibility to load the magnetic field 3-dimensional space map from an external source (file). Such a map can be either obtained by direct measurements or calculated by dedicated FEM programs (such as ANSYS, MagNet, Maxwell or similar). The successful use of these new modules is demonstrated by a very good agreement of neutron polarimetric experiments with performance of the spin turner with rotating magnetic field and an adiabatic gradient RF-flipper simulated by VITESS using calculated 3-dimensional field maps (using MagNet) and magnetic field mapping, respectively.

1. Introduction

Powerful Monte Carlo (MC) instrument simulation codes play a very important role in the context of the design and optimization of neutron scattering instrumentation. Particularly, comprehensive MC simulations have become a primary tool for developers of polarized neutron instrumentation. Although analytic calculations are sufficient in simple cases of the ideal geometry of magnetic field arrangements, mostly to check new concepts, MC simulations allow considering arbitrary complex geometries of real neutron scattering instruments.

Spin coordinates have been included in three open-source neutron simulation packages, VITESS [1], McStas [2] and NISP [3], during their creation. NISP contains polarization tools allowing for the simulation of the neutron spin precession in constant magnetic field and in magnetic field with variable field direction, however does not allow for simulations with the variable magnitude of a magnetic field. McStas allows for the polarization handling in constant magnetic fields; on-going developments aiming simulations in variable magnetic fields have been reported at this workshop.

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VITESS has become a very comprehensive polarized neutron simulation package since a new approach allowing for the simulations of neutron spin dynamics in time-dependent, both in magnitude and direction, magnetic fields has been introduced [4]. Now VITESS facilitates simulations of the neutron spin dynamics in practically all polarized neutron devices (the RF neutron flipper, the adiabatic gradient RF flippers and the Drabkin resonator, etc.) [5]. Consequently, it has made simulations of the performance of all kind of neutron spin-echo (NSE) instrumentation using them possible (generic NSE, neutron resonance spin-echo (NRSE), rotating and time-gradient magnetic fields NSE and MIEZE spectrometers, as well as NSE-based diffractometers SESANS and SERGIS) (see [5] and references therein].

However, up to present VITESS modules developed for the simulations with polarized neutrons do not allow for the use of real magnetic field distributions, but only ones given by a few analytical functions (sinusoidal, triangular, rectangular). To achieve flexibility of the VITESS for simulations of *real* instruments it is becoming imperative to have the possibility to load the magnetic field description from an external source (file). Such description can be either the 3-dimensional magnetic field map measured experimentally or the 3-dimensional field distribution that was calculated analytically or simulated by dedicated programs (such as ANSYS, MagNet, Maxwell or similar).

In this article we will present the modification of the VITESS modules allowing for simulations of the performance of a neutron spin turner based on a rotating magnetic field and a real adiabatic RF-flipper, as well as the results of simulations of real devices that are in good agreement with neutron experiments.

2. VITESS modules for simulations with imported magnetic field distributions

A standard VITESS module is defined over the space slab limited by input and output planes. For the VITESS modules handling time-dependent (both in magnitude and direction) magnetic fields this space is divided into rectangular blocks (called “domains”) (Figure 1a), in which the magnetic field is considered to be a constant during the neutron propagation across them [4]. Since the neutron spin in VITESS is considered as a classical torque the change in the space orientation of the spin vector is calculated as the result of the Larmor precession around the magnetic field vector $\boldsymbol{B}(k)$ over the propagation time across the k-th domain.

The neutron spin components after the propagation across of the k-th domain are considered as the incoming components of the spin vector for the $(k+1)$-th domain and so on:

$$\left\{s_k^i\right\}_{out} = \left\{s_{k+1}^i\right\}_{in}, \qquad i = x,y,z \quad k = 1,\dots, N-1$$

For this approximation to be valid the number of domains N_i in each direction (i=x, y or z) should be large enough to satisfy the condition $\boldsymbol{B}(k)=const$ during the time of neutron propagation across these domains, i.e. the size of these domains has to be sufficiently small. Thus, the time-dependent magnetic field is represented as a histogram of $B(k)$ and we neglect changes of the magnetic field vector in domains during the neutron propagation time.

Practically, N_i should be so large that the final result (magnitudes of neutron spin components coming out of the field area) will not depend on the further increase of N_i (Figure 1b) [4]. It should be chosen by an iterative procedure, e.g. by doubling N_i for each subsequent iteration. The procedure is completed when such number of domains N_{max} are achieved that results of two subsequent iterations do not differ within the expected accuracy of the polarization measurements, usually 0.1%.

Up to present, all magnetic field distributions that are used in VITESS modules dealing with polarized neutrons have being given by analytical functions (sinusoidal, triangular, rectangular) calculated using a limited number of parameters. To use the above-mentioned VITESS algorithm for real magnetic fields, they have also to be given as the 3-dimensional array with the sufficiently large number of points. This array of magnetic field values can be either calculated by dedicated programs (FEM software as ANSYS, RADIA, MagNet, Maxwell, etc.) or measured experimentally.

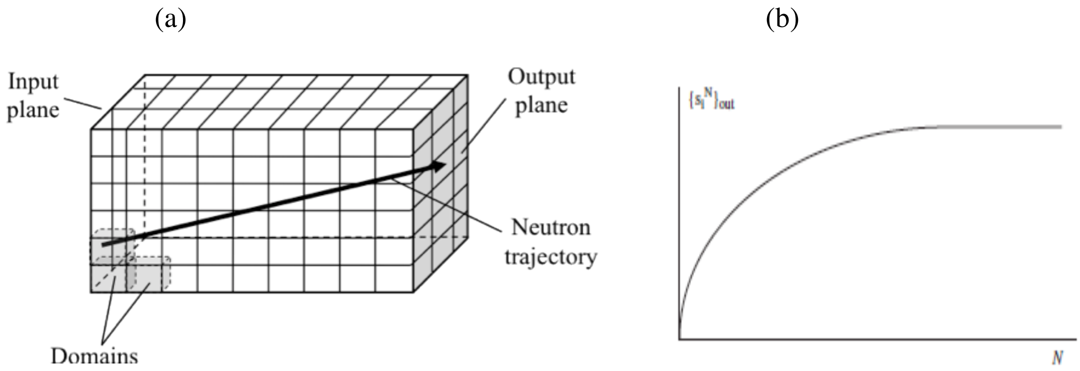

Figure 1. (a) Presentation of the field volume split into 3-dimensional array of domains and (b) the magnitude of simulated outgoing spin components vs. the number of slices *N*.

However, the number N_d of experimental (or calculated by an external software) points may not be sufficient for successful simulations. This is usually a case for spin-handling devices that uses the combination of permanent and time-dependent fields, e.g. RF-flippers. Generally, the steeper the time-dependence $\boldsymbol{B}(t)$ the larger N_d is supposed to be. Therefore, simulations of high-frequency devices require the field space to be split in a large number of domains in the neutron flight direction, usually far exceeding *N*.

We have modified the relevant VITESS modules in a way that allows them to accept external data files written in the format of the MagNet software (Infolityca.com) that we used for calculations of magnetic fields created by different "magnetic elements" (as coils and/or permanent magnets and magnetic screens) (see Figure3b in Sect. 3.1). Note that other FEM programs can also be used as their output files actually have the same structure; however one should pay attention to details of their format, that should be compatible with the MagNet/VITESS input format. In close future we will deliver the modification of the VITESS modules that will automatically choose the format for the import of data files according to the selection of FEM software made by user.

The MagNet software exports the calculated magnetic field as a data file, each line of which contains six columns: *x, y, z* coordinates and B_x, B_y, B_z components of the magnetic field. Each of the coordinates is changed successively from minimum to maximum values (one can imagine such a structure as three nested cycles). These coordinates are considered by VITESS as centres of domains; the number of domains in this case is the same as the number of lines in the file (note that domains in the VITESS structure are identical, so their centres are equidistant). Thus, only three nested cycles could be used to read the magnetic field data.

As it has been mentioned above, the simulations of high-frequency devices require a number of domains N_{max} that is usually exceeding the number of field values N_d measured experimentally or calculated by a FEM program by far. To match these numbers we introduce additional intermediate domains (in the directions of *x, y* and *z)* between two adjacent "main" domains determined by the imported data. The number of intermediate domains should be sufficient for successful simulations; the values of magnetic field in these new intermediate domains are obtained by interpolation (linear or B-spline) between "main" domains.

The physical consideration underlying such a procedure is the expected smoothness of the magnetic field distribution between the centres of "main" domains. In the case of experimental magnetic field maps, points for measurements are selected by an experimentalist in the assumption that the measured field distribution is a representative sampling of the true one, i.e. that no essential features (as jumps or extrema) are omitted. In the case of magnetic field maps calculated by a FEM program, the mesh for calculations is chosen automatically based on two criteria: to have a representative sampling (i.e. to provide the requested accuracy of calculations) and to minimize the number of points where the calculations have to be carried out. As the result the mesh is not homogeneous at all: its density is high at quick changes of the magnetic field vector (magnitude or direction) and low where the decay-like behaviour of the magnetic field magnitude or slow changes of the field direction take place. However, the MagNet software allows user to choose the regular mesh, which is excessive considering the amount of necessary information, but matches the input file format requested by VITESS.

3. Examples of the VITESS simulations with imported magnetic field distributions

3.1. Spin turner for the rotation magnetic fields NSE spectrometer

Neutron spin turners using rotating magnetic fields (RMF) are the key elements of the RMF NSE spectrometer [6]. They are thin devices, where the magnetic field is confined and rotated in the plane *yz* of the spin turner. In the ideal case the magnetic field is fully confined in the spin turner and there is no fringe magnetic field outside it. This is certainly not correct for the real device made of the finite size solenoidal coils (Figure2a), so that the scattered magnetic fields should be confined by the flux closing yokes made of 2mm thick μ-metal plates (Figure2b).

During the experiment carried out at the neutron polarimeter LAP of the Jülich Centre for Neutron Science (JCNS) installed at 4.5Å neutron beam [7], we have been able to measure all three components of the polarization vector passed through the set up consisting of two such spin turners separated by 10cm as a function of frequency ω of the applied sinusoidal electrical current. The result of measurements for the z component is presented in Figure3a together with the simulated (by the VITESS) performance for the case of ideal spin turners – although a sinusoidal dependence is reproduced, the mismatch of the amplitude definitely tells about the presence of fringe magnetic fields. Therefore, the magnetic field distribution in the real spin turner (i.e. two orthogonal coils with the winding density reduced towards the coils' periphery, surrounded by a number of μ-metal plates) was calculated using the MagNet software package and the results have been imported in the VITESS by the procedure described in Sect.2. The result of simulations with such a real magnetic field distribution (Figure3b) shows a good coincidence with the experiment and clearly demonstrates that the magnetic design has to be improved. The great advantage of this experiment is that now the validity of the chain MagNet -VITESS is experimentally confirmed, so that for further magnetic design work no neutron experiments are required till the test of the final version.

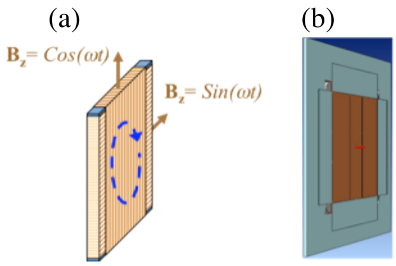

Figure 2. Spin turner made of two orthogonal solenoidal coils (a) and its MagNet model with the surrounding flux closing yokes (b).

3.2. Adiabatic RF flipper

The adiabatic gradient RF-flipper [8] (or adiabatic RF-flipper) consisting of a RF coil immersed in a continiously rising (gradient) permanent magnetic field (Figure 4a) has become one of most often used elements in polarized neutron scattering, as it is effectively flipping the neutron spin for all neutrons with the wavelength above the critical λ^*, that is especially valuable for the use at pulsed sources with basically wide-band spectrum neutron beams.

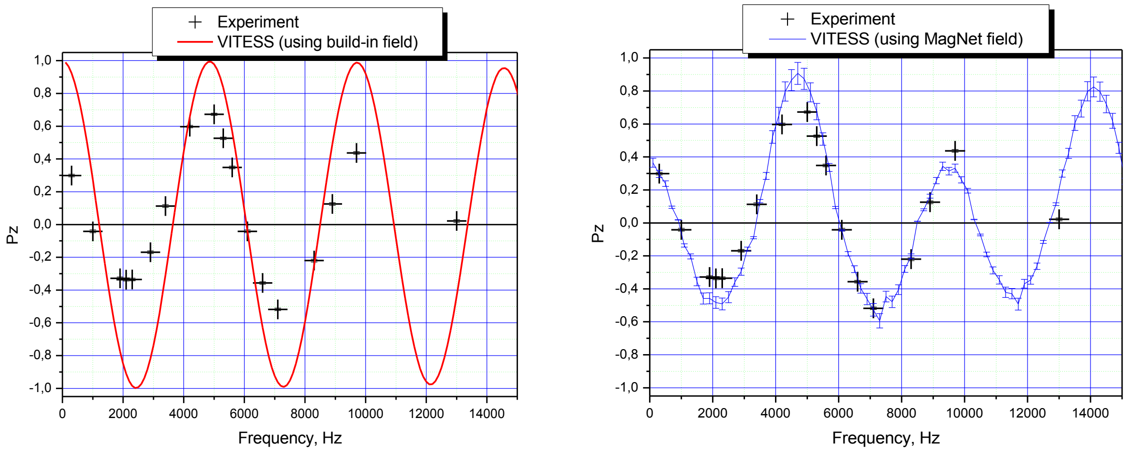

Figure 3. Frequency dependence of the *z*-component of the polarization in comparison with VITESS simulation using built-in (a) sinusoidal and (b) calculated by MagNet magnetic fields.

To maximize the flipper efficiency that may even exceed 99.99%, one should choose most suitable type of the gradient magnetic field. The simplest is the linear dependent field that rises from B_0-ΔB to B_0+ΔB over the flipper's length 2L (Figure 4a), that however results in less spin-flip efficiency than the cosinusoidally dependent field [9].

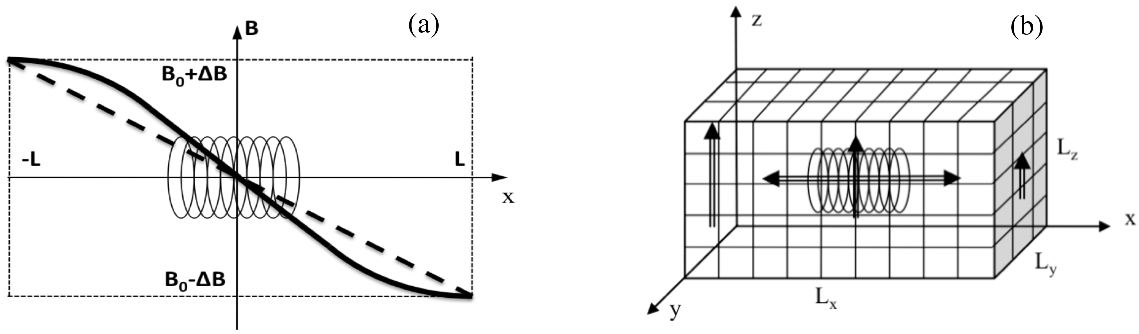

Figure 4. (a) Cosine and linear gradient magnetic fields in the adiabatic RF-flipper. (b) Magnetic field volume split in 9 x 5 x 3 domains used for simulations of the adiabatic RF-flipper.

The VITESS module for simulations of the adiabatic gradient flipper has been containing the built-in generator of both above-mentioned fields (with parameters defined by a user). Now we have also added to it the possibilty for the import of the magnetic field distrbution measured or calculated externally. This option is rather important not only because the exact linear or cosinusoidal magnetic field distributions can be hardly realized, but also because tough experimental conditions quite often do not allow for practical realization of such field distributions. Obviously, the possibility to estimate the expected efficiency of a "real" flipper by simulations is very desirable.

As an example we present here the simulations of a gradient spin flipper for the large cross-section neutron beam, (6 x 19) cm^2, that has been carried out prior to the neutron test of the flipper at the JCNS reflectometer MARIA [10]. The gradient field is created by a set of permanent magnets; the RF field is created by a solenoidal coil supplied by the AC current from a dedicated generator.

The magnetic field volume selected for further simulations – the parallelepiped with size L_x=40cm, L_y= 6cm, L_z=19cm - coincides in the cross-section (6cm x 19cm) with the size of the neutron beam propagating through the flipper along the *x*-axis. This volume is filled with the gradient magnetic field superimposed with the rotating (around *z*-axis) magnetic field created by the RF-coil of radius 2.5 cm and of length 20cm (Figure 4b). The measurements of the gradient magnetic field values have been conducted using a regular grid pattern 9 by 5 by 3 points along *x*-, *y*- and *z*-axes, respectively (Figure 5), and imported to VITESS as an external file. Transverse *y*- and *z*-components of the gradient field were found to be negligibly small with respect to B_z

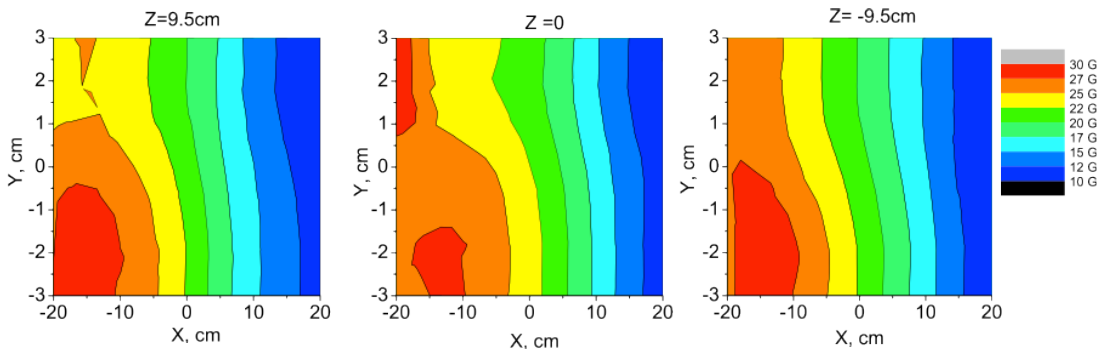

Figure 5. Y-X distributions of the gradient magnetic field in three horizontal cross-sections z=-9.5cm, z=0 and z=9.5cm (see Figure 4b).

The amplitude of the rotating field has been calculated using the standard formula describing the magnetic field strength B_z along the solenoid axis *x*:

$$B_z(x) = \frac{\mu_0 nI}{4}\left[\frac{x+l/2}{\sqrt{r^2+(x+l/2)^2}} - \frac{x-l/2}{\sqrt{r^2+(x-l/2)^2}}\right] \quad (1)$$

Here μ_0 is the permeability constant; *n* – the number of turns per unit length; *I*- the current in the solenoid; *r* and *l* – the radius and the length of the solenoid, respectively; *x* -the distance from the centre of the solenoid. Note an extra factor 2 in the denominator of Eq. (1): it reflects that the linear oscillating field in the solenoid is considered as a superposition of two counter rotating fields, whilst in the VITESS we are dealing with only one of these components with the same sense of rotation as the spin Larmor precession (the second component results in the Bloch-Siegert frequency shift [11] and is usually not relevant from the point of view of a neutron scattering instrument). Strictly speaking, one should also take into account transverse components B_x and B_y, that should be calculated using a FEM simulation program. We have neglected them in our case since they are much less than the z-component of the permanent field. The working parameters of the real flipper - the amplitude of the RF (rotating) magnetic field of 25 (12.5) Gauss and the frequency of 60 kHz - have been used for the simulations.

The nine points where the values of the permanent magnetic field were measured correspond to nine domains in x-direction that is no way sufficient for stable simulations. Therefore, the interpolation procedure described in Sect. 2 is applied. The number of domains, *N*, sufficient for simulations is determined from the stability of the simulated result shown in Figure 6, where the values of all three components P_x , P_y and P_z of the polarization vector are depicted in the dependence on *N* (time required for simulations for N≈400-500 and for 5 by 3 domains along *x*- and *y*-axes, respectively (see Figure 5)) at each wavelength is about 10-15 sec at a standard laptop). One can see that their values are not changed anymore beyond $N \approx 450$. Therefore, $N=500$ has been selected for final simulations, those results are shown in Figure 7 together with the result of the neutron test of such flipper at MARIA.

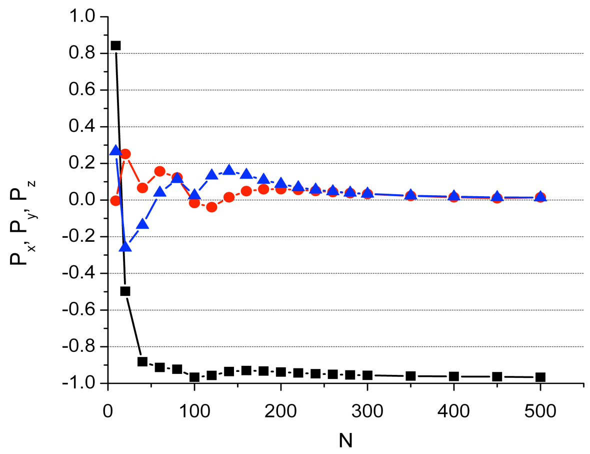

Figure 6. Simulated values of the components of the polarization vector in the dependence on the number of domains in x-direction. P_x –blue triangles, P_y –red circles, P_z – black squares.

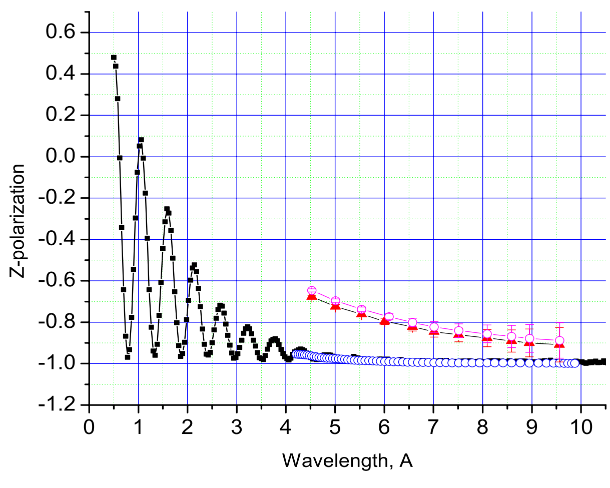

Figure 7. Flipping of the polarised neutron beam by the adiabatic RF flipper in the dependence on neutron wavelength. Full black squares - absolutely monochromatic neutron beam; hollow blue circles – neutron beam monochromatized by the velocity selector ($\Delta\lambda/\lambda=10\%$); hollow pink circles - polarization calculated by taking into account the non-perfect polarization of the incident beam and the non-perfect polarization efficiency of the ^{3}He spin filter; full pink triangles - the experimentally measured neutron polarization.

Simulations with absolutely monochromatic ($\Delta\lambda/\lambda=0$) neutron beam (full black squares) show the expected oscillating behaviour of the spin-flipped polarization (Figure 7). In reality, such behaviour is not observed because of the final monochromatization ($\Delta\lambda/\lambda=10\%$) of the used neutron beam (hollow blue circles), but one can see that the flipper works very efficiently for neutrons with the wavelength above the critical one $\lambda^* = 4.5$Å. The overall beam polarization (hollow pink circles) can be calculated from the latter curve by taking into account the non-perfect polarization of the incident beam and the non-perfect polarization efficiency of the ^{3}He spin filter used for the polarization analysis of a large neutron beam. This final result of VITESS simulations has to be compared with the experimentally measured polarization (depicted as full pink triangles in Figure 7). One can see rather good coincidence in the wavelength dependences of simulated and experimental curves, when slightly better, about 2%, absolute polarization obtained in the experiment is most probably caused by an error in the knowledge of the absolute polarization efficiency of the ^{3}He spin filter and the incident beam polarization.

4. Conclusions

When "ideal" magnetic field distributions (sinusoidal, triangular or rectangular) are sufficient for the VITESS simulations of the performance of practically all components constituting polarized neutron instrumentation, the main practical interest is in the use of real magnetic field distributions that may significantly influence the performance of real polarized neutron instruments and is the key issue in the practical use of the simulation packages.

This problem is now solved – we have modified VITESS modules in a way that now they allow to import 3-dimensional (space) magnetic field maps, which can be either obtained by direct measurements or calculated by dedicated FEM programs. A very good agreement between neutron polarimetric experiments and simulations carried out by VITESS using magnetic field maps calculated by the MagNet software is achieved.

The next step in this direction will be an extension of the data import option to others popular software packages for the magnetic simulations, such as ANSYS and RADIA. Further on, we will develop an approach allowing for simulations of performance of different instrument components (e.g. mirrors, flippers) deepened into the magnetic field.

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