McStas Union components for simulating multiple scattering

Mads Bertelsen, Kim Lefmann
University of Copenhagen
mads.bertelsen@gmail.com

Talk at DMSC November 17th 15.30

Monte Carlo ray tracing packages like McStas and Vitess have been the workhorse for modern neutron scattering instrumentation design, and are excellent for simulating the intended path of the neutron beam. This is sufficient for simulating the signal expected at the detector with a certain sample, but the current implementations have severe limitations when it comes to predicting the background from the unintended paths through the instrument. The problem originates from the basic assumption that a neutron instrument can be built from spatially isolated components, where the neutron will be propagated through these in a certain order specified by the user. In this way, contributions from all other possible orders of components are ignored.

We present a new set of McStas components called Union components that are able to overcome these limitations by allowing every possible multiple scattering path between them, much like the NISP implementation by P.A. Seeger. This way it is possible to model parts of the instrument where the linear succession of components is a good approximation with the existing set of McStas components, while using this new approach only in places where multiple possible neutron paths are expected.

The code splits the typical task of a McStas component into smaller parts: scattering processes and geometries. It is then possible to place such geometries in the McStas simulation and assign them a list of scattering processes such as incoherent scattering, powder scattering, single crystal diffraction and the like. The new ray tracing core will weigh each of these appropriately and natively perform multiple scattering between all added geometries and processes. The geometries can even overlap each other to create complicated shapes like a sample with the entire sample holder and cryostat around it, where each material will have appropriate absorption cross section and scattering processes. Adding a new scattering process is easier than creating a regular McStas component, as one only needs to describe the scattering cross section and a single scattering event.

The major obstacle to overcome when allowing all possible paths is to maintain a low execution time. This was done by analyzing the entire geometry before the actual ray tracing, resulting in a simple logical network which avoid unnecessary computations.

The talk will introduce the Union components and demonstrate new possibilities that allow for virtual experiments on a new level.

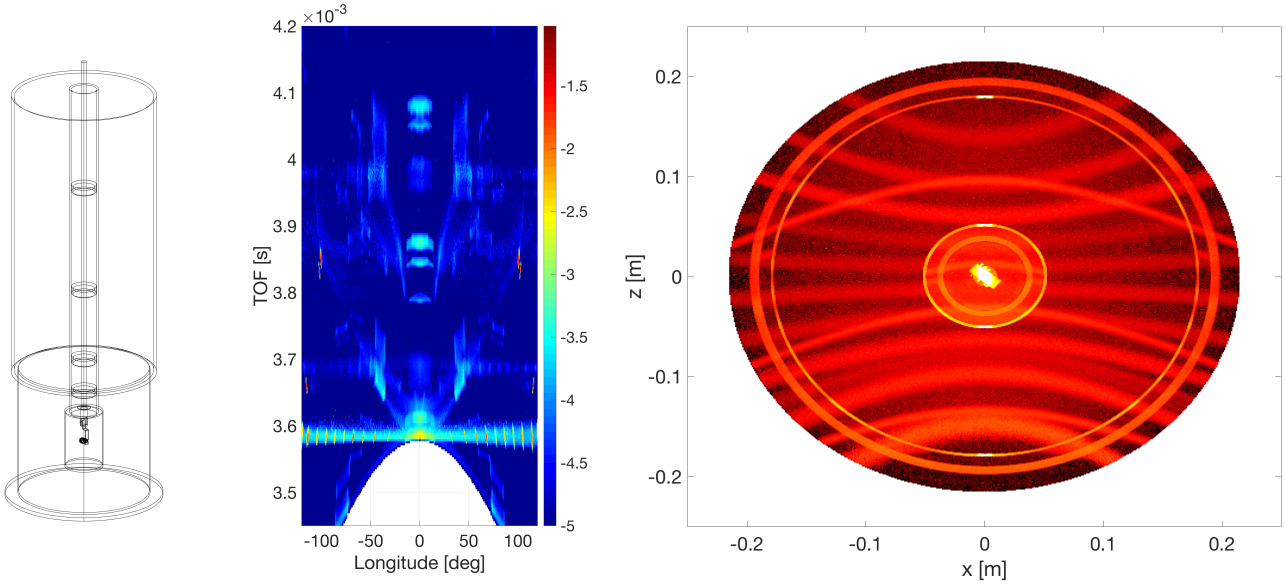

Figure 1: Left: Depiction of cryostat/sample model. Center: Time of flight banana monitor showing spurions. Right: Histogram over scattering locations in cryostat as seen from above.