New features in McStas

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Agenda

New features in McStas 2.0

McStas 2.1 and beyond...

New project areas

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Core / runtime highlights

- Backward compatibility 1: Some backward-compatibility is lost in the new version of the codegeneration, as we no longer use the information defined in the component STATE_PARAMETERS and POLARISATION_PARAMETERS macros. A warning is issued in case of components using these macros
- **Backward compatibility 2**: We have standardized naming of component parameters see the file NOMENCLATURE installed in the McStas library. The code generation will give error messages of e.g. using xw and yh where one should now be using xwidth and yheight.
- **Polarization 1:** Support for tabulated magnetic fields. New code for handling fast interpolation in sparse data is included in the share/interpolation/ area. A new version of the SE example.instr takes use of this feature.
- **Polarization 2:** We allow overlapping magnetic fields. All components that use the PROP_ routines for propagation implicitly allows larmor precession.
- Future keyword: ASSEMBLY allowing `metacomponents'



Future support tool situation

•Basic calc/sim functionality support still provided by C

Perl tools are there - but should be abandoned



•GUI widgets likely wxwidgets or Qt

- •High-level support tools provided using e.g.

•Johan Brinch done the first developments in this direction for McStas 2.0 New features in McStas - Berlin MC school 2013









Modernized build/package system - McStas 2.0

•CMake+CPack replace ./configure && make && home grown scripts • Supported platforms:



Modernized build/package system - McStas 2.1

- CMake+CPack replace ./configure && make && home grown scripts
- Supported platforms:

Metapackages!!!

Easy to install on Linux systems via dependency-requirements, i.e.

apt-get install mcstas-suite apt-get install mcstas-suite-perl apt-get install mcstas-suite-python

Meta-package now defined on the Mac

Will come for 2.1 on windows also... will allow install without internet connection





Component highlights

- - Sample_nxs.comp from Mirko Boin, HZB. Diffraction/imaging oriented sample where one defines the structure
- by means of the NXS crystallography library which is now also included with McStas. Comes with the test-
- instruments Test_Sample_nxs_diffraction.instr and Test_Sample_nxs_imaging.instr. NOTE: Special compilation
- required, see instrument source codes!
- - Elliptic_guide_gravity.comp from Henrik Carlsen, NBI. Analytical approach to describing an elliptical guide
- geometry where gravity is taken into account. Included in the Reflectometer.instr from Anette Vickery, NBI.
- - Suite of SANS-samples from Martin Cramer Pedersen, NBI. Various approaches to describing SANS diffraction
- e.g. using the PDB data bank. Component names are SANSShells.comp SANSPDBFast.comp SANSPDB.comp
- SANSNanodiscsWithTagsFast.comp SANSNanodiscsWithTags.comp SANSNanodiscsFast.comp SANSNanodiscs.comp
- SANSLiposomes.comp SANSEllipticCylinders.comp SANSCylinders.comp SANSCurve.comp SANSSpheres.comp. Included
- (some as comments) in the TestSANS.instr.
- - **SANSQMonitor.comp** also from Martin Cramer Pedersen, NBI. Q-monitor for SANS also included in TestSANS.instr.
- - **TOF2Q_cyIPSD_monitor** from Anette Vickery, NBI. Time-of-flight vs. q monitor of cylindrical shape. Included
- in the Reflectometer.instr test instrument.
- - **SNS_source_analytic.comp** from Franz X. Gallmeier, SNS. Smooth-fit description of the SNS-moderators. Fits are
- derived from the same underlying raw-data as the ordinary SNS_source.comp is using directly with linear
- interpolation.
- - Brilliance_monitor.comp from Peter Willendrup, DTU Fysik. Monitor for easy evaluation of mean and instantaneous
- source brilliance for source comparison. Used in the ESS_brilliance.instr test instrument.
- - **TOF_PSD_monitor_rad.comp** from Kim Lefmann, KU. Derived from PSD_monitor_rad by Henrich Frielinghaus, FZJ.
- Position-sensitive TOF monitor with radially averaging.
- - **PSD_TOF_monitor.comp** from Peter Willendrup, DTU Fysik. PSD-monitor with a number of independent time-slices.
- Derived from PSD_monitor by Kim Lefmann, KU.
- - Source_gen4.comp from Jonas O Birk, NBI and Uwe Filges PSI. Version of source_gen with PSI-specific changes,
- e.g. a high-energy tail contribution. Included in the RITA-II.instr from Linda Udby, NBI.
- - Absorber.comp from Peter Willendrup, DTU Fysik. Slab of perfectly absorbing material. Included in the RITA-II.instr
- from Linda Udby, NBI.
- - PSD_monitor_psf.comp and PSD_monitor_psf_eff.comp from Kim Lefmann and Linda Udby, KU. Two derivatives of
- PSD_monitor.comp both with gaussian point-spread-function and _eff with a 1/k efficiency parameter. Included
- in the RITA-II.instr from Linda Udby, NBI.
- • Virtual_mcnp_ss_input.comp and Virtual_mcnp_ss_output.comp from Esben Klinkby, DTU Nutech. Allows to read and write
- MCNP/MCNPX 'source surfaces'. For use in simulations where neutrons need transport in both codes.
- • Virtual_mcnp_ss_Guide.comp from Esben Klinkby, DTU Nutech. Single guide piece sitting in a 'sandwich' between
- an input and an output MCNP/X source surface.
- - ESS_moderator_long.comp patches from Kim Lefmann KU (multiple-pulses, TOF-focusing) and Esben Klinkby DTU Nutech
- (geometry and spectrum from ESS MCNPX models). Thanks to Klaus Lieutenant from Vitess/HZB for providing adjusted
- parameters for the 'Mezei moderator' and a wavelength-dependent corretion term.

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FOCT 427-75



The 1.12c ESS source (released)



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Either cold or thermal Flat, rectangular source

2001 cold and thermal brightness

NEXMA



The 2.0 ESS source (released)







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EUROPEAN SPALLATION SOURCE





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The 2.0a source (in the pipe)



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Overview of full monolith, including in-pile optics, shielding etc.



[Identification | Description | Input parameters | Output parameters | Links]

The Brilliance_monitor Component

Special "Brilliance" monitor of FIXED size 1x1cm. If used in the right setting, will output "instantaneous" and "mean" brilliances in units of Neutrons/cm^2/ster/AA/s. Conditions for proper units:

- Use a with a source of area 1x1cm
- The source must illuminate/focus to an area of 1x1cm a 1m distance
- Parametrise the Brilliance_monitor with the frequency of the source
- To not change the source TOF distribution, place the Brilliance monitor close to the source!

with a source of area 1x1cm illuminating/focusing to an area of 1x1cm a 1m distance, this monitor will output "instantaneous" and "mean" brilliances in units of Neutrons/cm^2/ster/AA/s

Identification

- Author: Peter Willendrup, derived from TOF_lambda_monitor.comp
- Origin: DTU Physics
- Date: May 23, 2012
- Version: 1.1

Description

Here is an example of the use of the component. Note how the mentioned Unit conditions are implemented in instrument code.

```
COMPONENT Source = ESS moderator long(
   l_low = lambdamin, l_high = lambdamax, dist = 1, xw = 0.01, yh = 0.01,
   freq = 14, T=50, tau=287e-6, tau1=0, tau2=20e-6,
   n=20, n2=5, d=0.00286, chi2=0.9, I0=6.9e11, I2=27.6e10,
  branch1=0, branch2=0.5, twopulses=0, size=0.01)
AT (0, 0, 0) RELATIVE Origin
COMPONENT BRIL = Brilliance_monitor(nlam=196,nt=401,filename="bril.sim",
        t 0=0,t 1=4000,lambda 0=lambdamin,
        lambda 1=lambdamax, Freg=14)
AT (0,0,0.000001) RELATIVE Source
```

Input parameters

Parameters	in	bol	dface	are
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Name	Unit	Description		
nlam	1	Number of bins in wavelength	101	
nt	1	Number of bins in TOF	1001	
filename	string	Defines filenames for the detector images. Stored as: Peak_ <filename> and Mean_<filename></filename></filename>		
t_0	us	Minimum time		
t_1	us	Maximum time	20000	
lambda_0	AA	Minimum wavelength detected	0	
lambda_1	AA	Maximum wavelength detected	20	
restore_neutron	1	If set, the monitor does not influence the neutron state		
Freq	Hz	Source frequency. Use freq=1 for reactor source		

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e required; the others are optional.

Brilliance_monitor output



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Easy way to get brilliance curves



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Interface to iFit

- Interface-code for the iFit data analysis package http://ifit.mccode.org
- Visualisation and analysis of simulation data and instrument (like Matlab but no need for the license)
- Suite of optimizers (see tomorrows exercise on that topic)



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	iFit: a sir	nple
	E. Fa	urhi, <i>ILL/L</i>
 Purpose Obtaining the package What's in the box The iData objects (iFit/@il The iFunc objects (iFit/@il The optimization library (il The fit functions/models (ii) The lower level import row The documentation (iFit/D) Example data files (iFit/Da) Interfaces with other softw Ok, let's start ! For beginners Help me ! Credits and Disclaimer 	Data): the core data set Func): the core model Fit/Optimizers) Fit/Models) tines (iFit/Loaders) ocs) ta) are and Graphical front-er	nds (iFit/O
	W	elcome to
	"Simple	e methods
Purpose		
The <i>iFit</i> library (pronounce [<i>eye-fit</i>]) is without Matlab license (stand-alone ver Any text file can be imported straight at though not all methods do work for the	a set of methods to load, a sion). It does not currently way, and a set of binary fi se). Any model can be ass	inalyze, pl / include a les are sup embled fo
iFit can also be used transparently from	Python / NumPy. Refer t	o our <mark>PyF</mark>
The spirit of the library is to include ob	ect definitions, with a set	of method

















Coollaboration

KU/ESS-DMSC, DTU Fysik, Mantid

McStas + Mantid integration

- COMPONENT nD_Mantid_1 = Monitor_nD(٠
- options ="mantid square x limits=[-0.2 0.2] bins=128 y limits=[-0.2 0.2] bins=128, neutron pixel t, list all neutrons",
- xmin = -0.2,
- xmax = 0.2,
- ymin = -0.2,
- ymax = 0.2,

 restore_neutron = 1, filename = "bank01_events.dat") 					Display Settings Save image	
00			M M	antidPlot – untitled		- 1,8e-18 - 1,7e-18
	A o B S	A > / 6 2		Lucida Grande	* 0	- 1,6e-18 - 1,5e-18
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Velcome to Mantid - Manipulation and Analysis Toolkit for istrument Data araView is not available revious initialization of Python failed, cannot retry. badMcStasEventNexus started badMcStasEventNexus successful, Duration 0.48 seconds		Execute LoadMcStasEventNexus Algorithms > Algorithms > Arithmetic > CorrectionFunctions > Crystal > DataHandling > Diagnostics > Diffraction > Events > Examples		v Load v Load v	 1e-18 9e-19 8e-19 7e-19 6e-19 5e-19 4e-19 3e-19 2e-19 1e-19 0 Unear ‡ 	
						Time-of-flight 14139.3

Proof of concept solution: One detector geometry so far, yet general:

Allows to define an IDF XML instrument description using a standard McStas. NeXus needs to be installed for producing NeXus output.





Pick

Full 3D

Axis View

Mask

Z-

Instrument Tree

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Select th	e simulation and its param	neters. [List latest simulatio	ons]		<pre>BARNS=1.0 D_PHI=6.0 Dw=0.8 PACK=0.7 (reconfigure)</pre>
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	Choose simulation:	PSI_Focus PSI_DMC			
Ste	p 2: Configure parame	ters (Documentation)			
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	Dw:	0.8	Default: 0.8		
	PACK:	0.7	Default: 0.7		
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New Rietveld refinement methodology using McStas virtual experiment models

E. Farhi and J. Rodriguez-Carvajal, ILL

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Science path: conventional

Raw data



Conventional Rietveld



Picture from B. Fultz, DANSE



McStas with CrysFML calls Optimisation With - Berlin MC school 2013

Picture from B. Fultz, DANSE

Implementation overview

- We set-up a diffractometer model from its geometry. No 'effective' parameters. The model should contain a realistic detector geometry (incl. ³He gas).
- We define the sample as part of the diffractometer description, with structural parameters as input (CIF/CFL/ShelX).
- We get some measured data.
- We refine the structural parameters on the measurement, using an ad-hoc optimizer.







D2B (2008-3) #50023 NAC sample low resolution configuration

That's not perfect, but a reasonable fit. Much slower than traditional Rietzeld, hut no a-priori assumptions about peak shape or resolution.



People

•The success of the project is also about the people:

Present McStas team members



• K Lefmann



E Farhi



P Willendrup



E Knudsen



U Filges

Past McStas team members



• K Nielsen



PO Åstrand



K Lieutenant



P Christiansen

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J Brinch



