The philosophy of McStas*

Per-Olof Åstrand[1,2], Kim Lefmann[1] and Kristian Nielsen[1,†]
[1] Materials Research Department, Risø National Laboratory, DK-4000 Roskilde, Denmark
[2] Department of Chemistry, University of Copenhagen, Universitetsparken 5,
DK-2100 Copenhagen Ø, Denmark

Abstract

The design of the neutron ray-tracing package McStas is presented. In particular, aspects important for making a neutron ray-tracing program a useful tool for the neutron scattering community are discussed. Finally, some ideas on future development are discussed.

Introduction

It is in principle a rather trivial task to write a short ray-tracing program for studying the properties of a specific beam-component and indeed many such programs have been written over the years. To be a general tool for the neutron scattering community, however, some aspects of a simulation software have to be considered in detail:

- **Correctness**. Neutron scattering is an expensive technique because of the large-scale facility required for generating the neutrons. For a simulation program to play an important role in the design of for example the ESS instrumentation, it is required that the software has been tested and validated extensively.
- **Modularity**. Many different types of beam components and instruments exist and a modular structure of the software is required to make it possible for *users* to study new types of instruments and add additional beam components.
- **Efficiency**. Long simulations are required and it is therefore preferred that the simulation code is generated in C or Fortran which give an efficient executable.
- **User-friendly**. The software should be user-friendly in two different ways. It should be easy to get started to use the program and it should be possible also for the user to easily make extensions to the program.

An important initiative is to define a set of model instruments for validating simulation programs [1]. Around five simulation softwares participate in this project, including McStas [2–7], Vitess [8, 9] and Restrax [10, 11], and the first results for McStas are presented in this report [12]. In addition, some detailed simulations have been carried out comparing McStas and Restrax with favourable results [13–15].

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†Present address: Sifira A/S, Fredericiagade 16, DK-1310 Copenhagen K, Denmark

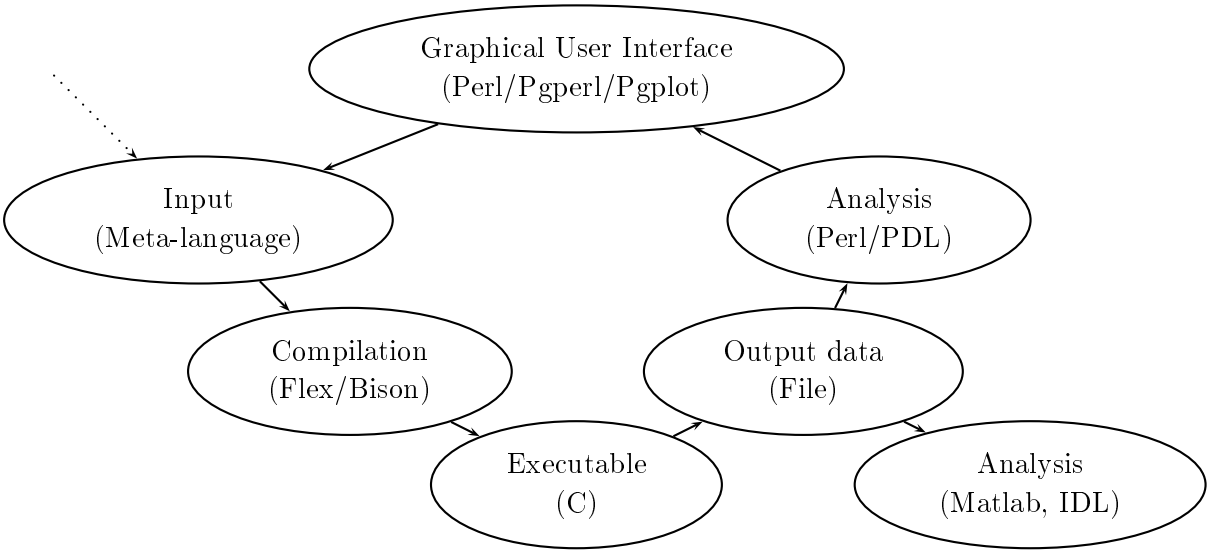

Figure 1: Schematic representation of the structure of McStas

Design of McStas

The McStas software was designed with these aspects in mind already from the start, and a version 1.0 was released in October 1998. In particular, the modularity of McStas has been considered in detail:

- Components are defined in separate files using a meta-language especially designed for the task.
- An instrument is defined by a set of components using the same meta-language.
- Many standard components (around 50) are available as a part of the McStas package, but it is in principle easy for users to implement additional components
- In particular, it is noted that all the physics is included in the component and instrument definitions, whereas the kernel handles the actual ray-tracing and local coordinate system transformations.

The structure of McStas is illustrated in Figure 1. The instrument input is given by editing the instrument file and specifying the simulation parameters either in the graphical user interface McGUI or at the command line. The instrument specification is compiled using the FLEX and Bison facilities and a C code is produced. The compilation ensures to some degree that the instrument specification is correct and the resulting C code gives an efficient executable. The resulting data from the simulation can either be analyzed with some basic McStas routines written in Perl or by the same methods an experiment is analyzed.

Version 1.4.2 of McStas contains 49 components [2], where examples of recent contributions include long- and short-pulse moderators for ESS. It is also noted that the McStas

components include virtual components acting as an interface to Vitess (`Vitess_input` and `Vitess_output`). Recently, a three-component model of the spin for modelling polarization instruments have been agreed on and the first components including polarisation will appear in McStas 1.5 to be released in September 2001.

To make a simulation software like McStas a useful tool for the neutron scattering community some points have to be considered in detail:

- Obviously, it is important that all the functionality is documented in detail in a user manual. A tutorial is crucial for new users to start running simulations.
- The interaction with the user community is preferrably handled by a web-page and an email-list. It should be emphasized that it is a time-demanding task to actually keep a web-page informative and up-to-date. It is not enough that a web-page exists, it also has to be of high quality!
- The graphical user interface is important for new users and users that only do simulations from time to time. Experienced users tend to prefer scripts where simulations may be automatized.
- It is of fundamental importance for a software addressing the scientific community that it is possible to extend the program. It should be easy for the *user* not only to define new types of instruments but also to include new physics (components). Also the source code should be available for modifications.

Simulation data is analyzed in principle in the same way as experimental data. In McStas, some Perl routines exist for some basic visualizations, but is the intention that McStas in the future will support the NeXus data format [16, 17]. Ideally, in the future the same standard tools can be used to analyze all simulations and experiments.

Simulations using McStas

McStas is used extensively also outside Risø National Laboratory and some of the recent work is mentioned here:

- The new guides on instruments at ILL have been simulated extensively [12, 14, 15, 18].
- Many of the new instruments at the FRM-II reactor in Munich have been simulated extensively.
  - The design of the time-of-flight spectrometer and diffractometer have been studied [19, 20].
  - The optical components of the structure powder diffractometer have been investigated [13].
  - The design of the thermal triple-axis spectrometer PUMA has been studied [21].

  - The neutron guide of the single-crystal diffractometer RESI has been optimized [22, 23].

- The RITA-2 instrument recently moved from Risø to PSI has been studied in simulations including a realistic model of the SINQ cold source [24].

- An entire inelastic neutron scattering experiment on RITA-1 at Risø has been simulated using the TASCOM interface to McStas [25].

- Loss mechanisms (including waviness and misalignments) in supermirror neutron guides have been simulated [26].

- The design of the proposed high-resolution inverse geometry spectrometer at SNS have been studied by simulation [27].

- The design of the guide CG1 at HFIR in Oak Ridge has been studied by simulations [28].

- Proposed high-resolution chopper spectrometers for the Joint Project in Japan have been investigated by simulations [29].

- Simulations have been carried out of a triple-axis spectrometer with neutron resonance spin-echo [30].

Prospects and future extensions

Many ideas exist for future extensions of McStas in particular and for simulations of neutron scattering instruments in general. Here, some ideas arising from discussions with the user community are listed.

- Calculation of correlation functions. Virtual monitors can be placed in principle everywhere in the instrument, and it is thus possible to correlate unexpected results with neutron properties at a component. Some support for this exist in the `Monitor_nD` and `PreMonitor_nD` components by Emmanuel Farhi. In addition, recently an option for labeling neutrons has been included and some spurious side-peaks of an experiment at the RITA-1 instrument at Risø was investigated [7].

- Automatic optimization of instrument parameters. It should be investigated if a Metropolis-like algorithm using adaptive importance sampling can be useful.

- Investigating stopping conditions for experiments. Currently, the only stopping condition in McStas is the number of neutron events. In line, with the work by R. McGreevy and coworkers in developing software for other stopping conditions in experiments (such as the precision for a requested property) [31], suitable stopping conditions should be investigated in simulations. It requires, however, extensions of the simulation software as illustrated in Figure 2. An instrument controller is required, for example written in Perl, that can be used to divide a simulation into several steps and analyse the

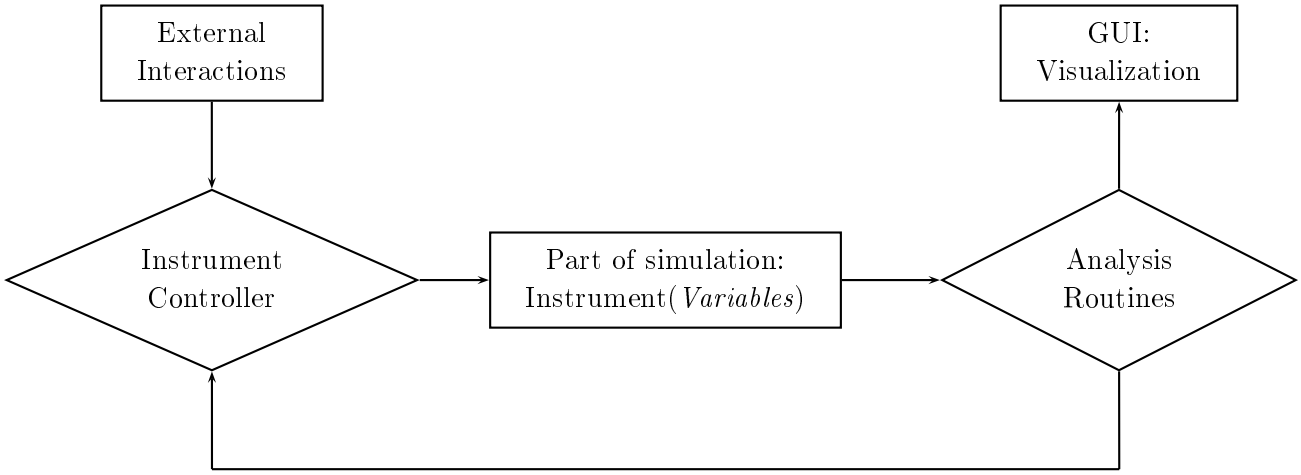

Figure 2: Schematic representation of a simulation controller

results of each step before it is decided if the simulation is continued. Obviously, an instrument controller being able to handle the results of many simulations would be useful in many cases, for example for automatic optimization of instrument parameters as mentioned in the previous entry.

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