



Publication Year	2018
Acceptance in OA	2020-10-14T10:29:19Z
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Publisher's version (DOI)	10.1117/12.2312272
Handle	http://hdl.handle.net/20.500.12386/27797
Serie	PROCEEDINGS OF SPIE
Volume	10699

The McXtrace AstroX toolbox: a general ray tracing software package for end to end simulation of X-ray optics for astronomical instrumentation

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ABSTRACT

McXtrace is a general, highly modular, X-ray tracing open source software package for simulating X-ray optics. While initially intended for simulating synchrotron beamlines, it has recently found use in astrophysics. Here it is being used to evaluate the projected performance of X-ray telescope designs. We present the software add-on toolbox "AstroX" to McXtrace containing all of the common optical elements found in satellite based X-ray telescopes. In addition, the toolbox contains detector and source models relevant for astronomical applications.

As an added benefit, users may exploit the heritage of McXtrace and use its beamline elements, to simulate characterization measurements of optical elements. McXtrace AstroX allows for simulation of X-rays telescopes based on different optical concepts such as nested mirror shells and Silicon Pore Optics technology. In this study we present examples of McXtrace AstroX use for ATHENA-, and NuSTAR-like telescope concepts.

Keywords: ATHENA, ray tracing, McXtrace, simulation, X-rays, SPO, effective area, mirror module

1. INTRODUCTION

The aim of this study is to demonstrate the use of McXtrace¹ to simulate the performance of X-ray telescopes, by extending the library with devices relevant for astronomical telescopes. Our goal is to realistically simulate X-ray optics taking into consideration all known physical processes affecting the performance of the telescope.

McXtrace is an open source Monte Carlo software package originally developed with the main objective of supporting optimisation of X-ray beam lines and is now used in several setups such as data analysis and experiments. For instance, McXtrace allows for modular simulations where each pore within a SPO mirror module can be traced and simulated.

We take advantage of the available database of X-ray elements already included in the McXtrace¹ package to build a ray tracing model of the ESA's next large X-ray mission called Advanced Telescope for High ENergy Astrophysics (ATHENA).² The ATHENA mission has its launch foreseen in 2028 and will address to two key astrophysical questions: "How does ordinary matter assemble into the large-scale structures we see today?" and "How do black holes grow and shape the Universe?".²

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2. MCXTRACE SETUP

McXtrace¹ itself is a general Monte Carlo ray tracing software package for performing simulations of X-ray optics and experiments.^{3–5} It has a very open modular structure, where it is quite simple to extend its capabilities with new optical modules. Thus, the optical devices associated with a space X-ray telescope can be modelled with minor effort and the rest of the simulation framework used as is.

In McXtrace, the optical setup, e.g. telescope, is described in a file with a defined language and structure. This defines optical parameters and spatial coordinates of the devices in the optical setup.

This description is automatically translated into a computer program in the c-language,⁶ which may be compiled and executed on the target platform which is to run the simulations. This procedure has a couple of advantages:

1. The executable is automatically optimised for the target platform.
2. The simulation code only contains the code actually used. A simulation of a telescope will not contain code describing the inner workings of a synchrotron undulator.⁷
3. Since a standard, c-code is produced by the system, the optics description may be extended at will by including c-code directly in the description.
4. McXtrace does not have to be installed on the target system. Instead the simulation c-code may be generated elsewhere, transferred to the target system, and compiled there. This way we can avoid installing anything special on the target system, e.g. supercomputer or cluster where restrictions may apply.

Although McXtrace can be run as a command line tool (which is convenient for e.g. HPC cluster installations) it comes with a GUI, including a plotting tool, and a visual ray tracer (fig. 5).

Any McXtrace device, denoted *component*, corresponds to an independent, structured file containing c-code. In essence, this piece of code describes the interaction of a single X-ray with the device in the coordinate frame of the device. The McXtrace system then takes care of coordinate transforms between frames and X-ray transport between devices. As a result, the component codes generally get clear logical boundaries, making each piece of component code small and manageable. As an example the code written specifically for ATHENA modelling a parabolic SPO-pore is < 400 lines, including documentation.

An extra feature, is the ability to generate 3D-visual traces of X-rays as they travel through the telescope optics. This is shown for a single SPO-pore taken from the outermost ring of optical modules of the proposed ATHENA design in fig. 1.

McXtrace was originally designed for simulating X-ray scattering experiment simulations at large scale facilities. To better cater to the needs of telescope designers, we are in the process of developing an X-ray telescope toolbox based on McXtrace. The main idea is to have an add-on, open source library of components and examples relevant for telescope applications, which may be distributed and maintained by an independent community in its own pace.

In addition we have developed source models based on measured stellar objects and realistic detector models, including effects as quantum efficiency, to be included in the proposed library.

2.1 Installation procedures

McXtrace itself is by design multi-platform in the sense that it can run on any system which has a c-compiler. For the added convenience that the GUI provides a set of other dependencies must be met. In the cases of the major platforms these are provided by the McXtrace installation system. For Debian/Ubuntu and RedHat class GNU/Linux systems the standard package management are used. For Windows and MacOSX self-contained installation file must be downloaded, and installed in the usual manner on each platform. The AstroX toolbox is provided as a archive file that should be extracted into the McXtrace library. The next version of AstroX will follow the above procedure and use standard package installers.

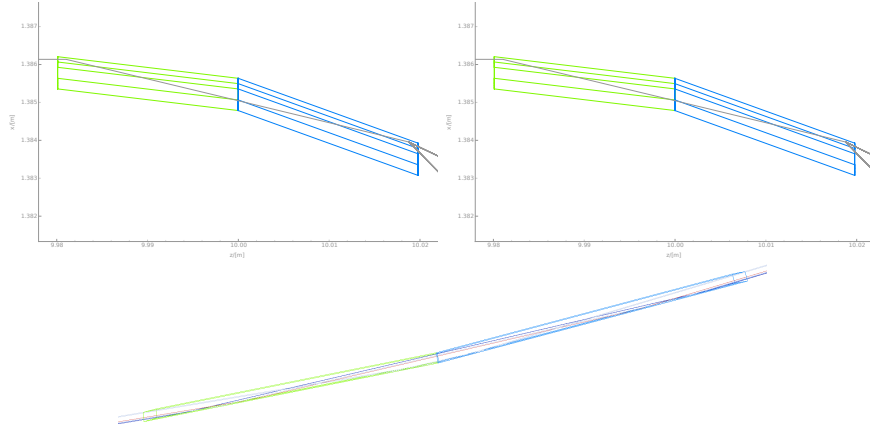


Figure 1. Visual 3D-traces of rays through a single pore of a SPO setup. The pore is the central pore of one of the outermost modules in the proposed ATHENA-optic. Top plots show a single ray being traced projected onto the XZ- (left) and YZ-planes (right) respectively. The bottom plot shows a range of ray being traced through a fully 3d visual representation of the pore. The parabolic and hyperbolic part of the pore is shown in green and blue respectively.

2.2 AstroX component library contents

The current version of AstroX contains the following components (fig. 2) targeting various types of X-ray telescope optics and auxiliary devices:

Shell A single, circular cross section, mirror shell, with either a parabolic, hyperbolic, and conical profile along the optical axis.

Ring A stack of mirror shells (a.k.a. a meta-shell), with either parabolic, hyperbolic, or conical profiles.

Pore A single pore with sidewalls and with either parabolic, hyperbolic, or conical profile along the optical axis. The sidewalls can have non-zero reflectivity. This is the most basic building block of an SPO-optic.

Mirror Module A block containing a set of identical pores. This is the basic block that forms the optic of ATHENA.

Stellar Object A type of source model that takes a heat map from a stellar object as input. This is to provide a means of answering questions like: What would I see if I pointed my proposed telescope towards e.g. the Crab.

Detector A spatially resolved monitor with built-in scintillator efficiency.

Also included are a set of example telescopes:

Conical_NuSTAR-like A set of conical shells resembling NuSTAR.

Wolter_I_Shell A true Wolter-I telescope built from single shells.

Wolter_I_Pore A true Wolter-I telescope built from individual pores.

Wolter_I_Ring A true Wolter-I telescope built from sets of meta-shells.

Wolter_I_MM A true Wolter-I telescope built from SPO mirror modules.

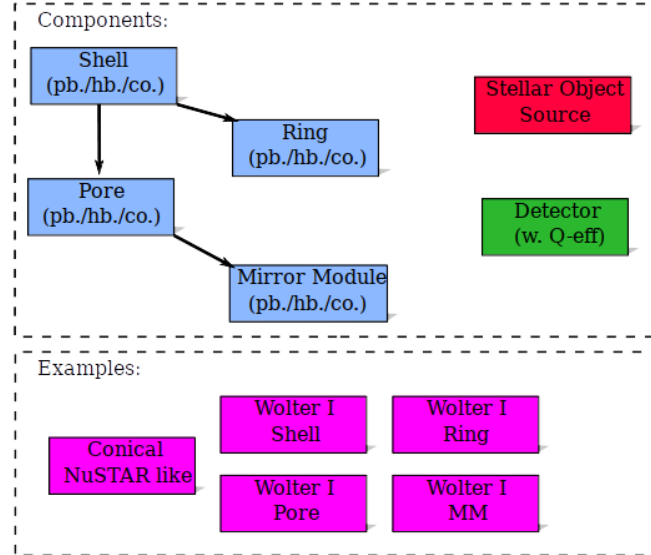


Figure 2. The contents of the AstroX toolbox version 1.0. The blue boxes constitute optics components, green and red indicate source and detector modules, respectively. Example telescope simulations included in the library are indicated in purple. Arrows indicate inheritance. E.g. A **Pore** may be seen as a **Shell** with side-walls, and A **Ring** (or meta-shell) may be seen as a special set of Shells. Further modules will be added in later versions of the toolbox.

2.3 SPO-Modules (ATHENA-like)

Flexibility of the code is crucial as several aspects of the geometry are still under investigation.⁸ The variables considered as input parameters are: pore width and height (so far assumed to be 0.830 mm and 0.605 mm, figure 1), rib width (0.17 mm), rib pitch (1.0 mm), silicon wafer thickness (0.775 mm), membrane thickness (0.17 mm), SPO plate width, SPO length, height of mirror modules (number of stacked plates: 68 reflecting plates), number of mirror modules per row, position of mirror module within the optics, mid radius of mirror modules, parabolic radius and hyperbolic radius for each set of SPOs, telescope’s focal length (12 m), Ir/B₄C bilayer coating throughout the whole optic, and average surface roughness of the coating (assumed to be 0.45 nm).^{9–11}

Using the latest available documentation on ATHENA as input,¹² we have simulated X-rays travelling through one set of pores (parabolic and hyperbolic) for each mirror module within one petal. For each of the 177 mirror modules we ray traced the very central pore of the module. That means that we ray traced one pore per mirror module and assumed that the results for that one central pore is representative of the performance of the given mirror module. The performance of the pore within the mirror module is simulated individually based on its geometry and position. The results of pores are then combined to obtain the total telescope performance.

Figure 3 shows the simulated transverse intensity distribution at 1keV energy for a SPO-realization of a true Wolter-I representation of an ATHENA-like telescope at two points along the optical axis. The first point is shortly after the optic, the second at the focal point. The SPOs are considered perfectly smooth, true to figure, and perfectly aligned. Misalignment of SPOs can be targeted by built in features of McXtrace. We simply add an additional translation and/or rotation to the placement of the SPO mirror-module, or even individual pore.

Figure 1 shows a SPO pore set in McXtrace. Here we observe the pore geometry along the Z-axis (focal axis). An example of parabolic (purple) and hyperbolic (grey) pores is seen along with the double reflection of a traced photon. The representation of the position of each mirror module considered for simulation is also seen.

To simulate the effective area of a telescope based on mirror modules like ATHENA, one may use the **Wolter_I_mm** example included in AstroX. As a side-output the model stores the reflectivities encountered by the rays as they pass through the telescope. As the total opening area of the mirror module is known we may compute the effective area as:

$$A_{eff} = \sum_i^N A_{MM\#i,proj} \overline{R_{pa} R_{hy}}$$

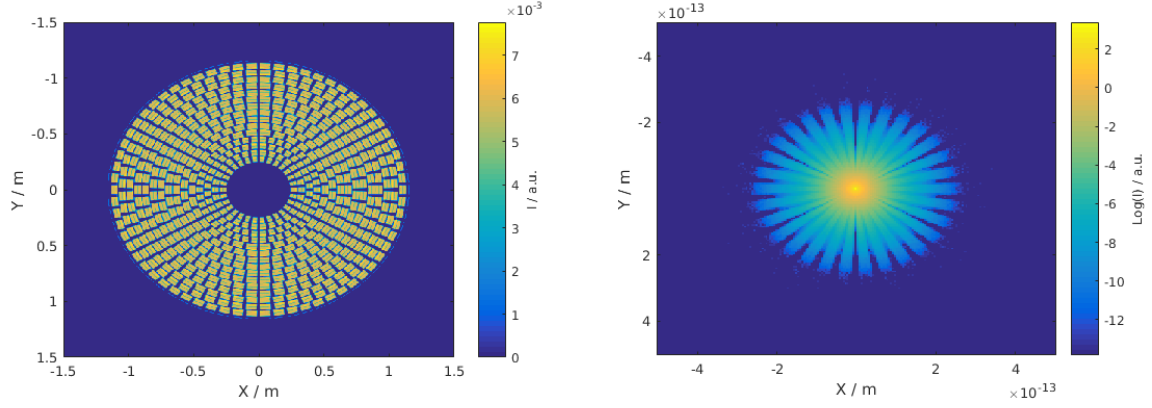


Figure 3. Transverse intensity distributions. Left: Shortly after the optic. The optics structure is clearly reflected in the pattern, including the gap in the the middle of the SPO mirror modules. Right: At the focal point (12m). For clarity we plot the $\log(I)$. The radial structure of the optics is reflected in the pattern, but note that the axis limits $\ll \lambda$.

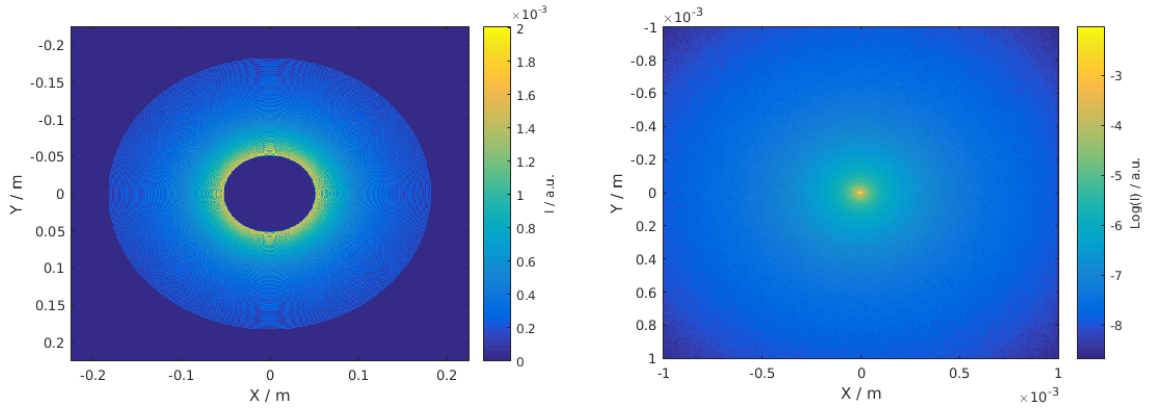


Figure 4. Transversal intensity distribution for a NuSTAR-like telescope, with conical, concentric shells with radii ranging from $\approx 55\text{mm}$ to $\approx 19\text{mm}$. Right: Shortly after the optic, Left: At the focal point. For clarity we plot $\log(I)$

where $\overline{R_{pa}R_{hy}}$ is the weighted mean of parabolic multiplied by hyperbolic reflectivities encountered by all the rays, and $A_{MM,\#i,proj}$ is the projected area of the i :th mirror module.

2.4 Concentric conical shells (NuSTAR-like)

Using the module Shell and/or Ring, which can be seen as direct generalizations of Pore and Mirror Module respectively, we may easily target the geometry as found in NuSTAR,¹³ A shell is imply a Pore with no side walls covering the full circle. This is an approximation as the NuSTAR telescope was built using quarter-circle plates. Also, the spacers that separate have the mirrors have been neglected, for the current simulation

NuSTAR is a built upon a conical approximation to a Wolter I, so we use the conical version of Shell optics as opposed to a combination of parabolic and hyperbolic objects. We show in figurefig. 4 the intensity distribution at the focal point. A simple moment analysis of the pattern at the focal point shows a HPD of arc seconds. By default McXtrace computes the first and second moment of the data registered on a detector, from which e.g. the HPD may be inferred.

ACKNOWLEDGMENTS

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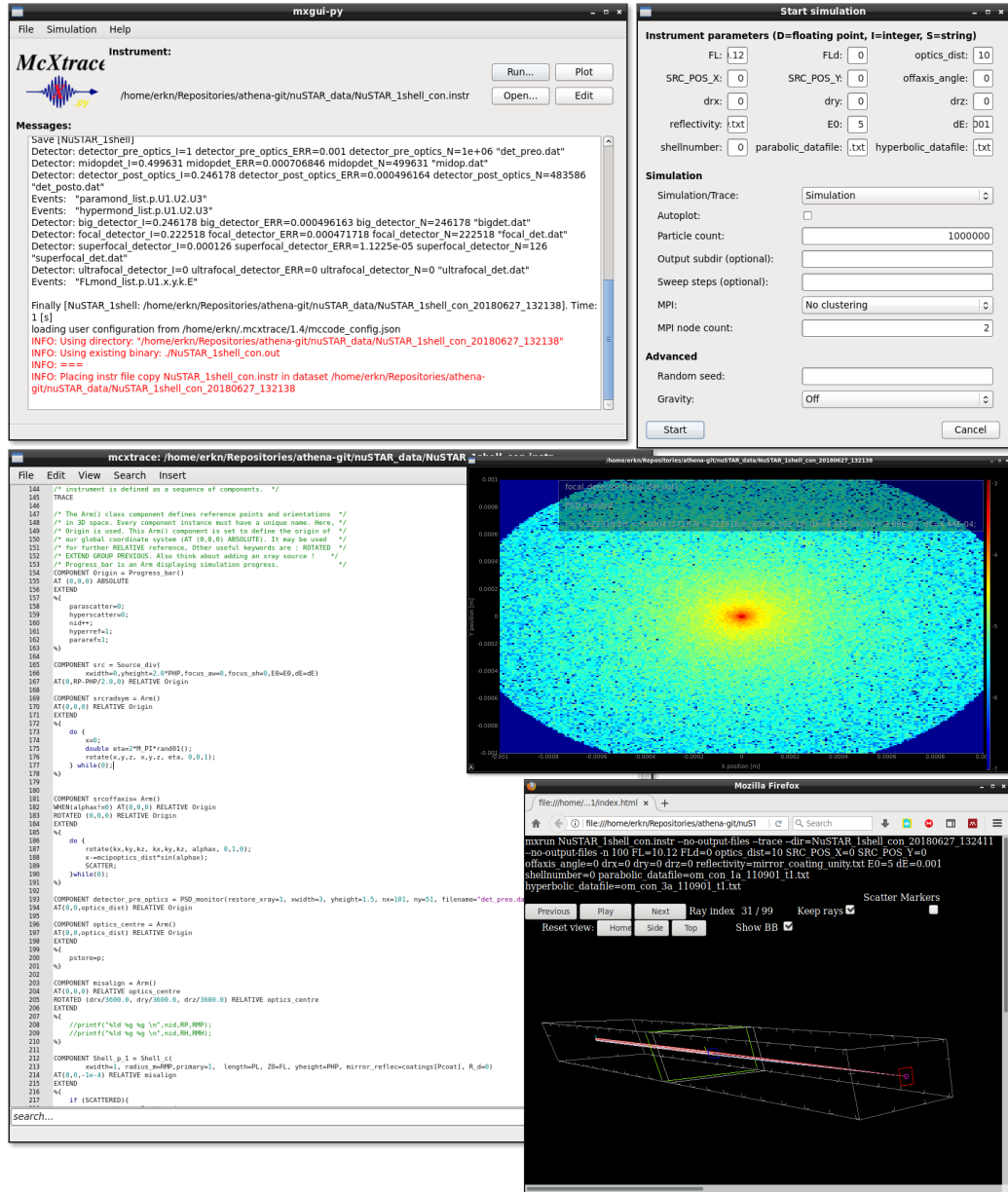


Figure 5. Screenshots of the McXtrace GUI. We show examples of the main window (top left), the editor window (bottom left), the run-dialog (top right), the built-in plotting tool (mid right), and the built-in 3D visual tracer (bottom right).

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