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McStas 1.1: A tool for building neutron Monte Carlo simulations

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Abstract

McStas is a project to develop general tools for the creation of simulations of neutron scattering experiments. In this paper, we briefly introduce McStas and describe a particular application of the program: the Monte Carlo calculation of the resolution function of a standard triple axis neutron scattering instrument. The method compares well with the analytical calculations of Popovici.

Keywords: Monte Carlo simulations, Neutron instruments, Resolution function

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With the very high complexity and price of current neutron scattering instrumentation, the knowledge gained by accurate numerical simulation has become essential, both for choosing the right design when building new instruments and for using them in an efficient way. The Risø package McStas is a software tool constructed to enable scientists to create and run such simulations with a minimum of effort [1,2]. McStas has its own high-level meta-language, which is designed especially for positioning components within an instrument, and a compiler from the McStas language to ANSI C. McStas is equipped with a number of front-ends to control the simulations (e.g. for scanning), for displaying the simulation results, and for visualizing the neutron paths (e.g. for debugging).

McStas version 1.0 was released in October 1998, with an update (version 1.1) in March 1999. The McStas project is open to the neutron community; the source code and component library may be freely downloaded, and users may contribute new code back to the project. Updates are made available on the project home page [1]. The current component library includes continuous and pulsed sources, supermirror guides and benders, slits, Soller collimators, and filters, monochromator/analyzer crystals with off-cut surface and anisotropic mosaic, powder and vanadium samples, disk and Fermi choppers, velocity selectors, and a wide variety of detectors. It is also simple for users to add their own components. McStas is currently in use at Risø, Kjeller, München, ILL, ISIS, PSI, Argonne, NIST, Ansto, and JAERI.

In this paper, we demonstrate the calculation of the resolution function of an instrument using McStas. The intensity, I, observed in a general neutron experiment may be written as [3]

$$I(Q_0,\omega_0) = \int R(Q_0+\Delta Q,\omega_0+\Delta\omega)\sigma(Q_0+\Delta Q,\omega_0+\Delta\omega)d(\Delta Q)d(\Delta\omega), \qquad (1)$$

where σ is the scattering cross section. R is the resolution function, which is given by

$$R(Q,\omega) = \int_{\mathrm{path}} P(Q,\omega,\mathrm{path}), \qquad (2)$$

where $P(Q,\omega,\mathrm{path})$ is the transmission probability for a neutron along the given path and the integral is over all possible paths with the given energy and momentum transfer.

In the standard analytical treatment of a triple-axis instrument by Cooper and Nathans, the analyzer and monochromator crystals are both assumed to have Gaussian mosaic rocking curves, and the collimators to have Gaussian transmissions. This leads to the well known Gaussian resolution ellipsoid [3]. In McStas we calculate for each initial neutron state the *neutron weight,* p, in the detector, the expected value of which is proportional to the transmission probability. This allows us to perform a Monte Carlo integral of Eq. (2) simultaneous for the relevant intervals of Q and ω. We utilize a sample component where $\sigma(Q,\omega)$ is constant and a detector component which directly measures (Q,ω,p) for each neutron. This method is similar to the one used in the current version of RESTRAX [4], a Monte Carlo program specific to triple-axis spectrometers.

The resolution front-end allows analysis and visualization of the results in various ways. As an example, we have simulated the standard triple-axis spectrometer TAS1 at Risø at a nominal incoming energy of 5 meV, $(Q,\omega) = (1.0\ \text{Å}^{-1}, 1.0\ \text{meV})$. Figure 1 shows histograms of the resolution function along the four axes (Q_x along the scattering vector, Q_y perpendicular in the horizontal scattering plane, Q_z vertically, and ω energy transfer). Also available are two and three dimensional visualizations of the resolution ellipsoid, and computations of the resolution matrix and Bragg widths. The resulting Bragg widths agree to within 10% with a standard calculation used on the Popovici extension of the Cooper-Nathans formalism [5].

By using the presented Monte Carlo method, it is possible to calculate the resolution function of any instrument — not just the Gaussian triple-axis of Cooper and Nathans. This makes the method invaluable for developing and using advanced neutron spectrometers, like RITA at Risø [6].

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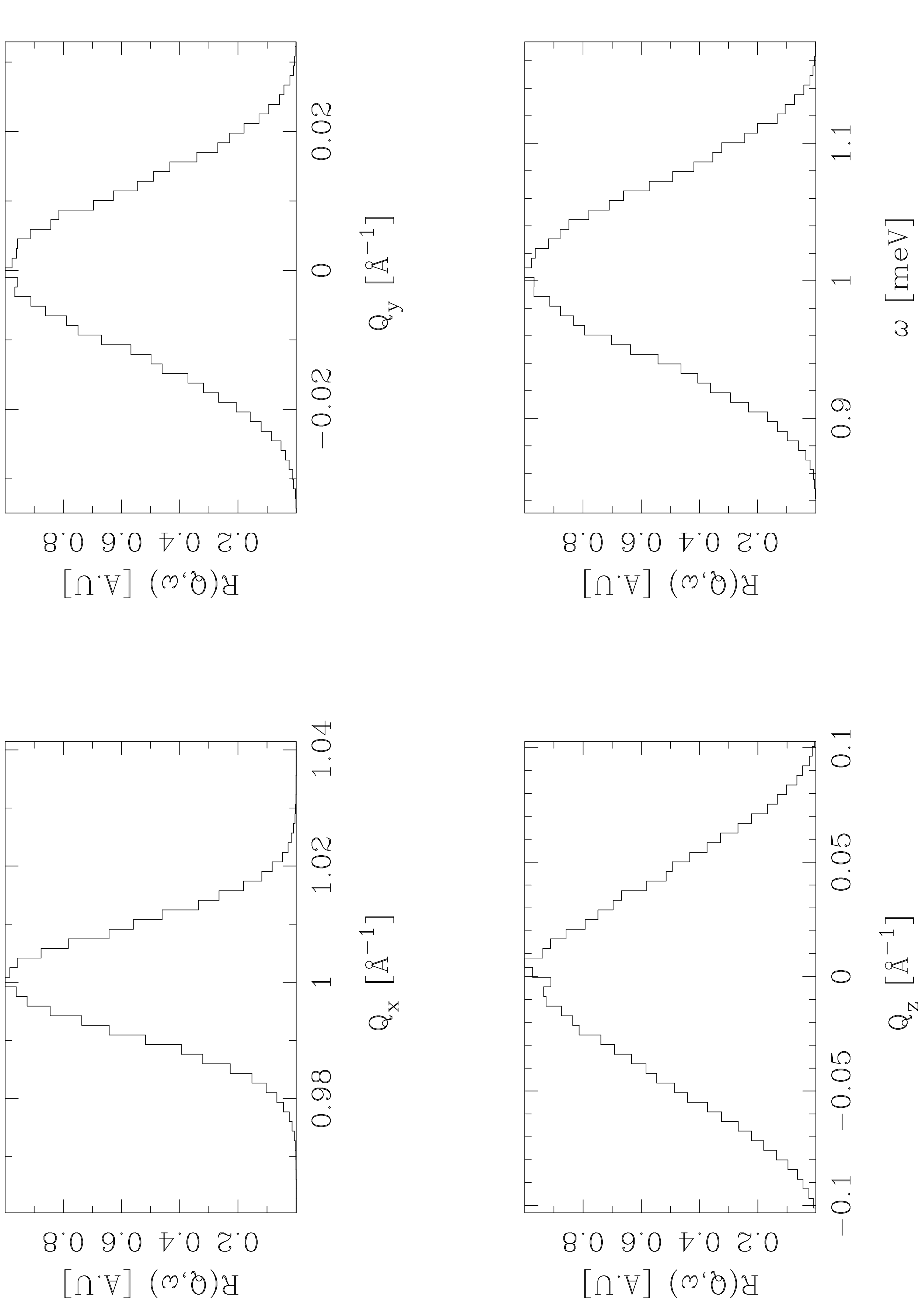
FIGURES

FIG. 1. Histograms of the resolution function at TAS1 along the four axes Q_x, Q_y, Q_z, and ω. The incident energy is 5.0 meV and all collimations are 60'.



R(Q,ω) [A.U]
0.2 0.4 0.6 0.8
Q_y [Å^-1]
−0.02 0 0.02
ω [meV]
0.9 1 1.1
Q_x [Å^-1]
0.98 1 1.02 1.04
Q_z [Å^-1]
−0.1 −0.05 0 0.05 0.1