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User and Programmers Guide to the Neutron Ray-Tracing Package McStas, Version 1.8

**Peter Willendrup, Emmanuel Farhi, Kim Lefmann,
Per-Olof Åstrand, Marc Hagen and Kristian Nielsen**

**Risø National Laboratory, Roskilde, Denmark
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Abstract

The software package McStas is a tool for carrying out Monte Carlo ray-tracing simulations of neutron scattering instruments with high complexity and precision. The simulations can compute all aspects of the performance of instruments and can thus be used to optimize the use of existing equipment, design new instrumentation, and carry out virtual experiments. McStas is based on a unique design where an automatic compilation process translates high-level textual instrument descriptions into efficient ANSI-C code. This design makes it simple to set up typical simulations and also gives essentially unlimited freedom to handle more unusual cases.

This report constitutes the reference manual for McStas, and, together with the manual for the McStas components, it contains full documentation of all aspects of the program. It covers the various ways to compile and run simulations, a description of the meta-language used to define simulations, and some example simulations performed with the program.

This report documents McStas version 1.8, released January 29th, 2004

The authors are:

Kim Lefmann <kim.lefmann@risoe.dk>
Materials Research Department, Risø National Laboratory, Roskilde, Denmark

Peter Kjær Willendrup <peter.willendrup@risoe.dk>
Materials Research Department, Risø National Laboratory, Roskilde, Denmark

Emmanuel Farhi <farhi@ill.fr>
Institut Laue-Langevin, Grenoble, France

Mark Hagen <mhz@ansto.gov.au>
Australian Nuclear Science and technology Organization, Sydney, Australia

as well as authors who left the project:

Per-Olof Åstrand <per-olof.aastrand@risoe.dk>
Materials Research Department, Risø National Laboratory, Roskilde, Denmark

Kristian Nielsen <kn@sifira.dk>
Materials Research Department, Risø National Laboratory, Roskilde, Denmark
Present address: Sifira A/S, Copenhagen, Denmark,

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Contents

Preface and acknowledgements **6**

1 Introduction to McStas **7**
1.1 Background . . . 7
1.1.1 The goals of McStas . . . 8
1.2 The design of McStas . . . 8
1.3 Overview . . . 10

2 New features in McStas versions 1.7 - 1.8 **11**
2.1 General . . . 11
2.2 Kernel . . . 11
2.3 Run-time . . . 12
2.4 Components and Library . . . 13
2.5 Documentation . . . 14
2.6 Example instruments . . . 14
2.7 Tools, installation . . . 15
2.8 Future extensions . . . 16

3 Installing McStas **17**
3.1 Licensing . . . 17
3.2 Installing support Apps . . . 17
3.2.1 C compiler . . . 17
3.2.2 Gui tools (Perl + Tk) . . . 18
3.2.3 Plotting backends (All platforms) . . . 18
3.3 Getting McStas . . . 19
3.4 Source code build . . . 19
3.4.1 Windows build . . . 19
3.4.2 Unix build . . . 20
3.5 Binary install, Linux . . . 21
3.6 Binary install, Windows . . . 21
3.7 Finishing and Testing the McStas distribution . . . 22

4 Running McStas **23**
4.1 Brief introduction to the graphical user interface . . . 23
4.1.1 New releases of McStas . . . 26
4.2 Running the instrument compiler . . . 27

4.2.1 Code generation options . . . 28
4.2.2 Specifying the location of files . . . 28
4.2.3 Embedding the generated simulations in other programs . . . 29
4.2.4 Running the C compiler . . . 29
4.3 Running the simulations . . . 30
4.3.1 Choosing a data file format . . . 31
4.3.2 Basic import and plot of results . . . 31
4.3.3 Interacting with a running simulation . . . 32
4.3.4 Optimizing a simulation . . . 34
4.4 Using simulation front-ends . . . 35
4.4.1 The graphical user interface (mcgui) . . . 36
4.4.2 Running simulations with automatic compilation (mcrun) . . . 41
4.4.3 The `gscan` front-end . . . 42
4.4.4 Graphical display of simulations (mcdisplay) . . . 42
4.4.5 Plotting the results of a simulation (mcplot) . . . 43
4.4.6 Plotting resolution functions (mcresplot) . . . 44
4.4.7 Creating and viewing the library and component/instrument help (mcdoc) . . . 45
4.4.8 Translating McStas components for Vitess (mcstas2vitess) . . . 46
4.4.9 Translating McStas results files between Matlab and Scilab formats 46
4.5 Analyzing and visualizing the simulation results . . . 46

5 The McStas kernel and meta-language 49
5.1 Notational conventions . . . 49
5.2 Syntaxical conventions . . . 50
5.3 Writing instrument definitions . . . 51
5.3.1 The instrument definition head . . . 53
5.3.2 The `DECLARE` section . . . 53
5.3.3 The `INITIALIZE` section . . . 54
5.3.4 The `TRACE` section . . . 54
5.3.5 The `SAVE` section . . . 56
5.3.6 The `FINALLY` section . . . 56
5.3.7 The end of the instrument definition . . . 57
5.3.8 Code for the instrument `vanadium_example.instr` . . . 57
5.4 Writing component definitions . . . 59
5.4.1 The component definition header . . . 59
5.4.2 The `DECLARE` section . . . 61
5.4.3 The `SHARE` section . . . 61
5.4.4 The `INITIALIZE` section . . . 62
5.4.5 The `TRACE` section . . . 62
5.4.6 The `SAVE` section . . . 63
5.4.7 The `FINALLY` section . . . 65
5.4.8 The `MCDISPLAY` section . . . 65
5.4.9 The end of the component definition . . . 66
5.4.10 A component example: Slit . . . 66
5.4.11 McDoc, the McStas library documentation tool . . . 68

6 Monte Carlo Techniques and simulation strategy **70**
6.1 The neutron weight, p . . . 70
6.1.1 Statistical errors of non-integer counts . . . 71
6.2 Weight factor transformations during a Monte Carlo choice . . . 72
6.2.1 Focusing components . . . 72
6.3 Transformation of random numbers . . . 73

7 The component library **75**
7.1 A short overview of the McStas component library . . . 75

8 Instrument examples **80**
8.1 A test instrument for the component V_sample . . . 80
8.1.1 Scattering from the V-sample test instrument . . . 80
8.2 The triple axis spectrometer TAS1 . . . 80
8.2.1 Simulated and measured resolution of TAS1 . . . 82
8.3 The time-of-flight spectrometer PRISMA . . . 84
8.3.1 Simple spectra from the PRISMA instrument . . . 86

A Libraries and conversion constants **88**
A.1 Run-time calls and functions . . . 88
A.1.1 Neutron propagation . . . 88
A.1.2 Coordinate and component variable retrieval . . . 89
A.1.3 Coordinate transformations . . . 90
A.1.4 Mathematical routines . . . 91
A.1.5 Output from detectors . . . 91
A.1.6 Ray-geometry intersections . . . 92
A.1.7 Random numbers . . . 92
A.2 Reading a data file into a vector/matrix (Table input) . . . 92
A.3 Monitor_nD Library . . . 94
A.4 Adaptative importance sampling Library . . . 94
A.5 Vitess import/export Library . . . 94
A.6 Constants for unit conversion etc. . . . 95

B The McStas terminology **96**

Bibliography **97**

Index and keywords **97**

Preface and acknowledgements

This document contains information on the Monte Carlo neutron ray-tracing program McStas version 1.8, an update to the initial release in October 1998 of version 1.0 as presented in Ref. [1]. The reader of this document is supposed to have some knowledge of neutron scattering, whereas only little knowledge about simulation techniques is required. In a few places, we also assume familiarity with the use of the C programming language and UNIX/Linux.

It is a pleasure to thank Prof. Kurt N. Clausen for his continuous support to this project and for having initiated McStas in the first place. Essential support has also been given by Prof. Robert McGreevy. We have also benefited from discussions with many other people in the neutron scattering community, too numerous to mention here.

This project has been supported by the European Union, initially through the "XENNI" network and "Cool Neutrons" RTD program, later through the "SCANS" network, and today the "MCNSI" network package.

In case of any errors, questions, or suggestions, contact the authors at `mcstas@risoe.dk` or consult the McStas WWW home page [2].

If you **appreciate** this software, please subscribe to the `neutron-mc@risoe.dk` email list, send us a smiley message, and contribute to the package.

McStas 1.8 contributors

Several people outside the core developer team have been contributing to McStas 1.8:

- Dickon Champion and Stuart Ansell, ISIS: `ISIS_moderator`. Dickon also contributed his model of the ISIS HET instrument plus a test instrument for the moderator component. Dickon also assisted in various debugging.
- Uwe Filges, PSI: `Guide_tapering` and a model of the PSI FOCUS instrument
- Ross Stewart, ILL: New `Guide_curved`
- Chris Ling, ILL: ILL D9 instrument
- Lise Arleth, RISØ: Helped the developer team regarding the new `Sans_spheres` component

Thank you guys! This is what McStas is all about!

Chapter 1

Introduction to McStas

Efficient design and optimization of neutron spectrometers are formidable challenges. Monte Carlo techniques are well matched to meet these challenges. When McStas version 1.0 was released in October 1998, except for the NISP/MCLib program [3], no existing package offered a general framework for the neutron scattering community to tackle the problems currently faced at reactor and spallation sources. The McStas project was designed to provide such a framework.

McStas is a fast and versatile software tool for neutron ray-tracing simulations. It is based on a meta-language specially designed for neutron simulation. Specifications are written in this language by users and automatically translated into efficient simulation codes in ANSI-C. The present version supports both continuous and pulsed source instruments, and includes a library of standard components with in total around 90 components. These enable to simulate all kinds of neutron scattering instruments (diffractometers, triple-axis, reflectometers, time-of-flight, small-angle, back-scattering,...).

The McStas package is written in ANSI-C and is freely available for down-load from the McStas web-page [2]. The package is actively being developed and supported by Risø National Laboratory and the Institut Laue Langevin. The system is well tested and is supplied with several examples and with an extensive documentation, including a separate component manual.

1.1 Background

The McStas project is the main part of a major effort in Monte Carlo simulations for neutron scattering at Risø National Laboratory. Simulation tools were urgently needed, not only to better utilize existing instruments (*e.g.* RITA-1 and RITA-2 [4–6]), but also to plan completely new instruments for new sources (*e.g.* the Spallation Neutron Source, SNS [7] and the European Spallation Source, ESS [8]). Writing programs in C or Fortran for each of the different cases involves a huge effort, with debugging presenting particularly difficult problems. A higher level tool specially designed for the needs of simulating neutron instruments is needed. As there was no existing simulation software that would fulfill our needs, the McStas project was initiated. In addition, the ILL required an efficient and general simulation package in order to achieve renewal of its instruments and guides. A significant contribution to both the component library and the McStas kernel itself was

developed at the ILL and included in the package, in agreement with the original McStas authors.

1.1.1 The goals of McStas

Initially, the McStas project had four main objectives that determined the design of the McStas software.

Correctness. It is essential to minimize the potential for bugs in computer simulations. If a word processing program contains bugs, it will produce bad-looking output or may even crash. This is a nuisance, but at least you know that something is wrong. However, if a simulation contains bugs it produces wrong results, and unless the results are far off, you may not know about it! Complex simulations involve hundreds or even thousands of lines of formulae, making debugging a major issue. Thus the system should be designed from the start to help minimize the potential for bugs to be introduced in the first place, and provide good tools for testing to maximize the chances of finding existing bugs.

Flexibility. When you commit yourself to using a tool for an important project, you need to know if the tool will satisfy not only your present, but also your future requirements. The tool must not have fundamental limitations that restrict its potential usage. Thus the McStas systems needs to be flexible enough to simulate different kinds of instruments (e.g. triple-axis, time-of-flight and possible hybrids) as well as many different kind of optical components, and it must also be extensible so that future, as yet unforeseen, needs can be satisfied.

Power. "*Simple things should be simple; complex things should be possible*". New ideas should be easy to try out, and the time from thought to action should be as short as possible. If you are faced with the prospect of programming for two weeks before getting any results on a new idea, you will most likely drop it. Ideally, if you have a good idea at lunch time, the simulation should be running in the afternoon.

Efficiency. Monte Carlo simulations are computationally intensive, hardware capacities are finite (albeit impressive), and humans are impatient. Thus the system must assist in producing simulations that run as fast as possible, without placing unreasonable burdens on the user in order to achieve this.

1.2 The design of McStas

In order to meet these ambitious goals, it was decided that McStas should be based on its own meta-language, specially designed for simulating neutron scattering instruments. Simulations are written in this meta-language by the user, and the McStas compiler automatically translates them into efficient simulation programs written in ANSI-C.

In realizing the design of McStas, the task was separated into four conceptual layers:

1. Modeling the physical processes of neutron scattering, *i.e.* the calculation of the fate of a neutron that passes through the individual components of the instrument (absorption, scattering at a particular angle, etc.)

2. Modeling of the overall instrument geometry, mainly consisting of the type and position of the individual components.

3. Accurate calculation, using Monte Carlo techniques, of instrument properties such as resolution function from the result of ray-tracing of a large number of neutrons. This includes estimating the accuracy of the calculation.

4. Presentation of the calculations, graphical or otherwise.

Though obviously interrelated, these four layers can be treated independently, and this is reflected in the overall system architecture of McStas. The user will in many situations be interested in knowing the details only in some of the layers. For example, one user may merely look at some results prepared by others, without worrying about the details of the calculation. Another user may simulate a new instrument without having to reinvent the code for simulating the individual components in the instrument. A third user may write an intricate simulation of a complex component, e.g. a detailed description of a rotating velocity selector, and expect other users to easily benefit from his/her work, and so on. McStas attempts to make it possible to work at any combination of layers in isolation by separating the layers as much as possible in the design of the system and in the meta-language in which simulations are written.

The usage of a special meta-language and an automatic compiler has several advantages over writing a big monolithic program or a set of library functions in C, Fortran, or another general-purpose programming language. The meta-language is more *powerful*; specifications are much simpler to write and easier to read when the syntax of the specification language reflects the problem domain. For example, the geometry of instruments would be much more complex if it were specified in C code with static arrays and pointers. The compiler can also take care of the low-level details of interfacing the various parts of the specification with the underlying C implementation language and each other. This way, users do not need to know about McStas internals to write new component or instrument definitions, and even if those internals change in later versions of McStas, existing definitions can be used without modification.

The McStas system also utilizes the meta-language to let the McStas compiler generate as much code as possible automatically, letting the compiler handle some of the things that would otherwise be the task of the user/programmer. *Correctness* is improved by having a well-tested compiler generate code that would otherwise need to be specially written and debugged by the user for every instrument or component. *Efficiency* is also improved by letting the compiler optimize the generated code in ways that would be time-consuming or difficult for humans to do. Furthermore, the compiler can generate several different simulations from the same specification, for example to optimize the simulations in different ways, to generate a simulation that graphically displays neutron trajectories, and possibly other things in the future that were not even considered when the original instrument specification was written.

The design of McStas makes it well suited for doing "what if..." types of simulations. Once an instrument has been defined, questions such as "what if a slit was inserted",

"what if a focusing monochromator was used instead of a flat one", "what if the sample was offset 2 mm from the center of the axis" and so on are easy to answer. Within minutes the instrument definition can be modified and a new simulation program generated. It also makes it simple to debug new components. A test instrument definition may be written containing a neutron source, the component to be tested, and whatever detectors are useful, and the component can be thoroughly tested before being used in a complex simulation with many different components.

The McStas system is based on ANSI-C, making it both efficient and portable. The meta-language allows the user to embed arbitrary C code in the specifications. *Flexibility* is thus ensured since the full power of the C language is available if needed.

1.3 Overview

The McStas system documentation consists of the following major parts:

- A short list of new features introduced in this McStas release appears in chapter 2
- Chapter 3 explains how to obtain, compile and install the McStas compiler, associated files and supportive software
- Chapter 4 includes a brief introduction (section 4.1) as well a section (4.2) on running the compiler to produce simulations. Section 4.3 explains how to run the generated simulations. A number of front-end programs are used to run the simulations and to aid in the data collection and analysis of the results. These user interfaces are described in section 4.4.
- The McStas meta-language is described in chapter 5. This chapter also describes a set of library functions and definitions that aid in the writing of simulations. See appendix A for more details.
- Chapter 6 concerns Monte Carlo techniques and simulation strategies in general
- The McStas component library contains a collection of well-tested, as well as user contributed, beam components that can be used in simulations. The McStas component library is documented in a separate manual and on the McStas web-page [2], but a short overview of these components is given in chapter 7.1 of the Manual.
- A collection of example instrument definitions is described in chapter 8 of the Manual.

A list of library calls that may be used in component definitions appears in appendix A, and an explanation of the McStas terminology can be found in appendix B of the Manual.. Plans for future extensions are presented on the McStas web-page [2] as well as in section **??**.

Chapter 2

New features in McStas versions 1.7 - 1.8

Many new features have been implemented in McStas version 1.8 since version 1.5 (no version 1.6. manual was written, the most important being that McStas can now compile and run in a Windows enviroment. The list of changes given here may be particularly useful to experienced McStas users who do not wish to read the whole manual, searching only for new features. A global upward compatibility exists for all changes, and thus all previous components and instruments should work as before. Changes are labelled as 1.7 or 1.8 to indicate in which McStas version they appeared.

Important note for Windows users: It is a known problem that some of the McStas tools do not support filenames / directories with spaces. We are working on a more general approach to this problem, which will hopefully be solved in the next release.

2.1 General

As of McStas version 1.8 the license covering the McStas package is the GNU General Pubclic License. See `http://www.gnu.org` for details.

2.2 Kernel

The following changes concern the 'Kernel' (i.e. the McStas meta-language and program). See the dedicated chapter in the *User manual* for more details.

- McStas can now compile for Windows!
- Instrument parameters may now have default values, the same way as components do (appeared in 1.8).
- An instrument source file may contain `EXTEND` %{ ...}% C blocks just after the usual `AT` ... `ROTATED` ... keywords, to extend the behaviour of existing components, without touching their code. All local component variables are available. This may for instance be used to add a new 'color' to neutrons, i.e. assign a new characteristic variable to the neutron (appeared in 1.7).

- Component instances in an instrument file may be `GROUP`'ed into exclusive assembly, i.e. only one component of the group will intercept the neutron ray, the rest will be skipped. This is useful for multi monochromators multi detectors, multiple collimators, etc. After the `ROTATED` keyword, the keyword `GROUP` should be added followed by a group name (e.g. `GROUP` MyGroup) (appeared in 1.7).
- The instrument and components may have string (`char*`) setting parameters. For components, their length is limited to 1024 characters (appeared in 1.7).
- In both components and instruments, the `FINALLY` section, that is executed at the end of simulations, has been supplemented with a new `SAVE` section. This latter is executed at simulation end (just before the `FINALLY` section), but also each time an intermediate save is required (e.g. when a 'kill -USR2 $pid' is used under Unix, see section 2.3) (appeared in 1.7).
- Components may have a `SHARE` section, which is imported only once per type of component. `SHARE` has the same role as `DECLARE`, but is useful when several instances of the same component is used in a single simulation (appeared in 1.7).
- The component files may have some `%include` inside '%{ }%' `DECLARE` or `SHARE` C blocks. The files to include are searched locally, and then in the library. If an extension is found, only the specified file is included, else both .h and .c are embedded unless the –no-runtime has been specified. As in previous releases, the instrument files can embed external files, both in C blocks and in the instrument parts (`DECLARE`, etc.) (appeared in 1.7).
- The `PREVIOUS` keyword, to be used after `RELATIVE` in place of component instance names refers to the preceeding component, and does not require to actually know its name. Similarly the `PREVIOUS(n)` keyword refers to the n-th preceeding component (appeared in 1.8).

2.3 Run-time

Some important modifications were done to the 'Run-time' library (i.e. the functions used in the instrument program). Some details may be found in *Running* chapter of the *User manual* as well as in the appendix A.

- A global gravitation handling is now available, by setting the `-g` flag.
- Many output formats are available for data. Use the `--format="format"` flag, e.g. `--format="Scilab"`. The default format is McStas/PGPLOT, but may be specified globally using the `MCSTAS_FORMAT` environment variable. See section 4.3.2 for details (appeared in 1.7).
- It is possible to save 3D data arrays, by calling the DETECTOR_OUT_3D macro. (handled as 2D by `mcplot` by ignoring the 3rd dimension) (appeared in 1.7).
- The C type of the 'number of events' array in monitors (usually named `L_N`) was changed from `int` to `double`, to avoid overflow. All 'home-made' monitors should be updated accordingly (appeared in 1.7).

- The `USR2` signal generates an intermediate save for all monitors, during the simulation (executes the `SAVE` section). The `USR1` signal still gives informations (appeared in 1.7).
- New `randvec_target_rect` and `randvec_target_rect_angular` functions now focus on a rectangle (more efficient than the former `randvec_target_sphere`) (appeared in 1.7 and 1.8).

2.4 Components and Library

We here list some of the new components (found in the McStas `lib` directory) which are detailed in the *Component manual*, also mentioned in the *Component Overview* of the *User Manual*.

- All components now have a valid header for `mcdoc` automatic documentation, as well as usage example.
- `contrib` This directory now contains contributed components. Those that will be found to be highly stable will then go into the other component categories. Contributed components (`Guide_honeycomb`, `Guide_tapering`, `Guide_curved`, `ISIS_moderator`) have been placed there (appeared in 1.7 and 1.8).
- `data` This directory now contains example data files mainly for Laue diffraction, transmission and reflection files.
- `doc` The documentation is now included in the `doc` directory.
- `example` A new `example` directory contains instrument examples, available from the `mcgui` 'Neutron site' menu Tool.
- `misc` Updated `Vitess_input` and `Vitess_output` components according to Vitess ¿= 2.3 Neutron structure.
- `misc` A `Progress_bar` component may be positioned anywhere in the simulation and displays the simulation percentage. It may also save temporary data files regularly so that one can have a look (using `mcplot`) at the results on-the-fly before the end of the simulation.
- `monitors` The `Monitor_nD` component may be used as a replacement for all monitors. It may have automatic limits mode for either all or selected monitored variables. It may also plot banana monitors for `mcdisplay` and monitor something else than the intensity, e.g. the mean energy on a XY psd (appeared in 1.7). A bug (atan2) was corrected in `PSD_monitor_4PI`.
- `obsolete` Some components were renamed by categories for better sorting. Old components are still available, but not maintained anymore. We highly encourage to avoid using these when writing new instrument definitions.
- `optics` components were renamed by categories, starting with Guide_..., Monochromator_..., Filter_... etc so that sorting is easier (appeared in 1.7).

- `optics` Monochromator_curved can read reflectivity and transmission tables (appeared in 1.7).
- `optics` Guide_gravity can handle a 2D array of channels, and has options for subdivisions in length, chamfers and wavyness.
- `optics` Filter_gen can read a table from a file and affect the neutron beam (replaces the obsolete `Flux_adapter`). It may act as a filter or a source (appeared in 1.7).
- `optics` Bugs were corrected in the following components: Bender, Chopper, Guide_channeled. Some similar components were gathered. New components were added: Guide_gravity, Guide_wavy, Filter_gen.
- `samples` can now target towards any component, given its index (no need to compute `target_x|y|z` vector, use e.g. `target_index=1`). Position an `Arm` at the focusing position when targetting to centered components (appeared in 1.7).
- `samples` Rectangular focusing has been implemented (instead of circular) in most components. More sample shapes are available. A bug has been corrected in Single_crystal. A Powder2 component (2 rings) has been added. Sans_spheres is a new sample component for small angle scattering. Phonon_simple is a new sample for phonon scattering. (appeared in 1.8).
- `share` Many dedicated libraries are now available as shared code for reading tables, handling data files and monitors. These are C functions to be `%included` into components (see e.g. `MCSTAS/monitors/Monitor_nD.comp`) (appeared in 1.7).
- `sources` The `Source_gen` and `Source_Maxwell_3` components may now simulate all kinds of continuous neutron sources. Some bugs were corrected in most sources in order to have an isotropic neutron emission. The `Virtual_input` and `Virtual_output` may load and save neutron event files (beware the size of the generated files !). Format may be text or binary (appeared in 1.7).

2.5 Documentation

As of McStas 1.8 an improved tutorial has been integrated into to the graphical user interface of McStasṪhe content of the tutorial is also available in appendix **??**.

2.6 Example instruments

As mentioned above, McStas 1.8 has various improvements regarding distribution of instruments. Firstly, `mcgui` has a new special menu for instruments distributed with McStasand secondly instruments can now have default values and thirdly a new McStas tutorial has integrated into the user interface. These three new features together proves a solid starting point for new users of McStasṪo further increase the value of the package, we have decided to include selveral example instruments contributed by McStas users. The full list of example instruments are

- `vanadium_example`, improved version used in the McStas tutorial.
- `linup-1-linup-7`, legacy instruments of the Risø TAS1 instrument from a historical release of McStas.
- `h8_test`, model of the Brookhaven H8 triple-axis, written by McStas team member Emmanuel Farhi
- `ILL_D9`, a model of the ILL D9 hot four-circle diffractometer, contributed by Chris Ling
- `Hetfull`, a model of the ISIS HET spectrometer, contributed by Dickon Champion
- `focus_psi`, a model of the PSI FOCUS spectrometer, contributed by Uwe Filges
- `prisma2`, a model of the ISIS prisma2 spectrometer, written by Kristian Nielsen and Mark Hagen from a historical release of McStas.
- Test instruments `ISIStest` for testing the new `ISIS_moderator` component, `SANS` for testing the new `Sans_spheres` component and `Test_Phonon` for testing the new `Phonon_simple` component, all contributed by the corresponding component authors.

2.7 Tools, installation

A renewal of most McStas Tools, used to edit and display instrument or results, has been undertaken, aiming at proposing alternatives to the Perl+PerlTk+PGPLOT+PDL libraries.

Quite a lot of work was achieved in order to solve the installation problems that have been encoutered so far. A fully working McStas distribution now only requires a C compiler, perl, perl-Tk and one of Matlab, Scilab and (PGPLOT, perl-DL). The Plotlib Scilab library has been included in the package, and does not need to be installed separately anymore.

This has improved significantly the portability of McStas and thus simplified the installation of the package. Details about the installation and the available tools are given in the *Installing McStas* chapter of the *User Manual*.

- The list of required packages for a complete McStas installation is now a C compiler, Perl, PerlTk and Scilab or Matlab.
- Matlab, Scilab and IDL may read directly McStas results if the simulation was executed with the `--format="..."` option (see 2.3 changes). The former PGPLOT interface is still supported (appeared in 1.7).
- `mcgui` can now perform `mcrun`-like parameter scans directly from the gui (appeared in 1.8).
- `mcgui` has now a 'Neutron site' menu which enables to load directly one of the instrument examples (appeared in 1.8).

- `mcrun` can generate scan results in all formats (appeared in 1.8).
- `mcrun` has a McStas self test procedure available (appeared in 1.8).
- `mcplot`, `mcdisplay`, `mcgui` are now less dependent on the `perl/PDL/pgplot` installed versions and fully work with Matlab/Scilab (appeared in 1.7).
- `mcplot` can plot a single simulation data file.
- `mcplot`, `mcresplot`, `mcdisplay` can output GIF, PS and color PS files. They also have integrated help (-h options), and may generate output files in a non interactive mode (read data, create output file, exit) (appeared in 1.7).
- `mcplot` and `mcdisplay` work with Matlab, PGPLOT and Scilab plotters (depends on the `MCSTAS_FORMAT` environment variable, or -pPLOTTER option, or PGPLOT if not set) (appeared in 1.7).
- `mcplot` may display parameter scan step results in all formats (appeared in 1.8).
- `mcstas2vitess` enables to convert a McStas component into a Vitess [9] one (appeared in 1.7).
- `mcresplot` can plot projections of the 4D resolution function of an instrument obtained from the `Res_sample` and `Res_monitor` components. In version 1.8, it only works with the McStas/PGPLOT format, but a port for Scilab/Matlab is under way (appeared in 1.7).
- `mcdoc` can now display the pdf version of the manual, an HTML catalog of the current library, as well as help for single components. The `mcdoc` functions have been closely integrated into `mcgui` (appeared in 1.7).
- `mcdoc` can document automatically instruments in the same way as components (appeared in 1.8).
- `mcconvert` is a new tool to convert McStas result text files from Matlab to Scilab, and from Scilab to Matlab formats (appeared in 1.8).

2.8 Future extensions

The following features are planned for the oncoming releases of McStas:

- Support for Matlab and Scilab in `mcresplot`.
- Support for MPI (parallel processing library) in the runtime
- Language extension 'JUMP' for enabeling loops, 'teleporting' etc. in instrument descriptions.
- Concentric components.
- Polarised components and magnetic field computation components.
- Optimize a set of parameters for a better flux and/or resolution on a given monitor.

Chapter 3

Installing McStas

The information in this chapter is also available as a separate html/ps/pdf document in the `install_docs/` folder of your McStas installation package.

3.1 Licensing

The conditions on the use of McStas can be read in the files `LICENSE` and `LICENSE.LIB` in the distribution. Essentially, McStas may be used and modified freely, and copies of the McStas source code may be distributed to others. New or modified component and instrument files may be shared by the user community, and we shall be glad to include user contributions in the package.

3.2 Installing support Apps

To get a fully functional McStas installation, a few support applications are required. Essentially, you will need a C compiler, Perl and Perl-Tk, as well as a plotter such as Matlab, Scilab or PGPLOT (which we do not support but is still functional). These should better be installed before McStas.

Under Windows, we recommand to avoid using spaces when specifying the location of packages during their installation.

3.2.1 C compiler

The C compiler is used for building the instrument simulation executable, which does the hard job. It is called transparently by the mcgui and mcrun McStas tools.

- Win32: Bloodshed Dev-C++ (Win32). To install Bloodshed Dev-C++, download the installer package from

  http://www.bloodshed.net/dev/devcpp.html.

  When installed, add the `C:\Dev-Cpp\bin` directory to your PATH using

  'Start/Settings/Control Panel/System/Advanced/Environment Variables'.

- Unix/Linux: standard C compiler. Most Unix/Linux systems come with a system C compiler, usually named 'cc' or 'gcc'. In case this would not be the case, install such a compiler from Linux packages (RedHat, SuSe or Debian), or compile it from scratch.

3.2.2 Gui tools (Perl + Tk)

The McStas tools are written using the Perl language, with calls to the perl-Tk library.

- Win32:
  - Get and install the ActivePerl package from http://www.activestate.com/Products/Download/Register.plex?id=ActivePerl (Registration not required) This package provides Perl and Perl-Tk. IMPORTANT: Get the 'msi' type package!
  - Optionally, get and install the ActiveTcl package from http://www.activestate.com/Products/Download/Register.plex?id=ActiveTcl (Registration not required) This package provides Tcl/Tk.
  - You may need to update/install the Microsoft Windows Installer. Get it from Windows Support Downloads at http://www.microsoft.com/.
  - Make sure that during installation, you have requested to attach the .pl and .tcl extensions to Perl and Tcl, and the `C:\Perl\bin` is in the PATH.
- Unix/Linux:
  - Install Perl, Tcl/Tk and perl-Tk. Prebuilt packages exist for most Linux distributions and also most other Unix-like operating systems. You will find these packages at http://freshmeat.net/, http://www.rpmfind.net/linux/RPM/ (for SuSe and RedHat) and using Fink Commander (for Mac OS X). Some Linux like system do not provide perl-Tk as an RPM/Debian file. You will then have to compile it from the source code (with ./configure; make; make install).
  - Consult the McStas webpage at http://mcstas.risoe.dk for updated links to the source code distributions.

3.2.3 Plotting backends (All platforms)

For plotting with McStas, different support packages can be used:

- PGPLOT/PDL (perl-PDL)/pgperl (perl-PGPLOT) (Unix only) - Binary builds of the packages exist for various Linux distributions (for instance Debian comes with prebuilt versions). Prebuilt versions also exist for some commercial Unix'es. Refer to distributor/vendor for documentation. The packages can also be built from source using some (in many cases much) effort. See the PGPLOT documentation for further details. You may need to define the `PGPLOT_DIR` variable to the location of the Pgplot library.

- Matlab (Some Unix/Win32) - refer to http://www.mathworks.com. Matlab licenses are rather costly, but discount programmes for university and research departments exist.

- Scilab (Unix/Win32/Mac...) - a free 'Matlab-like' package, available from http://www-rocq.inria.fr/scilab/.
  On Windows systems, Scilab should be installed in a directory such as `C:\Scilab` (do NOT use spaces in names) and you should then add the `C:\Scilab\bin` directory to your PATH using

  'Start/Settings/Control Panel/System/Advanced/Environment Variables'.

3.3 Getting McStas

The McStas package is available in three different distribution packages, from the project website at http://mcstas.risoe.dk, e.g.

- `mcstas-1.8-src.tar.gz`
  Source code package for building McStas on (at least) Linux and Windows 2000. This package should compile on most Unix platforms with an `ANSI-c` compiler. - Refer to section 3.4

- `mcstas-1.8-i686-unknown-Linux.tar.gz`
  Binary package for Linux systems, currently built on Debian GNU/Linux 3.0 'woody'. Should work on most Linux setups. - Refer to section 3.5

- `mcstas-1.8-i686-unknown-Win32.zip`
  Binary package for Win32 systems, currently built on Microsoft Windows 2000 professional, using the `gcc` 2.95 compiler from Bloodshed Dev-C++ 5 Beta 7 - Refer to section 3.6

3.4 Source code build

The McStas package is beeing co-developed for mainly Linux and Windows systems, however the Linux build instructions below will work on most Unix systems, including Mac OS X). For an updated list of platforms on which McStas has been built, refer to the project website.

3.4.1 Windows build

- Start by unpacking the `mcstas-1.8-src.tar.gz` package using e.g. Winzip.

- Compile the McStas package using the `build.bat` script of the `mcstas-1.8` directory you just unpacked. Follow the on screen instructions.

- When the build has been done (e.g. `mcstas.exe` has been produced), proceed to install (Section 3.6).

3.4.2 Unix build

McStas uses autoconf to detect the system configuration and creates the proper Makefiles needed for compilation. On Unix-like systems, you should be able to compile and install McStas using the following steps:

1. Unpack the sources to somewhere convenient and change to the source directory:
   gunzip -c mcstas-1.8-src.tar.gz — tar xf -
   cd mcstas-1.8/

2. Configure and compile McStas:
   ./configure
   make

3. Install McStas (as superuser):
   make install

The installation of McStas in step 3 by default installs in the /usr/local/ directory, which on most systems requires superuser (root) privileges. To install in another directory, use the –prefix= option to configure in step 2. For example,

```
./configure –prefix=/home/joe
```

will install the McStas programs in /home/joe/bin/ and the library files needed by McStas in /home/joe/lib/mcstas/.

In case ./configure makes an incorrect guess, some environment variables can be set to override the defaults:

- The CC environment variable may be set to the name of the C compiler to use (this must be an ANSI C compiler). This will also be used for the automatic compilation of McStas simulations in mcgui and mcrun.

- CFLAGS may be set to any options needed by the compiler (eg. for optimization or ANSI C conformance). Also used by mcgui/mcrun.

- PERL may be set to the path of the Perl interpreter to use.

To use these options, set the variables before running ./configure. Eg.

```
setenv PERL /pub/bin/perl5
./configure
```

It may be necessary to remove configure's cache of old choices first:

```
rm -f config.cache
```

If you experience any problems, or have some questions or ideas concerning McStas, please contact peter.willendup@risoe.dk or the McStas mailing list at neutron-mc@risoe.dk.

You should try to make sure that the directory containing the McStas binaries (mcstas, gscan, mcdisplay, etc.) is contained in the PATH environment variable. The default directory is /usr/local/bin, which is usually, but not always, included in PATH. Alternatively, you can reference the McStas programs using the full path name, ie.

```
/usr/local/bin/mcstas my.instr
perl /usr/local/bin/mcrun -N10 -n1e5 mysim -f output ARG=42
perl /usr/local/bin/mcdisplay --multi mysim ARG=42
```

This may also be necessary for the front-end programs if the install procedure could not determine the location of the perl interpreter on your system.

If McStas is installed properly, it should be able to find the files it needs automatically. If not, you should set the MCSTAS environment variable to the directory containing the runtime files "mcstas-r.c" and "mcstas-r.h" and the standard components (*.comp). Use one of

```
MCSTAS=/usr/local/lib/mcstas; export MCSTAS # sh, bash
setenv MCSTAS /usr/local/lib/mcstas         # csh, tcsh
```

3.5 Binary install, Linux

Should be very easy, simply start from 'make install' in Section 3.4.

3.6 Binary install, Windows

- Start by unpacking the `mcstas-1.8-i686-unknown-Win32.zip` package using e.g. Winzip.
- Execute the `install.bat` installation script. Follow the on screen instructions.
- Set the required (see output of `install.bat`) environment variables using

  'Start/Settings/Control Panel/System/Advanced/Environment Variables'

  - `PATH` Append e.g. `C:\mcstas\bin`
  - `MCSTAS` Create it as e.g. `C:\mcstas\lib`

It is important that Perl is correctly installed to execute all the McStas tools (e.g. mcdoc.pl, mcrun.pl, mcgui.pl, ...). Create a shortcut of the `C:\mcstas\bin\mcgui.pl` on your Desktop (the icon should be a yellow dot). Whenever launched from the Windows Command window (cmd), you must specify the .pl extension to all McStas Perl script commands (e.g. 'mcrun.pl' and 'mcgui.pl', not 'mcrun' or 'mcgui') except for `mcstas` itself.

Actually, the modifications to your environnement variables should be

- `PATH` Append e.g.
  `C:\mcstas\bin;c:\Program Files\Scilab-2.7.2\bin;C:\Perl\bin\;C:\Dev-Cpp\bin;`
- `MCSTAS` Create it as e.g. `C:\mcstas\lib`

using menu item 'Start/Settings/Control Panel/System/Advanced/Environment Variables'. On some Windows systems, it may be necessary to logout/login (no need to restart the computer) to make these changes active for the whole session.

3.7 Finishing and Testing the McStas distribution

The `examples` directory of the distribution contains a set of instrument examples. These are used for the McStas self test procedure, which is executed with

```
mcrun --test
```

This test takes a few minutes to complete, and ends with a short report on the installation itself, the simulation accuracy and the plotter check.

You should now be able to use McStas. For some examples to try, see the examples/ directory. Start 'mcgui' (mcgui.pl on Windows), and select one of the examples in the 'Neutron Sites' menu.

Chapter 4

Running McStas

This chapter describes usage of the McStas simulation package. Refer to Chapter 3 for installation instructions. In case of problems regarding installation or usage, the McStas mailing list [2] or the authors should be contacted.

Important note for Windows users: It is a known problem that some of the McStas tools do not support filenames / directories with spaces. We are working on a more general approach to this problem, which will hopefully be solved in the next release.

To use McStas, an instrument definition file describing the instrument to be simulated must be written. Alternatively, an example instrument file can be obtained from the `examples/` directory in the distribution or from another source.

The structure of McStas is illustrated in Figure 4.1.

The input files (instrument and component files) are written in the McStas meta-language and are edited either by using your favourite editor or by using the built in editor of the graphical user interface (`mcgui`).

Next, the instrument and component files are compiled using the McStas compiler using the FLEX and Bison facilities to produce a C program[1].

The resulting C program can then be compiled with a C compiler and run in combination with various front-end programs for example to present the intensity at the detector as a motor position is varied.

The output data may be analyzed in the same way as regular experiments are analyzed by using Matlab, Scilab [10] or IDL or by using the Perl routines included in McStas.

4.1 Brief introduction to the graphical user interface

This section gives an ultra-brief overview of how to use McStas once it has been properly installed. It is intended for those who do not read manuals if they can avoid it. For details on the different steps, see the following sections. This section uses the `vanadium_example.instr` file supplied in the `examples/` directory of the McStas distribution.

To start the graphical user interface of McStas, run the command `mcgui` (`mcgui.pl` on Windows). This will open a window with some menus etc., see figure 4.2.

[1] Note that since release 1.7 of McStas, FLEX and Bison need not be installed on your computer.

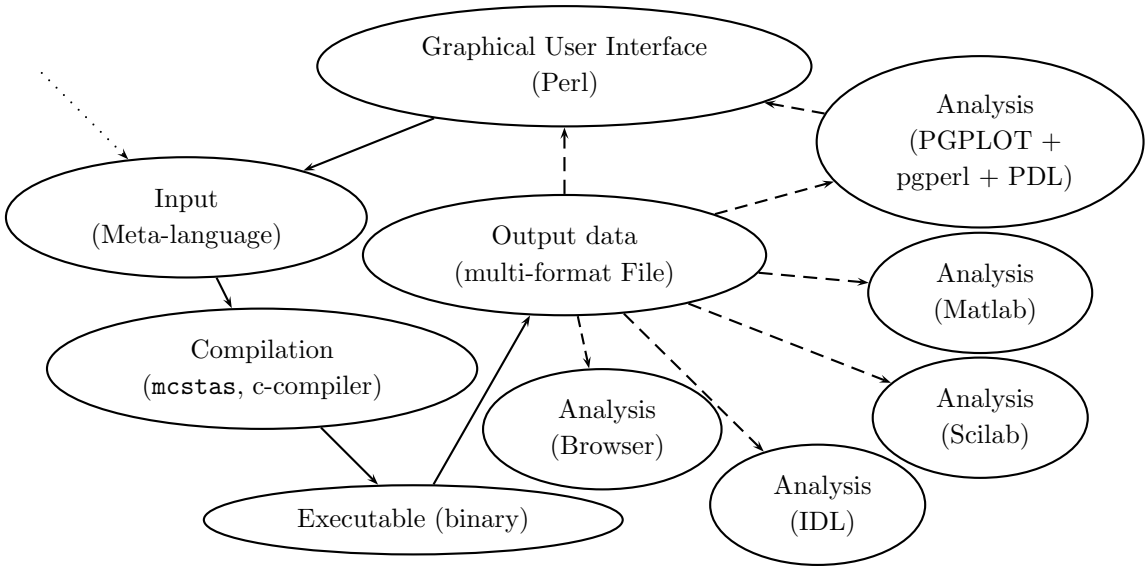

Figure 4.1: An illustration of the structure of McStas .

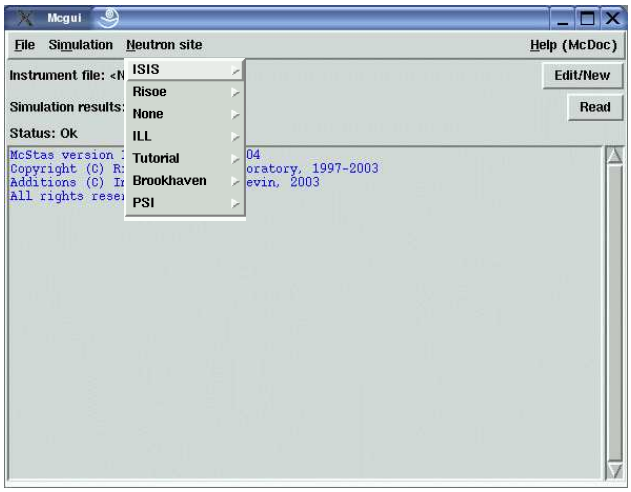

Figure 4.2: The graphical user interface `mcgui`.

To load an instrument, select “Tutorial” from the “Neutron site” menu and open the file `vanadium_example`. Next, check that the current plotting backend setting (select “Choose backend” from the “Simulation” menu) corresponds to your system setup. The default setting can be adjusted as explained in Chapter 3

- by editing the `tools/perl/mcstas_config.perl` setup file of your installation
- by setting the `MCSTAS_FORMAT` environment variable.

Next, select “Run simulation” from the “Simulation” menu. McStas will translate the definition into an executable program and pop up a dialog window. Type a value for the “ROT” parameter (*e.g.* 90), check the “Plot results” option, and select “Start”. The simulation will run, and when it finishes after a while the results will be plotted in a window. Depending on your chosen plotting backend, the presented graphics will resemble one of those shown in figure 4.3. When using the Scilab or Matlab backends, full 3D view

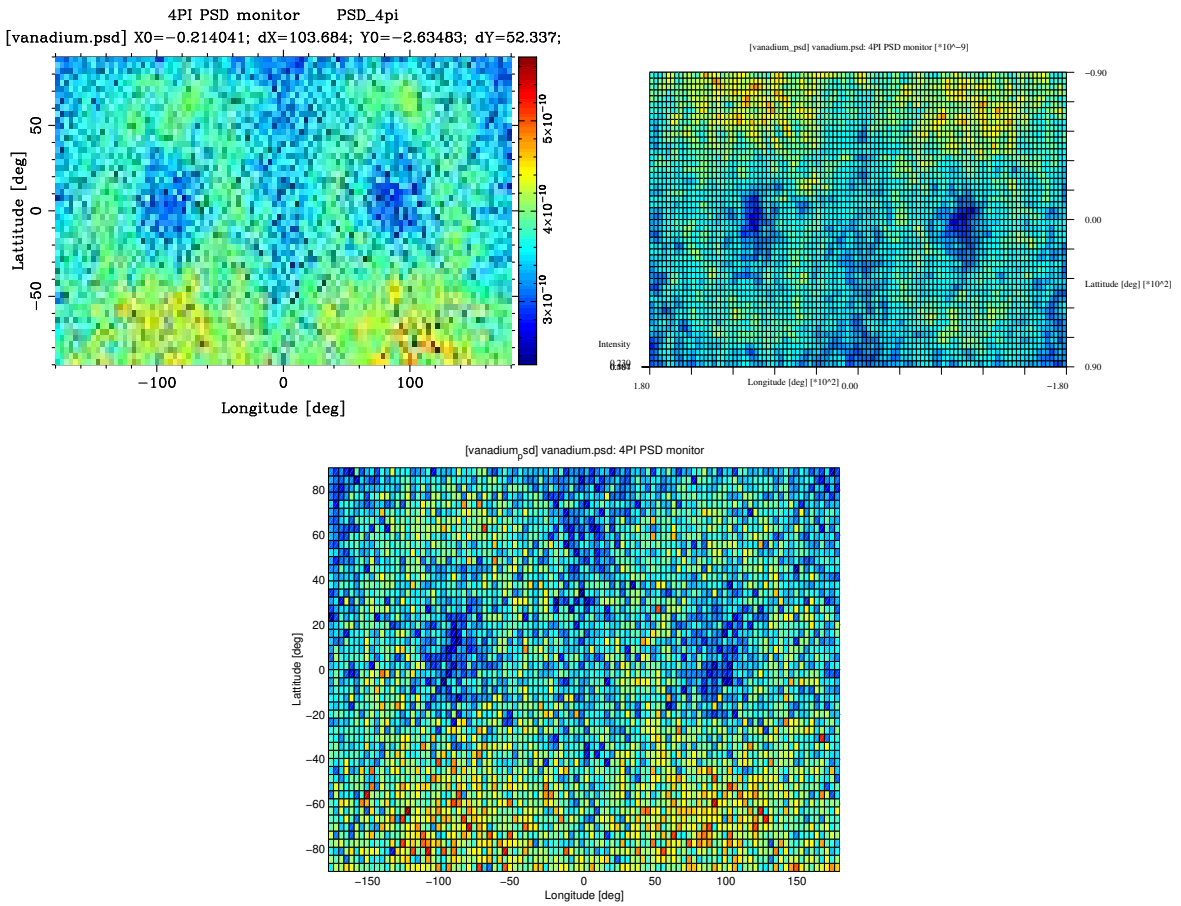

Figure 4.3: Output from `mcplot` with PGPLOT, Scilab and Matlab backends

of plots and different display possibilities are available. Use the attached McStas window menus to control these. Features are quite self explanatory. For other options, execute `mcplot --help` (`mcplot.pl --help` on windows) to get help.

To debug the simulation graphically, repeat the steps but check the “Trace” option instead of the “Simulate” option. A window will pop up showing a sketch of the instrument. Depending on your chosen plotting backend, the presented graphics will resemble one of those shown in figures 4.4-4.6.

For a slightly longer gentle introduction to McStas, see the McStas tutorial (available from [2]), and as of version 1.8 built into the `mcgui` help menu. For more technical details, read on from section 4.2

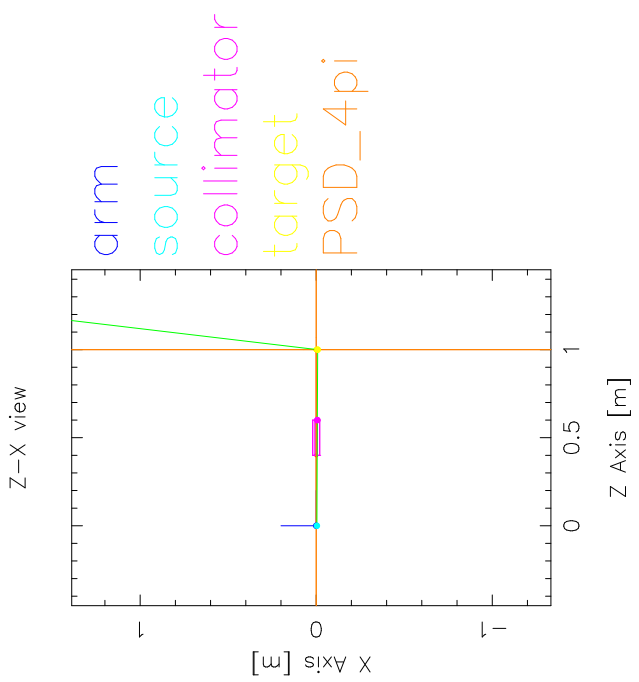

Figure 4.4: Output from `mcdisplay` with PGPLOT backend. The left mouse button starts a new neutron, the middle button zooms, and the right button resets the zoom. The Q key quits the program.

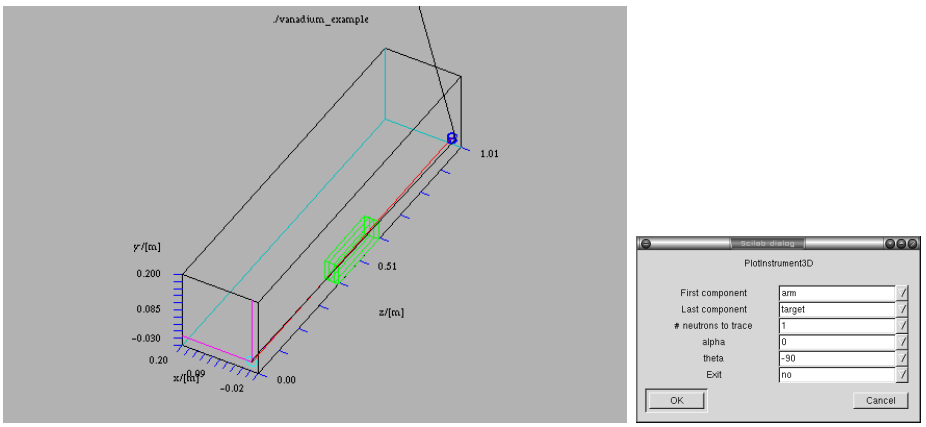

Figure 4.5: Output from `mcdisplay` with Scilab backend. Display can be adjusted using the dialogbox (right).

4.1.1 New releases of McStas

Releases of new versions of a software can today be carried out more or less continuously. However, users do not update their software on a daily basis, and as a compromise we have adopted the following policy of McStas .

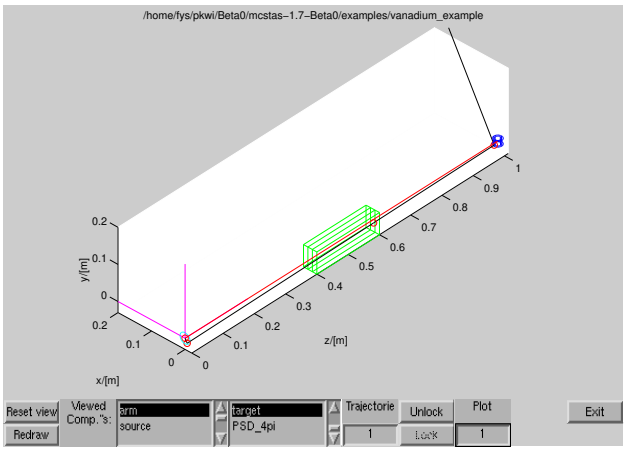

Figure 4.6: Output from `mcdisplay` with Matlab backend. Display can be adjusted using the window buttons.

- A version 1.8.x will contain bug fixes and new functionality. A new manual will, however, not be released and the modifications are documented on the McStas webpage. The extensions of the forthcoming version 1.8.x are also listed on the web, and new versions may be released quite frequently when it is requested by the user community.

- A version 1.9 will contain an updated manual. It will typically be released once or twice a year in connection to for example a McStas workshop.

4.2 Running the instrument compiler

This section describes how to run the McStas compiler manually. Often, it will be more convenient to use the front-end program `mcgui` (section 4.4.1) or `mcrun` (section 4.4.2). These front-ends will compile and run the simulations automatically.

The compiler for the McStas instrument definition is invoked by typing a command of the form

```
mcstas name.instr
```

This will read the instrument definition `name.instr` which is written in the McStas metalanguage. The compiler will translate the instrument definition into a Monte Carlo simulation program provided in ANSI-C. The output is by default written to a file in the current directory with the same name as the instrument file, but with extension `.c` rather than `.instr`. This can be overridden using the `-o` option as follows:

```
mcstas -o code.c name.instr
```

which gives the output in the file `code.c`. A single dash '`-`' may be used for both input and output filename to represent standard input and standard output, respectively.

4.2.1 Code generation options

By default, the output files from the McStas compiler are in ANSI-C with some extensions (currently the only extension is the creation of new directories, which is not possible in pure ANSI-C). The use of extensions may be disabled with the `-p` or `--portable` option. With this option, the output is strictly ANSI-C compliant, at the cost of some slight reduction in capabilities.

The `-t` or `--trace` option puts special "trace" code in the output. This code makes it possible to get a complete trace of the path of every neutron through the instrument, as well as the position and orientation of every component. This option is mainly used with the `mcdisplay` front-end as described in section 4.4.4.

The code generation options can also be controlled by using preprocessor macros in the C compiler, without the need to re-run the McStas compiler. If the preprocessor macro `MC_PORTABLE` is defined, the same result is obtained as with the `--portable` option of the McStas compiler. The effect of the `--trace` option may be obtained by defining the `MC_TRACE_ENABLED` macro. Most Unix-like C compilers allow preprocessor macros to be defined using the `-D` option, eg.

```
cc -DMC_TRACE_ENABLED -DMC_PORTABLE ...
```

Finally, the `--verbose` option will list the components and libraries beeing included in the instrument.

4.2.2 Specifying the location of files

The McStas compiler needs to be able to find various files during compilation, some explicitly requested by the user (such as component definitions and files referenced by `%include`), and some used internally to generate the simulation executable. McStas looks for these files in three places: first in the current directory, then in a list of directories given by the user, and finally in a special McStas directory. Usually, the user will not need to worry about this as McStas will automatically find the required files. But if users build their own component library in a separate directory or if McStas is installed in an unusual way, it will be necessary to tell the compiler where to look for the files.

The location of the special McStas directory is set when McStas is compiled. It defaults to `/usr/local/lib/mcstas` on Unix-like systems and `C:\mcstas\lib` on Windows systems, but it can be changed to something else, see section 3 for details. The location can be overridden by setting the environment variable `MCSTAS`:

```
setenv MCSTAS /home/joe/mcstas
```

for csh/tcsh users, or

```
export MCSTAS=/home/joe/mcstas
```

for bash/Bourne shell users. For Windows Users, you should define the `MCSTAS` from the menu 'Start/Settings/Control Panel/System/Advanced/Environment Variables' by creating `MCSTAS` with the value `C:\mcstas\lib`

To make McStas search additional directories for component definitions and include files, use the `-I` switch for the McStas compiler:

```
mcstas -I/home/joe/components -I/home/joe/neutron/include name.instr
```

Multiple `-I` options can be given, as shown.

4.2.3 Embedding the generated simulations in other programs

By default, McStas will generate a stand-alone C program, which is what is needed in most cases. However, for advanced usage, such as embedding the generated simulation in another program or even including two or more simulations in the same program, a stand-alone program is not appropriate. For such usage, the McStas compiler provides the following options:

- `--no-main` This option makes McStas omit the `main()` function in the generated simulation program. The user must then arrange for the function `mcstas_main()` to be called in some way.
- `--no-runtime` Normally, the generated simulation program contains all the run-time C code necessary for declaring functions, variables, etc. used during the simulation. This option makes McStas omit the run-time code from the generated simulation program, and the user must then explicitly link with the file `mcstas-r.c` as well as other shared libraries from the McStas distribution.

Users that need these options are encouraged to contact the authors for further help.

4.2.4 Running the C compiler

After the source code for the simulation program has been generated with the McStas compiler, it must be compiled with the C compiler to produce an executable. The generated C code obeys the ANSI-C standard, so it should be easy to compile it using any ANSI-C (or C++) compiler. *E.g.* a typical Unix-style command would be

```
cc -O -o name.out name.c -lm
```

The `-O` option typically enables the optimization phase of the compiler, which can make quite a difference in speed of McStas generated simulations. The `-o name.out` sets the name of the generated executable. The `-lm` options is needed on many systems to link in the math runtime library (like the cos() and sin() functions).

Monte Carlo simulations are computationally intensive, and it is often desirable to have them run as fast as possible. Some success can be obtained by adjusting the compiler optimization options. Here are some example platform and compiler combinations that have been found to perform well (up-to-date information will be available on the McStas WWW home page [2]):

- Intel x86 ("PC") with Linux and GCC, using options `gcc -O3`.
- Intel x86 with Linux and EGCS (GCC derivate) using options `egcc -O6`.
- Intel x86 with Linux and PGCC (pentium-optimized GCC derivate), using options `gcc -O6 -mstack-align-double`.

- HPPA machines running HPUX with the optional ANSI-C compiler, using the options `-Aa +Oall -Wl,-a,archive` (the `-Aa` option is necessary to enable the ANSI-C standard).
- SGI machines running Irix with the options `-Ofast -o32 -w`

A warning is in place here: it is tempting to spend far more time fiddling with compiler options and benchmarking than is actually saved in computation times. Even worse, compiler optimizations are notoriously buggy; the options given above for PGCC on Linux and the ANSI-C compiler for HPUX have been known to generate *incorrect code* in some compiler versions. McStas actually puts an effort into making the task of the C compiler easier, by in-lining code and using variables in an efficient way. As a result, McStas simulations generally run quite fast, often fast enough that further optimizations are not worthwhile. Also, optimizations are higly time and memory consuming during compilation, and thus may fail when dealing with large instrument descriptions (e.g. more that 100 elements). The compilation process is simplified when using components of the library making use of shared libraries (see `SHARE` keyword in chapter 5).

4.3 Running the simulations

Once the simulation program has been generated by the McStas compiler and an executable has been obtained with the C compiler, the simulation can be run in various ways. The simplest way is to run it directly from the command line or shell:

```
./name.out
```

Note the leading dot, which is needed if the current directory is not in the path searched by the shell. When used in this way, the simulation will prompt for the values of any instrument parameters such as motor positions, and then run the simulation. Default instrument parameter values (see section 5.3), if any, will be indicated and entered when hitting the `Return` key. This way of running McStas will only give data for one spectrometer setting which is normally sufficient *e.g.* for a time-of-flight spectrometer, but not for a triple-axis spectrometer where a scan over various spectrometer settings is required. Often the simulation will be run using one of several available front-ends, as described in the next section. These front-ends help manage output from the potentially many detectors in the instruments, as well as running the simulation for each data point in a scan.

The generated simulations accept a number of options and arguments. The full list can be obtained using the `--help` option:

```
./name.out --help
```

The values of instrument parameters may be specified as arguments using the syntax *name=val*. For example

```
./vanadium_example.out ROT=90
```

The number of neutron histories to simulate may be set using the `--ncount` or `-n` option, for example `--ncount=2e5`. The initial seed for the random number generator is by default chosen based on the current time so that it is different for each run. However, for debugging

purposes it is sometimes convenient to use the same seed for several runs, so that the same sequence of random numbers is used each time. To achieve this, the random seed may be set using the `--seed` or `-s` option.

By default, McStas simulations write their results into several data files in the current directory, overwriting any previous files stored there. The `--dir=`*dir* or `-d`*dir* option causes the files to be placed instead in a newly created directory *dir* (to prevent overwriting previous results an error message is given if the directory already exists). Alternatively, all output may be written to a single file *file* using the `--file=`*file* or `-f`*file* option (which should probably be avoided when saving in binary format, see below).

The complete list of options and arguments accepted by McStas simulations appears in table 4.1.

4.3.1 Choosing a data file format

Data files contain header lines with information about the simulation from which they originate. In case the data must be analyzed with programs that cannot read files with such headers, they may be turned off using the `--data-only` or `-a` option.

The format of the output files from McStas simulations is described in more detail in section 4.5. It may be chosen either with `--format=FORMAT` for each simulation or globally by setting the MCSTAS_FORMAT environment variable. The available format list is obtained using the `name.out --help` option, and shown in table 4.2. McStas can presently generate many formats, including the original McStas/PGPLOT and the new Scilab and Matlab formats. All formats, except the McStas/PGPLOT, may eventually support binary files, which are much smaller and faster to import, but are platform dependent. The simulation data file extensions are appended automatically, depending on the format. For example:

```
./vanadium_example.out ROT=90 --format="Scilab_binary"
```

or more generally (for bash/Bourne shell users)

```
export MCSTAS_FORMAT="Matlab"
./vanadium_example.out ROT=90
```

4.3.2 Basic import and plot of results

The previous example will result in a `mcstas.m` file, that may be read directly from Matlab (using the *sim file* function)

```
matlab> s=mcstas;
matlab> s=mcstas('plot')
```

The first line returns the simulation data as a single structure variable, whereas the second one will additionally plot each detector separately. This also equivalently stands for Scilab (using the `get_`*sim file* function, the 'exec' call is required in order to compile the code)

```
scilab> exec('mcstas.sci', -1); s=get_mcstas();
scilab> exec('mcstas.sci', -1); s=get_mcstas('plot')
```

and for IDL

`-s` *seed* `--seed=`*seed*	Set the initial seed for the random number generator. This may be useful for testing to make each run use the same random number sequence.
`-n` *count* `--ncount=`*count*	Set the number of neutron histories to simulate. The default is 1,000,000.
`-d` *dir* `--dir=`*dir*	Create a new directory *dir* and put all data files in that directory.
`-f` *file* `--file=`*file*	Write all data into a single file *file*. Avoid when using binary formats.
`-a` `--data-only`	Do not put any headers in the data files.
`-h` `--help`	Show a short help message with the options accepted, available formats and the names of the parameters of the instrument.
`-i` `--info`	Show extensive information on the simulation and the instrument definition it was generated from.
`-t` `--trace`	This option makes the simulation output the state of every neutron as it passes through every component. Requires that the `-t` (or `--trace`) option is also given to the McStas compiler when the simulation is generated.
`--no-output-files`	This option disables the writing of data files (output to the terminal, such as detector intensities, will still be written).
`-g` `--gravitation`	This option toggles the gravitation handling for the whole neutron propagation within the instrument.
`--format=`*FORMAT*	This option sets the data format for result files from monitors
param=*value*	Set the value of an instrument parameter, rather than having to prompt for each one.

Table 4.1: Options accepted by McStas simulations

```
idl> s=mcstas()
idl> s=mcstas(/plot)
```

See section 4.4.5 for an other way of plotting simulation results using the `mcplot` front-end.

4.3.3 Interacting with a running simulation

Once the simulation has started, it is possible, under Unix, Linux and Mac OS X systems, to interact with the on-going simulation.

McStas attaches a signal handler to the simulation process. In order to send a signal to the process, the process-id *pid* must be known. Users may look at their running processes with the Unix 'ps' command, or alternatively process managers like 'top' and 'gtop'. If a *file.out* simulation obtained from McStas is running, the process status command should output a line ressembling

```
<user> 13277 7140 99 23:52 pts/2    00:00:13 file.out
```

`McStas`	.sim	Original format for PGPLOT plotter (may be used with -f and -d options)
`PGPLOT`		
`Scilab`	.sci	Scilab format (may be used with -f and -d options)
`Scilab_binary`		Scilab format with external binary files (may be used with -d option). Also toggles -a option.
`Matlab`	.m	Matlab format (may be used with -f and -d options)
`Matlab_binary`		Matlab format with external binary files (may be used with -d option). Also toggles -a option.
`IDL`	.pro	IDL format. *Must* be used with -f option.
`IDL_binary`		IDL format with external binary files (may be used with -d option). Also toggles -a option.
`XML`	.xml	XML/NeXus format (may be used with -f and -d options).
`HTML`	.html	HTML format (generates a web page, may be used with -f and -d options).

Table 4.2: Available formats supported by McStas simulations.

where `user` is your loggin name. The *pid* is there '13277'.

Once known, it is possible to send one of the signals listed in table 4.3 using the 'kill' unix command (or the functionalities of your process manager), e.g.

```
kill -USR2 13277
```

This will result in a message showing status (here 33 % achieved), as well as the position in the instrument of the current neutron.

```
# McStas: [pid 13277] Signal 12 detected SIGUSR2 (Save simulation)
# Simulation: file (file.instr)
# Breakpoint: MyDetector (Trace) 33.37 % (  333654.0/ 1000000.0)
# Date      : Wed May  7 00:00:52 2003
# McStas: Saving data and resume simulation (continue)
```

followed by the list of detector outputs (integrated counts and files). Finally, sending a `kill 13277` (which is equivalent to `kill -TERM 13277`) will end the simulation before the initial 'ncount' preset.

A typical usage example would be, for instance, to save data during a simulation, plot or analyze it, and decide to interupt the simulation earlier if the desired statistics has been achieved. This may be done automatically using the `Progress_bar` component.

Whenever simulation data is generated before end (or the simulation is interupted), the 'ratio' field of the monitored data will provide the level of achievement of the computation (for instance '3.33e+05/1e+06');

Additionally, any system error will result in similar messages, giving indication about the occurence of the error (in which component ? in which section ?). Whenever possible, the simulation will *try* to save the data before ending. Most errors appear when writing a new component, in the `INITIALIZE`, `TRACE` or `FINALLY` sections. Memory errors usually

`USR1`	Request informations (status)
`USR2`	Request informations and performs an intermediate saving of all monitors (status and save). This triggers the execution of all `SAVE` sections (see chapter 5).
`INT, TERM`	Save and exit before end (status)

Table 4.3: Signals supported by McStas simulations.

show up when C pointers have not been allocated/unallocated before usage, whereas mathematical errors are set when, for instance, dividing per zero.

4.3.4 Optimizing a simulation

There are various other ways to speed-up a simulation

- Optimize the compilation of the instrument, as explained in section 4.2.4.
- Divide simulation into parts using a file for saving or generating neutron events. This way, a guide may be simulated only once, saving the neutron events getting out from it as a file, which is being read quickly by the second simulation part. Use the Virtual_input and Virtual_output components for this technique.
- Use source optimizers like the components Source_adapt or Source_Optimizer. Such component may sometimes not be very efficient, when no neutron importance sampling can be achieved, or may even sometimes alter the simulation results. Be careful and always check results with a non-optimized computation.
- Complex components usually take into account additional small effects in a simulation, but are much longer to execute. Thus, simple components should be prefered whenever possible, at least to start with.

Additionally, the user may wish to optimize the parameters of a simulation (e.g. find the optimal curvature of a monochromator, or the best geometry of a given component). The user should write a function script or a program that

- inputs the simulation parameters, which are usually numerical values such as TT in the `prisma2` instrument from the `examples` directory of the package.
- builds a command line from these parameters.
- execute that command, and waits until the end of the computation.
- reads the relevant data from the monitors.
- outputs a simulation quality measurement from this data, usually the integrated counts or some peak width.

For instance, for the `prisma2` instrument we could write a function for Matlab (see section 4.5 for details about the Matlab data format) in order to study the effects of the TT parameter:

```
function y = instr_value(p)
  TT = p(1);     % p may be a vector/matrix containing many parameters
  syscmd = [ 'mcrun prisma2.instr -n1e5 TT=' num2str(TT) ...
             ' PHA=22 PHA1=-3 PHA2=-2 PHA3=-1 PHA4=0 PHA5=1' ...
             ' PHA6=2 PHA7=3 TTA=44 --format="Matlab binary"' ];
  system(syscmd); path(path) % execute simulation, and rehash files
  s = mcstas;     % get the simulation data, and the monitor data
  s = s.prisma2.m_mcstas.detector.prisma2_tof.signal;
  eval(s);        % we could also use the 'statistics' field
  y = -Mean;      % 'value' of the simulation
```

Then a numerical optimization should be available, such as those provided with Matlab, Scilab, IDL, and Perl-PDL high level languages. In this example, we may wish to maximize the `instr_value` function value. The `fminsearch` function of Matlab is a minimization method (that's why we have a minus sign for y value), and:

```
matlab> TT = fminsearch('instr_value', -25)
```

will determine the best value of TT, starting from -25 estimate, in order to minimize function `instr_value`, and thus maximize the mean detector counts.

The choice of the optimization routine, of the simulation quality value to optimize and the initial parameter guess all may have a large influence on the results. Be cautious and wise when interpreting the optimal guess.

4.4 Using simulation front-ends

McStas includes a number of front-end programs that extend the functionality of the simulations. A front-end program is an interface between the user and the simulations, running the simulations and presenting the output in various ways to the user.

The list of available McStas front-end programs may be obtained from the `mcdoc --tools` command:

```
McStas Tools
   mcstas        Main instrument compiler
   mcrun         Instrument maker and execution utility
   mcgui         Graphical User Interface instrument builder
   mcdoc         Component library documentation generator/viewer
   mcplot        Simulation result viewer
   mcdisplay     Instrument geometry viewer
   mcresplot     Instrument resolution function viewer
   mcstas2vitess McStas to Vitess component translation utility
   mcconvert     Matlab <-> Scilab script conversion tool
When used with the -h flag, all tools display a specific help.
SEE ALSO: mcstas, mcdoc, mcplot, mcrun, mcgui, mcresplot, mcstas2vitess
DOC:      Please visit http://neutron.risoe.dk/mcstas/
```

An extended set of front-end programs is planned for future versions of McStas, including a NeXus data format option [11].

4.4.1 The graphical user interface (mcgui)

The front-end `mcgui` provides a graphical user interface that interfaces the various parts of the McStas package. It is started using simply the command

```
mcgui
```

The mcgui (mcgui.pl on Windows) program may optionally be given the name of an instrument file.

When the front-end is started, a main window is opened (se figure 4.2). This window displays the output from compiling and running simulations, and also contains a few menus and buttons. The main purpose of the front-end is to edit and compile instrument definitions, run the simulations, and visualize the results.

The menus

The "File" menu has the following features:

Open instrument selects the name of an instrument file to be used.

Edit current opens a simple editor window for editing the current instrument definition. This function is also available from the "Edit" button to the right of the name of the instrument definition in the main window.

Spawn editor This starts the editor defined in the environment variable `VISUAL` or `EDITOR` on the current instrument file. It is also possible to start an external editor manually; in any case `mcgui` will recompile instrument definitions as necessary based on the modification dates of the files on the disk.

Compile instrument forces a recompile of the instrument definition, regardless of file dates. This is for example useful to pick up changes in component definitions, which the front-end will not notice automatically. See section 3 for how to override default C compiler options.

Clear output erases all text in the window showing output of compilations and simulations.

Quit exits the graphical user interface front-end.

The "Simulation" menu has the following features:

Read old simulation prompts for the name of a file from a previous run of a McStas simulation (usually called `mcstas.sim`). The file will be read and any detector data plotted using the `mcplot` front-end. The parameters used in the simulation will also be made the defaults for the next simulation run. This function is also available using the "Read" button to the right of the name of the current simulation data.

Run simulation opens the run dialog window, explained further below.

Plot results plots (using `mcplot`) the results of the last simulation run or loaded.

Choose backend selection of plotting backend (PGPLOT/Matlab/Scilab). Opens the choose backend dialog shown in figure 4.7. All formats are chosen as full text, but a 'Use binary files' option is possible.

The "Neutron Site" menu contains a list of template/example instruments as found in the McStas library, sorted by neutron site. When selecting one of these, a local copy of the instrument description is transfered to the active directory (so that users have modification rights). One may then view its source (Edit) and use it directly for simulations/trace (3D View).

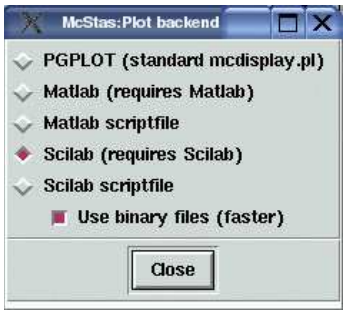

Figure 4.7: The choose backend dialog in `mcgui`.

The "Help" menu has the following features, through use of `mcdoc` and a web browser. To customize the used web browser, set the `BROWSER` environment variable. If `BROWSER` is not set, `mcgui` uses `netscape` on Unix and the default browser on Windows.

McStas web page calls `mcdoc --web`, brings up the McStas website in a web browser.

McStas User manual calls `mcdoc --manual`, brings up the local pdf version of this manual, using a web browser.

McStas Component manual calls `mcdoc --comp`, brings up the local pdf version of the component manual, using a web browser.

Component doc index displays the component documentation using the component `index.html` index file.

Generate component index (re-)generates locally the component `index.html`.

Test McStas installtion launches a self test procedure to check that the McStas package is installed properly, generates accurate results, and may use the plotter to display the results.

single menu point, "McStas web-page", which attempts to open a Netscape window with the McStas web-page. This obviously requires that Netscape is properly installed on the computer.

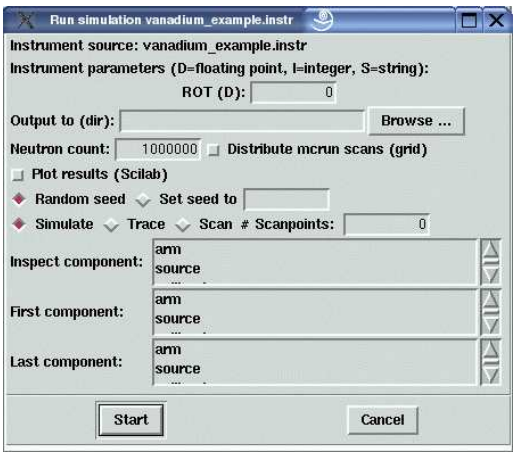

Figure 4.8: The run dialog in `mcgui`.

The run dialog

The run dialog is used to run simulations. It allows the entry of instrument parameters as well as the specifications of options for running the simulation (see section 4.3 for details). It also allows to run the `mcdisplay` (section 4.4.4) and `mcplot` (section 4.4.5) front-ends together with the simulation.

The meaning of the different fields is as follows:

Instrument parameters allows the setting of the values for the input parameters of the instrument. The type of each instrument parameter is given in parenthesis after each name. Floating point numbers are denoted by (D) (for the C type "`double`"), (I) denotes integer parameters, and (S) denotes strings.

Output to allows the entry of a directory to store the resulting data files in (like the `--dir` option). If no name is given, the results are put in the current directory, to be overwritten by the next simulation.

Neutron count sets the number of neutron histories to simulate (the `--ncount` option).

Distribute mcrun scans (grid) is an experimental option to distribute scan steps on a set of machines using *ssh* connexions. To use this option you will need

- A set of unix machines of the same architecture (binary compatible).
- `ssh` access from the master node (where McStas is installed) to the slaves through e.g. dsa keys *without* a password.
- The machine names listed in the file `.mcstas-hosts` in your home directory on the master node, one node pr. line.

Warning: This option is considered *experimental* - i.e., you are welcome to use it, but be ready for trouble. Note also that this is a unix only option in `mcgui`, it **does not** work on windows.

Plot results – if checked, the `mcplot` front-end will be run after the simulation has finished, and the plot dialog will pop up (see below).

Random seed/Set seed to selects between using a random seed (different in each simulation) for the random number generator, or using a fixed seed (to reproduce results for debugging).

Simulate/Trace selects between running the simulation normally, or using the `mcdisplay` front-end.

Inspect component will trace neutron trajectories that only reach a given component (e.g. sample or detector).

First component seletcs the first component to plot (default is first) in order to define a region of interest.

Last component seletcs the last component to plot (default is first) in order to define a region of interest.

Start runs the simulation.

Cancel aborts the dialog.

Before running the simulation, the instrument definition is automatically compiled if it is newer than the generated C file (or if the C file is newer than the executable). The executable is assumed to have a `.out` suffix in the filename.

The plot dialog

This dialog only shows-up when using the McStas/PGPLOT plotter. Other plotters have attached menus to control graphics and file exports.

Monitors and detectors lists all the one- and two-dimensional detectors in the instrument. By double-clicking, one plots the data in the plot window.

Plot plots the selected detector in the plot window, just like double-clicking its name.

Overview plot plots all the detectors together in the plot window.

B&W postscript prompts for a file name and saves the current plot as a black and white postscript file. This can subsequently be printed on a postscript printer.

Colour postscript creates a colour postscript file of the current plot.

Colour GIF creates a colour GIF file of the current plot.

Close ends the dialog.

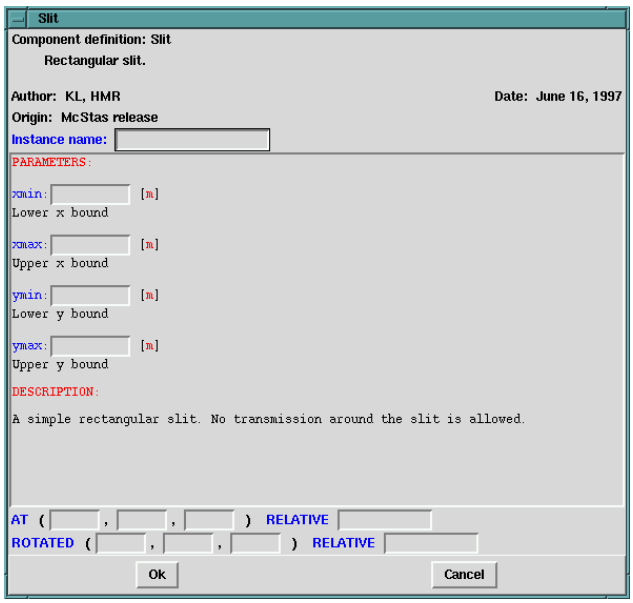

Figure 4.9: Component parameter entry dialog.

The editor window

The editor window provides a simple editor for creating and modifying instrument definitions. Apart from the usual editor functions, the "Insert" menu provides some functions that aid in the construction of the instrument definitions:

Instrument template inserts the text for a simple instrument skeleton in the editor window.

Component... opens up a dialog window with a list of all the components available for use in McStas. Selecting a component will display a description. Double-clicking will open up a dialog window allowing the entry of the values of all the parameters for the component (figure 4.9). See section 5.3 for details of the meaning of the different fields.

The dialog will also pick up those of the users own components that are present in the current directory when `mcgui` is started. See section 5.4.11 for how to write components to integrate well with this facility.

Type These menu entries give quick access to the entry dialog for the various components available.

To use the `mcgui` front-end, the programs Perl and Perl/Tk must be properly installed on the system.

Additionally, if the McStas/PGPLOT back-end is used for data format, PGPLOT, PgPerl, and PDL will be required. It may be necessary to set the `PGPLOT_DIR` and `PGPLOT_DEV` environment variable; consult the documentation for PGPLOT on the local system in case of difficulty.

4.4.2 Running simulations with automatic compilation (mcrun)

The `mcrun` front-end (mcrun.pl on Windows) provides a convenient command-line interface for running simulations with the same automatic compilation features available in the `mcgui` front-end. It also provides a facility for running a series of simulations while varying an input parameter, thereby replacing the old `gscan` front-end.

The command

`mcrun` *sim args* `...`

will compile the instrument definition *sim*`.instr` (if necessary) into an executable simulation *sim*`.out`. It will then run *sim*`.out`, passing the argument list *args*

The possible arguments are the same as those accepted by the simulations themselves as described in section 4.3, with the following extensions:

- The `-c` or `--force-compile` option may be used to force the recompilation of the instrument definition, regardless of file dates. This may be needed in case any component definitions are changed (in which case `mcrun` does not automatically recompile), or if a new version of McStas has been installed.

- The `-p` *file* or `--param=`*file* option may be used to specify a file containing assignment of values to the input parameters of the instrument definition. The file should consist of specifications of the form *name*`=`*value* separated by spaces or line breaks. Multiple `-p` options may be given together with direct parameter specifications on the command line. If a parameter is assigned multiple times, later assignments override previous ones.

- The `-N` *count* or `--numpoints=`*count* option may be used to perform a series of *count* simulations while varying one or more parameters within specified intervals. Such a series of simulations is called a *scan*. To specify an interval for a parameter X, it should be assigned two values separated with a comma. For example, the command

  ```
  mcrun sim.instr -N4 X=2,8 Y=1
  ```

  would run the simulation defined in `sim.instr` four times, with X having the values 2, 4, 6, and 8, respectively.

  After running the simulation, the results will be written to the file `mcstas.dat` by default. This file contains one line for each simulation run giving the values of the scanned input variables along with the intensity and estimated error in all detectors. Additionally, a file `mcstas.sci` (when using Scialb format) is written that can be read by the `mcplot` front-end to plot the results on the screen or in a Postscript file, see section 4.4.5.

- When doing a scan, the `-f` *file* and `--file=`*file* options make `mcrun` write the output to the files *file*`.dat` and *file*`.sim` instead of the default names.

- When doing a scan, the `-d` *dir* and `--dir=`*dir* options make `mcrun` put all output in a newly created directory *dir*. Additionally, the directory will have subdirectories `1`, `2`, `3`,... containing all data files output from the different simulations. When the

`-d` option is not used, no data files are written from the individual simulations (in order to save disk space).

- The `mcrun --test` command will test your McStas installation, accuracy and plotter.

The `-h` option will list valid options. The `mcrun` front-end requires a working installation of Perl to run.

4.4.3 The `gscan` front-end

The front-end `gscan` is obsolete from version 1.3 of McStas, and is included only for backwards compatibility. The front-end `mcrun` (section 4.4.2) includes all the functionality of the old `gscan` front-end and should be used instead.

4.4.4 Graphical display of simulations (mcdisplay)

The front-end `mcdisplay` (mcdisplay.pl on Windows) is a graphical debugging tool. It presents a schematic drawing of the instrument definition, showing the position of the components and the paths of the simulated neutrons through the instrument. It is thus very useful for debugging a simulation, for example to spot components in the wrong position or to find out where neutrons are getting lost.

To use the `mcdisplay` front-end with a simulation, run it as follows:

```
mcdisplay sim args ...
```

where `sim` is the name of either the instrument source *sim*`.instr` or the simulation program *sim*`.out` generated with McStas, and *args ...* are the normal command line arguments for the simulation, as explained above. The `-h` option will list valid options.

The drawing back-end program may be selected among PGPLOT, Matlab and Scilab using either the -p*PLOTTER* option or using the current `MCSTAS_FORMAT` environment variable. For instance, calling

```
mcdisplay -pScilab ./vanadium_example.out ROT=90
```

or (`csh`/`tcsh` syntax)

```
setenv MCSTAS_FORMAT Scilab
mcdisplay ./vanadium_example.out ROT=90
```

will output graphics using Scilab. The `mcdisplay` front-end can also be run from the `mcgui` front-end. Examples of plotter appearence for `mcdisplay` is shown in figures 4.4-4.6.

McStas/PGPLOT back-end This will view the instrument from above. A multi-display that shows the instrument from three directions simultaneously can be shown using the `--multi` option:

```
mcdisplay --multi sim.out args ...
```

Click the left mouse button in the graphics window or hit the space key to see the display of successive neutron trajectories. The 'P' key saves a postscript file containing the current display that can be sent to the printer to obtain a hardcopy; the 'C' key produces color postscript. To stop the simulation prematurely, type 'Q' or use control-C as normal in the window in which `mcdisplay` was started.

To see details in the instrument, it is possible to zoom in on a part of the instrument using the middle mouse button (or the 'Z' key on systems with a one- or two-button mouse). The right mouse button (or the 'X' key) resets the zoom. Note that after zooming, the units on the different axes may no longer be equal, and thus the angles as seen on the display may not match the actual angles.

Another way to see details while maintaining an overview of the instrument is to use the `--zoom=`*factor* option. This magnifies the display of each component along the selected axis only, *e.g.* a Soller collimator is magnified perpendicular to the neutron beam but not along it. This option may produce rather strange visual effects as the neutron passes between components with different coordinate magnifications, but it is occasionally useful.

When debugging, it is often the case that one is interested only in neutrons that reach a particular component in the instrument. For example, if there is a problem with the sample one may prefer not to see the neutrons that are absorbed in the monochromator shielding. For these cases, the `--inspect=`*comp* option is useful. With this option, only neutrons that reach the component named *comp* are shown in the graphics display.

The `mcdisplay` front-end will then require the Perl, the PGPLOT, and the PGPerl packages to be installed. It may be necessary to set the `PGPLOT_DIR` and `PGPLOT_DEV` environment variable; consult the documentation for PGPLOT on the local system in case of difficulty.

Matlab and Scilab back-ends A 3D view of the instrument, and various operations (zoom, export, print, trace neutrons, ...) is available from dedicated Graphical User Interfaces. The `--inspect` option may be used (see previous paragraph), as well as the `--first` and `--last` options to specify a region of interest.

The `mcdisplay` front-end will then require the Perl+PGPLOT, and either Scilab or Matlab to be installed.

See section 5.4.8 for how to make new components work with the `mcdisplay` front-end.

4.4.5 Plotting the results of a simulation (mcplot)

The front-end `mcplot` (mcplot.pl on Windows) is a program that produces plots of all the detectors in a simulation, and it is thus useful to get a quick overview of the simulation results.

In the simplest case, the front-end is run simply by typing

```
mcplot
```

This will plot any simulation data stored in the current directory, which is where simulations put their results by default. If the `--dir` or `--file` options have been used (see section 4.3), the name of the file or directory should be passed to mcplot, *e.g.* "`mcplot` *dir*" or "`mcplot` *file*". It is also possible to plot one single text (not binary) data file from a given monitor, passing its name to mcplot.

The drawing back-end program may be selected among PGPLOT, Matlab and Scilab using either the -p*PLOTTER* option (e.g. `mcplot -pScilab file`) or using the current `MCSTAS_FORMAT` environment variable. Moreover, the drawing back-end program will also be set depending on the *file* extension (see table 4.2).

It should be emphasized that `mcplot` may *only* display simulation results with the format that was chosen during the computation. Indeed, if you request data in a given format from a simulation, you will only be able to display results using that same drawing back-end. Anyway, the `mcconvert` utility may convert a McStas data file between Matlab and Scilab formats (see section 4.4.9).

The `mcplot` front-end can also be run from the `mcgui` front-end.

The initial display shows plots for each detector in the simulation. Examples of plotter appearence for `mcplot` is shown in figures 4.4-4.3.

McStas/PGPLOT back-end Clicking the left mouse button on a plot produces a full-window version of that plot. The 'P' key saves a postscript file containing the current plot that can be sent to the printer to obtain a hardcopy; the 'C' key produces color postscript. The 'Q' key quits the program (or CTRL-C in the controlling terminal may be used as normal).

To use the `mcplot` front-end with PGPLOT, the programs Perl, PGPLOT, PgPerl, and PDL must all be properly installed on the system. It may be necessary to set the `PGPLOT_DIR` and `PGPLOT_DEV` environment variable; consult the documentation for PGPLOT on the local system in case of difficulty.

Matlab and Scilab back-ends A dedicated McStas/Mcplot Dialog or menu attached to the plotting window is available, and provides many operations (duplication, export, colormaps, ...). The corresponding 'mcplot' Matlab and Scilab functions may be called from these language prompt with the same method as in section 4.3, e.g:

```
matlab> s=mcplot;
matlab> help mcplot
scilab> s=mcplot();
matlab or scilab> s=mcplot('mcstas.m');
matlab or scilab> mcplot(s);
```

A full parameter scan simulation result, or simply one of its scan steps may be displayed using the 'Scan step' menu item. When the `+nw` option is specified, a separate Matlab or Scilab window will appear (instead of being launched in the current terminal). This will then enable Java support under Matlab and Tk support under Scilab, resulting in additional menus and tools.

To use the `mcplot` front-end, the programs Perl, and either Scilab or Matlab are required.

4.4.6 Plotting resolution functions (mcresplot)

The `mcresplot` front-end is used to plot the resolution function, particularly for triple-axis spectrometers, as calculated by the Res_sample component. It requires to have a Res_monitor component further in the instrument description (at the detector position).

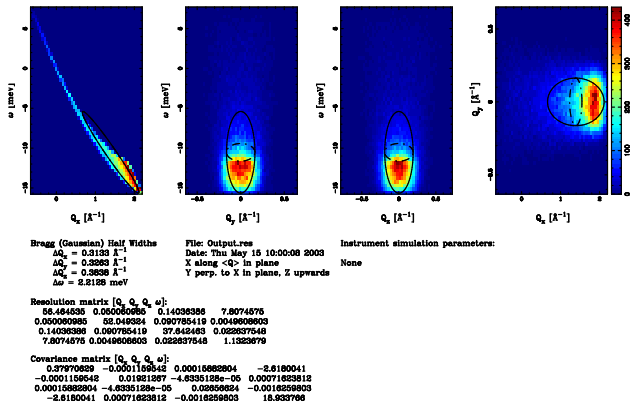

Figure 4.10: Output from `mcresplot` with PGPLOT backend. Use P, C and G keys to write hadrcopy files.

This front-end has been included in the release since it may be useful despite its somewhat rough user interface.

The `mcresplot` front-end is launched with the command

```
mcresplot file
```

Here, *file* is the name of a file output from a simulation using the Res_monitor component.

This front-end currently only works with the PGPLOT plotter, but ports for Matlab and Scilab may be written in the future.

The front-end will open a window displaying projections of the 4-dimensional resolution function $R(\boldsymbol{Q}, \omega)$. The covariance matrix of the resolution function, the resolution along each projection axis and the resulting resolution matrix are also shown, as well as the instrument name and parameters used for the simulation. This is mainly useful for triple-axis spectrometers.

To use the `mcresplot` front-end, the programs Perl, PGPLOT, PgPerl, and PDL must all be properly installed on the system.

4.4.7 Creating and viewing the library and component/instrument help (mcdoc)

McStas provides an easy way to generate automatically an HTML help page about a given component or instrument, or the whole McStas library.

```
mcdoc
mcdoc comp—instr
mcdoc -l
```

The first example generates an *index.html* catalog file using the available components and instruments (both locally, and in the McStas library. When called with the `--show` or `-s` option, the library catalog of components is opened using the `BROWSER` environment variable (e.g. netscape, konqueror, nautilus, MSIE, mozilla, ...).

Alternatively, if a component or instrument *comp* is specified, it will be searched within the library, and an HTML help will be created for all available components matching *comp*. When using the `-s`, the help will be opened. If the `BROWSER` is not defined, the help is displayed as text in the current terminal. This latter output may be forced with the `-t` or `--text` option.

The last example will list the name and action of all McStas tools (same as `--tools` option).

Additionally, the `--web`, `--manual` and `--comp` options will open the McStas web site page, the User Manual (this document) and the Component Manual, all requiring `BROWSER` to be defined. Finally, the `--help` option will display the command help, as usual.

See section 5.4.11 for more details about the McDoc usage and header format. To use the `mcdoc` front-end, the program Perl should be available.

4.4.8 Translating McStas components for Vitess (mcstas2vitess)

Any McStas component may be translated for usage with Vitess (starting from version 2.3). The syntax is simply

`mcstas2vitess` *file.comp*

This will create a Vitess module of the given component. To use the `mcstas2vitess` front-end, the program Perl should be available.

4.4.9 Translating McStas results files between Matlab and Scilab formats

If you have been running a McStas simulation with Scilab output, but finally plan to look at the results with Matlab, or the contrary, you may use

`mcconvert` *file.m—sci*

to simply translate one file format the other. This works only for the text files of course. The binary files need not be translated.

4.5 Analyzing and visualizing the simulation results

To analyze simulation results, one uses the same tools as for analyzing experimental data, *i.e.* programs such as IDL, Matlab and Scilab. The output files from simulations are usually simple text files containing headers and data blocks. If data blocks are empty they may be accessed refering to an external file indicated in the header. This file may also be a binary file (except with the original McStas/PGPLOT format), which does not contain any header (except if simulation is launched with `+a` option), but are in turn smaller in size and faster to import.

In order for the user to choose the data format, we recommand to set it *via* the MCSTAS_FORMAT environment variable, which will also make the front-end programs able to import and plot data and instrument consistently. The available format list is shown in table 4.2.

Note that the neutron event counts in detectors is typically not very meaningful except as a way to measure the performance of the simulation. Use the simulated intensity instead whenever analysing simulation data.

McStas and PGPLOT format The McStas original format, which is equivalent to the PGPLOT format, is simply columns of ASCII text that most programs should be able to read.

One-dimensional histogram detectors (time-of-flight, energy-sensitive) write one line for each histogram bin. Each line contains a number identifying the bin (*i.e.* the time-of-flight) followed by three numbers: the simulated intensity, an estimate of the statistical error as explained in section 6.1.1, and the number of neutron events for this bin.

Two-dimensional histogram detectors (position sensitive detectors) output M lines of N numbers representing neutron intensities, where M and N are the number of bins in the two dimensions. The two-dimentional detectors also store the error estimates and event counts as additional matrices.

Single-point detectors output the neutron intensity, the estimated error, and the neutron event count as numbers on the terminal. (The results from a series of simulations may be combined in a data file using the `mcrun` front-end as explained in section 4.4.2).

Both one- and two-dimentional detector output by default start with a header of comment lines, all beginning with the '`#`' character. This header gives such information as the name of the instrument used in the simulation, the values of any instrument parameters, the name of the detector component for this data file, *etc.* The headers may be disabled using the `--data-only` option in case the file must be read by a program that cannot handle the headers.

In addition to the files written for each one- and two-dimensional detector component, another file (by default named `mcstas.sim`) is also created. This file is in a special McStas ASCII format. It contains all available information about the instrument definition used for the simulation, the parameters and options used to run the simulation, and the detector components present in the instrument. It is read by the `mcplot` front-end (see section 4.4.5). This file stores the results from single detectors, but by default contains only pointers (in the form of file names) to data for one- and two-dimensional detectors. By storing data in separate files, reading the data with programs that do not know the special McStas file format is simplified. The `--file` option may be used to store all data inside the `mcstas.sim` file instead of in separate files.

Matlab, Scilab and IDL formats These formats write automatically scripts containing the data as a structure, as well as in-line import and plot functions for the selected language. Usage examples are given in section 4.3. Thus, it is not necessary to write a load routine for each format, as the script is itself a program that knows how to handle the data. Alternatively, using `mcplot` with Matlab and Scilab plotters provide additional functionalities from menus and dialogs (see section 4.4.5).

When imported through the data generated script (see section 4.3), or using `mcplot` (see section 4.4.5), a single variable may be created into the Matlab, Scilab or IDL base workspace. This variable is a *structure* constituting a data tree containing many fields, some of them being themselves structures. Field names are the initial names from the instrument (components, files, ...), transformed into valid variable names, e.g containing

only letters, digits and the '_' character, except for the first character which may only be a letter, or the 'm' letter[2]. In this tree, you will find the monitor names, which fields contain the monitored data. The usual structure is

s.*instrument*.*simulation*.*comp_name*.*file_name*

For instance, reading the data from a 'test' instrument using Matlab format will look like

```
matlab> s=mcstas; % or mcplot mcstas.m from the terminal
matlab> s
s =
     Format: 'Matlab with text headers'
        URL: 'http://neutron.risoe.dk'
     Editor: 'farhi on pcfarhi'
    Creator: 'test (test.instr) McStas 1.7 - May. 14, 2003 simulation'
       Date: 1.0529e+09
       File: './mcstas'
       test: [1x1 struct]
    EndDate: 1.0529e+09
      class: 'root'
matlab> s.test.m_mcstas.monitor1.monitor1_y_kz
ans =
          ...
          Date:       1.0529e+09
          File:       'monitor1.y_kz'
          type:       'array_2d(20, 10)'
          ...
          ratio:      '1e+06/1e+06'
          signal:     'Min=0; Max=5.54051e-10; Mean= 6.73026e-13;'
          statistics: 'X0=0.438302; dX=0.0201232; Y0=51019.6; dY=20557.1;'
          ...
matlab> eval(s.test.m_mcstas.monitor1.monitor1_y_kz);
matlab> dX
ans =
          0.0201232
```

The latter example accesses the data from the 'monitor1.y_kz' file written by the 'monitor1' component in the 'test' instrument during the './mcstas' simulation. You may evaluate directly the 'signal' and 'statistics' fields of the structure to obtain useful informations.

HTML, XML/NeXus and NeXus formats Both HTML and XML/NeXus formats are available. The former may be viewed using any web browser (Netscape, Internet Explorer, Nautilus), while the latter may be browsed for instance using Internet Explorer (Windows and Mac OS) or GXMLViewer and KXMLEditor (under Linux).

A future version of McStas will support output in the NeXus format [11].

[2]For instance in most case, the simulation location is './mcstas.m' which turns into field 'm_mcstas'.

Chapter 5

The McStas kernel and meta-language

Instrument definitions are written in a special McStas meta-language which is translated automatically by the McStas compiler into a C program which is in turn compiled to an executable that performs the simulation. The meta-language is custom-designed for neutron scattering and serves two main purposes: (i) to specify the interaction of a single neutron with a single optical component, and (ii) to build a simulation by constructing a complete instrument from individual components.

For maximum flexibility and efficiency, the meta-language is based on C. Instrument geometry, propagation of neutrons between the different components, parameters, data input/output etc. is handled in the meta-language and by the McStas compiler. Complex calculations are written in C embedded in the meta-language description of the components. It is possible to set up an instrument from existing components and run a simulation without writing a single line of C code, working entirely in the meta-language. On the other hand, the full power of the C language is available for special-purpose setups in advanced simulations, and for computing neutron trajectories in the components.

Apart from the meta-language, McStas also includes a number of C library functions and definitions that are useful for neutron ray-tracing simulations. The definitions available for users coding components are listed in appendix A. The list includes functions for computing the intersection between a flight-path and various objects (such as cylinders and spheres), functions for generating random numbers with various distributions, functions for reading or writing informations from/to data files, convenient conversion factors between relevant units, etc.

The McStas meta-language was designed to be readable, with a verbose syntax and explicit mentioning of otherwise implicit information. The recommended way to get started with the meta-language is to start by looking at the examples supplied with McStas, modifying them as necessary for the application at hand.

5.1 Notational conventions

Simulations generated by McStas use a semi-classical description of the neutron to compute the neutron trajectory through the instrument and its interaction with the different

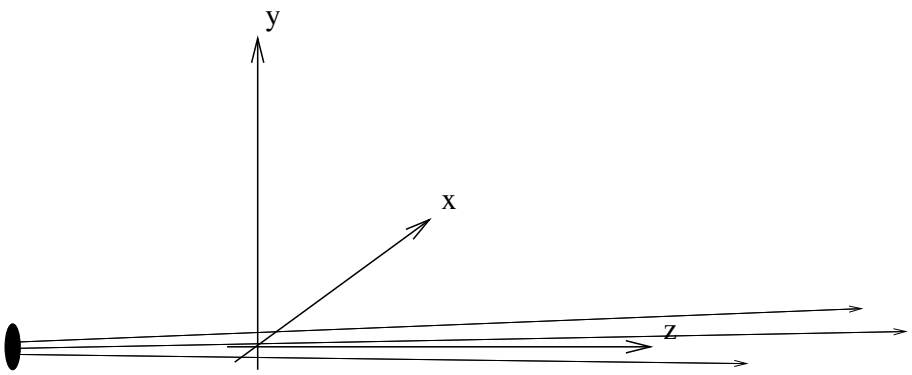

Figure 5.1: conventions for the orientations of the axis in simulations.

components. The effect of gravity is taken into account either in particular components, or more generaly when setting an execution flag (`-g`) to perform gravitation computation.

An instrument consists of a list of components through which the neutron passes one after the other. The order of components is thus significant since McStas does not automatically check which component is the next to interact with the neutron at a given point in the simulation.

The instrument is given a global, absolute coordinate system. In addition, every component in the instrument has its own local coordinate system that can be given any desired position and orientation (though the position and orientation must remain fixed for the duration of a single simulation). By convention, the z axis points in the direction of the beam, the x axis is perpendicular to the beam in the horizontal plane pointing left as seen from the source, and the y axis points upwards (see figure 5.1). Nothing in McStas enforces this convention, but if every component used different conventions the user would be faced with a severe headache! It is therefore recommended that this convention is followed by users implementing new components.

In the instrument definitions, units of length (*e.g.* component positions) are given in meters and units of angles (*e.g.* rotations) are given in degrees. The state of the neutron is given by its position (x, y, z) in meters, its velocity (v_x, v_y, v_z) in meters per second, the time t in seconds, and the two parameters s_1 and s_2 that are obsolete and should not be used. A three-component representation of the spin, (s_x, s_y, s_z), normalized to one, is used. In addition, the outgoing neutron has an associated weight p which is used to model fractional neutrons in the Monte Carlo simulation. $p = 0.2$ means that a single neutron following this path has a 20% chance of reaching the present position without being absorbed or scattered away from the instrument. Alternatively, one may regard a ray of neutrons and p is the fraction of neutrons following the considered path.

5.2 Syntaxical conventions

Comments follow the normal C syntax "`/* ... */`". C++ style comments "`// ...`" may also be used.

Keywords are not case-sensitive, for example "`DEFINE`", "`define`", and "`dEfInE`" are all equivalent. However, by convention we always write keywords in uppercase to distinguish them from identifiers and C language keywords. In contrast, McStas identifiers (names), like C identifiers and keywords, *are* case sensitive, another good reason to use a consistent case convention for keywords. All McStas keywords are reserved, and thus should not be used as C variable names. The list of these reserved keywords is shown in table 5.1.

It is possible, and usual, to split the input instrument definition across several different files. For example, if a component is not explicitly defined in the instrument, McStas will search for a file containing the component definition in the standard component library (as well as in the current directory and any user-specified search directories, see section 4.2.2). It is also possible to explicitly include another file using a line of the form

```
%include "file"
```

Beware of possible confusion with the C language "`#include`" statement, especially when it is used in C code embedded within the McStas meta-language. Files referenced with "`%include`" are read when the instrument is translated into C by the McStas compiler, and must contain valid McStas meta-language input (and possibly C code). Files referenced with "`#include`" are read when the C compiler generates an executable from the generated C code, and must contain valid C.

Embedded C code is used in several instances in the McStas meta-language. Such code is copied by the McStas compiler into the generated simulation C program. Embedded C code is written by putting it between the special symbols `%{` and `%}`, as follows:

```
%{
        ... Embedded C code ...
%}
```

The "`%{`" and "`%}`" must appear on a line by themselves (do not add comments after). Additionally, if a "`%include`" statement is found *within* an embedded C code block, the specified file will be included from the 'share' directory of the standard component library (or from the current directory and any user-specified search directories) as a C library, just like the usual "`#include`" *but only once*. For instance, if many components require to read data from a file, they may all ask for "`%include "read_table-lib"`" without duplicating the code of this library. If the file has no extension, both `.h` and `.c` files will be searched and included, otherwise, only the specified file will be imported. The McStas 'run-time' shared library is included by default (equivalent to "`%include "mcstas-r"`" in the `DECLARE` section). For an example of `%include`, see the monitors/Monitor_nD component.

5.3 Writing instrument definitions

The purpose of the instrument definition is to specify a sequence of components, along with their position and parameters, which together make up an instrument. Each component is given its own local coordinate system, the position and orientation of which may be specified by its translation and rotation relative to another component. An example is given in section 5.3.8 and some additional examples of instrument definitions can be found on the McStas web-page [2] and in the `example` directory.

Keyword	Scope	Meaning
ABSOLUTE	I	Indicates that the AT and ROTATED keywords are in the absolute coordinate system.
AT	I	Indicates the position of a component in an instrument definition.
DECLARE	I,C	Declares C internal instrument or component variables.
DEFINE - INSTRUMENT - COMPONENT	I,C	Starts an instrument or component definition. (each associated parameter may have default values)
DEFINITION	C	Defines component parameters that are constants (like C #define).
END	I,C	Ends the instrument or component definition.
EXTEND	I	Extends the TRACE section of a component in an instrument definition.
FINALLY	I,C	Embeds C code to execute when simulation ends (also executes the SAVE section).
GROUP	I	Defines an exclusive group of components.
%include	I,C	Imports an instrument part, a component or a piece of C code (when within embedded C).
INITIALIZE	I,C	Embeds C code to be executed when starting.
MCDISPLAY	C	Embeds C code to display a geometric representation of a component.
OUTPUT	C	Defines internal variables to be public and protected symbols (usually all those of DECLARE).
PARAMETERS	C	Defines a class of component parameter.
POLARISATION	C	Defines neutron polarisation coordinates.
PREVIOUS	C	Refers to a previous component position/orientation.
RELATIVE	I	Indicates that the AT and ROTATED keywords are relative to an other component.
ROTATED	I	Indicates the orientation of a component in an instrument definition.
SAVE	I,C	Embedded C code to execute when saving data.
SETTING	C	Defines component parameters that are variables (double, int, char*).
SHARE	C	Declares global functions and variables to be used by all components.
STATE	C	Defines neutron state coordinates.
TRACE	I,C	Lists the components or embedded C code to execute during simulation.

Table 5.1: Reserved McStas keywords. Scope is 'I' for instrument and 'C' for component definitions.

5.3.1 The instrument definition head

`DEFINE INSTRUMENT` *name* $(a_1, a_2, \ldots)$

This marks the beginning of the definition. It also gives the name of the instrument and the list of instrument parameters. Instrument parameters describe the configuration of the instrument, and usually correspond to setting parameters of the components. A motor position is a typical example of an instrument parameter. The input parameters of the instrument constitute the input that the user (or possibly a front-end program) must supply when the generated simulation is started.

By default, the parameters will be floating point numbers, and will have the C type `double` (double precision floating point). The type of each parameter may optionally be declared to be `int` for the C integer type or `char *` for the C string type. The name `string` may be used as a synonym for `char *`, and floating point parameters may be explicitly declared using the name `double`. The following example illustrates all possibilities:

```
DEFINE INSTRUMENT test(d1, double d2, int i, char *s1, string s2)
```

Here `d1` and `d2` will be floating point parameters of C type `double`, `i` will be an integer parameter of C type `int`, and `s1` and `s2` will be string parameters of C type `char *`. The parameters of an instrument may be given default values. Parameters with default values are called *optional parameters*, and need not be given an explicit value when the instrument simulation is executed. When executed without any parameter value in the command line (see section 4.3), the instrument asks for all parameter values, but pressing the `Return` key selects the default value (if any). When used with at least one parameter value in the command line, all non specified parameters will have their value set to the default one (if any). A parameter is given a default value using the syntax "*param* `=` *value*". For example

```
DEFINE INSTRUMENT test(d1 = 1, string s2="hello")
```

Here `d1` is an optional parameter and if no value is given explicitly, "1" will be used.

Optional parameters can greatly increase the convenience for users of instruments for which some parameters are seldom changed or of unclear signification to the user. Also, if all instrument parameters have default values, then the simple command `mcdisplay test.instr` will show the instrument view without requesting any other input, which is usually a good starting point to study the instrument design.

5.3.2 The `DECLARE` section

```
DECLARE
%{
      ... C declarations of global variables etc. ...
%}
```

This gives C declarations that may be referred to in the rest of the instrument definition. A typical use is to declare global variables or small functions that are used elsewhere in the instrument. The `%include ''file''` keyword may be used to import a specific component definition or a part of an instrument. The `DECLARE` section is optional.

5.3.3 The INITIALIZE section

```
INITIALIZE
%{
        ... C initializations. ...
%}
```

This gives code that is executed when the simulation starts. This section is optional.

5.3.4 The TRACE section

The TRACE keyword starts a section giving the list of components that constitute the instrument. Components are declared like this:

COMPONENT *name* = *comp*($p_1 = e_1, p_2 = e_2, \ldots$)

This declares a component named *name* that is an instance of the component definition named *comp*. The parameter list gives the setting and definition parameters for the component. The expressions $e_1, e_2, \ldots$ define the values of the parameters. For setting parameters arbitrary ANSI-C expressions may be used, while for definition parameters only *constant* numbers, strings, names of instrument parameters, or names of C identifiers are allowed (see section 5.4.1 for details of the difference between definition and setting parameters). To assign the value of a general expression to a definition parameter, it is necessary to declare a variable in the DECLARE section, assign the value to the variable in the INITIALIZE section, and use the variable as the value for the parameter.

The McStas program takes care to rename parameters appropriately in the output so that no conflicts occur between different component definitions or between component and instrument definitions. It is thus possible (and usual) to use a component definition multiple times in an instrument description.

The McStas compiler will automatically search for a file containing a definition of the component if it has not been declared previously. The definition is searched for in a file called "*name*.comp", "*name*.cmp", or "*name*.com". See section 4.2.2 for details on which directories are searched. This facility is often used to refer to existing component definitions in standard component libraries. It is also possible to write component definitions in the main file before the instrument definitions, or to explicitly read definitions from other files using %include (not within embedded C blocks).

The position of a component is specified using an AT modifier following the component declaration:

AT (x, y, z) RELATIVE *name*

This places the component at position (x, y, z) in the coordinate system of the previously declared component *name*. Placement may also be absolute (not relative to any component) by writing

AT (x, y, z) ABSOLUTE

Any C expression may be used for x, y, and z. The AT modifier is required. Rotation is achieved similarly by writing

ROTATED (ϕ_x, ϕ_y, ϕ_z) RELATIVE *name*

This will result in a coordinate system that is rotated first the angle ϕ_x (in degrees) around the x axis, then ϕ_y around the y axis, and finally ϕ_z around the z axis. Rotation may also be specified using ABSOLUTE rather than RELATIVE. If no rotation is specified, the default is $(0, 0, 0)$ using the same relative or absolute specification used in the AT modifier. The *position* of a component depends on its definition. Usually, it will be the input window position (e.g. for guide-like components), or the center position for cylindrical/spherical components. Thus, the next component position will be most of the time set to the previous component AT position increased by its size/radius along the z axis.

The PREVIOUS keyword is a generic name to refer to the previous component in the simulation. Moreover, the PREVIOUS(n) keyword will refer to the n-th previous component, starting from the current component, so that PREVIOUS is equivalent to PREVIOUS(1). This keyword should be used after the RELATIVE keyword, but not for the first component instance of the instrument description.

AT (x, y, z) RELATIVE PREVIOUS ROTATED (ϕ_x, ϕ_y, ϕ_z) RELATIVE PREVIOUS(2)

Invalid PREVIOUS references will be assumed to be absolute placement.

The order and position of components in the TRACE section does not allow components to overlap, except for particular cases (see the GROUP keyword below). Indeed, many components of the McStas library start by propagating the neutron event to the begining of the component itself. Anyway, when the corresponding propagation time is found to be negative (*i.e.* the neutron is already *after* the component, and has thus passed the 'active' position), the neutron event is ABSORBed, resulting in a zero intensity and event counts after a given position. Such situations may arise e.g. when positioning some components not one after the other (nested, in parallel, or overlapping), for instance in a multiple crystal monochromator (they are then side by side). One would then like the neutron to interact with *one of* the components and then continue after this group of components. In order to handle such arrangements, groups are defined by appending the GROUP modifier

GROUP *name*

to all involved component declarations. All components of the same named group are tested one after the other, until one of them interacts (uses the SCATTER macro). The selected component acts on the neutron, and the rest of the group is skipped. Such groups are thus exclusive (only one of the elements is active). If no component of the group could intercept the neutron, it is ABSORBed. If you wish not to absorb these neutrons, you may end each group by a large monitor, which will eventually catch neutrons that were not caught by previous components of the group.

It is sometimes desirable to slighlty modify an existing component of the McStas library. One would usually make a copy of the component, and extend the code of its TRACE section. McStas provides an easy way to change the behaviour of existing components in an instrument definition without duplicating files, using the EXTEND modifier

```
EXTEND
%{
      ... C code executed after the component TRACE section ...
%}
```

The embeded C code is appended to the component `TRACE` section, and all its internal variables (as well as all the instrument variables) may be used. This component declaration modifier is of course optional. Within a `GROUP`, *all* `EXTEND` sections of the group are executed. In order to discriminate components that are active from those that are skipped, one may use the SCATTERED flag, which is set to zero when entering each component or group, and incremented when the neutron is SCATTERed, as in the following example

```
COMPONENT name0 = comp(p1 = e1, p2 = e2, ...)
   AT (0, 0, 0) ABSOLUTE
COMPONENT name1 = comp(...)
   AT (x, y, z) RELATIVE name0
   ROTATED (φx, φy, φz) RELATIVE name0
   GROUP GroupName EXTEND
   %{
       if (SCATTERED) printf("I scatter"); else printf("I do not scatter");
   %}
COMPONENT name2 = comp(...)
   AT (x, y, z) RELATIVE name0
   ROTATED (φx, φy, φz) RELATIVE name0
   GROUP GroupName
```

Components *name1* and *name2* are at the same position. If the first one intercepts the neutron (and has a SCATTER within its `TRACE` section), the SCATTERED variable becomes true, the code extension will result in printing "I scatter", and the second component will be skipped. Thus, we recommand to make use of the SCATTER keyword each time a component 'uses' the neutron (scatters, detects, ...).

5.3.5 The `SAVE` section

```
SAVE
%{
        ... C code to execute each time a temporary save is required ...
%}
```

This gives code that will be executed when the simulation is requested to save data, for instance when receiving a USR2 signal (on Unix systems), or using the `Progress_bar` component with intermediate savings. This section is optional.

5.3.6 The `FINALLY` section

```
FINALLY
%{
        ... C code to execute at end of simulation ...
%}
```

This gives code that will be executed when the simulation has ended. When existing, the `SAVE` section is first executed. This section is optional. A simulation may be requested to

end before all neutrons have been traced when recieving a TERM or INT signal (on Unix systems), or with Control-C.

5.3.7 The end of the instrument definition

The end of the instrument definition is marked using the keyword

```
END
```

5.3.8 Code for the instrument `vanadium_example.instr`

An instrument definition taken from the `examples` directory is given as an example.

```
/*******************************************************************************
*
* McStas, neutron ray-tracing package
*         Copyright 1997-2002, All rights reserved
*         Risoe National Laboratory, Roskilde, Denmark
*         Institut Laue Langevin, Grenoble, France
*
* Instrument: vanadium_example
*
* %Identification
* Written by: KN and KL
* Date: 1998
* Origin: Risoe
* Release: McStas 1.1
* Version: 0.1
* %INSTRUMENT_SITE: Tutorial
*
* A test instrument using a vanadium cylinder
*
* %Description
* This instrument shows the vanadium sample scattering anisotropy.
* This is an effect of attenuation of the beam in the cylindrical sample.
*
* Example: mcrun vanadium_example.instr ROT=0
*
* %Parameters
* INPUT PARAMETERS:
* ROT: (deg) Rotation angle of the PSD monitor
*
* %Link
* The McStas User manual
* The McStas tutorial
*
* %End
*******************************************************************************/
/* The line below defines the 'name' of our instrument */
/* Here, we have a single input parameter, ROT         */
DEFINE INSTRUMENT vanadium_example(ROT=0)

/* The DECLARE section allows us to declare variables  */
/* in c syntax. Here, coll_div (collimator divergence) */
/* is set to 60 degrees...                             */
DECLARE
```

```
%{
  double coll_div = 60;
%}

/* Here comes the TRACE section, where the actual      */
/* instrument is defined....                           */
TRACE

/* The Arm() class component defines reference points  */
/* in 3D space. Every component instance must have a   */
/* unique name. Here, arm is used. This Arm() component*/
/* is set to define the origin of our global coordinate*/
/* system (AT (0,0,0) ABSOLUTE)                        */
COMPONENT arm = Arm() AT (0,0,0) ABSOLUTE

/* Next, we need some neutrons. Let's place a neutron  */
/* source. Refer to documentation of Source_flat to    */
/* understand the different input parameters.          */
/* The source component is placed RELATIVE to the arm  */
/* component, meaning that modifying the position or   */
/* orientation of the arm will also affect the source  */
/* component (and other components after that one...   */
COMPONENT source = Source_flat(radius = 0.015, dist = 1,
  xw=0.024, yh=0.015, E0=5, dE=0.2)
 AT (0,0,0) RELATIVE arm

/* Here we have a collimator - or Soller - placed to   */
/* improve beam divergence.                            */
/* The component is placed at a distance RELATIVE to   */
/* a previous component...                             */
COMPONENT collimator = Collimator_linear(len = 0.2,
  divergence = coll_div, xmin = -0.02, xmax = 0.02,
  ymin = -0.03, ymax = 0.03)
  AT (0, 0, 0.4) RELATIVE arm

/* We also need something to 'shoot at' - here a sample*/
/* made from vanadium - an isotrope scatterer. Options */
/* are available to restrict the solid angle in which  */
/* neutrons are emitted (no need to simulate anything  */
/* that we know for sure will not gain us more insight)*/
/* Other options for smart targeting are available -   */
/* refer to component documentation for info.          */
COMPONENT target = V_sample(radius_i = 0.008, radius_o = 0.012,
  h = 0.015, focus_r = 0, pack = 1,
  target_x = 0, target_y = 0, target_z = 1)
  AT (0,0,1) RELATIVE arm

/* Here, a secondary arm - or reference point, placed  */
/* on the sample position. The ROT parameter above     */
/* defines rotation of this arm (and components        */
/* relative to the arm)                                */
COMPONENT arm2 = Arm()
  AT (0,0,0) RELATIVE target
  ROTATED (0,ROT,0) relative arm

/* For data output, let us place a detector. This      */
```

```
/* detector is not very realistic, since it is sphere  */
/* shaped and has a 10 m radius, but has the advantage */
/* that EVERYTHING emitted from the sample will be     */
/* picked up. Notice that this component changes       */
/* orientation with the ROT input parameter of the     */
/* instrument.                                         */
COMPONENT PSD_4pi = PSD_monitor_4PI(radius=10, nx=101, ny=51,
  filename="vanadium.psd")
  AT (0,0,0) RELATIVE target ROTATED (ROT,0,0) RELATIVE arm2
END
```

5.4 Writing component definitions

The purpose of a component definition is to model the interaction of a neutron with the component. Given the state of the incoming neutron, the component definition calculates the state of the neutron when it leaves the component. The calculation of the effect of the component on the neutron is performed by a block of embedded C code. One example of a component definition is given in section 5.4.10, and all component definitions can be found on the McStas web-page [2].

There exists a large number of functions and constants available in order to write efficient components. Look at the appendix A for neutron propagation functions, geometric intersection time computations, vector operators, random number and vector generation, physical constants, coordinate retrieval and operations, file generation routines (for monitors), data file reading, ...

5.4.1 The component definition header

`DEFINE COMPONENT` *name*

This marks the beginning of the definition, and defines the name of the component.

`DEFINITION PARAMETERS` $(d_1, d_2, \ldots)$
`SETTING PARAMETERS` $(s_1, s_2, \ldots)$

This declares the definition and setting parameters of the component. The parameters define the characteristics of the component, and can be accessed from the `SAVE`, `FINALLY`, and `MCDISPLAY` sections (see below), as well as in `EXTEND` sections of the instrument definition (see section 5.3).

Setting parameters are translated into C variables usually of type `double` in the generated simulation program, so they are usually numbers. Definition parameters are translated into `#define` macro definitions, and so can have any type, including strings, arrays, and function pointers.

However, because of the use of `#define`, definition parameters suffer from the usual problems with C macro definitions. Also, it is not possible to use a general C expression for the value of a definition parameter in the instrument definition, only constants and variable names may be used. For this reason, setting parameters should be used whenever possible.

There are a few cases where the use of definition parameters instead of setting parameters makes sense. If the parameter is not numeric, nor a character string (*i.e.* an array, for

example), a setting parameter cannot be used. Also, because of the use of `#define`, the C compiler can treat definition parameters as constants when the simulation is compiled. For example, if the array sizes of a multidetector are definition parameters, the arrays can be statically allocated in the component `DECLARE` section. If setting parameters were used, it would be necessary to allocate the arrays dynamically using *e.g.* `malloc()`.

Setting parameters may optionally be declared to be of type `int` and `char *`, just as in the instrument definition (see section 5.3).

`OUTPUT PARAMETERS` $(s_1, s_2, \ldots)$

This declares a list of C identifiers that are output parameters for the component. Output parameters are used to hold values that are computed by the component itself, rather than being passed as input. This could for example be a count of neutrons in a detector or a constant that is precomputed to speed up computation. Output parameters will typically be declared as C variables in the `DECLARE` section, see section 5.4.2 below for an example.

The `OUTPUT PARAMETERS` section is optional.

`STATE PARAMETERS` $(x, y, z, v_x, v_y, v_z, t, s_1, s_2, p)$

This declares the parameters that define the state of the incoming neutron. The task of the component code is to assign new values to these parameters based on the old values and the values of the definition and setting parameters. Note that s_1 and s_2 are obsolete and cannot be used.

`POLARISATION PARAMETERS` (s_x, s_y, s_z)

This line is necessary only if the component handles polarisation of neutrons and thus modifies the spin vector. For an instrument to handle polarisation correctly, it is only required that *one* of the components contains this line.

Optional component parameters

Just as for instrument parameters, the definition and setting parameters of a component may be given a default value. Parameters with default values are called *optional parameters*, and need not be given an explicit value when the component is used in an instrument definition. A parameter is given a default value using the syntax "*param* `=` *value*". For example

```
SETTING PARAMETERS (radius, height, pack = 1)
```

Here `pack` is an optional parameter and if no value is given explicitly, "1" will be used[1].

Optional parameters can greatly increase the convenience for users of components with many parameters that have natural default values which are seldom changed. Optional parameters are also useful to preserve backwards compatibility with old instrument definitions when a component is updated. New parameters can be added with default values that correspond to the old behavior, and existing instrument definitions can be used with the new component without changes.

[1] In contrast, if no value is given for `radius` or `height`, an error message will result.

However, optional parameters should not be used in cases where no general natural default value exists. For example, the length of a guide or the size of a slit should not be given default values. This would prevent the error messages that should be given in the common case of a user forgetting to set an important parameter.

5.4.2 The DECLARE section

```
DECLARE
%{
        ... C code declarations (variables, definitions, functions)...
        ... These are usually OUTPUT parameters to avoid name conflicts ...
%}
```

This gives C declarations of global variables etc. that are used by the component code. This may for instance be used to declare a neutron counter for a detector component. This section is optional.

Note that any variables declared in a `DECLARE` section are *global*. Thus a name conflict may occur if two instances of a component are used in the same instrument. To avoid this, variables declared in the `DECLARE` section should be `OUTPUT` parameters of the component because McStas will then rename variables to avoid conflicts. For example, a simple detector might be defined as follows:

```
DEFINE COMPONENT Detector
OUTPUT PARAMETERS (counts)
DECLARE
%{
  int counts;
%}
...
```

The idea is that the `counts` variable counts the number of neutrons detected. In the instrument definition, the `counts` parameter may be referenced using the `MC_GETPAR` C macro, as in the following example instrument fragment:

```
COMPONENT d1 = Detector()
...
COMPONENT d2 = Detector()
...
FINALLY
%{
  printf("Detector counts: d1 = %d, d2 = %d\n",
         MC_GETPAR(d1,counts), MC_GETPAR(d2,counts));
%}
```

5.4.3 The SHARE section

```
SHARE
%{
```

```
... C code shared declarations (variables, definitions, functions)...
... These should not be OUTPUT parameters ...
%}
```

The SHARE section has the same role as DECLARE except that when using more than one instance of the component, it is inserted *only once* in the simulation code. No occurence of the items to be shared should be in the OUTPUT parameter list (not to have McStas rename the identifiers). This is particularly useful when using many instances of the same component (for instance guide elements). If the declarations were in the DECLARE section, McStas would duplicates it for each instance (making the simulation code bigger). A typical example is to have shared variables, functions, type and structure definitions that may be used from the component TRACE section. For an example of SHARE, see the samples/Single_crystal component. The %include ''file'' keyword may be used to import a shared library. The SHARE section is optional.

5.4.4 The INITIALIZE section

```
INITIALIZE
%{
... C code initialization ...
%}
```

This gives C code that will be executed once at the start of the simulation, usually to initialize any variables declared in the DECLARE section. This section is optional.

5.4.5 The TRACE section

```
TRACE
%{
... C code to compute neutron interaction with component ...
%}
```

This performs the actual computation of the interaction between the neutron and the component. The C code should perform the appropriate calculations and assign the resulting new neutron state to the state parameters.

The C code may also execute the special macro ABSORB to indicate that the neutron has been absorbed in the component and the simulation of that neutron will be aborted. When the neutron state is changed or detected, for instance if the component simulates multiple events (for example multiple reflections in a guide, or multiple scattering in a powder sample), the special macro SCATTER should be called. This does not affect the results of the simulation in any way, but it allows the front-end programs to visualize the scattering events properly, and to handle component GROUPs in an instrument definition (see section 5.3.4). The SCATTER macro should be called with the state parameters set to the proper values for the scattering event. For an example of SCATTER, see the optics/Channeled_guide component.

5.4.6 The SAVE section

```
SAVE
%{
        ... C code to execute in order to save data ...
%}
```

This gives code that will be executed when the simulation is requested to save data, for instance when receiving a USR2 signal (on Unix systems, see section 4.3). This might be used by monitors and detectors in order to write results.

In order to work properly with the common output file format used in McStas, all monitor/detector components should use standard macros for outputting data in the SAVE or FINALLY section, as explained below. In the following, we use $N = \sum_i p_i^0$ to denote the count of detected neutron events, $p = \sum_i p_i$ to denote the sum of the weights of detected neutrons, and $p2 = \sum_i p_i^2$ to denote the sum of the squares of the weights, as explained in section 6.1.1.

Single detectors/monitors The results of a single detector/monitor are written using the following macro:

```
DETECTOR_OUT_0D(t, N, p, p2)
```

Here, t is a string giving a short descriptive title for the results, *e.g.* "Single monitor".

One-dimensional detectors/monitors The results of a one-dimensional detector/ monitor are written using the following macro:

```
DETECTOR_OUT_1D(t, xlabel, ylabel, xvar, xmin, xmax, m,
                &N[0], &p[0], &p2[0], filename)
```

Here,

- t is a string giving a descriptive title (*e.g.* "Energy monitor"),
- *xlabel* is a string giving a descriptive label for the X axis in a plot (*e.g.* "Energy [meV]"),
- *ylabel* is a string giving a descriptive label for the Y axis of a plot (*e.g.* "Intensity"),
- *xvar* is a string giving the name of the variable on the X axis (*e.g.* "E"),
- $x_{\min}$ is the lower limit for the X axis,
- $x_{\max}$ is the upper limit for the X axis,
- m is the number of elements in the detector arrays,
- $\&N[0]$ is a pointer to the first element in the array of N values for the detector component (or NULL, in which case no error bars will be computed),
- $\&p[0]$ is a pointer to the first element in the array of p values for the detector component,

- &*p2*[0] is a pointer to the first element in the array of *p2* values for the detector component (or NULL, in which case no error bars will be computed),

- *filename* is a string giving the name of the file in which to store the data.

Two-dimensional detectors/monitors The results of a two-dimensional detector/ monitor are written to a file using the following macro:

DETECTOR_OUT_2D(*t*, *xlabel*, *ylabel*, $x_{\min}$, $x_{\max}$, $y_{\min}$, $y_{\max}$, m, n, &*N*[0][0], &*p*[0][0], &*p2*[0][0], *filename*)

Here,

- t is a string giving a descriptive title (*e.g.* "PSD monitor"),

- *xlabel* is a string giving a descriptive label for the X axis in a plot (*e.g.* "X position [cm]"),

- *ylabel* is a string giving a descriptive label for the Y axis of a plot (*e.g.* "Y position [cm]"),

- $x_{\min}$ is the lower limit for the X axis,

- $x_{\max}$ is the upper limit for the X axis,

- $y_{\min}$ is the lower limit for the Y axis,

- $y_{\max}$ is the upper limit for the Y axis,

- m is the number of elements in the detector arrays along the X axis,

- n is the number of elements in the detector arrays along the Y axis,

- &*N*[0][0] is a pointer to the first element in the array of N values for the detector component,

- &*p*[0][0] is a pointer to the first element in the array of p values for the detector component,

- &*p2*[0][0] is a pointer to the first element in the array of *p2* values for the detector component,

- *filename* is a string giving the name of the file in which to store the data.

Note that for a two-dimensional detector array, the first dimension is along the X axis and the second dimension is along the Y axis. This means that element (i_x, i_y) can be obtained as $p[i_x * n + i_y]$ if p is a pointer to the first element.

Three-dimensional detectors/monitors The results of a three-dimensional detector/monitor are written to a file using the following macro:

DETECTOR_OUT_3D(t, *xlabel*, *ylabel*, *zlabel*, *xvar*, *yvar*, *zvar*, $x_{\min}$, $x_{\max}$, $y_{\min}$, $y_{\max}$, $z_{\min}$, $z_{\max}$, m, n, p
&N[0][0][0], &p[0][0][0], &*p2*[0][0][0], *filename*)

The meaning of parameters is the same as those used in the 1D and 2D versions of DETECTOR_OUT. The available data format currently save the 3D arrays as 2D, with the 3rd dimension specified in the *type* field of the data header.

5.4.7 The FINALLY section

```
FINALLY
%{
      ... C code to execute at end of simulation ...
%}
```

This gives code that will be executed when the simulation has ended. This might be used to free memory and print out final results from components, *e.g.* the simulated intensity in a detector.

5.4.8 The MCDISPLAY section

```
MCDISPLAY
%{
      ... C code to draw a sketch of the component ...
%}
```

This gives C code that draws a sketch of the component in the plots produced by the `mcdisplay` front-end (see section 4.4.4). The section can contain arbitrary C code and may refer to the parameters of the component, but usually it will consist of a short sequence of the special commands described below that are available only in the MCDISPLAY section. When drawing components, all distances and positions are in meters and specified in the local coordinate system of the component.

The MCDISPLAY section is optional. If it is omitted, `mcdisplay` will use a default symbol (a small circle) for drawing the component.

The `magnify` command This command, if present, must be the first in the section. It takes a single argument: a string containing zero or more of the letters "x", "y" and "z". It causes the drawing to be enlarged along the specified axis in case `mcdisplay` is called with the `--zoom` option. For example:

```
magnify("xy");
```

The `line` command The `line` command takes the following form:

line(x_1, y_1, z_1, x_2, y_2, z_2)

It draws a line between the points (x_1, y_1, z_1) and (x_2, y_2, z_2).

The `multiline` command The `multiline` command takes the following form:

`multiline(`n`, `x_1`, `y_1`, `z_1`, ..., `x_n`, `y_n`, `z_n`)`

It draws a series of lines through the n points (x_1, y_1, z_1), (x_2, y_2, z_2), ..., (x_n, y_n, z_n). It thus accepts a variable number of arguments depending on the value of n. This exposes one of the nasty quirks of C since *no* type checking is performed by the C compiler. It is thus very important that all arguments to `multiline` (except n) are valid numbers of type `double`. A common mistake is to write

```
multiline(3, x, y, 0, ...)
```

which will silently produce garbage output. This must instead be written as

```
multiline(3, (double)x, (double)y, 0.0, ...)
```

The `circle` command The `circle` command takes the following form:

`circle(`*plane*`, `x`, `y`, `z`, `r`)`

Here *plane* should be either `"xy"`, `"xz"`, or `"yz"`. The command draws a circle in the specified plane with the center at (x, y, z) and the radius r.

5.4.9 The end of the component definition

```
END
```

This marks the end of the component definition.

5.4.10 A component example: Slit

A simple example of the component `Slit` is given.

```
/*******************************************************************************
*
* McStas, neutron ray-tracing package
*         Copyright 1997-2002, All rights reserved
*         Risoe National Laboratory, Roskilde, Denmark
*         Institut Laue Langevin, Grenoble, France
*
* Component: Slit
*
* %I
* Written by: Kim Lefmann and Henrik M. Roennow
* Date: June 16, 1997
* Version: $Revision: 1.18 $
* Origin: Risoe
* Release: McStas 1.6
*
* Rectangular/circular slit.
*
* %D
* A simple rectangular or circular slit. You may either
```

```
* specify the radius (circular shape), or the rectangular bounds.
* No transmission around the slit is allowed.
*
* Example: Slit(xmin=-0.01, xmax=0.01, ymin=-0.01, ymax=0.01)
*          Slit(radius=0.01)
*
* %P
* INPUT PARAMETERS
*
* radius: Radius of slit in the z=0 plane, centered at Origo (m)
* xmin: Lower x bound (m)
* xmax: Upper x bound (m)
* ymin: Lower y bound (m)
* ymax: Upper y bound (m)
*
* %E
*******************************************************************************/


DEFINE COMPONENT Slit
DEFINITION PARAMETERS ()
SETTING PARAMETERS (xmin=0, xmax=0, ymin=0, ymax=0,radius=0)
STATE PARAMETERS (x,y,z,vx,vy,vz,t,s1,s2,p)

INITIALIZE
%{
  if (xmin == 0 && xmax == 0 && ymin == 0 & ymax == 0 && radius == 0)
    { fprintf(stderr,"Slit: %s: Error: give geometry\n", NAME_CURRENT_COMP); exit(-1); }

%}

TRACE
%{
    PROP_Z0;
    if (((radius == 0) && (x<xmin || x>xmax || y<ymin || y>ymax))
    || ((radius != 0) && (x*x + y*y > radius*radius)))
      ABSORB;
    else
      SCATTER;
%}

MCDISPLAY
%{
  double xw, yh;
  magnify("xy");
  xw = (xmax - xmin)/2.0;
  yh = (ymax - ymin)/2.0;
  multiline(3, xmin-xw, (double)ymax, 0.0,
            (double)xmin, (double)ymax, 0.0,
            (double)xmin, ymax+yh, 0.0);
  multiline(3, xmax+xw, (double)ymax, 0.0,
            (double)xmax, (double)ymax, 0.0,
            (double)xmax, ymax+yh, 0.0);
  multiline(3, xmin-xw, (double)ymin, 0.0,
            (double)xmin, (double)ymin, 0.0,
            (double)xmin, ymin-yh, 0.0);
```

```
  multiline(3, xmax+xw, (double)ymin, 0.0,
            (double)xmax, (double)ymin, 0.0,
            (double)xmax, ymin-yh, 0.0);
%}

END
```

5.4.11 McDoc, the McStas library documentation tool

McStas includes a facility called McDoc to help maintain good documentation of components and instruments. In the component source code, comments may be written that follow a particular format understood by McDoc. The McDoc facility will read these comments and automatically produce output documentation in various forms. By using the source code itself as the source of documentation, the documentation is much more likely to be a faithful and up-to-date description of how the component/instrument actually works.

Two forms of documentation can be generated. One is the component entry dialog in the `mcgui` front-end, see section 4.4.1. The other is a collection of web pages documenting the components and instruments, handled via the `mcdoc` front-end (see section 4.4.7), and the complete documentation for all available McStas components and instruments may be found at the McStas webpage [2], and in the McStas library (see 7.1). This latter is accessible from the `mcgui` 'Help' menu.

Note that McDoc-compliant comments in the source code are no substitute for a good reference manual entry. The mathematical equations describing the physics and algorithms of the component should still be written up carefully for inclusion in the component manual. The McDoc comments are useful for describing the general behaviour of the component, the meaning and units of the input parameters, etc.

The format of the comments in the library source code

The format of the comments understood by McDoc is mostly straight-forward, and is designed to be easily readable both by humans and by automatic tools. McDoc has been written to be quite tolerant in terms of how the comments may be formatted and broken across lines. A good way to get a feeling for the format is to study some of the examples in the existing components and instruments. Below, a few notes are listed on the requirements for the comment headers:

The comment syntax uses `%IDENTIFICATION`, `%DESCRIPTION`, `%PARAMETERS`, `%LINKS`, and `%END` keywords to mark different sections of the documentation. Keywords may be abbreviated, *e.g.* as `%IDENT` or `%I`.

- In the `%IDENTIFICATION` section, `author:` (or `written by:` for backwards compatibility with old comments) denote author; `date:`, `version:`, and `origin:` are also supported. Any number of `Modified by:` entries may be used to give the revision history. The `author:`, `date:`, etc. entries must all appear on a single line of their own. Everything else in the identification section is part of a "short description" of the component.
- In the `%PARAMETERS` section, descriptions have the form "*name*`:` `[`*unit*`]` *text*" or "*name*`:` *text* `[`*unit*`]`". These may span multiple lines, but subsequent lines must

be indented by at least four spaces. Note that square brackets `[]` should be used for units. Normal parenthesis are also supported for backwards compatibility, but nested parenthesis do not work well.

- The `%DESCRIPTION` section contains text in free format. The text may contain HTML tags like `<IMG>` (to include pictures) and `<A>...</A>` (for links to other web pages, but see also the `%LINK` section). In the generated web documentation pages, the text is set in `<PRE>...</PRE>`, so that the line breaks in the source will be obeyed.
- Any number of `%LINK` sections may be given; each one contains HTML code that will be put in a list item in the link section of the description web page. This usually consists of an `<A HREF="..."> ... </A>` pointer to some other source of information.
- Optionally, an `%INSTRUMENT_SITE` section followed by a single word is used to sort *instruments* by origin/location in the 'Neutron Site' menu in `mcgui`.
- After `%END`, no more comment text is read by McDoc.

Chapter 6

Monte Carlo Techniques and simulation strategy

This chapter explains the simulation strategy and the Monte Carlo techniques used in McStas. We first explain the concept of the neutron weight factor, and discuss the statistical errors in dealing with sums of neutron weights. Secondly, we give an expression for how the weight factor should transform under a Monte Carlo choice and specialize this to the concept of focusing components. Finally, we present a way of generating random numbers with arbitrary distributions.

6.1 The neutron weight, p

A totally realistic semi-classical simulation will require that each neutron is at any time either present or not (it might be ABSORB'ed or lost in another way). In many setups, *e.g.* triple axis spectrometers, only a small fraction of the initial neutrons will ever be detected, and simulations of this kind will therefore waste much time in dealing with neutrons that get lost.

An important way of speeding up calculations is to introduce a neutron weight for each simulated neutron and to adjust this weight according to the path of the neutron. If *e.g.* the reflectivity of a certain optical component is 10%, and only reflected neutrons are considered in the simulations, the neutron weight will be multiplied by 0.10 when passing this component, but every neutron is allowed to reflect in the component. In contrast, the totally realistic simulation of the component would require in average ten incoming neutrons for each reflected one.

Let the initial neutron weight be p_0 and let us denote the weight multiplication factor in the j'th component by π_j. The resulting weight factor for the neutron after passage of the whole instrument is equal to the product of all the contributions

$$p = p_0 \prod_{j=1}^{n} \pi_j. \tag{6.1}$$

For convenience, the value of p is updated within each component.

Simulation by weight adjustment is performed whenever possible. This includes

- Transmission through filter.
- Transmission through Soller blade collimator (in the approximation which does not take each blade into account).
- Reflection from monochromator (and analyser) crystals with finite reflectivity and mosaicity.
- Scattering from samples.

6.1.1 Statistical errors of non-integer counts

In a typical simulation, the result will consist of a count of neutrons with different weights.[1] One may write the counting result as

$$I = \sum_i p_i = N\overline{p}, \tag{6.2}$$

where N is the number of neutrons in the detector and the vertical bar denote averaging. By performing the weight transformations, the (statistical) mean value of I is unchanged. However, N will in general be enhanced, and this will improve the statistics of the simulation.

To give some estimate of the statistical error, we proceed as follows: Let us first for simplicity assume that all the counted neutron weights are almost equal, $p_i \approx \overline{p}$, and that we observe a large number of neutrons, $N \geq 10$. Then N almost follows a normal distribution with the uncertainty $\sigma(N) = \sqrt{N}$ [2]. Hence, the statistical uncertainty of the observed intensity becomes

$$\sigma(I) = \sqrt{N}\overline{p} = I/\sqrt{N}, \tag{6.3}$$

as is used in real neutron experiments (where $\overline{p} \equiv 1$). For a better approximation we return to Eq. (6.2). Allowing variations in both N and $\overline{p}$, we calculate the variance of the resulting intensity, assuming that the two variables are independent and both follow a Gaussian distribution.

$$\sigma^2(I) = \sigma^2(N)\overline{p}^2 + N^2\sigma^2(\overline{p}) = N\overline{p}^2 + N^2\sigma^2(\overline{p}). \tag{6.4}$$

Assuming that the individual weights, p_i, follow a Gaussian distribution (which in many cases is far from the truth) we have $N^2\sigma^2(\overline{p}) = \sigma^2(\sum_i p_i) = N\sigma^2(p_i)$ and reach

$$\sigma^2(I) = N\left(\overline{p}^2 + \sigma^2(p_i)\right). \tag{6.5}$$

The statistical variance of the p_i's is estimated by $\sigma^2(p_i) \approx (N-1)^{-1}(\sum_i p_i^2 - N\overline{p}^2)$. The resulting variance then reads

$$\sigma^2(I) = \frac{N}{N-1}\left(\sum_i p_i^2 - \overline{p}^2\right). \tag{6.6}$$

[1] The sum of these weights is an estimate of the mean number of neutrons hitting the monitor (or detector) in a "real" experiment where the number of neutrons emitted from the source is the same as the number of simulated neutrons.

[2] This is not correct in a situation where the detector counts a large fraction of the neutrons in the simulation, but we will neglect that for now.

For large values of N, this is very well approximated by the simple expression

$$\sigma^2(I) \approx \sum_i p_i^2. \tag{6.7}$$

In order to compute the intensities and uncertainties, the detector components in McStas thus must keep track of $N = \sum_i p_i^0$, $I = \sum_i p_i^1$, and $M_2 = \sum_i p_i^2$.

6.2 Weight factor transformations during a Monte Carlo choice

When a Monte Carlo choice must be performed, *e.g.* when the initial energy and direction of the neutron is decided at the source, it is important to adjust the neutron weight so that the combined effect of neutron weight change and Monte Carlo probability equals the actual physical properties of the component.

Let us follow up on the example of a source. In the "real" semi-classical world, there is a distribution (probability density) for the neutrons in the six dimensional (energy, direction, position) space of $\Pi(E, \mathbf{\Omega}, \mathbf{r}) = dP/(dEd\mathbf{\Omega}d^3\mathbf{r})$ depending upon the source temperature, geometry *etc.* In the Monte Carlo simulations, the six coordinates are for efficiency reasons in general picked from another distribution: $f_{\mathrm{MC}}(E, \mathbf{\Omega}, \mathbf{r}) \neq \Pi(E, \mathbf{\Omega}, \mathbf{r})$, since one would *e.g.* often generate only neutrons within a certain parameter interval. However, we must then require that the weights are adjusted by a factor π_j (in this case: $j = 1$) so that

$$f_{\mathrm{MC}}(E, \mathbf{\Omega}, \mathbf{r})\pi_j(E, \mathbf{\Omega}, \mathbf{r}) = \Pi(E, \mathbf{\Omega}, \mathbf{r}). \tag{6.8}$$

For the sources present in version 1.4, only the $(\mathbf{\Omega}, \mathbf{r})$ dependence of the correction factors are taken into account.

The weight factor transformation rule Eq. (6.8) is of course also valid for other types of Monte Carlo choices, although the probability distributions may depend upon different parameters. An important example is elastic scattering from a powder sample, where the Monte-Carlo choices are the scattering position and the final neutron direction.

It should be noted that the π_j's found in the weight factor transformation are multiplied by the π_j's found by the weight adjustments described in subsection 6.1 to yield the final neutron weight given by Eq. (6.1).

6.2.1 Focusing components

An important application of weight transformation is focusing. Assume that the sample scatters the neutrons in many directions. In general, only neutrons flying in some of these directions will stand any chance of being detected. These directions we call the *interesting directions*. The idea in focusing is to avoid wasting computation time on neutrons scattered in the uninteresting directions. This trick is an instance of what in Monte Carlo terminology is known as *importance sampling*.

If *e.g.* a sample scatters isotropically over the whole 4π solid angle, and all interesting directions are known to be contained within a certain solid angle interval $\Delta\mathbf{\Omega}$, only these solid angles are used for the Monte Carlo choice of scattering direction. According to Eq. (6.8), the weight factor will then have to be changed by the (fixed) amount $\pi_j =$

$|\Delta\mathbf{\Omega}|/(4\pi)$. One thus ensures that the mean simulated intensity is unchanged during a "correct" focusing, while a too narrow focusing will result in a lower (*i.e.* wrong) intensity, since one cuts away neutrons that would otherwise have counted.

One could also think of using adaptive importance sampling, so that McStas during the simulations will determine the most interesting directions and gradually change the focusing according to that. A first implementation of this idea is found in the Source_adapt component.

6.3 Transformation of random numbers

In order to perform the Monte Carlo choices, one needs to be able to pick a random number from a given distribution. However, most random number generators only give uniform distributions over a certain interval. We thus need to be able to transform between probability distributions, and we here give a short explanation on how to do this.

Assume that we pick a random number, x, from a distribution $\phi(x)$. We are now interested in the shape of the distribution of the transformed $y = f(x)$, assuming $f(x)$ is monotonous. All random numbers lying in the interval $[x; x + dx]$ are transformed to lie within the interval $[y; y+f'(x)dx]$, so the resulting distribution must be $\phi(y) = \phi(x)/f'(x)$.

If the random number generator selects numbers uniformly in the interval $[0; 1]$, we have $\phi(x) = 1$, and one may evaluate the above expression further

$$\phi(y) = \frac{1}{f'(x)} = \frac{d}{dy} f^{-1}(y). \tag{6.9}$$

By indefinite integration we reach

$$\int \phi(y)dy = f^{-1}(y) = x, \tag{6.10}$$

which is the essential formula for finding the right transformation of the initial random numbers. Let us illustrate with a few examples of transformations used within the McStas components.

The circle For finding a random point within the circle of radius R, one would like to choose the polar angle from a uniform distribution in $[0; 2\pi]$ and the radius from the normalised distribution $\phi(r) = 2r/R^2$. The polar angle is found simply by multiplying a random number with 2π. For the radius, we like to find $r = f(x)$, where again x is the generated random number. Left side of Eq. (6.10) gives $\int \phi(r)dr = \int 2r/R^2 dr = r^2/R^2$, which should equal x. Hence $r = R\sqrt{x}$.

Exponential decay In a simple time-of-flight source, the neutron flux decays exponentially after the initial activation at $t = 0$. We thus want to pick an initial neutron emission time from the normalised distribution $\phi(t) = \exp(-t/\tau)/\tau$. Use of Eq. (6.10) gives $x = -\exp(-t/\tau)$, which is a number in the interval $[-1; 0]$. If we want to pick a positive random number instead, we will have to change sign by $x_1 = -x$ and thus reach $t = -\tau \ln(x_1)$.

The sphere For finding a random point on the surface of the unit sphere, one needs to determine the two angles, (θ, ψ). As for a circle, ψ is chosen from a uniform distribution in $[0; 2\pi]$. The probability distribution of θ should be $\phi(\theta) = \sin(\theta)$ (for $\theta \in [0; \pi/2]$), whence $\theta = \cos^{-1}(x)$.

Chapter 7

The component library

This chapter has been removed from the manual and will instead be published in a separate manual describing the McStas components. The McStas component manualis edited by the McStas authors and it will include contributions from users writing components. As a complement to the McStas component manual, you may use the `mcdoc -s` command to obtain the on-line component documentation and refer to the McStas web-page [2] where all components are documented using the McDoc system.

7.1 A short overview of the McStas component library

This section gives a quick overview of available McStas components provided with the distribution, in the `MCSTAS` library. The location of this library is detailed in section 4.2.2. All of them are thought to be reliable, eventhough no absolute guaranty may be given concerning their accuracy.

The `contrib` directory of the library contains components that were given by McStas users, but are not validated yet.

Additionally the `obsolete` directory of the library gathers components that were renamed, or considered to be outdated. Anyway, they still all work as before.

The `mcdoc` front-end (section 4.4.7) enables to display both the catalog of the McStas library, e.g using:

```
mcdoc --show
```

as well as the documentation of specific components, e.g with:

```
mcdoc --text name
mcdoc --show file.comp
```

The first line will search for all components matching the *name*, and display their help section as text, where as the second example will display the help corresponding to the *file.comp* component, using your BROWSER setting, or as text if unset. The `--help` option will display the command help, as usual.

MCSTAS/sources	Description
Adapt_check	Optimization specifier for the Source_adapt component.
ESS_moderator_long	Parametrised pulsed source for modelling ESS long pulses.
ESS_moderator_short	A parametrised pulsed source for modelling ESS short pulses.
Moderator	A simple pulsed source for time-of-flight.
Monitor_Optimizer	To be used after the Source_Optimizer component.
Source_Maxwell_3	Source with up to three Maxwellian distributions
Source_Optimizer	A component that optimizes the neutron flux passing through the Source_Optimizer in order to have the maximum flux at the Monitor_Optimizer position.
Source_adapt	Neutron source with adaptive importance sampling.
Source_div	Neutron source with Gaussian divergence.
Source_flat	A circular neutron source with flat energy spectrum and arbitrary flux.
Source_flat_lambda	Neutron source with flat wavelength spectrum and arbitrary flux.
Source_flux	An old variant of the official Source_flux_lambda component.
Source_flux_lambda	Neutron source with flat wavelength spectrum and user-specified flux.
Source_gen	Circular/squared neutron source with flat or Maxwellian energy/wavelength spectrum (possibly spatially gaussian).
Virtual_input	Source-like component that generates neutron events from an ascii/binary 'virtual source' file (for Virtual_output).
Virtual_output	Detector-like component that writes neutron state (for Virtual_input).

Table 7.1: Source components of the McStas library.

MCSTAS/optics	Description
Arm	Arm/optical bench
Beamstop	Rectangular/circular beam stop.
Bender	Models a curved neutron guide (shown straight).
Chopper	Disk chopper.
Chopper_Fermi	Fermi Chopper with curved slits.
Collimator_linear	A simple analytical Soller collimator (with triangular transmission).
Filter_gen	This components may either set the flux or change it (filter-like), using an external data file.
Guide	Neutron guide.
Guide_channeled	Neutron guide with channels (bender section).
Guide_gravity	Neutron guide with gravity. Can be channeled and focusing.
Guide_wavy	Neutron guide with gaussian waviness.
Mirror	Single mirror plate.
Monochromator_curved	Double bent multiple crystal slabs with anisotropic gaussian mosaic.
Monochromator_flat	Flat Monochromator crystal with anisotropic mosaic.
Selector	A velocity selector (helical lamella type) such as V_selector component.
Slit	Rectangular/circular slit.
V_selector	Velocity selector.

Table 7.2: Optics components of the McStas library.

MCSTAS/samples	Description
Powder1	General powder sample with a single scattering vector.
Powder2	General powder sample with a two scattering vectors.
Res_sample	Sample for resolution function calculation.
Sans_spheres	Sample for Small Angle Neutron Scattering - hard spheres in thin solution, mono disperse.
Single_crystal	Mosaic single crystal with multiple scattering vectors.
V_sample	Vanadium sample.

Table 7.3: Sample components of the McStas library.

MCSTAS/monitors	Description
DivLambda_monitor	Divergence/wavelength monitor.
DivPos_monitor	Divergence/position monitor (acceptance diagram).
Divergence_monitor	Horizontal+vertical divergence monitor.
EPSD_monitor	A monitor measuring neutron intensity vs. position, x, and neutron energy, E.
E_monitor	Energy-sensitive monitor.
Hdiv_monitor	Horizontal divergence monitor L_monitor Wavelength-sensitive monitor.
Monitor	Simple single detector/monitor.
Monitor_4PI	Monitor that detects ALL non-absorbed neutrons.
Monitor_nD	This component is a general Monitor that can output 0/1/2D signals (Intensity or signal vs. [something] and vs. [something] ...).
PSD_monitor	Position-sensitive monitor.
PSD_monitor_4PI	Spherical position-sensitive detector.
PSDcyl_monitor	A 2D Position-sensitive monitor. The shape is cylindrical with the axis vertical. The monitor covers the whole cylinder (360 degrees).
PSDlin_monitor	Rectangular 1D PSD, measuring intensity vs. vertical position, x.
PreMonitor_nD	This component is a PreMonitor that is to be used with one Monitor_nD, in order to record some neutron parameter correlations.
Res_monitor	Monitor for resolution calculations.
TOFLambda_monitor	Time-of-flight/wavelength monitor.
TOF_cylPSD_monitor	Cylindrical (2pi) PSD Time-of-flight monitor.
TOF_monitor	Rectangular Time-of-flight monitor.
TOFlog_mon	Rectangular Time-of-flight monitor with logarithmic time binning.

Table 7.4: Monitor components of the McStas library.

MCSTAS/misc	Description
Progress_bar	A simulation progress bar. May also trigger intermediate SAVE.
Vitess_input	Read neutron state parameters from VITESS neutron file.
Vitess_output	Write neutron state parameters to VITESS neutron file.

Table 7.5: Miscellaneous components of the McStas library.

MCSTAS/contrib	Description
Al_window	Aluminium window in the beam.
Collimator_ROC	Radial Oscillationg Collimator (ROC).
Guide_curved	Non focusing continuous curved guide (shown curved).
Guide_tapering	Rectangular tapered guide (parabolic, elliptic, sections ...).
FermiChopper	Fermi Chopper with rotating frame.
Filter_graphite	Pyrolytic graphite filter (analytical model).
Filter_powder	Box-shaped powder filter based on Single_crystal (unstable).
Guide_honeycomb	Neutron guide with gravity and honeycomb geometry. Can be channeled and focusing.
He3_cell	Polarised 3He cell.
Monochromator_2foc	Double bent monochromator with multiple slabs.
SiC	SiC multilayer sample for reflectivity simulations.

Table 7.6: Contributed components of the McStas library.

MCSTAS/share	Description
adapt_tree-lib	Handles a simulation optimisation space for adatative importance sampling. Used by the Source_adapt component.
mcstas-r	Main Run-time library (always included).
monitor_nd-lib	Handles multiple monitor types. Used by Monitor_nD, Res_monitor, ...
read_table-lib	Enables to read a data table (text/binary) to be used within an instrument or a component.
vitess-lib	Enables to read/write Vitess event binary files. Used by Vitess_input and Vitess_output

Table 7.7: Shared libraries of the McStas library. See Appendix A for details.

MCSTAS/data	Description
*.lau	Laue pattern file, as issued from Crystallographica or FullProf. Data: [h k l Mult. d-space 2Theta F-squared]
*.trm	transmission file, typically for monochromator crystals and filters. Data: [k (Angs-1) , Transmission (0-1)]
*.rfl	reflectivity file, typically for mirrors and monochromator crystals. Data: [k (Angs-1) , Reflectivity (0-1)]

Table 7.8: Data files of the McStas library.

MCSTAS/examples	Description
*.instr	This directory contains example instruments, accessible throught the `mcgui` "Neutron site" menu.

Table 7.9: Instrument example files of the McStas library.

Chapter 8

Instrument examples

Here, we give a short description of three selected instruments. We present the McStas versions of the Risø standard triple axis spectrometer TAS1 (8.2) and the ISIS time-of-flight spectrometer PRISMA (8.3). Before that, however, we present one example of a component test instrument: the instrument to test the component **V_sample** (8.1). These instrument files are included in the McStas distribution in the `examples/` directory. All the instrument examples there-in may be executed automatically throught the McStas self-test procedure (see section 3.7). It is also our intention to extend the list of instrument examples extensively and perhaps publish them in a separate report.

8.1 A test instrument for the component V_sample

This instrument is one of many test instruments written with the purpose of testing the individual components. We have picked this instrument both because we would like to present an example test instrument and because it despite its simplicity has produced quite non-trivial results, also giving rise to the McStas logo.

The instrument consists of a narrow source, a 60' collimator, a V-sample shaped as a hollow cylinder with height 15 mm, inner diameter 16 mm, and outer diameter 24 mm at a distance of 1 m from the source. The sample is in turn surrounded by an unphysical 4π-PSD monitor with 50×100 pixels and a radius of 10^6 m. The set-up is shown in figure 8.1.

8.1.1 Scattering from the V-sample test instrument

In figure 8.2, we present the radial distribution of the scatting from an evenly illuminated V-sample, as seen by a spherical PSD. It is interesting to note that the variation in the scattering intensity is as large as 10%. This is an effect of attenuation of the beam in the cylindrical sample.

8.2 The triple axis spectrometer TAS1

With this instrument definition, we have tried to create a very detailed model of the conventional cold-source triple-axis spectrometer TAS1 at Risø National Laboratory. Un-

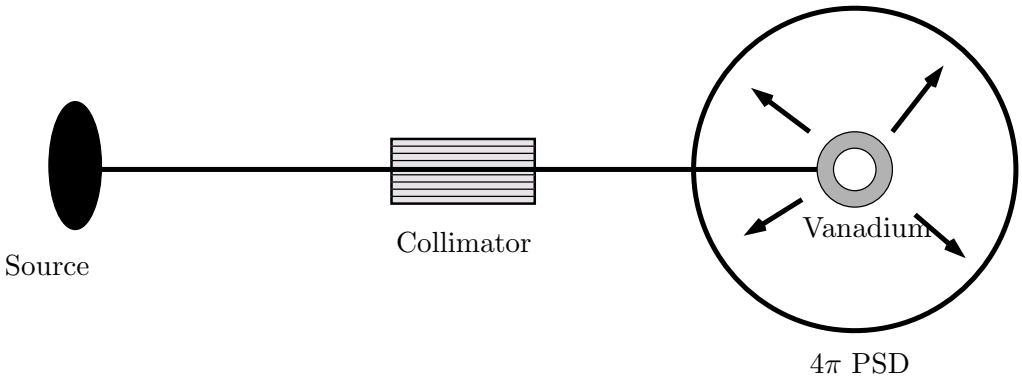

Figure 8.1: A sketch of the test instrument for the component V_sample.

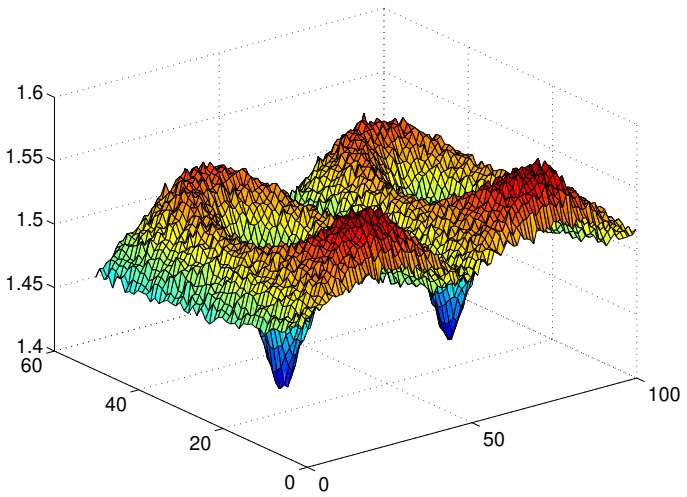

Figure 8.2: Scattering from a V-sample, measured by a spherical PSD. The sphere has been transformed onto a plane and the intensity is plotted as the third dimension. A colour version of this picture is found on the title page of this manual.

fortunately, no neutron scattering is performed at Risø anymore, but it still serves as a good example. Except for the cold source itself, all components used have quite realistic properties. Furthermore, the overall geometry of the instrument has been adapted from the detailed technical drawings of the real spectrometer. The TAS 1 simulation is the first detailed work performed with the McStas package.For further details see reference [12].

At the spectrometer, the channel from the cold source to the monochromator is asymmetric, since the first part of the channel is shared with other instruments. In the instrument definition, this is represented by three slits. For the cold source, we use a flat energy distribution (component **Source_flat**) focusing on the third slit.

The real monochromator consist of seven blades, vertically focusing on the sample. The angle of curvature is constant so that the focusing is perfect at 5.0 meV (20.0 meV for 2nd order reflections) for a 1×1 cm^2 sample. This is modeled directly in the instrument definition using seven **Monochromator** components. The mosaicity of the pyrolytic graphite crystals is nominally 30' (FWHM) in both directions. However, the simulations indicated that the horisontal mosaicities of both monochromator and analyser were more likely 45'. This was used for all mosaicities in the final instrument definition.

The monochromator scattering angle, in effect determining the incoming neutron energy, is for the real spectrometer fixed by four holes in the shielding, corresponding to the energies 3.6, 5.0, 7.2, and 13.7 meV for first order neutrons. In the instrument definition, we have adapted the angle corresponding to 5.0 meV in order to test the simulations against measurements performed on the spectrometer.

The exit channel from the monochromator may on the spectrometer be narrowed down from initially 40 mm to 20 mm by an insert piece. In the simulations, we have chosen the 20 mm option and modeled the channel with two slits to match the experimental set-up.

In the test experiments, we used two standard samples: An Al_2O_3 powder sample and a vanadium sample. The instrument definitions use either of these samples of the correct size. Both samples are chosen to focus on the opening aperture of collimator 2 (the one between the sample and the analyser). Two slits, one before and one after the sample, are in the instrument definition set to the opening values which were used in the experiments.

The analyser of the spectrometer is flat and made from pyrolytic graphite. It is placed between an entry and an exit channel, the latter leading to a single detector. All this has been copied into the instrument definition, where the graphite mosaicity has been set to 45'.

On the spectrometer, Soller collimators may be inserted at three positions: Between monochromator and sample, between sample and analyser, and between analyser and detector. In our instrument definition, we have used 30', 28', and 67' collimators on these three positions, respectively.

An illustration of the TAS1 instrument is shown in figure 8.3. Test results and data from the real spectrometer are shown in Appendix 8.2.1.

8.2.1 Simulated and measured resolution of TAS1

In order to test the McStas package on a qualitative level, we have performed a very detailed simulation of the conventional triple axis spectrometer TAS1, Risø. The measurement series constitutes a complete alignment of the spectrometer, using the direct beam and scattering from V and Al_2O_3 samples at an incoming energy of 20.0 meV, using

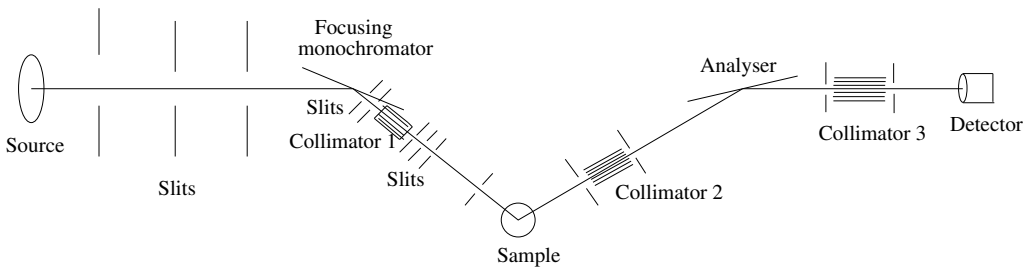

Figure 8.3: A sketch of the TAS1 instrument.

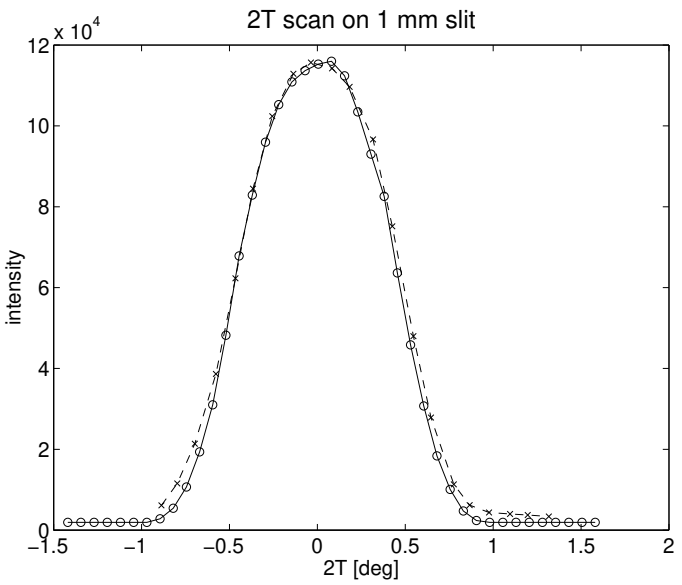

Figure 8.4: Scans of $2\theta_s$ in the direct beam with 1 mm slit on the sample position. "×": measurements, "o": simulations Collimations: open-30'-open-open.

the second order scattering from the monochromator. In the instrument definitions, we have used all available information about the spectrometer. However, the mosaicities of the monochromator and analyser are set to 45' in stead of the quoted 30', since we from our analysis believe this to be much closer to the truth.

In these simulations, we have tried to reproduce every alignment scan with respect to position and width of the peaks, whereas we have not tried to compare absolute intensities. Below, we show a few comparisons of the simulations and the measurements.

Figure 8.4 shows a scan of $2\theta_s$ on the collimated direct beam in two-axis mode. A 1 mm slit is placed on the sample position. Both the measured width and non-Gaussian peak shape are well reproduced by the McStas simulations.

In contrast, a simulated $2\theta_a$ scan in triple-axis mode on a V-sample showed a surprising offset from zero, see Figure 8.5. However, a simulation with a PSD on the sample position showed that the beam center was 1.5 mm off from the center of the sample, and this was

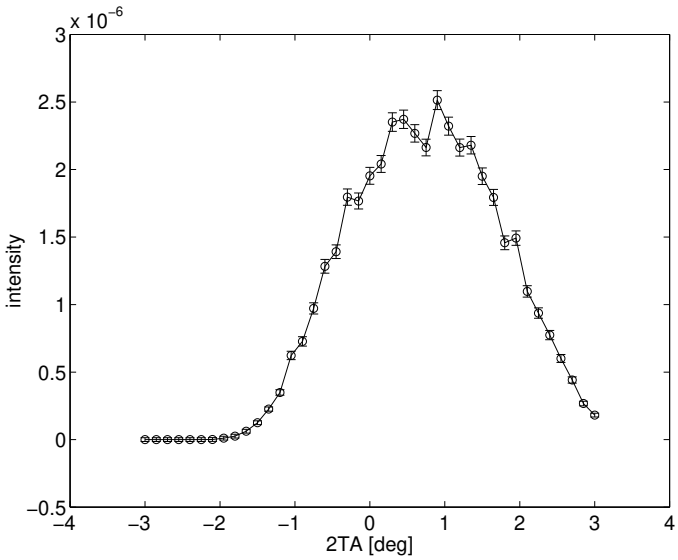

Figure 8.5: First simulated $2\theta_a$ scan on a vanadium sample. Collimations: open-30'-28'-open.

important since the beam was no wider than the sample itself. A subsequent centering of the beam resulted in a nice agreement between simulation and measurements. For a comparison on a slightly different instrument (analyser-detector collimator inserted), see Figure 8.6.

The result of a $2\theta_s$ scan on an Al_2O_3 powder sample in two-axis mode is shown in Figure 8.7. Both for the scan in focusing mode $(+\ -\ +)$ and for the one in defocusing mode $(+\ +\ +)$ (not shown), the agreement between simulation and experiment is excellent.

As a final result, we present a scan of the energy transfer $E_a = \hbar\omega$ on a V-sample. The data are shown in Figure 8.8.

8.3 The time-of-flight spectrometer PRISMA

In order to test the time-of-flight aspect of McStas, we have in collaboration with Mark Hagen, ISIS, written a simple simulation of a time-of-flight instrument loosely based on the ISIS spectrometer PRISMA. The simulation was used to investigate the effect of using a RITA-style analyser instead of the normal PRISMA backend.

We have used the simple time-of-flight source **Tof_source**. The neutrons pass through a beam channel and scatter off from a vanadium sample, pass through a collimator on to the analyser. The RITA-style analyser consists of seven analyser crystals that can be rotated independently around a vertical axis. After the analysers we have placed a PSD and a time-of-flight detector.

To illustrate some of the things that can be done in a simulation as opposed to a real-life experiment, this example instrument further discriminates between the scattering off each individual analyser crystal when the neutron hits the detector. The analyser component is modified so that a global variable `neu_color` keeps track of which crystal scatters the

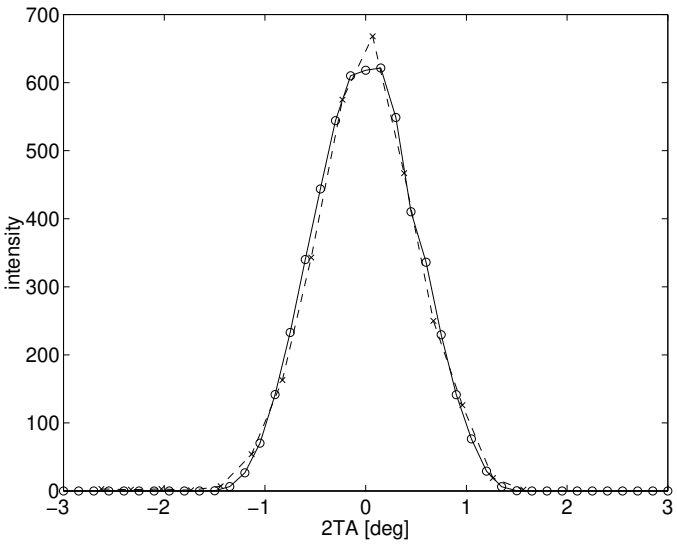

Figure 8.6: Corrected $2\theta_a$ scan on a V-sample. Collimations: open-30'-28'-67'. "×": measurements, "o": simulations.

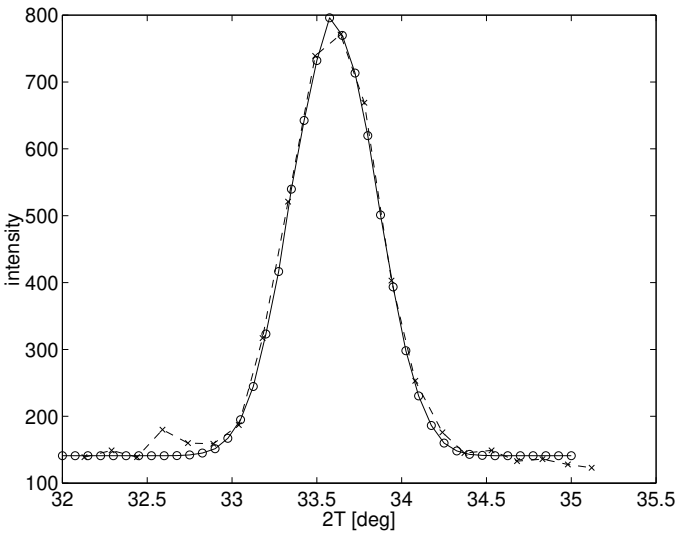

Figure 8.7: $2\theta_s$ scans on Al_2O_3 in two-axis, focusing mode. Collimations: open-30'-28'-67'. "×": measurements, "o": simulations. A constant background is added to the simulated data.

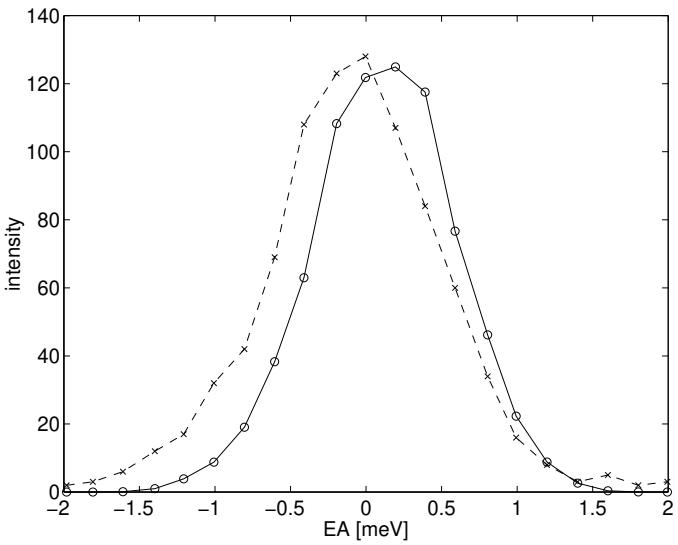

Figure 8.8: Scans of the analyser energy on a V-sample. Collimations: open-30'-28'-67'. "×": measurements, "o": simulations.

neutron. The detector component is then modified to construct seven different time-of-flight histograms, one for each crystal (see the source code for the instrument for details). One way to think of this is that the analyser blades paint a color on each neutron which is then observed in the detector. An illustration of the instrument is shown in figure 8.9. Test results are shown in Appendix 8.3.1.

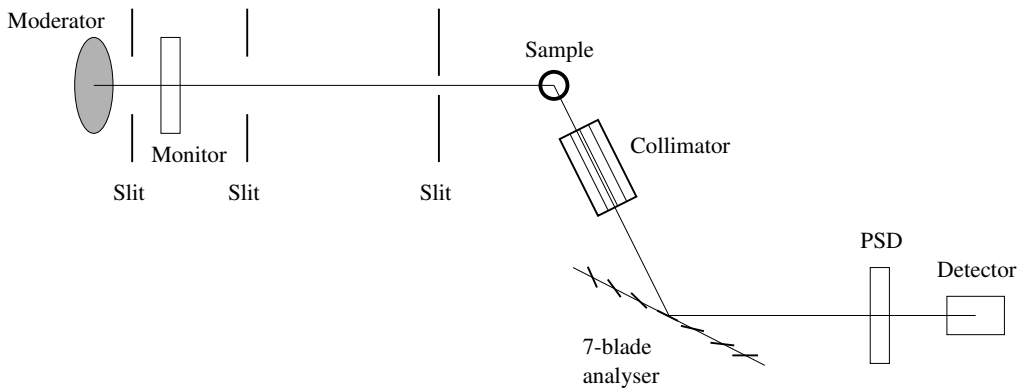

Figure 8.9: A sketch of the PRISMA instrument.

8.3.1 Simple spectra from the PRISMA instrument

A plot from the detector in the PRISMA simulation is shown in Figure 8.10. These results were obtained with each analyser blade rotated one degree relative to the previous one. The separation of the spectra of the different analyser blades is caused by different energy

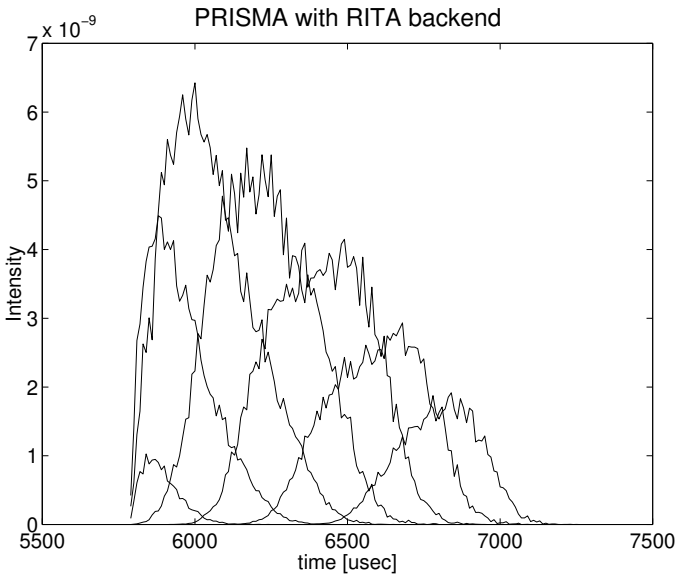

Figure 8.10: Test result from PRISMA instrument using "coloured neutrons". Each graph shows the neutrons scattered from one analyser blade.

of scattered neutrons and different flight path length from source to detector. We have not performed any quantitative analysis of the data at this time.

Appendix A

Libraries and conversion constants

The McStas Library contains a number of built-in functions and conversion constants which are useful when constructing components. These are stored in the `share` directory of the `MCSTAS` library.

Within these functions, the 'Run-time' part is available for all component/instrument descriptions. The other parts (see table 7.7) are dynamic, that is they are not pre-loaded, but only imported once when a component requests it using the `%include` McStas keyword. For instance, within a component C code block, (usually SHARE or DECLARE):

```
%include "read_table-lib"
```

will include the 'read_table-lib.h' file, and the 'read_table-lib.c' (unless the `--no-runtime` option is used with `mcstas`). Similarly,

```
%include "read_table-lib.h"
```

will *only* include the 'read_table-lib.h'. The library embedding is done only once for all components (like the SHARE section). For an example of implementation, see the Res_monitor component.

Here, we present a short list of both each of the library contents and the run-time features.

A.1 Run-time calls and functions

Here we list a number of preprogrammed macros which may ease the task of writing component and instrument definitions.

A.1.1 Neutron propagation

- **ABSORB**. This macro issues an order to the overall McStas simulator to interrupt the simulation of the current neutron history and to start a new one.
- **PROP_Z0**. Propagates the neutron to the $z = 0$ plane, by adjusting (x, y, z) and t. If the neutron velocity points away from the $z = 0$ plane, the neutron is absorbed. If component is centered, in order to avoid the neutron to be propagated there, use the `_intersect` functions to determine intersection time(s), and then a `PROP_DT` call.

- **PROP_DT**(dt). Propagates the neutron through the time interval dt, adjusting (x, y, z) and t.

- **PROP_GRAV_DT**(dt, Ax, Ay, Az). Like **PROP_DT**, but it also includes gravity using the acceleration (Ax, Ay, Az). In addition, to adjusting (x, y, z) and t also (vx, vy, vz) is modified.

- **SCATTER**. This macro is used to denote a scattering event inside a component, see section 5.4.5. It should be used e.g to indicate that a component has 'done something' (sctattered or detected). This does not affect the simulation at all, and is mainly used by the `MCDISPLAY` section and the `GROUP` modifier (see 5.3.4 and 5.4.8). See also the SCATTERED variable (below).

A.1.2 Coordinate and component variable retrieval

- **MC_GETPAR**(). This may be used in the finally section of an instrument definition to reference the output parameters of a component. See page 61 for details.

- **NAME_CURRENT_COMP** gives the name of the current component as a string.

- **POS_A_CURRENT_COMP** gives the absolute position of the current component. A component of the vector is referred to as POS_A_CURRENT_COMP.i where i is x, y or z.

- **ROT_A_CURRENT_COMP** and **ROT_R_CURRENT_COMP** give the orientation of the current component as rotation matrices (absolute orientation and the orientation relative to the previous component, respectively). A component of a rotation matrice is referred to as ROT_A_CURRENT_COMP$[m][n]$, where m and n are 0, 1, or 2.

- **POS_A_COMP**(*comp*) gives the absolute position of the component with the name *comp*. Note that *comp* is not given as a string. A component of the vector is referred to as POS_A_COMP(*comp*).i where i is x, y or z.

- **ROT_A_COMP**(*comp*) and **ROT_R_COMP**(*comp*) give the orientation of the component *comp* as rotation matrices (absolute orientation and the orientation relative to its previous component, respectively). Note that *comp* is not given as a string. A component of a rotation matrice is referred to as ROT_A_COMP(*comp*)$[m][n]$, where m and n are 0, 1, or 2.

- **INDEX_CURRENT_COMP** is the number (index) of the current component (starting from 1).

- **POS_A_COMP_INDEX**(*index*) is the absolute position of component *index*. POS_A_COMP_INDEX (INDEX_CURRENT_COMP) is the same as POS_A_CURRENT_COMP. You may use POS_A_COMP_INDEX (INDEX_CURRENT_COMP+1) to make, for instance, your component access the position of the next component (this is usefull for automatic targeting). A component of the vector is referred to as

POS_A_COMP_INDEX(*index*).*i* where i is x, y or z. **POS_R_COMP_INDEX** works the same, but with relative coordinates.

- **STORE_NEUTRON**($index, x, y, z, vx, vy, vz, t, sx, sy, sz, p$) stores the current neutron state in the trace-history table, in local coordinate system. *index* is usually INDEX_CURRENT_COMP. This is automatically done when entering each component of an instrument.

- **RESTORE_NEUTRON**($index, x, y, z, vx, vy, vz, t, sx, sy, sz, p$) restores the neutron state to the one at the input of the component *index*. To ignore a component effect, use RESTORE_NEUTRON (INDEX_CURRENT_COMP, $x, y, z, vx, vy, vz, t, sx, sy, sz, p$) at the end of its TRACE section, or in its EXTEND section. These neutron states are in the local component coordinate systems.

- **SCATTERED** is a variable set to 0 when entering a component, which is incremented each time a SCATTER event occurs. This may be used in the `EXTEND` sections (always executed when existing) to branch action depending if the component acted or not on the current neutron.

- **extend_list**(n, &*arr*, &*len*, *elemsize*). Given an array *arr* with *len* elements each of size *elemsize*, make sure that the array is big enough to hold at least n elements, by extending *arr* and *len* if necessary. Typically used when reading a list of numbers from a data file when the length of the file is not known in advance.

- **mcset_ncount**(n). Sets the number of neutron histories to simulate to n.

- **mcget_ncount**(). Returns the number of neutron histories to simulate (usually set by option `-n`).

- **mcget_run_num**(). Returns the number of neutron histories that have been simulated until now.

A.1.3 Coordinate transformations

- **coords_set**(x, y, z) returns a Coord structure (like POS_A_CURRENT_COMP) with x, y and z members.

- **coords_get**(P, &x, &y, &z) copies the x, y and z members of the Coord structure P into x, y, z variables.

- **coords_add**(a, b), **coords_sub**(a, b), **coords_neg**(a) enable to operate on coordinates, and return the resulting Coord structure.

- **rot_set_rotation**(*Rotation t*, ϕ_x, ϕ_y, ϕ_z) Get transformation for rotation first ϕ_x around x axis, then ϕ_y around y, then ϕ_z around z. t should be a 'Rotation' ([3][3] 'double' matrix).

- **rot_mul***(Rotation t1, Rotation t2, Rotation t3)* performs $t3 = t1.t2$.

- **rot_copy***(Rotation dest, Rotation src)* performs $dest = src$ for Rotation arrays.

- **rot_transpose***(Rotation src, Rotation dest)* performs $dest = src^t$.

- **rot_apply***(Rotation t, Coords a)* returns a Coord structure which is $t.a$

A.1.4 Mathematical routines

- **NORM**(x, y, z). Normalizes the vector (x, y, z) to have length 1.

- **scalar_prod**$(a_x, a_y, a_z, b_x, b_y, b_z)$. Returns the scalar product of the two vectors (a_x, a_y, a_z) and (b_x, b_y, b_z).

- **vecprod**$(a_x, a_y, a_z, b_x, b_y, b_z, c_x, c_y, c_z)$. Sets (a_x, a_y, a_z) equal to the vector product $(b_x, b_y, b_z) \times (c_x, c_y, c_z)$.

- **rotate**$(x, y, z, v_x, v_y, v_z, \varphi, a_x, a_y, a_z)$. Set (x, y, z) to the result of rotating the vector (v_x, v_y, v_z) the angle φ (in radians) around the vector (a_x, a_y, a_z).

- **normal_vec**$(\&n_x, \&n_y, \&n_z, x, y, z)$. Computes a unit vector (n_x, n_y, n_z) normal to the vector (x, y, z).

A.1.5 Output from detectors

- **DETECTOR_OUT_0D**(...). Used to output the results from a single detector. The name of the detector is output together with the simulated intensity and estimated statistical error. The output is produced in a format that can be read by McStas front-end programs. See section 5.4.7 for details.

- **DETECTOR_OUT_1D**(...). Used to output the results from a one-dimentional detector. See section 5.4.7 for details.

- **DETECTOR_OUT_2D**(...). Used to output the results from a two-dimentional detector. See section 5.4.7 for details.

- **DETECTOR_OUT_3D**(...). Used to output the results from a three-dimentional detector. Arguments are the same as in DETECTOR_OUT_2D, but with the additional z axis (the signal). Resulting data files are treated as 2D data, but the 3rd dimension is specified in the *type* field.

- **mcheader_out***(FILE *f,char *parent, int m, int n, int p, char *xlabel, char *ylabel, char *zlabel, char *title, char *xvar, char *yvar, char *zvar, double x1, double x2, double y1, double y2, double z1, double z2, char *filename)* appends a header file using the current data format setting. Signification of parameters may be found in section 5.4.7. Please contact the authors in case of perplexity.

- **mcinfo_simulation***(FILE *f, mcformat, char *pre, char *name)* is used to append the simulation parameters into file f (see for instance the Res_monitor component). Internal variable $mcformat$ should be used as specified. Please contact the authors in case of perplexity.

A.1.6 Ray-geometry intersections

- **box_intersect**(&t_1, &t_2, x, y, z, v_x, v_y, v_z, d_x, d_y, d_z). Calculates the (0, 1, or 2) intersections between the neutron path and a box of dimensions d_x, d_y, and d_z, centered at the origin for a neutron with the parameters (x, y, z, v_x, v_y, v_z). The times of intersection are returned in the variables t_1 and t_2, with $t_1 < t_2$. In the case of less than two intersections, t_1 (and possibly t_2) are set to zero. The function returns true if the neutron intersects the box, false otherwise.

- **cylinder_intersect**(&t_1, &t_2, x, y, z, v_x, v_y, v_z, r, h). Similar to **box_intersect**, but using a cylinder of height h and radius r, centered at the origin.

- **sphere_intersect**(&t_1, &t_2, x, y, z, v_x, v_y, v_z, r). Similar to **box_intersect**, but using a sphere of radius r.

A.1.7 Random numbers

- **rand01**(). Returns a random number distributed uniformly between 0 and 1.

- **randnorm**(). Returns a random number from a normal distribution centered around 0 and with $\sigma = 1$. The algorithm used to get the normal distribution is explained in [13], chapter 7.

- **randpm1**(). Returns a random number distributed uniformly between -1 and 1.

- **randvec_target_circle**(&v_x, &v_y, &v_z, &$d\Omega$, aim_x, aim_y, aim_z, r_f). Generates a random vector (v_x, v_y, v_z), of the same length as $(\mathrm{aim}_x, \mathrm{aim}_y, \mathrm{aim}_z)$, which is targeted at a *disk* centered at $(\mathrm{aim}_x, \mathrm{aim}_y, \mathrm{aim}_z)$ with radius r_f (in meters), and perpendicular to the *aim* vector.. All directions that intersect the sphere are chosen with equal probability. The solid angle of the sphere as seen from the position of the neutron is returned in $d\Omega$. This routine was previously called **randvec_target_sphere** (which still works).

- **randvec_target_rect_angular**(&v_x, &v_y, &v_z, &$d\Omega$, aim_x, aim_y, aim_z,$height, width, Rot$) does the same as randvec_target_circle but targetting at a rectangle with angular dimensions *height* and *width* (in **radians**, not in degrees as other angles). The rotation matrix *Rot* is the coordinate system orientation in the absolute frame, usually ROT_A_CURRENT_COMP.

- **randvec_target_rect**(&v_x, &v_y, &v_z, &$d\Omega$, aim_x, aim_y, aim_z,$height, width, Rot$) is the same as randvec_target_rect_angular but *height* and *width* dimensions are given in meters. This function is useful to target at a guide entry window.

A.2 Reading a data file into a vector/matrix (Table input)

The `read_table-lib` provides functionalities for reading text (and binary) data files. To use this library, add a `%include "read_table-lib"` in your component definition DECLARE or SHARE section. Available functions are:

- **Table_Init**(&$Table$) and **Table_Free**(&$Table$) initialize and free allocated memory blocks

- **Table_Read**(&$Table$, $filename$, *block*) reads numerical block number *block* (0 for all) data from *text* file $filename$ into $Table$. The block number changes when the numerical data changes its size, or a comment is encoutered (lines starting by '`# ; % /`'). If the data could not be read, then $Table.data$ is NULL and $Table.rows = 0$. You may then try to read it using Table_Read_Offset_Binary.

- **Table_Rebin**(&$Table$) rebins $Table$ rows with increasing, evenly spaced first column (index 0), e.g. before using Table_Value.

- **Table_Read_Offset**(&$Table$, $filename$, *block*, &$offset$, n_{rows}) does the same as Table_Read except that it starts at offset $offset$ (0 means begining of file) and reads n_{rows} lines (0 for all). The $offset$ is returned as the final offset reached after reading the n_{rows} lines.

- **Table_Read_Offset_Binary**(&$Table$, $filename$, *type*, *block*, &$offset$, n_{rows}, $n_{columns}$) does the same as Table_Read_Offset, but also specifies the *type* of the file (may be "float" or "double"), the number n_{rows} of rows to read, each of them having $n_{columns}$ elements. No text header should be present in the file.

- **Table_Info**($Table$) print information about the table $Table$.

- **Table_Index**($Table, m, n$) reads the $Table[m][n]$ element.

- **Table_Value**($Table, x, n$) looks for the closest x value in the first column (index 0), and extracts in this row the n-th element (starting from 0). The first column is thus the 'x' axis for the data.

The format of text files is free. Lines starting by '`# ; % /`' characters are considered to be comments. Data blocks are vectors and matrices. Block numbers are counted starting from 1, and changing when a comment is found, or the column number changes. For instance, the file 'MCSTAS/data/BeO.trm' (Transmission of a Berylium filter) looks like:

```
# BeO transmission, as measured on IN12
# Thickness: 0.05 [m]
# [ k(Angs-1) Transmission (0-1) ]
# wavevector multiply
1.0500  0.74441
1.0750  0.76727
1.1000  0.80680
...
```

Binary files should be of type "float" (i.e. REAL*32) and "double" (i.e. REAL*64), and should *not* contain text header lines. These files are plateform dependent (little or big endian).

The $filename$ is first searched into the current directory (and all user additional locations specified using the `-I` option, see section 4.2.2), and if not found, in the `data`

sub-directory of the `MCSTAS` library location. This way, you do not need to have local copies of the McStas Library Data files (see table 7.8).

A usage example for this library part may be:

```
t_Table rTable;       % declares a t_Table structure
char file="BeO.trm";  % a file name
double x,y;

Table_Init(&rTable);  % initialize the table to empty state
Table_Read(&rTable, file, 1); % reads the first numerical block
Table_Info(rTable);   % display table informations
...
x = Table_Index(rTable, 2,5);  % reads the 3rd row, 6th column element
                               % of the table. Indexes start at zero in C.
y = Table_Value(rTable, 1.45,1);  % looks for value 1.45 in 1st column (x axis)
                                  % and extract 2nd column value of that row
Table_Free(&rTable);  % free allocated memory for table
```

Additionally, if the block number (3rd) argument of **Table_Read** is 0, all blocks will be catenated. The **Table_Value** function assumes that the 'x' axis is the first column (index 0). Other functions are used the same way with a few additional parameters, e.g. specifying an offset for reading files, or reading binary data.

You may look into, for instance, the Monochromator_curved component, or the Virtual_input component for other implementation examples.

A.3 Monitor_nD Library

This library gathers a few functions used by a set of monitors e.g. Monitor_nD, Res_monitor, Virtual_output, ... It may monitor any kind of data, create the data files, and may display many geometries (for `mcdisplay`). Refer to these components for implementation examples, and ask the authors for more details.

A.4 Adaptative importance sampling Library

This library is currently only used by the components Source_adapt and Adapt_check. It performs adaptative importance sampling of neutrons for simulation efficiency optimization. Refer to these components for implementation examples, and ask the authors for more details.

A.5 Vitess import/export Library

This library is used by Vitess_input, Vitess_output components, as well as the `mcstas2vitess` utility (see section 4.4.8). Refer to these components for implementation examples, and ask the authors for more details.

A.6 Constants for unit conversion etc.

The following predefined constants are useful for conversion between units

Name	Value	Conversion from	Conversion to
DEG2RAD	$2\pi/360$	Degrees	radians
RAD2DEG	$360/(2\pi)$	Radians	degrees
MIN2RAD	$2\pi/(360 \cdot 60)$	Minutes of arc	radians
RAD2MIN	$(360 \cdot 60)/(2\pi)$	Radians	minutes of arc
V2K	$10^{10} \cdot m_{\mathrm{N}}/\hbar$	Velocity (m/s)	**k**-vector (Å^{-1})
K2V	$10^{-10} \cdot \hbar/m_{\mathrm{N}}$	**k**-vector (Å^{-1})	Velocity (m/s)
VS2E	$m_{\mathrm{N}}/(2e)$	Velocity squared (m^2 s^{-2})	Neutron energy (meV)
SE2V	$\sqrt{2e/m_{\mathrm{N}}}$	Square root of neutron energy (meV$^{1/2}$)	Velocity (m/s)
FWHM2RMS	$1/\sqrt{8\log(2)}$	Full width half maximum	Root mean square (standard deviation)
RMS2FWHM	$\sqrt{8\log(2)}$	Root mean square (standard deviation)	Full width half maximum
MNEUTRON	$1.67492E-27kg$	Neutron mass	
HBAR	$1.05459E-34Js$	Planck constant	
PI	3.14159265358979323846	π	

Further, we have defined the constants **PI**= π and **HBAR**= $\hbar$.

Appendix B

The McStas terminology

This is a short explanation of phrases and terms which have a specific meaning within McStas. We have tried to keep the list as short as possible with the risk that the reader may occasionally miss an explanation. In this case, you are more than welcome to contact the authors.

- **Arm** A generic McStas component which defines a frame of reference for other components.
- **Component** One unit (*e.g.* optical element) in a neutron spectrometer.
- **Definition parameter** An input parameter for a component. For example the radius of a sample component or the divergence of a collimator.
- **Input parameter** For a component, either a definition parameter or a setting parameter. These parameters are supplied by the user to define the characteristics of the particular instance of the component definition. For an instrument, a parameter that can be changed at simulation run-time.
- **Instrument** An assembly of McStas components defining a neutron spectrometer.
- **McStas** Monte Carlo Simulation of Triple Axis Spectrometers (the name of this project).
- **Output parameter** An output parameter for a component. For example the counts in a monitor. An output parameter may be accessed from the instrument in which the component is used using `MC_GETPAR`.
- **Run-time** C code, contained in the files `mcstas-r.c` and `mcstas-r.h` included in the McStas distribution, that declare functions and variables used by the generated simulations.
- **Setting parameter** Similar to a definition parameter, but with the restriction that the value of the parameter must be a number.

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Index

Code generation options, 26
Comments, 48
Components, 11, 52
Coordinate system, 48

Data format, 10, 29, 44, 45

Embedded C code, 49, 51, 52, 54
Environment variable
  BROWSER, 43, 73
  EDITOR, 34
  MCSTAS, 26, 73, 86, 91
  MCSTAS_CC, 15
  MCSTAS_CFLAGS, 15
  MCSTAS_FORMAT, 10, 15, 22, 29, 40, 42, 44
  PGPLOT_DEV, 38, 41, 42
  PGPLOT_DIR, 38, 41, 42

Gravitation, 48

Installing, 13, 15, 40
Instruments, 49

Kernel, 9, **47**
Keyword, 49

  %include, 26, 49, 86
  ABSOLUTE, 52
  AT, 52
  COMPONENT, 52
  DECLARE, 10, 51, 59
  DEFINE
    COMPONENT, 57
    INSTRUMENT, 51
  DEFINITION PARAMETERS, 57
  END, 55, 64
  EXTEND, 9, 53, 87
  FINALLY, 10, 54, 63
  GROUP, 10, 53, 87
  INITIALIZE, 52, 60
  MCDISPLAY, 63, 87
  OUTPUT PARAMETERS, 58, 59
  POLARISATION PARAMETERS, 58
  PREVIOUS, 10, 53
  RELATIVE, 52
  ROTATED, 52
  SAVE, 10, 54, 61
  SETTING PARAMETERS, 57
  SHARE, 10, 60, 86
  STATE PARAMETERS, 58
  TRACE, 52, 60

Library, **86**
  adapt_tree-lib, 92
  Components, 11, 26, 43, 44, 53, **73**
    contrib, 11, 73, 77
    data, 11, 77, 91
    doc, 11
    misc, 11, 76
    monitors, 11, 76
    obsolete, 11, 73
    optics, 11, 12, 75
    samples, 12, 75
    share, 12, 47, 49, 77, 86
    sources, 12, 74
  Instruments, 11, 77
  mcstas-r, *see* Library/Run-time
  monitor_nd-lib, 92
  read_table-lib (Read_Table), 49, **90**
  Run-time, 10, 27, 47, 49, 77, **86**
    ABSORB, 60, 86
    DETECTOR_OUT, 10, 61
    MC_GETPAR, 59, 87
    NAME_CURRENT_COMP, 87
    POS_A_COMP, 87
    POS_A_CURRENT_COMP, 87

PROP_DT, 86
PROP_GRAV_DT, 86
PROP_Z0, 86
randvec_target_rect, 11
RESTORE_NEUTRON, 87
ROT_A_COMP, 87
ROT_A_CURRENT_COMP, 87
SCATTER, 53, 54, 60, 86
SCATTERED, 54, 87
STORE_NEUTRON, 87
Shared, *see* Library/Components/share
vitess-lib, 44, 92

Neutron state and units, 48

Parameters
Definition, 52, 57
Instruments, 10, 28, 39, 51
Optional, default value, 9, 28, 51, 58
Scans, 39
Setting, 10, 52, 57

Signal handler, **30**
INT signal, 55
TERM signal, 55
USR1 signal, 11
USR2 signal, 10, 54
Simulation optimization, 27, 32

Testing the distribution, 15
Tools, 13, 21
gscan (obsolete), 40
IDL, 13, 30, 45
Matlab, 13, 29, 41, 42, 44, 45
mcconvert, 14, **44**
mcdisplay, **40**
mcdoc, 14, **43**, 66, 73
mcgui, 21, 25, **34**, 40, 42
mcplot, 11, 14, 30, 39, **41**
mcresplot, 14, **42**
mcrun, 14, 25, **39**
mcstas2vitess, 14, **44**, 92
Perl libraries, 13, 38, 41–43
Scilab, 13, 29, 41, 42, 44, 45

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Peter Kjær Willendrup, Emmanuel Farhi, Kim Lefmann, Per-Olof Åstrand, Mark Hagen and Kristian Nielsen

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Abstract (Max. 2000 char.)

The software package McStas is a tool for carrying out Monte Carlo ray-tracing simulations of neutron scattering instruments with high complexity and precision. The simulations can compute all aspects of the performance of instruments and can thus be used to optimize the use of existing equipment, design new instrumentation, and carry out virtual experiments. McStas is based on a unique design where an automatic compilation process translates high-level textual instrument descriptions into efficient ANSI-C code. This design makes it simple to set up typical simulations and also gives essentially unlimited freedom to handle more unusual cases.

This report constitutes the reference manual for McStas, and, together with the manual for the McStas components, it contains full documentation of all aspects of the program. It covers the various ways to compile and run simulations, a description of the meta-language used to define simulations, and some example simulations performed with the program.

Descriptors

Neutron Instrumentation; Monte Carlo Simulation; Software

Available on request from:
Information Service Department, Risø National Laboratory
(Afdelingen for Informationsservice, Forskningscenter Risø)
P.O. Box 49, DK–4000 Roskilde, Denmark
Phone +45 4677 4004, Telefax +45 4677 4013