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McXtrace

McXtrace - An X-ray Monte Carlo Ray-tracing software package

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Abstract

We present plans and very early designs for a software package, simulating X-ray instrumentation. The package, McXtrace, is spun off from the McStas package[1], and modified to apply to X-rays. Where possible the code base is identical, inherenting the modularity and flexibility of the parent package, which has been proven in the neutron scattering community through a decade.

Funding is secured for a concentrated effort for the next few years[2], intending to go far beyond existing packages, partly by inviting the community to contribute by coding their own modules.

Conversion from McStas

The code structure of McStas is basically divided into 3 parts:

Instrument Consists of Components. May simply be a list of components in the setup with their coordinates in the McStas-meta language, but may also include complex programming. Users are required to write such a file - assisted by GUI/helper applications.

Component Where "physics" happen. Inside components the interactions between neutrons/X-rays and matter are described. Some users who wish to contribute and/or develop new features (not yet in the library components) write these. Often components are initiated by users and completed and maintained by the McStas/McXtrace team. As components are usually no more than ≈ 300 lines of code, this is usually a manageble task, even for non-specialized programmers[a].

Kernel The Kernel takes care of positioning the bits and pieces of an neutron/X-ray experimental setup and handles beam transport. No users need to bother about this.

[a]such as physicists

In the same manner, the process of spinning off McXtrace from McStas occurs on the same three levels. On the Kernel level the transport mechanisms are edited to reflect the properties of an X-ray photon vs. a neutron.

NEUTRON	X-RAY PHOTON
$\mathrm{n} = (\mathbf{r}, \mathbf{v}, p, t, \mathbf{s})$	$\tilde{\mathrm{p}} = (\mathbf{r}, \mathbf{k}, p, \phi, \mathbf{E})$
→ time domain propagation	→ freq. domain propagation
• magnetic field/spin polarization	• optical polarization
• gravitational field	• phase propagation/wave optics

Ray-tracing vs., wave optics

Seen from the perspective of a single neutron/x-ray photon, the particle travels from device to device, or in the laguage of McStas/McXtrace *from component to component*, where the kernel takes care of transport inbetween components. The Kernel itself sees components at "black boxes". Inside a component code (generally written in c) may do anything and everything do the particle. The upshot of this is that inside a component, indeed a different mode of transport may be employed. For instance, inside a single crystal component the ray is considered to be a wave which interacts with the crystal and exits the component as a (possibly) modified ray (Figure 1.).

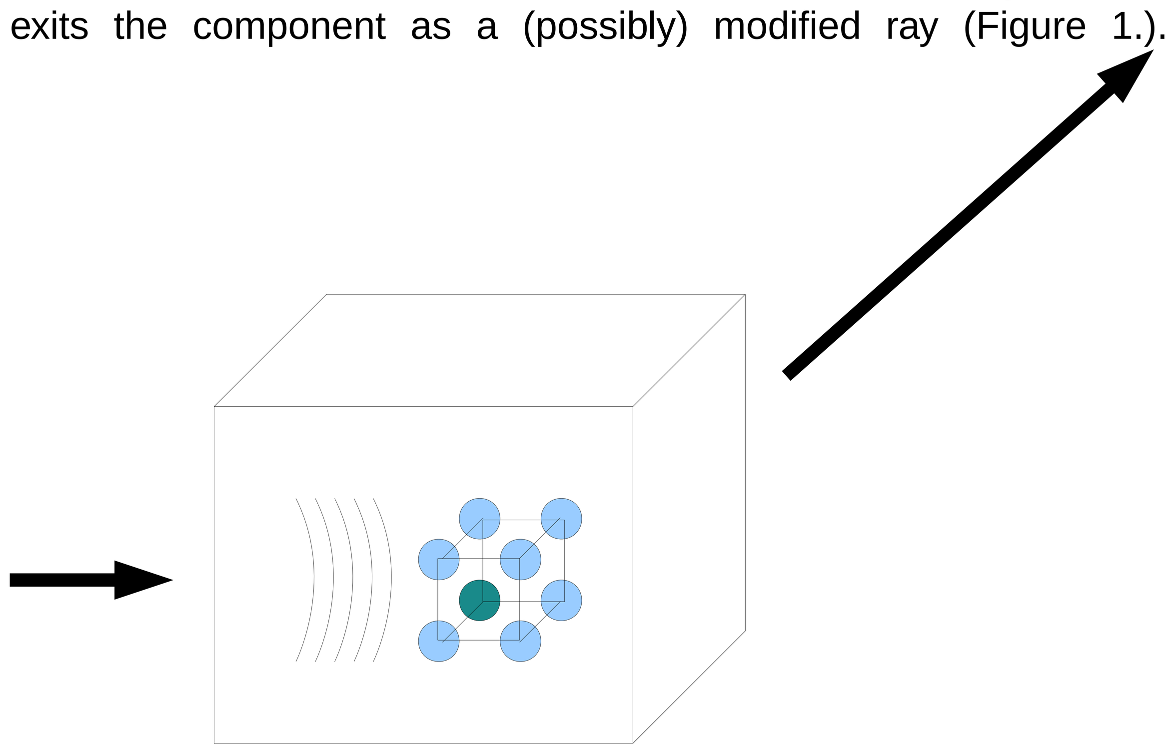
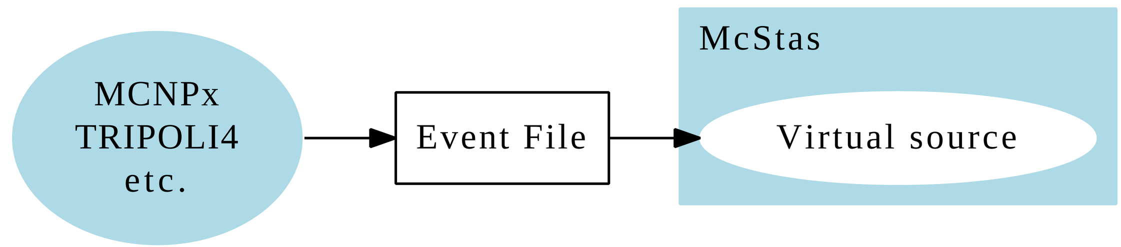


Figure 1: Schematic of the Single crystal component in McStas/McXtrace. A ray enters the component, inside the component it is treated as a wave and, on exit, is converted back to a ray again

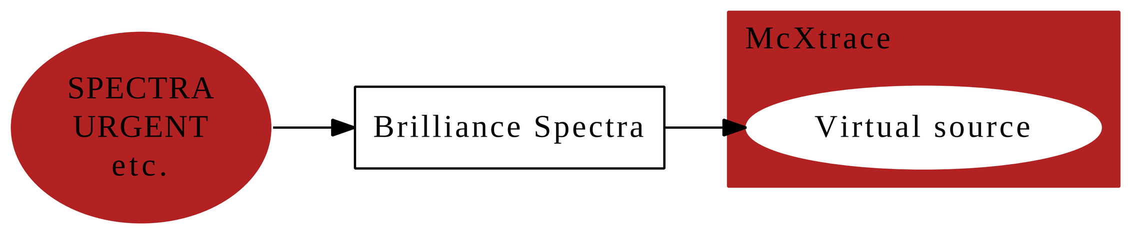
Tie-ins with established software packages

General philosophy: If soneome does it well already - interface, don't reinvent *but* have very simple models in-house. In terms of sources for instance the structure is:

NEUTRON



X-RAY PHOTON



Another example of this kind of interfacing is the single crystal sample component where input generally comes from a crystallographic program such as "Crystallographica"[3].

1st batch of Target instruments

A set of three target instruments have been set for the first phase of the project with increased complexity as we go along.

Low Budget Monochromatic Beamline

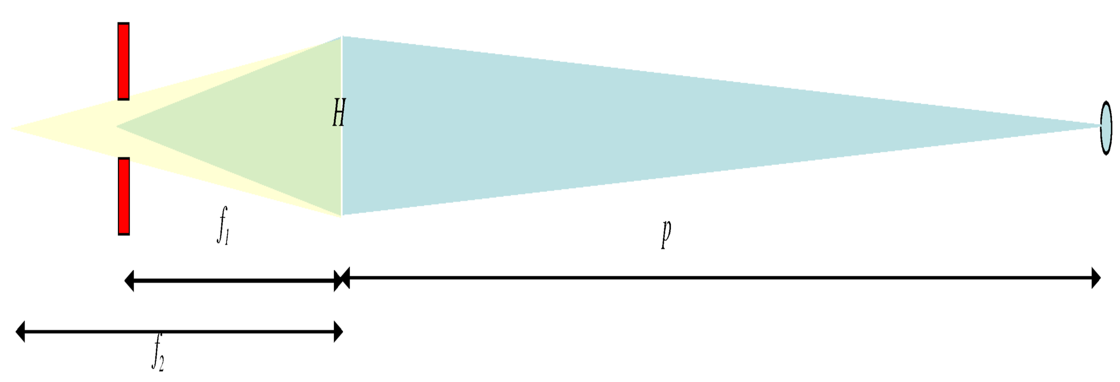
The 1st target insrument is a proposed Low-cost monchormatic beamline, where monochromaticity is provided by a simple slit and a Be-lens. The slit is set in the focal point of the lens for the targeted wavelength, λ_0. In principle, wavelengths $\neq \lambda_0$ will be absorbed in the slit. Due to its simplicity this kind of arrangement would be very cheap compared to other, more sofisticated solutions.

If we denote the lens aperture H, the source size σ, the images size in the focal point becomes: $h = (f_1/p)\sigma$. Further, for the lens

$$(\lambda_1 f_1)^{(1/2)} = (\lambda_2 f_2)^{(1/2)} = c$$

. Thus, we may write the energy resolution as:

$$\frac{h}{H} = \frac{f_2 - f_1}{f_2} = \frac{\frac{c^2}{\lambda_2} - \frac{c^2}{\lambda_1}}{\frac{c^2}{\lambda_2}} = \frac{E_2 - E_1}{E_2} = \frac{\Delta E}{E} \Rightarrow \frac{\Delta E}{E} = \frac{f_1}{p}\frac{\sigma}{H}$$



As example: given

$$\frac{f_1}{p} = \frac{1}{10}; \; H = 0.8mm; \; \sigma = 0.08mm;$$

we get

$$\frac{\Delta E}{E} = 1\%$$

SAXS

Laboratory equipment may also be simulated using this approach. A collaboration agreement is setup with an external company to model their Small Angle Xray Scattering product.[a]

Figure 2: Picture of the JJ-X-Ray SAX machine.

[a]The 1st fundamental milestone of the McXtrace project entails a detailed simulationof this setup

ESRF, ID11

The insertion device Beamline ID11 at the European Synchrotron Radiation Facility[4], hosts the 3DXRD-microscope[5].[a] It is a well chosen target instrukent since it consists of a fairly complex setup with many different optical options, yet one where the differnet objects easily may be thought of as discrete entities or components. Figures and show most of the components that need to be modelled in order ot have a complete description of the beamline.

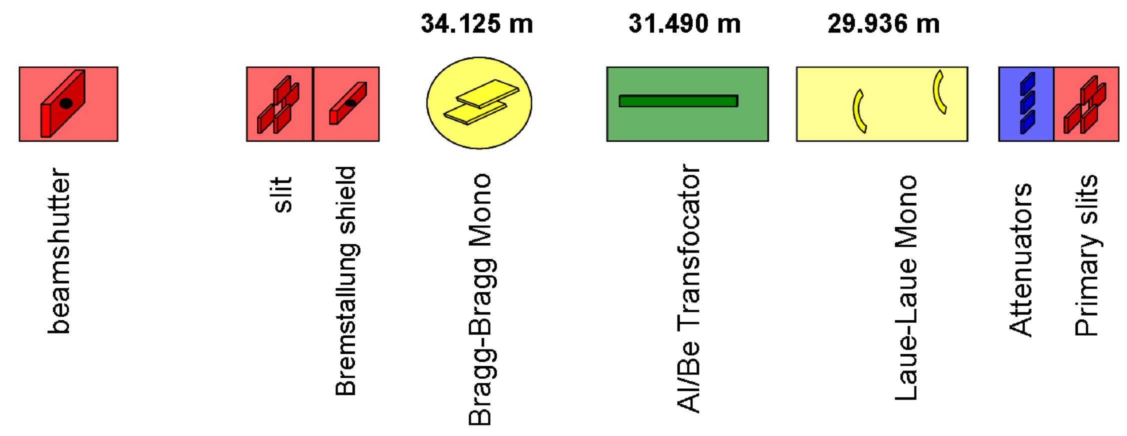


Figure 3: Schematic drawing of the primary optics elements of beamline ID11 (ESRF).

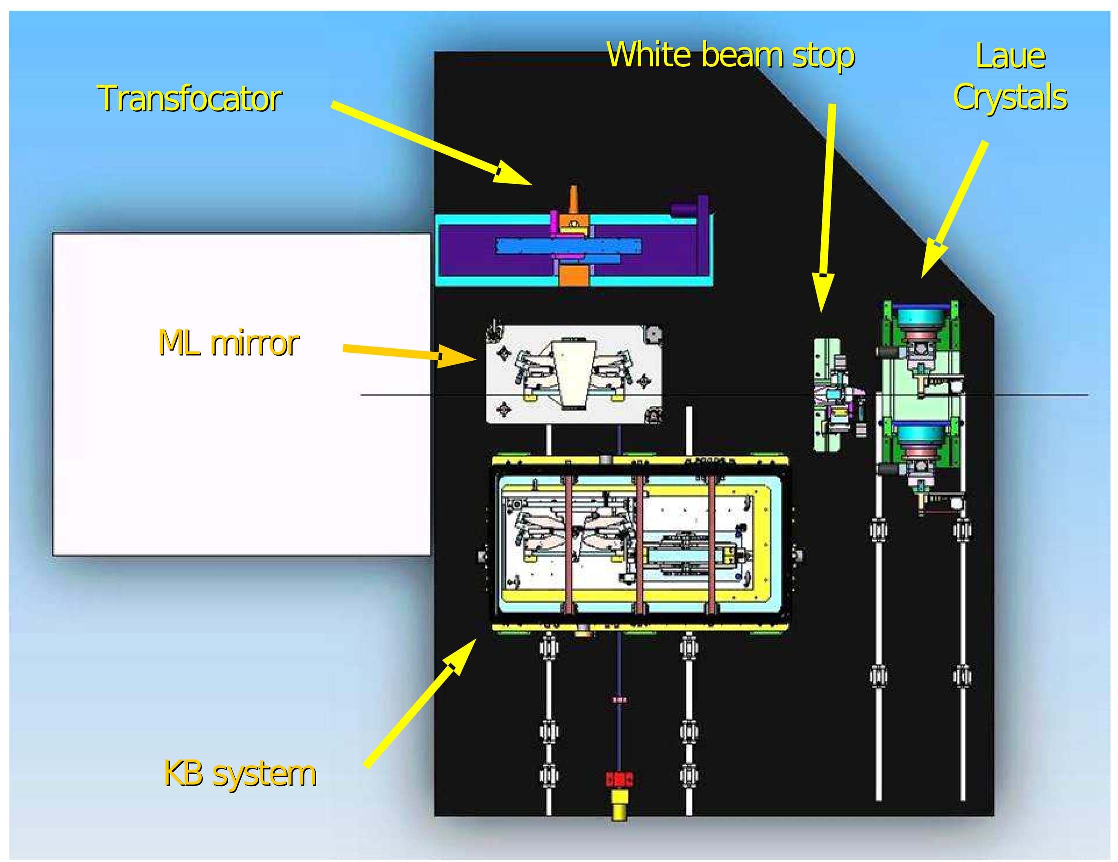


Figure 4: Schematic drawing of the secondary optics elements of beamline ID11 (ESRF).

In addition to this we need several different types of area detector components, as well as various types of sample components, including polycrystals.

[a]The 2nd fundamental milestone of the McXtrace project entails a detailed simulation of this setup

References

[1] *McStas* project website at http://www.mcstas.org

[2] *McXtrace* project website at http://www.mcxtrace.org

[3] *Crystallographica* website at http:www.crystallographica.com

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[5] H.F. Poulsen, *Three-Dimensional X-Ray Diffraction Microscopy*, Springer Verlag, 2004.

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