McStas developments for ESS simulation work

Willendrup, Peter Kjær; Klinkby, Esben Bryndt; Nielsen, Johan Sejr Brinch; Hansen, Britt Rosendahl; Bergbäck Knudsen, Erik; Udby, L.; Lefmann, Kim; Filges, U.; Farhi, E.

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Abstract

The neutron Monte Carlo ray-trace package McStas[1],[3] is developed in collaboration between Department of Physics at Technical University of Denmark (DTU), Institut Laue-Langevin (ILL), the Niels Bohr Institute at University of Copenhagen (KU) and Paul Scherrer Institute (PSI).

Through the Danish and Swiss inkind work packages, McStas is used intensively for simulation work toward future instruments at the European Spallation Source (ESS)[1]. The framework of these work packages, ESS-dependent developments of the software has been done. This poster presents the features of McStas release 2.0 (expected release in May 2012) as well as new developments toward better integration with neutronics codes, such as MCNPX[5], used within the ESS work packages relating to target and moderator development.

Repository of source brilliances

In collaboration with the Vitess team[6], we will be benchmarking a "representative" description of neutron sources/moderators[1].

New components

A number of updated components have been developed for the ESS collaboration. This paragraph shows a few.

New tool layer components

For the soon-to-be-released McStas 2.0, a replacement for the Perl toolset will be provided. The replacement is built on Python.

Below, advantages and drawbacks of the various implemented McStas-MCNPX coupling solutions are tabulated.

Cross comparison

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<td>Supermirror</td>
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This utility is very useful to McStas. The tool has a database backend and server-side cookbook solution, importing the INSIS school in Frascati this summer.

Interoperability with IFI, optimizers

The IFI package by Emmanuel Farhi is becoming a powerful Matlab package and very useful addon to McStas. Importing your simulation data is easy:

Running simulations and optimizations from within IFI are also possible.

McStas-MCNPX interfaces

At DTU NuTech, E. Klinkby is working on coupling McStas and MCNPX[5]. The work aims at better computation tools for neutronics and beamlines, e.g. for estimates of shielding need along the long guide of the ESS.

References

[4] see e.g. http://www-ess-academie.eu

Next Release: 2.0

McStas 2.0 - preview code via http://www.mcstas.org/svn

• Uniformized parameter naming across components (breaks some backward compatibility for user-instruments)
• New feature in the meta-language for placing a grid of similar components - practical for e.g. large array of samples
• Likely a new tool layer, likely python based (replacing perl+Th+pypet+PGPLOT) - dedicated staff working on this
• Split infrastructure for core package, components and tools. Allows to only install core package and want tool layer.
• Updated web interface solution - dedicated staff working on this
• All components support polarized neutron simulations
• Up-to-date documentation for the polarized neutron methods
• Standardized method for neutron propagation in tabulated magnetic fields (e.g. from Radio or Isklev)
• Possibility for needing magnetic fields, e.g. for stray fields
• A richer suite of example instruments with more thorough testing of components
• Support for any shape in our sample components and some optics components, facilitated via Geoview/OFF format
• Interface-code for the IFI data analysis package. Through IFI, a new set of optimizers of type genetic algorithm / swarm etc.
• Expected release in May 2012
• SVN version fully functional, only docs and a few features missing!