Raytrace of Neutron Optical Systems with RESTRAX

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Abstract. RESTRAX is an advanced software package for raytrace simulations of neutron optical systems. This chapter reviews the techniques used by its efficient raytrace code, namely sampling strategy, numerical optimizations and details of the random-walk technique used to simulate transport through neutron optical components. In addition, raytrace simulations of resolution functions and model spectra for three-axis neutron spectrometers are briefly described.

4.1 Introduction

Raytrace simulation permits realistic modeling of neutron optics components as well as of complete neutron scattering instruments. While development of neutron raytrace software goes back to the 1970s (MCLIB library, [1]), it has been significantly accelerated by the advent of powerful desktop computers in 1990s and has lead to the creation of several software packages capable of realistic modeling of most of modern neutron optics devices. They include the programs NISP [2] based on the MCLIB library, IDEAS [3], McStas [4], VITESS [5] or RESTRAX [6]. Of course, Monte Carlo (MC) simulation always involves a trade-off between the level of physical reality implemented in the description of neutron transport and computing speed. Consequently, these programs differ in both the physical models underlying simulation of particular components and the structure of their code, depending on the different purposes for which they have been written. While some put emphasis on modularity (McStas, VITESS, NISP), which permits one to easily incorporate new components and to test new ideas of experimental techniques, others, like RESTRAX, trade part of their flexibility for a highly efficient sampling strategy permitting to gain several orders of magnitude in computing speed.

In the first part of this chapter, we review some principles and methods, upon which the efficient raytrace code used by the RESTRAX package is based, namely sampling strategy, numerical optimizations, and details of the

1 The RESTRAX package is available at http://omega.ujf.cas.cz/restrax
random-walk technique used to simulate neutron transport through neutron optical components. This part is followed by a brief description of the ray-tracing method used to simulate resolution functions of three-axis neutron spectrometers.

4.2 About the RESTRAX Code

The RESTRAX package actually consists of two independent modules. One is designed specifically to simulate three-axis spectrometers (TASs) and includes tools for simulation of resolution functions, convolutions, data fitting, and a set of modules implementing different scattering functions. The other one, called SIMRES, is equipped with a raytrace code which simulates instrument components on a more detailed level and provides more flexibility in varying instrument configuration. In addition, functions for parameter space mapping and numerical optimizations are provided, which makes this module a useful tool for designing novel neutron optical components and instrument configurations.

4.2.1 Instrument Model

The instrument model has a closed structure of a three-axis neutron spectrometer with a fixed number and succession order of the optical elements (Fig. 4.1). Each of the elements is, however, described in considerable detail

Fig. 4.1. Instrument layout in SIMRES with positions of beam monitors