Athena end-to-end simulations

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ABSTRACT

We present an overview of the development of the end-to-end simulation programs for the instruments on the future European X-ray astronomy mission Athena. The overview includes the design considerations behind the simulation software and the current status and planned developments of the simulators for the X-ray Integral Field Unit and the Wide Field Imager.

Keywords: Athena, X-ray astronomy, end-to-end simulations, simulations, response matrices, mirror model, detector model, performance analysis

1. INTRODUCTION

Simulations are a crucial part of the development process of any future astronomical satellite mission, as a good simulation program represents a careful mathematical model of the planned instrumental setup well before the hardware has been built. During the mission proposal and the mission definition phases, science simulations allow scientists to gauge the scientific performance of the mission by showing them what the final data products of the mission such as spectra, images, or time series would look like. Monte Carlo simulations of the interaction of photons and particles with the satellite hardware done with programs such as GEANT4 are routinely used to estimate the expected particle background of a detector and to design the required shielding, while other simulations are used, e.g., to model the thermal environment or mechanical behavior of the instrument. During later stages of the mission development, such science simulations help trade off decisions between different instrument designs as they allow to gauge how these designs affect the performance of the mission.

In this contribution we present the status and design considerations for the end-to-end simulations of the future European X-ray mission *Athena*. The aim of end-to-end simulations is to model the scientific performance of the whole X-ray mission, considering all factors that are relevant for future users of the satellite. An end-to-end simulation therefore starts with a description of a real measurement, such as an astronomical observation or a laboratory setup, and then attempts to model the outcome of this experiment as precisely as possible. The final output of the simulation is typically a set of simulated data that closely resembles the data that will come out of the detector and that can then be processed with the mission specific data reduction software.

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Figure 1. Data flow diagram in a typical end-to-end simulation.

In the following we describe the design philosophy behind the end-to-end simulator for the *Athena* mission in greater detail. In Sect. 2.1 we explain the design considerations behind the end-to-end simulator in more detail as well as the SIXTE framework (9) in which it is developed. This introductory section is followed in Sects. 2.2 and 2.3 by a description of the preliminary design for the X-ray Integral Field Unit (X-IFU; 1; 2) and Wide Field Imager (WFI; 3) end-to-end simulations.

2. END-TO-END SIMULATIONS FOR ATHENA

2.1 Design Considerations: SIXTE

In the area of X-ray astronomy, a large number of different mission specific simulation programs exist. Examples are MARX (4) for *Chandra* (5), SciSim for *XMM-Newton* (6), NuSim for *NuStar* (7; 8), or simx developed by R.K. Smith (CfA) for *Astro-H* and other missions^{*}.

Common to all of these simulators is that their input is some kind of a source description, which for point sources is typically an X-ray spectrum and sometimes a lightcurve. Extended sources are either described by a simple parameterized shape (e.g., an ellipse where the major and minor axes and the position angle are given) or by an image. They then model the imaging process, either by ray tracing or by convolving the image with the point spread function of the X-ray optics, and then model the X-ray detection in the satellite's detectors. The output of the simulations are either PHA-files which can be further studied with standard X-ray analysis programs, or event lists which can be processed with the satellite specific software.

With the exception of simx, all existing X-ray simulators are mission specific. An important consequence of this is that the input into the simulator is not portable: if a user wants to see what a source looks like with different instruments, the full simulation has to be set up with the different simulators. This approach causes a significant overhead and is very error prone. Furthermore, because the design of many simulators is that of a single monolithic program, replacing parts of the simulation code, e.g., in order to improve how the photon detection is simulated, requires significant knowledge of the underlying code base.

During the course of the studies for *IXO*, *Athena*-L1, *Athena+*, *LOFT*, and *eROSITA*, we have developed the simulation framework SImulation of X-ray TElescopes (SIXTE) that tries to avoid these shortcomings. SIXTE is based on Monte Carlo simulations, where individual photons are propagated through the whole observation and detection chain. The advantage of this approach is that nonlinear behavior, such as pile up, can be easily implemented. The major disadvantage of the Monte Carlo approach is that it tends to be rather computing time intensive. However, with the availability of parallel computing facilities now being fairly standard even at smaller computer installations, this shortcoming is fading away quickly. In the following we give a brief summary of the major ideas behind SIXTE. A full description of the framework is given by Schmid et al. (9). All software developed for the framework is available for download under the GNU Public License at http://www.sternwarte.uni-erlangen.de/research/sixte/.

SIXTE has a modular design where mission dependent and independent parts are clearly separated and where all (software and data) interfaces are clearly defined. The advantage of this approach is that "mix and match" is easily possible. For example, all SIXTE modules use the same data format to specify an observation, and the low-level programs making up SIXTE are designed in a way that makes it easy to add new observatories or better instrument descriptions to the simulation package.

^{*}http://hea-www.harvard.edu/simx/

Figure 1 gives an overview of the setup of a typical SIXTE pipeline to simulate an observation, which consists of the following steps:

X-ray source catalog: The sources to be observed are specified in an X-ray source cataloge using the SIMPUT data format (10). SIMPUT is a generic, mission-independent format to specify properties of X-ray sources based on the FITS standard. A SIMPUT-data file contains a list of source positions, fluxes, spectra, and – optionally – light curves and images. SIMPUT is flexible enough to describe virtually all X-ray sources. It scales well enough from observations of single point sources to catalogs of millions of objects as required for simulating X-ray all sky surveys.

The SIXTE distribution provides command line tools to generate SIMPUT files for point sources based on best fit models obtained with XSPEC (11) or ISIS (12; 13). There is also a general SIMPUT library available that can be interfaced to more complicated simulation codes and other simulation codes[†]. For example, in the framework of the *Athena* study we have successfully combined the cosmological *N*-body simulation code of zuHone et al. (14) with this library to prepare simulations of *Athena* observations of cluster mergers based on these hydrodynamical models.

- **Photon generation:** Based on the SIMPUT catalog, the Monte Carlo simulation generates a list of photons emitted from all sources that are visible to the instrument. In order to save computing time, SIXTE takes into account the attitude information for the observation to determine the visibility of individual sources. The attitude is specified through a standard FITS attitude file. This approach allows SIXTE to simulate slews or model the pointing jitter. Simple tools are provided with the SIXTE distribution that allow to generate attitude files for typical cases (e.g., pointed observations and slews between two positions). As indicated in Fig. 1 further optimizations are possible. For example, if one does not want to simulate the details of the photon absorption processes, then it is possible to use the knowledge about the effective area curve to make sure that only photons are generated which will be detected by the instrument. In other words, photons which would be "stuck" in dead areas of the detector are already discarded as part of the photon generation rather than during the photon detection step below.
- **Photon imaging:** Once the photons which hit the instrument are generated, they are projected onto the X-ray detector during the photon imaging step. The baseline setup of SIXTE uses the energy and position dependent point spread function (PSF) of the X-ray optics of the mission, although in principle this module could also be replaced with a formal ray tracing code. Using the PSF, information about the vignetting, and the attitude file, during this step all photons are projected onto the detector. The output of this step is the impact list, which contains the arrival time, energy, and position of all photons hitting the detector.
- Photon detection: In the photon detection step an instrument model is used to convert the photon impact information into an event list of detected events that can then be processed with standard X-ray data analysis software such as the FTOOLS in order to produce the measured spectrum, lightcurve, or image. Depending on the level of realism that is to be achieved with the simulation, this step could consist of a very simple mapping of the photon energy into a Pulse Height Analyzer (PHA) channel based on the instrument's precalculated response matrix function (RMF), or it could be a very elaborate description of the detection process where the microphysics in the detector is simulated in detail. Furthermore, during this step the particle background is also taken into account.

SIXTE includes several different modules for the photon detection. A very useful SIXTE module is a general code to simulate the readout process for a variety of pixel based detectors such as Charge Coupled Devices or Active Pixel Sensors. While the photon detection process in this module is only described rudimentary based on the RMF, the module traces the charge cloud in the detector and includes a detailed model of the readout, including the shifting of charge through the detector. This part of the readout is described through files that are based on the eXtensible Markup Language (XML) and thus makes it very easy to study how different CCD readout strategies influence the pileup behavior of an imaging detector. Figure 2 shows an excerpt of the XML file describing the XMM-Newton EPIC-pn burst mode. EPIC-pn observations simulated with this module are remarkably similar to real observations. For example, the ratio between single and double events, i.e., events where the charge cloud produced by a photon is detected in one or two CCD pixels, follows exactly the measured ratio. When a source becomes too bright, pileup can occur where more than one photon hits the detector during one readout cycle in the same or neighboring

[†]For example, SIMPUT is also supported by simx.



Figure 2. XML specification of the readout mode of the XMM-Newton EPIC-pn burst mode as an example for specifications possible for X-ray CCDs (9).

pixels, leading to the erroneous detection of a higher energy single or double event. Pileup is detected during the EPIC data analysis as a deviation of the energy dependent ratio between single and double events. The simulator reproduces extremely well both the standard faint source single to double ratio as well as the deviations seen during pileup (9). Because of the flexibility of the CCD simulator, we have produced simulation pipelines for all data modes of the EPIC-pn and the EPIC-MOS cameras as well as for the *Suzaku* XIS detectors which can be used to plan observations of observations of bright sources with these missions. Programs are available within SIXTE to convert the output of the photon detection into a set of files corresponding to an *XMM-Newton* Observation Data File (ODF) set that can be processed with the standard *XMM-Newton* data analysis software.

The flexibility of the SIXTE package illustrated above means that it is ideally suited as a framework for the development of the end-to-end simulator for *Athena*. In the following two sections we describe the current status and next steps for the simulators for both instruments on *Athena* in greater details.

2.2 X-IFU: Status and Next Steps

The X-IFU (1; 2) is a transition edge sensor array providing simultaneously high energy resolution and imaging with good spatial resolution in the inner region of the field of view of *Athena*.

The current version of the end-to-end simulation module for the X-IFU describes the device with a set of response matrices which give a rough description of the 2.5 eV nominal energy resolution described by a Gaussian probability density and a good model for the detector sensitivity. The simulations include the baseline *Athena* effective area, with $\sim 2.1 \text{ m}^2$ at 1 keV and $\sim 0.26 \text{ m}^2$ at 6.5 keV. The simulation also includes a model for the two currently discussed optical blocking filters and allows to include a diffusor optics which can be used in observations of brighter sources to spread the source events over a larger region. Figures 3 and 4 show two examples for simulated X-IFU observations.

A simplified description of the detection process in a TES is that the absorption of a photon induces a change in temperature in the detector pixel, which is measured by a change of the current as the resistance of the material is strongly temperature dependent in this regime. The resulting signal is shown in the left panel of Fig. 5. Noise in the detector then results in pulse profiles similar to that shown on the right hand side of Fig. 5. In order to reconstruct the photon energy, the measured temperature profile is correlated with a library of template pulse profiles to find the best matching profile (15; 16). For this process to work the baseline current level in



Figure 3. Simulated observation of the Crab pulsar and nebula with X-IFU.



Figure 4. Simulation of an observation of a cluster merger with X-IFU (9). Blue: simulated data. Red: best fit model.



Figure 5. Theoretical temperature behavior of a TES pixel (left) and simulated reaction of a TES pixel to an incoming photon as a function of time (right; the signal is displayed in analog digital converter units of the pixel current).



the detector has to be determined to high precision. As the count rate of the observed X-ray sources increases, the average time between incoming events decreases, such that the determination of the background becomes more difficult. This results in a degradation of the precision with which the photon energy can be determined, and thus an effective degradation of the detector resolution. Based on initial simulations of a source with a constant brightness, we assume that for events with fluxes $\gtrsim 10 \,\mathrm{mCrab} 30\%$ of all events can be reconstructed with 2.5 eV resolution, 30% with a medium resolution of 4.5 eV, and 40% with a low resolution of 30 eV (1). Note that even these degraded events still have a resolution that is much higher than that of a silicon based CCD. At count rates corresponding to above 100 mCrab, 80% of the events will be measured with a low energy resolution of 30 eV while the remaining events are piled up and not usable for the analysis. We note that preliminary simulations show that these piled up events can be detected, i.e., they do not affect the measured spectrum but just reduce the efficiency of the detection process. We stress that these numbers are still preliminary, as they depend significantly on the details of the pulse reconstruction. Together with laboratory measurements, simulations such as the ones presented here will be used to optimize the reconstruction process.

The current, simplified version of the X-IFU simulator includes a model for the pixel layout of the detector as well as the filters discussed above. Event grading into low, medium, and high resolution events is based on the arrival time history of photons in a single pixel. In reality, the energy degradation of the TES is not step-wise but rather the energy resolution degrades smoothly. In order to simulate this effect, however, the microphysics of the TES has to be described in greater detail (see Fig. 6). In a first step, the microphysics will be simulated based on measured pulse profiles similar to those shown in Fig. 5. This approach results in pulse profiles as a function of time similar to the right hand side of Fig. 5. In addition, pulse matching and reconstruction algorithms are being developed to facilitate the event reconstruction. The aim is to use this setup as a testbed for the hardware implementation of the event reconstruction. Following this initial step the simulation will be extended to allow cross talk between pixels and in the analogue chain from the pixel matrix to the detector electronics. Finally, the simplified treatment of absorption in the detectors (which is currently represented by a simplified energy



Figure 7. Athena WFI simulation of the Chandra deep field south. The small gaps are due to the detector layout (9).

dependent detector efficiency) will be replaced by a full treatment of the photon absorption process.

2.3 WFI: Status and Next Steps

The Wide Field Imager is an active pixel sensor based on a set of depleted p-channel field effect transistors (DEPFET) embedded in $450 \,\mu\text{m}$ thick silicon bulk. The detector covers the full field of view of Athena.

The current version of the end-to-end simulation models this detector with a special setup of the CCD detector code described in Sect. 2.1 above. The efficiency of the detection and the energy redistribution is based assuming that the Fano limit can be reached. Event grading into single and double events is done with the standard SIXTE software, again as described above. The latter is of special importance, since the WFI will be the instrument of choice for bright source observations. The simulation software therefore implements different readout strategies for the device, including the windowing modes where only part of the detector is read out. We believe it to give a good representation of the detector behavior out to even very high fluxes of several Crab, see (3). The simulation code also includes the split of the WFI into an inner detector and four outer detectors discussed by Rau et al. (3). Figure 7 shows a simulation of the Chandra deep field south performed with the current setup, illustrating well the very good imaging performance of *Athena*.

The next steps in the WFI simulator development will address the currently simplified model for the absorption of photons in the detector (which is based on response matrices), which will be replaced by a Monte Carlo simulation in which the absorption of the primary photon is modeled directly and where solid state effects are included to model properly the energy resolution of the device from first principle.

3. SUMMARY

The end-to-end simulators described in the previous sections are already at a level that allows to describe the overall properties of the instruments on the *Athena* mission to quite some detail. The source code for all simulation programs mentioned here is available through the SIXTE web pages. Cutting edge versions of the programs are also available via a git repository as outlined on the WWW pages. Scientists interested in performing their own simulations are also invited to make use of the online version of the simulator available

Simulation Parameters
Instrument: X-IFU 💌
pointed Observation RA: 10.3 deg DEC: -5.5 deg
O Upload attitude file
Source Components Point source
RA: 10.298 deg DEC: -5.505 deg
components are additive
✓ Power law /: 2.1 Flux: 4.31 x 10-10 cgs
Black Body kT: keV Flux: x10-10 cgs
gal. Absorption I/H: 0.43 × 1022 cm-2
Energy band for fluxes: Emin: 1 keV - Emax. 10 keV
Exposure time: 10 ks 🕶 Tstart: 0 s
Returned Data Products
in in aye
Simulate Reset

Figure 8. WWW-interface for the Athena simulator.

at http://cetus.sternwarte.uni-erlangen.de/~athenasim/ (see Fig. 8). This online version allows users to easily simulate observations of point sources with simple spectra, but also allows the upload of SIMPUT catalogs in case more complicated simulations are required.

The next steps for both instruments will be to improve the modeling of the assumed detector physics, with the aim of getting a fully self-consistent model of both detectors. Combined with the **GEANT4** simulations of the detector background described elsewhere in this volume, these simulations will allow scientists to gauge directly the scientific performance of *Athena*, while it will also represent a simple way to gauge the implications of decisions made during the hardware development process onto this performance.

During the course of the development of *Athena* up to its launch in 2028, the end-to-end simulator will be in continuous development. This development will include the adaption of the simulator as the detector hardware is being better defined and understood. At the same time, modules of the end-to-end simulator will also be verified based on the behavior of the detectors in the laboratory as these become available. This approach will ensure that the end-to-end simulator is a faithful representation of *Athena* as the mission design evolves.

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