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.

Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

Workunit SD022DK General Simulations: McStas developments for ESS simulation work

P. Willendrup[1,6], E. Klinkby[2,6], J. Brinch[1,6], B. Rosendahl[1,6], E. Knudsen[1,6], L. Udby[3,6] ,K. Lefmann[3,6], U. Filges [4,7] and E. Farhi [5]

[1]Department of Physics, Technical University of Denmark, Denmark
[2]Center for Nuclear Technologies, Technical University of Denmark, Denmark
[3]Nano-Science Center, Niels Bohr Institute, University of Copenhagen, Denmark
[4]Paul Scherrer Institute, Switzerland
[5]Institut Laue-Langevin, France
[6]European Spallation Source (ESS) Collaboration, Denmark
[7]European Spallation Source (ESS) Collaboration, Switzerland

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 the 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)[4]. In the framework of these work packages, ESS-dedicated developments of the software has been done.

This poster presents the features of McStas release 2.0 (released 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 a benchmarked, “representative” description of neutron sources/moderators:

- ESS:
  - Cold: 2001 “Mezei moderator” and updated 2012, both running at 14Hz
  - Thermal: 2001 “Mezei moderator” running at 14Hz. Ultimo 2012 supplemented with updated moderator
- ISIS:
  - Cold moderators: TS1 and TS2 hydrogen moderators
  - Thermal moderators: TS1 water
- SNS:
  - Cold moderators: BL02 (McStas) and analytical model (Vitess), 1.4 MW
  - Thermal moderators: BL08 (McStas) and analytical model (Vitess), 1.4 MW
- ILL:
  - Cold moderators: Legacy Yellowbook (2001), Updated HCS/VCS average (2012)
  - Thermal moderators: Legacy Yellowbook (2001), Updated average (2012)
- Other steady-state sources: FRM-II, HZB, PSI cold and thermal

For each described moderator, the dataset will incude:

- Parameters needed for McStas and Vitess respectively
- Graphs (peak/mean brilliance) and graph data
- Simulation data used to generate the graphs
- Details to be aware of

No data is shown here as we are aiming at *correct* descriptions in the first release of these data. Further, we aim to re-release this type of data whenever updates arrive, hence the data will have a release tag.

New components

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

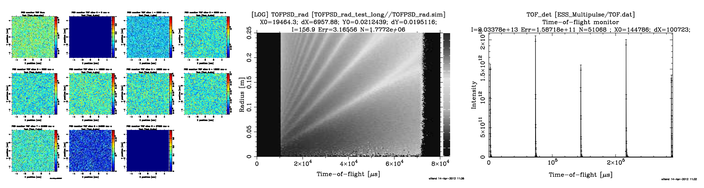

Figure 1: Left: PSD monitor with TOF axis, mean signal and 10 TOF slices shown. Middle: Radially averaging SANS monitor with TOF channel, here shown in log scale. Right: Updated ESS moderator with user-selectable number of pulses and time focusing option. See also MCNPX-related paragraph.

New tool layer components

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

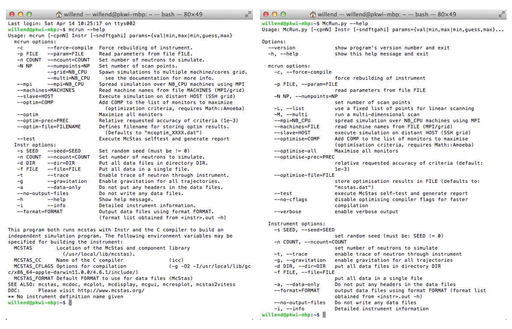

Figure 2: Left: Legacy mcrun.pl perl script options. Right: Replacement Python version. Currently 90% of the options are implemented.

We are also providing a replacement Python-based plotting tool via the matplotlib package

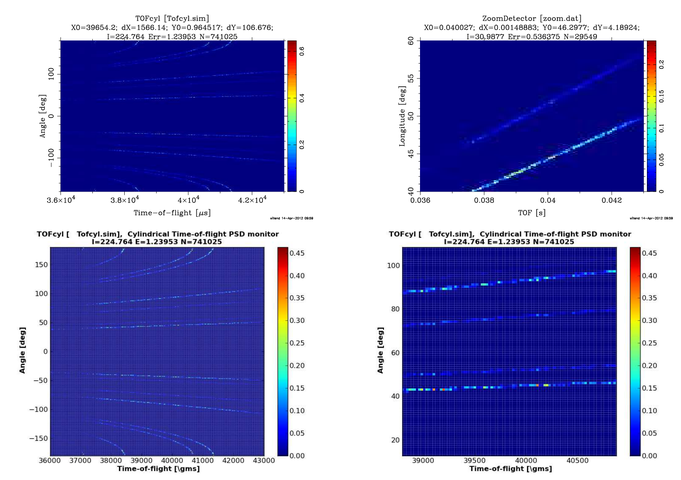

Figure 3: Top: Legacy PGPLOT visualization. "zooming" is not implemented in the tool, instead a smaller high-res monitor is added. Bottom: The new Python mcplot has many new features, including interactive zooming.

Web interface

A new development is a Python-based web frontend for McStas. The tool has a database backend and server-side cookies for storing parameters. Various security measures are taken into account. We expect to test this utility thorougly during the INSIS school in Frascati this summer.

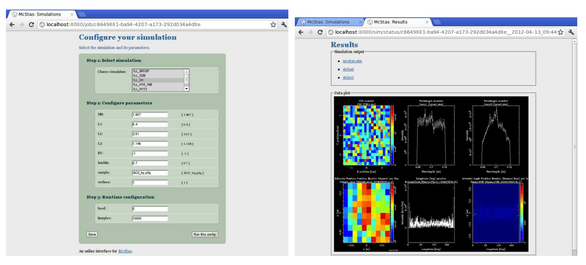

Figure 4: Left: Configuration options for the web frontend. Right: Example simulation output.

Interoperability with iFit, optimizers

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

```
To import a McStas simulation results, just use

>> results = iData('single_detector_file')
>> results = iData('directory')                    # import everything in the directory, including sim files (files may imported more than once)
>> results = iData('scan_directory/mcstas.dat') # for scans
>> results = iData('scan_directory/mcstas.sim') # for all files from the directory, uniquely.
```

Running simulations and optimizations from within iFit is also possible:

```
>> monitors=mcstas('templateDIFF', struct('RV',1), struct('ncount',1e6))
monitors =  array [1  5] iData objects:

Index      [Tag]      [Dimension]                    [File] [Last command]          [Label]
    1  id445199       [40  40]  'File Diff_Mono_XY_1299773321...'  id445199=load(iData,...  Diff_Mono_XY
    2  id445212       [40   1]  'File Diff_Mono_Lambda_129977...'  id445212=load(iData,...  Diff_Mono_...
    3  id445224       [40   1]  'File Diff_Sample_Lambda_1299...'  id445224=load(iData,...  Diff_Sampl...
    4  id445236       [360  40]  'File Diff_BananaTheta_129977...'  id445236=load(iData,...  Diff_Banan...
    5  id445248       [170  25]  'File Diff_BananaPSD_12997733...'  id445248=load(iData,...  Diff_Banan...
>> subplot(monitors)
```

```
>> [parameters, monitors]=mcstas('templateDIFF',struct('RV',1), ...
      struct('monitors','Banana','mode','optimize','optimizer','fminimfil'));
parameters =
    RV: 0.75
```

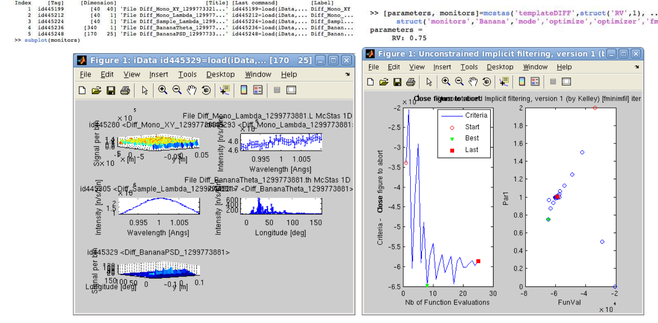

Figure 5: Left: Commands and output in simulate mode Right: Commands and output in optimize mode

McStas-MCNPX interfaces

At DTU NuTech, Esben Klinkby is working on coupling McStas and MCNPX[5]. The work aims at better computation tools for description of *advanced moderators* and integrated simulation of neutronics and beamlines, e.g. for estimates of shielding need along the long guides of the ESS.

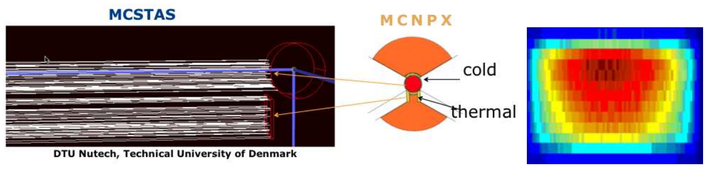

Figure 6: McStas component geometry (Left) corresponding to MCNPX geometry (Middle). Studied model is the current ESS Bilbao MCNPX model of the bi-spectral moderator. On the right panel an estimate of flux variation across the cylindrical cold moderator is shown. Target is above the moderator.

- Tally approach: Parameters fitted to MCNPX neutron distributions are transferred. Legacy approach, works only MCNPX⇒ McStas.
- Ptrac approach: Neutron events are stored in ASCII files, in practice works only MCNPX⇒ McStas.
- SSW/SSR approach: Neutron events crossing special surfaces are stored in binary files. Works MCNPX⇔ McStas.
- Compile: By slight modification to the McStas code, MCNPX and a McStas instrument file is compiled together. Works MCNPX⇔ McStas.
- Supermirror approach: Coherent scattering physics inspired from McStas is implemented directly within MCNPX.

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

Cross comparison

	Re-entry neutrons	Speed	Single neutron	Require License	Comments
Tally	No	Fast*	No	Yes/No	Should try to determine validity at least once
Ptrac	No	Fast*	Yes	Yes	Somewhat outdated by SSW/SSR
SSW/SSR	Yes	Fast*	Yes	Yes	Promising…
Compile	Yes	Slow	Yes	Yes	Generalizes poorly (auto gen c-code hacks)
Supermirror	Yes	Slow	yes	yes	Generalizes poorly (but who cares?)

*) The computational heavy MCNP/X calculation can be performed once-and-for-all

Current Production Release: 1.12c

McStas 1.12c - available at http://www.mcstas.org/download

- Released on June 3rd 2011
- Update release, the last in the 1.x series
- Fix of a bug in the rectangular focusing routine
- Introduction of –ncount as unsigned long long int in place of double. Using double could potentially lead simulations to "hang".
- If gnuplot is available at installation time, mcplot and mcgui can use this in place of PGPLOT.
- Various component and instrument bugfixes

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 analyzer arrays
- Likely a new tool layer, likely python based (replacing perl+Tk+pgperl+PGPLOT) - dedicated staff working on this
- Split infrastructure for core package, components and tools. Allows to only install core package and wanted 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 Radia or freefem)
- Possibility for nesting 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 Geomview OFF format
- Interface-code for the iFit data analysis package. Through iFit, 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!**

References

[1] K. Lefmann and K. Nielsen, *Neutron News* **10**, 20, (1999).

[2] P. Willendrup et al, *Physica B*, **350** (2004)

[3] http://www.mcstas.org

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

[5] D. B. Pelowitz, ed., *MCNPX User’s Manual, Version 2.5.0*, LA-CP-05-0369 (April 2005).

[6] Vitess project website at http://www.helmholtz-berlin.de/vitess

[7] iFit website at http://ifit.mccode.org

Keywords: McStas, Monte Carlo sim., Software, Neutrons, Instruments
PACS: 61.12-q, 05.10.Ln