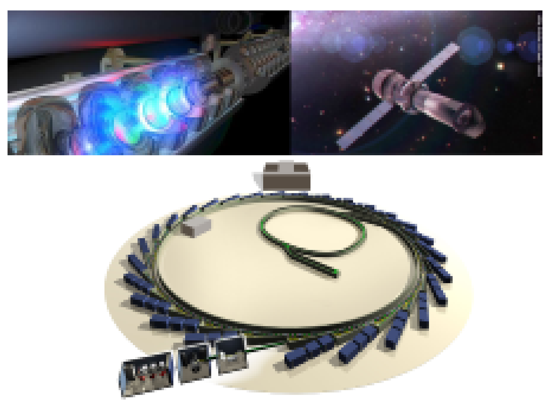

Latest results and features with McXtrace 1.4.

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Abstract

McXtrace[4, 1] is a Monte Carlo Ray tracing package for performing simulations of any kind of X-ray optical instrumentation or scattering experiment. We present the latest results obtained using the new release McXtrace version 1.4.
Some highlights of simulations using McXtrace include:

- McXtrace in space - simulations of an X-ray telescope satellite ATHENA[5]. McXtrace is being adopted as the general tool for simulating X-ray optics of the European Space Agency.
- A full beamline description of the DanMAX beamline at the MaxIV synchrotron. McXtrace is used to simulate the DanMAX beamline while it is being designed, not only supporting design choices, but in parallel also building a virtual facility.

New Features

Exciting new features in the latest release of McXtrace include:

- New Python/Qt-based GUI.
- Interface to the MCPL-fileformat.
- New components
  - A new polyphase/polycrystal sample model.
  - Mirror with heatbump.
  - Toroidal shape mirror.
  - Divergence monitors.
  - Capillary tube optic.
  - Synchrotron source models, incl. Bending Magnet, Wiggler, and Undulator.
  - Interfaces to other source codes (e.g. SPECTRA[3], SIMPLEX[2], adn GENESIS 1.3[7]).
- Better conformance to Debian standards.
- Example instrument with solvent scattering.
- Generalized reflectivity library.
- DEPENDENCY keyword - for simple handling of extra dependencies (for specialized components).

DanMAX

DanMAX is a combined Powder Diffraction, and Imaging beamline being constructed at the MAX IV synchtron in Lund, Sweden.

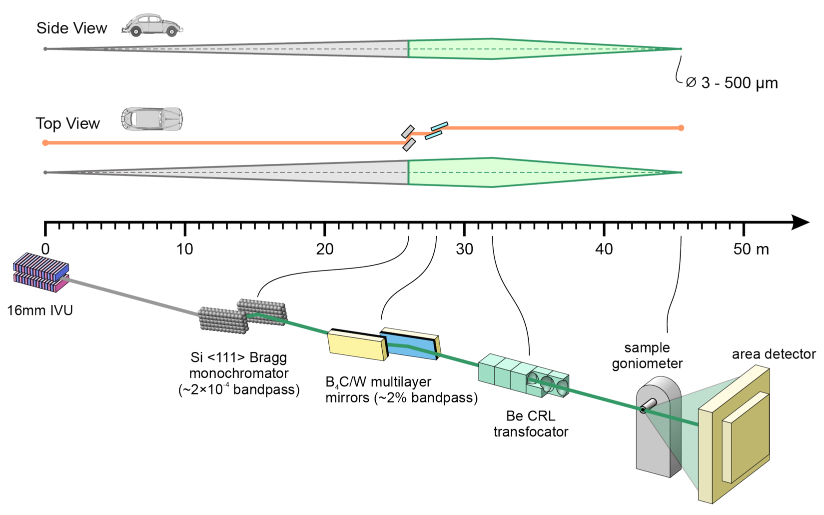

Figure 1: Cartoon of the DanMAX beamline optical concept.

The optical concept can provide "pink" (only multilayer mono) and monochromatic (using DCM) beam with a fixed output. Using both monochromators at the same time ensures higher harmonic rejection.
Parallel to the design process, a vitual version of the beamline is being built using McXtrace.

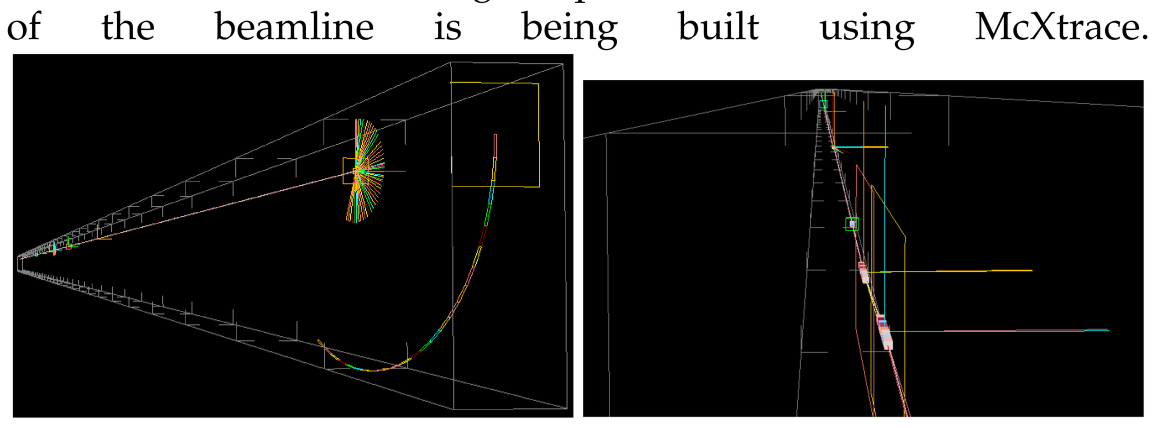

Figure 2: Ray tracing the full DanMAX model using McXtrace. Left) Beamline as seen from the powder diffraction strip detector; Right) Close-up of the double multilayer monochromator

DanMAX undulator

A new undulator model in McXtrace — applied to the parameters o fthe DanMAX undulator. 187, 16 mm periods with a minimum gap of 4 mm, yielding a peak magnetic field strength of $B \approx 0.9$ T.

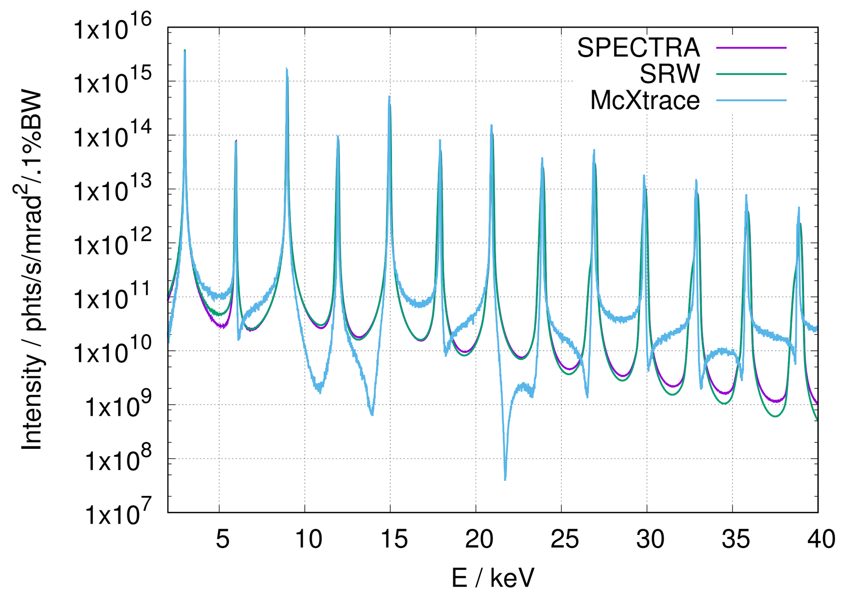

Figure 3: Simulated undulator spectrum for the proposed DanMAX-undulator tuned to a peak at 15 keV. Purple) Sim. with SPECTRA[3]; green) Sim. w. SRW[8]; blue) Sim. w. McXtrace[1].

MCPL

McXtrace supprts the MCPL (Monte Carlo Particle List) fileformat for event-mode operation.

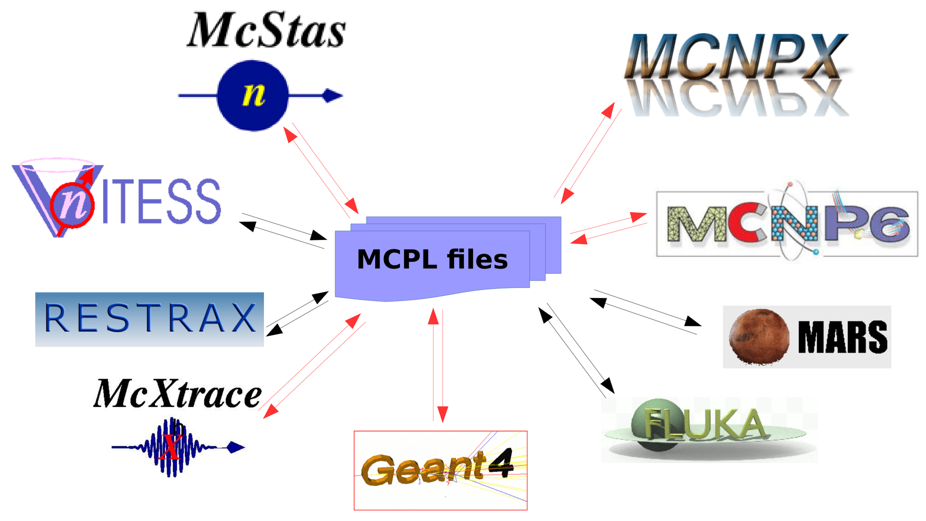

Figure 9: Connection diagram showing existing (red) and in-progress/in-preparation (black) interfaces to MCPL.

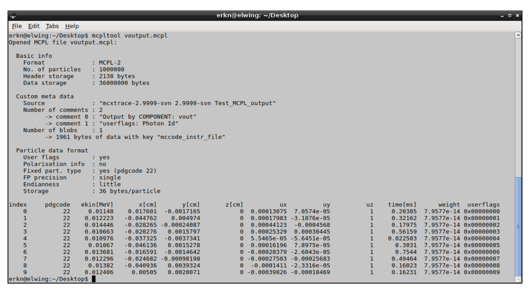

Figure 10: Screenshot of the output from mcpltool - i.e. the first 10 particles of an mcpl-file.

New GUI

A new Python/Qt based GUI is available for McXtrace.

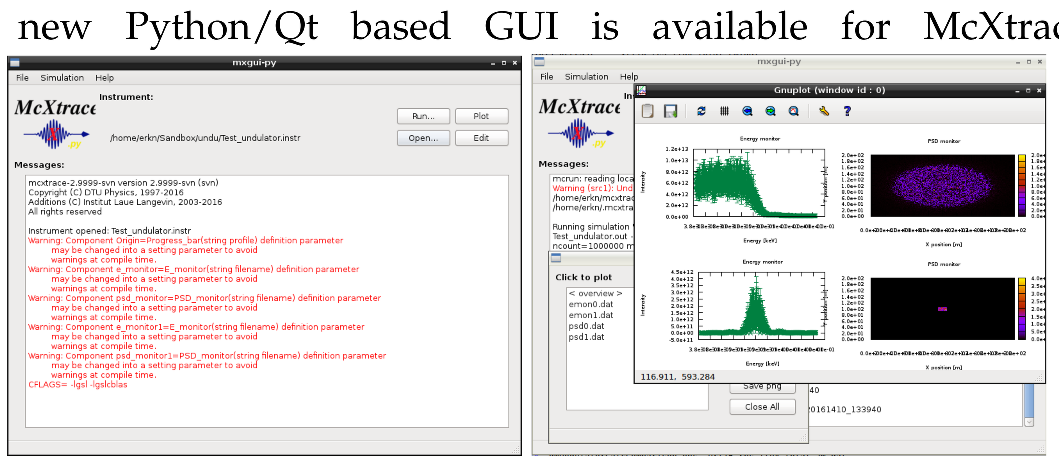

Figure 11: Examples of the new McXtrace python/Qt based GUI. Left) The main window. Right) plotting windows.

SPECTRA/SIMPLEX interfaces

Interfaces to the spectra and simplex codes[3, 2]. Input from simplex for FEL ray tracing. As single pulse may be ray traced through the beamline.

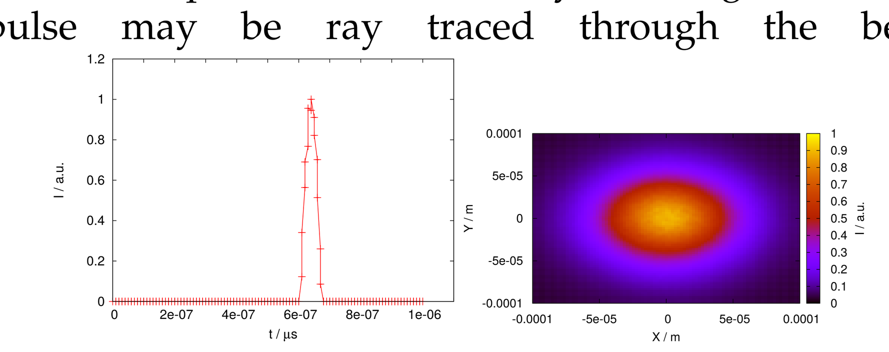

Figure 12: Single pulse from simplex traced to a detector by McXtrace. Left) Area plot of intensity integrated over time. Right) Intensity vs. time integrated spatially.

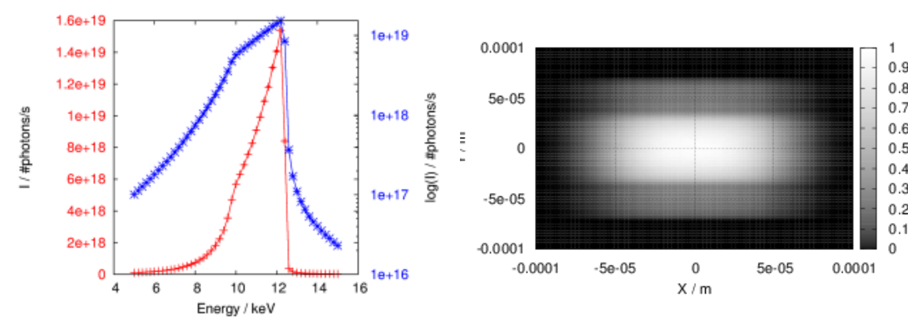

Figure 13: Example of a standard SPring-8 undulator simulated with SPECTRA/McXtrace. Left) Intensity vs. energy; Right) Spatial intensity distribution @15 keV.

ATHENA telescope

McXtrace is part of the design effort for the ESA ATHENA mission. ATHENA is an X-ray telescope scheduled for launch in 2028. The design is based on the concept of Silicon Pore Optics (SPO) where plates of Silicon with etched ribs are bent into paraboloid/hyperboloid meridionally, and cylindrical sagittally to form a true Wolter I optic.

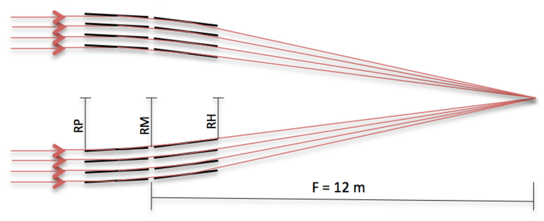

Figure 4: Schematic of the WolterI-optic. A parabolic surface feeds a hyperbolic.

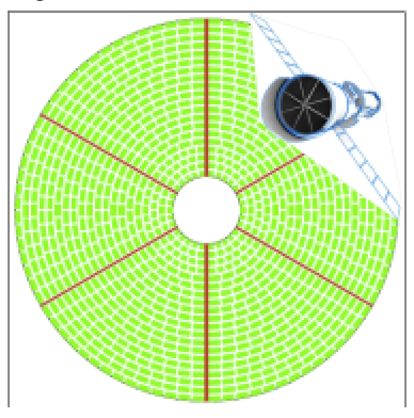

Figure 5: Sketch of the endface of the ATHENA optic facing the stellar object. Inset is a sketch of the satellite.

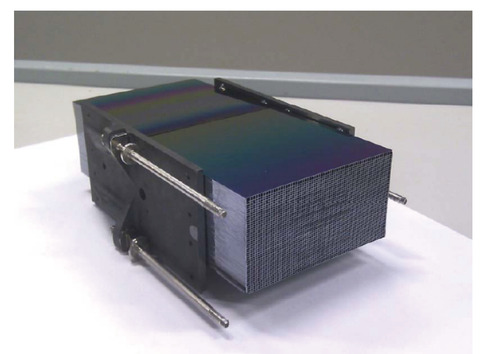

Figure 6: Picture of single mirror module. Cf. the green boxes in 5.

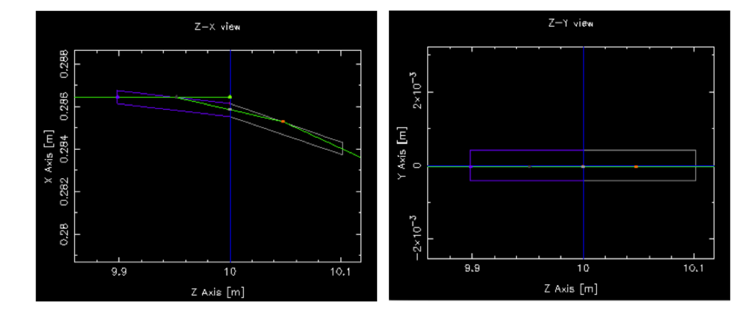

Figure 7: Projections of visual ray tracing through single pore of a single mirror module.

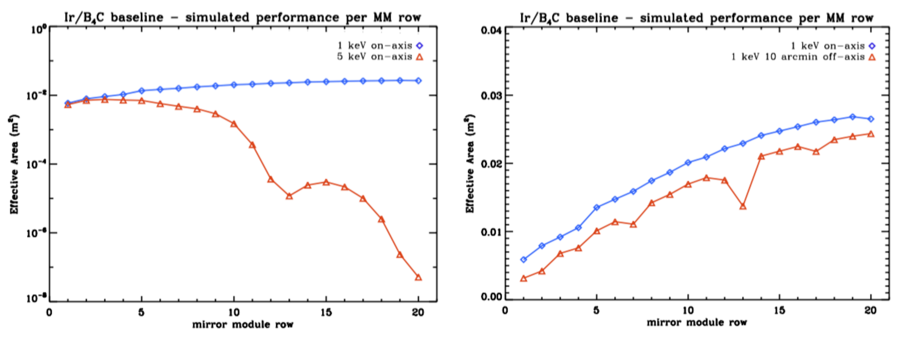

Figure 8: Performance evalauation of ATHENA optic. Left) Effective are for on-axis illumination; Right) Effective area for off-axis illumination.

ROOT interface

An interface to the CERN based mathematical framweork ROOT is now included with McXtrace.

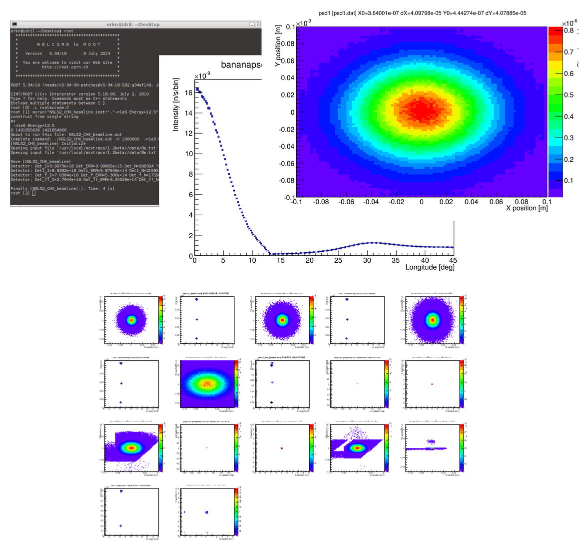

Figure 14: Various screenshots of the ROOT interface in action.

References

References

[1] *McXtrace website*. 2016. URL: http://www.mcxtrace.org.

[2] *SIMPLEX*. 2016. URL: http://radiant.harima.riken.go.jp/simplex.

[3] *SPECTRA*. 2016. URL: http://radiant.harima.riken.go.jp/spectra.

[4] E. B. Knudsen et al. "McXtrace: a Monte Carlo software package for simulating X-ray optics, beamlines and experiments". In: *Journal of Applied Crystallography* 46.3 (2013), pp. 679–696.

[5] *ATHENA mission homepage*. URL: http://http://www.the-athena-x-ray-observatory.eu/.

[6] *EUCALL website*. URL: https://www.eucall.eu.

[7] *GENESIS 1.3 website*. URL: http://genesis.web.psi.ch/index.html.

[8] *SRW github site*. URL: https://github.com/ochubar/SRW.

FUTURE: SimEX integration,

Ray tracing integration with the SimEX[6] platform for XFEL simulations. The SimEX platform is general platform for performing Source-to-End simulations at X-ray Free Electron laser facilites supported by the EU under the EUCALL initiative. We will provide a plugin such that McXtrace may interoperate with the SimEX platform, creating a versatile tool with which to explore the new possibilities created by the FEL X-ray sources.