RefleX User Manual

Version 3.0

Stéphane Paltani & Claudio Ricci
Astronomy & Astrophysics, 2017, 607, A31

January 25, 2023

Abstract

REFLEX is a ray-tracing code designed for X-ray photons (energies from about 100 eV up to about 1 MeV). Photons can be generated with different source geometries and different emission spectrum. The photons encounter different user-specified objects. The following processes are implemented: photo-ionization, Compton scattering on free electrons, Compton scattering on bound electrons, Rayleigh scattering, K-shell and L-shell fluorescence and dust absorption and scattering. REFLEX can output its results in a very versatile way, either in text form, in a FITS binary table, in user-defined spectra, histograms or in FITS images.

Contents

1 What's new in RefleX 3.0?

This is a major release, with the addition of some physical processes, in particular dust extinction.

Physics

- Added dust absorption and scattering according to [7].
- Improvement in Rayleigh scattering angular redistribution, which is now treated element by element.
- H_2 photo-electric cross-section from [28] and [27].
- Added a virtual particle called `REFLEXINO` that has no interaction with matter

Geometry

- Added emission in an annulus.
- A rotation can be applied to any object.
- Added `Millimeter` and `Micrometer` legnth units.

Output

- RefleX is now able to create histograms of any photon properties.
- Spectra of individual objects (or collections of objects) can be generated, instead of spectra of the whole system only.
- Source coordinates and position angle can be specified for easier comparison with real images.
- Verbosity can be controlled using the names of the processes.
- Event file is now written in a binary FITS table.

Control

- Documentation has been largely improved.
- Numerical issues when computing the exit of photons are now solved in a more clever way, which essentially guarantees that photons cannot get stuck anymore. `MARGIN` is now obsolete (a warning is issued). `MAXINT` can still be set, but will probably be made obsolete in the future.
- RefleX can now resume a simulation that was terminated in order to increase the number of photons.
- Variable parameters can now be passed on the command line, in order to modify the values in a parameter file on the fly.
- `ABUNDMIN` is now obsolete (a warning is issued), as it does not lead to any significant gain in computation time with the new implementation of the selection of interactions introduced in RefleX 2.0.

Bug fixes

- Minor initialization issue in vector normalization.
- Fixed a bug affecting the calculation of some interactions with a disc.
- Fixed a bug that made a disc with an infinitesimal (but sometimes significant) hole in the center.
- Fixed a bug affecting the calculation of some interactions with a cone or hollow cone.
- Multi-threading is now fully functional.

2 Invocation

ReflеX is called the following way:

```
reflex [ %varname=value ]* [ parameter_file ]* [2> logfile]
```

An arbitrary (larger than or equal to 0) number of parameter files with file names `parameter_file` can be passed on the command line; they will be processed sequentially. `parameter_file` should not contain spaces. If the `parameter_file` parameter is left out, the file `reflex.par` is used. ReflеX produces a detailed log file in output using the standard error `stderr`; in order to keep the log in the file `logfile`, a redirection of file descriptor 2 might be necessary.

Any number of variables with names `%varname` can be passed through the command line. Variables are identified with the prefix `%`. Spaces are not allowed either in `%varname`, `value` or around the `=`. ReflеX will then search for any occurence of `%varname` in the parameter files and replace them with `value`. No interpretation of `value` is performed by ReflеX; the substitution is performed as a string. The following command line:

```
reflex %DENSE=1e20 my_parameter_file.par
```

will replace the following line in the file `my_parameter_file.par`

```
DENSITY %DENSE
```

with

```
DENSITY 1e20
```

3 Bugs

Please report any issue about ReflеX to `Stephane.Paltani@unige.ch`

4 Basic principles

[Adapted from [20]]
ReflеX aims at simulating the physical processes of propagation of X-rays, which we define as photons with energies from about 0.1 keV to about 1 MeV) through matter around the central

engine of AGN. REFLEX uses Monte Carlo simulations to track individual photons. The simulated photons interact with the matter through all the physical processes selected by the user (with sensible defaults), until the photon dies, is down scattered to an energy below a chosen termination energy or exits the system.

The ray-tracing simulation consists of four separate engines that are closely connected: photon creation, geometrical and matter content description, photon propagation, and physical processes.

REFLEX records the full list of events that are experienced by each photon, although the level of detail is configurable to allow the user to manage the quantity of information produced. This allows us, for instance, to select photons that crossed a particular object or experienced a particular physical process. The time of flight of the photon is also recorded, allowing the user to perform timing studies.

The simulation is geometrically bounded by the `WORLD`, which is a sphere with a user-defined radius centered on the origin. All processes occurring outside of `WORLD` are ignored and ray tracing stops when a photon reaches `WORLD`.

In general, a REFLEX simulation requires:

- Exactly one source geometry with one spectral shape, and optionally a flux.
- Exactly one domain in which the simulation takes place, called "World".
- Any number of objects.
- The compositions and densities of these objects.
- The physical processes that need to be simulated, if different from the default (all processes, except polarization).
- Either a number of photons, or a time limit
- Any number of directives on how to output the results.
- Optionally, some control parameters that affect the working of REFLEX.

The order of the commands is not frozen, but in some cases the order is very important. For instance, when am object is created, it will use the composition, density and physical processes that are currently defined, so these definitions must take place before creating the object.

4.1 Units and conventions

A number of units and conventions are used by REFLEX:

- The lengths can be expressed either in meter, centimeter, micrometer, light-year, light-second, or parsec.
- Densities can be expressed either in any of the length unit to the power $^{-3}$.
- Time is in seconds.
- Energies and temperatures are in eV.
- Angles are expressed in degrees.
- The X axis of Cartesian coordinates (1,0,0) is the polar vector $(90, 0)$. The Z axis of Cartesian coordinates (0,0,1) is the polar vector $(0, x)$ (x is arbitrary).

4.2 Source

The first step of the REFLEX Monte Carlo simulation is the creation of photons. REFLEX generates photons until either a number of photons have been simulated, a time limit has been reached, or the simulation is terminated by the user (for instance by typing Ctrl+C). A photon, described by its time, position, direction, and energy, is created according to the source that is defined by the user. The source has a geometry and a spectral shape. Optionally, it can have a luminosity. It can be placed anywhere in the simulation.

All photons are created at time $t = 0$. The position and directions are drawn at random following the spectral distribution and geometry selected by the user. For each geometry, the photon is emitted randomly within a sector whose opening can vary between 0° (unidirectional) and 180° (isotropic). The photon energy is drawn randomly from several possible distributions chosen by the user.

Optionally, the user can set the intrinsic source luminosity in a given energy range. This implies that the redshift of the source is provided. Cosmology can be set by providing H_0, Ω_M and Ω_Λ. The default is the Planck 2018 cosmology [21]: $H_0 = 67.4\,\mathrm{km\ s{-}1\ Mpc{-}1}$, $\Omega_M = 0.315$ and $\Omega_\Lambda = 0.685$. Setting the luminosity and redshift is mandatory if the user wants to compute photon fluxes in cm^{-2} s^{-1} keV^{-1} or energy fluxes in keV cm^{-2} s^{-1} keV^{-1}. The time needed for a real source to generate the requested number of photons and the photon flux associated to each event are provided in the log output of REFLEX (through `stderr`). This photon flux is in cm^{-2} s^{-1}.

4.3 Objects

REFLEX allows the user to define complex geometries for the surrounding material by assembling independent building blocks. An arbitrary number of objects can be set up by the user. Each object is characterized by a position, geometrical shape, size, composition, and hydrogen density; physical conditions may also differ from object to object. Different geometrical shapes with arbitrary sizes are available. The objects can also be named, so that they can be identified in the tracking of the events; in addition, this allows the user to investigate the radiation coming from specific objects.

Objects can can be placed anywhere within the domain of simulation, and their orientation can be specified arbitrarily. The domain of the simulation is defined by a special object called WORLD, which is an empty sphere centered on (0,0,0); ray-tracing stops when a photon hits its boundary, and the photon can be "observed". The 'observer' can be located at any place on `WORLD` (although 'imaging detectors' can be placed at other locations as well).

Several kinds of objects can be set in REFLEX. They are shown in Figure 1.

4.4 Composition

In addition to their shape and size, objects are given a chemical composition and a density. A composition is defined by the number density ratios of all elements from $Z = 2$ (helium) to $Z = 30$ (zinc) compared to hydrogen. The density is the number density of Hydrogen atom within the object. Each object can have different compositions and hydrogen number densities. Several compositions have been predefined similarly to those available in XSPEC. The metallicity (abundance of elements with $Z > 2$) can be modified for all elements and the number density ratio of each element can be tuned individually to simulate arbitrary chemical compositions. The fraction of molecular hydrogen can also be defined.

The composition and density must be defined before creating an object. Indeed, the object will inherit the currently defined composition. Subsequent changes in the composition and density

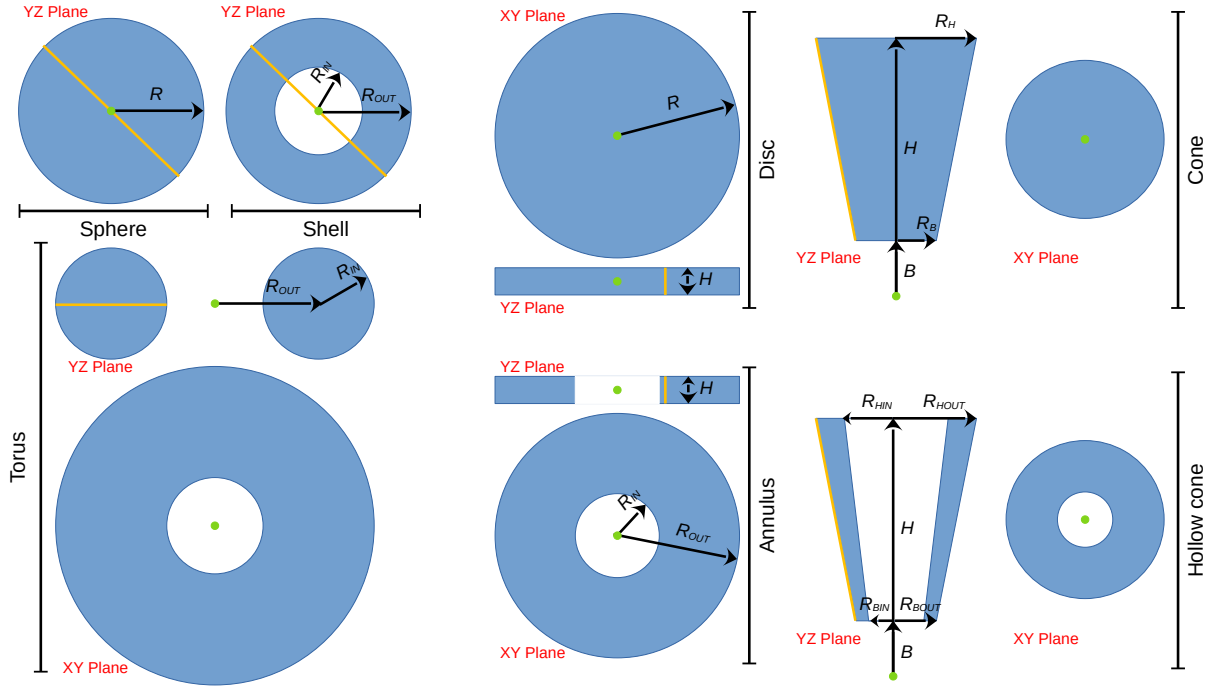

Figure 1: Objects available in REFLEX with their parameters. The image show the sections of the objects along the YZ and XY planes. The green dots indicate the reference point of the object. The yellow line indicate where the column density is measured.

will not affect this object, as REFLEX computes and stores in the object all the cross-sections for all physical processes at all considered energies. All subsequently created objects inherit the same properties, until the user changes these properties, without needing to recompute the cross-sections. Therefore, if several objects are created with different composition, it is recommended to create all objects with a given composition before changing it. This does not apply when only the density changes, which does not require changing the cross-sections. Thus, when creating a large number of objects (e.g., a clumpy structure), the storage and computation time needed for the cross-sections remains negligible even if the density of the objects changes every time. However, if the composition or physical conditions change for all objects the time to compute all cross-sections and the amount of memory needed to store the information will increase. In such (presumably rare) situation, the user can decrease the resolution of the grid of energies used to compute the cross-sections.

Starting with REFLEX 3.0, a new component in the composition is dust. Only one (binary) type of dust is considered, following [7]. It consists of graphite (pure Carbon) and silicate $MgFeSiO_4$. In order to add dust in a simulation, a dust-free composition must first be selected. The only parameter is then the Fe depletion factor, which is the fraction of Fe atoms that are in the form of dust. These atoms (as well as the corresponding fraction of C, O, Mg and Si atoms) are removed from the gas, so that changing depletion does not change the numbers of atoms of each element in the object. Depletion cannot be larger than 1; however, with some compositions, other atoms (typically Si) are depleted before iron, so that the maximum depletion is lower than 1 in some cases.

5 Physical processes

REFLEX implements several physical processes that take place when an X-ray photon crosses matter. We do not attempt to simulate all physical processes, but restrict ourselves to the few that are the most significant, similar to what has been the case in other models such as PEXRAV [16], PEXMON [19] and MYTORUS [18]. In order to provide insight into the physical mechanisms, each process can be turned on and off and the processes that have taken place are recorded for each simulated photon.

5.1 Atomic configuration

Two physical configurations can be selected by setting the 'temperature' of the medium: If the temperature is cold, all electrons are bound to atoms; this is the atomic configuration. If the temperature is 'warm', Hydrogen and Helium atoms are fully ionized. Electrons from other elements are ignored; this is the free-electron configuration. This configuration is used to match those use in other models, e.g. `pexrav` or `MYTorus`. Each object can use a different configuration. In the cold case, some user-specified fraction of Hydrogen is in the form of molecular Hydrogen, while in the warm case, all H_2 is destroyed.

5.2 Compton and Rayleigh scattering

Compton scattering is the inelastic (incoherent) interaction between a photon and a free electron. In the low-energy limit, the scattering becomes quasi-elastic, and is approximated by the Thomson scattering. The Compton scattering cross-section is given by the Klein-Nishina relativistic differential cross-section. REFLEX implements the full Klein-Nishina cross-section for free electrons, although the user can disable both the Klein-Nishina correction and inelastic scattering, for educational purposes. Several models, such as PEXRAV [16], assume that all H and He atoms are fully ionized, and scattering occurs only on these free electrons, neglecting the electrons bound on metallic atoms. The same physical configuration can be selected by the user in REFLEX; this the "warm" configuration. In this configuration, molecular hydrogen is destroyed.

However, electrons bound to atoms have a different behavior with respect to scattering of photons. REFLEX can therefore adopt a different physical configuration, that we refer to as the "cold" configuration, which takes into account the bound state of electrons. We include in REFLEX binding correction terms for Compton scattering, called incoherent scattering functions, computed by [12] as an energy- and Z-dependent multiplicative term on the Klein-Nishina cross-section. These corrections are also available in the EPDL97 library[1], and strongly decrease the cross-section for Compton scattering at low energy, which is essentially replaced by coherent (Rayleigh) scattering.

Rayleigh scattering is a coherent scattering on atoms due to their polarizability. Contrarily to Compton scattering, the atom is neither ionized nor excited. Rayleigh scattering cross-sections are significantly larger than the Compton scattering cross-sections at low energy, up to several tens of keV for heavy nuclei. The angular distribution is identical to that of Compton scattering in the low-energy limit, but becomes strongly forward-scattering in the X-ray domain. In the "cold" configuration, REFLEX implements Rayleigh scattering, unless disabled by the user. The Rayleigh cross-sections and the angular distributions have been taken from [12].

[1] https://www-nds.iaea.org/epdl97/

Coherent and incoherent scattering on molecular hydrogen, H_2, is also included in REFLEX in the "cold" configuration using the cross-sections of [12]. The fraction of hydrogen in molecular form can be set in REFLEX.

Several recent models already include the corrections for scattering on bound electrons [13, 10]. Applying these corrections has been shown to make a difference of up to 25% in the reflected spectrum at 1 keV, the effect becoming negligible around and above 10 keV [13].

5.3 Photoelectric absorption

Photoelectric absorption by bound electrons is another important process affecting transmission and reprocessing of X-rays. We use here the cross-sections determined from the analytic fits for each shell of the 30 elements provided by [26] and [25]; the cross-sections are computed using the Hartree-Dirac-Slater formalism and are thoroughly checked with existing laboratory measurements. In the current implementation, only neutral atoms are considered, although the analytic representations cover all ionization stages.

The use of analytic functions allows us to avoid performing any interpolation in functions that have sharp edges. The cross-sections are calculated on the fly when the photon is created or when its energy changes, for instance after Compton scattering, at the precise photon energy. The cross-sections are calculated separately for each shell, which allows us to keep track of the shell responsible for the photoelectric absorption.

Photo-electric cross-sections for H_2 molecular hydrogen in previous versions were taken to be twice those of atomic hydrogen. We use now the results from [28], with the modification below 85 eV introduced in [27]. We note that, above 300 eV, H_2 photo-electric cross-sections are now 2.8 times larger than the atomic hydrogen ones.

5.4 Fluorescence

When photoionization occurs, an electron is kicked out of the atom. The vacancy is filled by another electron from an outer electronic shell. Usually, the excess energy is transmitted to an outer-shell electron, which is then ejected. No further photon is emitted, and the simulation simply terminates. This process is known as the Auger effect.

In other cases, a fluorescence photon is emitted at an energy equal to the difference between the outer-shell energy level of the electron having filled the gap and the energy level of the vacancy. It is emitted in a random direction at the location of the interaction. The probabilities of such transitions, the fluorescence yields, which depend strongly on the atomic number of the element, have been taken from LBNL X-ray Data Booklet [24]; in particular, the Fe Kα/Fe Kβ ratio is 8.147. The energy levels of a number of X-ray fluorescence lines have been measured in the laboratory by [5] and are therefore more accurate than the LBNL ones; we use these measured energies when available, otherwise the EPDL89 library [6] is used. All transition probabilities are from EPDL89.

Only fluorescence from K and L shells has been implemented. The L-shell fluorescence lines are considerably weaker and have energies below 1.2 keV, but some lines are astrophysically relevant, as iron L-shell fluorescence has already been detected in an AGN [8]. The Coster-Kronig process is not implemented. The full list of K-shell fluorescence lines with the adopted fluorescence yields and energy levels is presented in Appendix B.

5.5 Dust

The presence of dust in the medium introduces several new physical processes. Dust in REFLEX is described in detail in [22]. The parameters defining dust are however even more numerous than those defining the properties of the gas phase. Indeed dust is not only defined by the densities of the different atoms, but also by the types of molecules and crystalline structures, as well as the full distribution of grain sizes. The complexity is way too high to be probed by numerical simulations. For this reason, only a simple, fixed dust model is considered within REFLEX, following [7], which consists of a mix of Carbon grains in graphite crystalline structure and of olivine silicate grains $Mg_{2x}Fe_{2(1-x)}SiO_4$. According to [7], Mg and Fe are both equally represented in the dust phase of the Milky Way, thus olivine is globally in the form $MgFeSiO_4$. In addition, there is about four Carbon atoms in the dust phase for each Silicon atom. The grain size distributions for graphite and olivine adopted in [7] are power law shaped with cut-offs at 0.01 and 0.164 μm, respectively. In addition, the graphite distribution presents two additional log-normal components centered at 3.5 and 30 Å respectively. The adopted densities of graphite and silicate grains are 2.24 and 3.5 gcm^{-3}, respectively.

Three physical processes are specific to the presence of dust in the X-rays, and are implemented in REFLEX:

- Scattering on dust grains. While Rayleigh scattering can be considered as scattering on particles of sizes of the same order of magnitude as, or smaller than, the wavelength of the incoming photon, dust particles are significantly larger than the photon wavelength, but not so large that scattering becomes normal optical reflection. Scattering on dust is described by Mie theory and anomalous diffraction theory; it is elastic, and mostly forward-scattering, with the median scattering angle decreasing as the photon energy increases. Cross-sections and differential cross-sections are provided in Draine (2003a).

- NEXAFS (Near-Edge X-ray Absorption Fine Structure). The crystalline arrangement of the atoms in dust grains affects the photo-ionization absorption cross-sections near the X-ray edges very close to the transition energy. The photo- ionization absorption cross-sections in dust used in REFLEX are also obtained from Draine (2003a), which includes the effect of NEXAFS.

- Self-shielding is another process that affects the photo-ionization absorption cross-sections of dust, and is the effect by which some atoms are hidden from X-ray radiation. This is due to the fact that atoms in dust are very strongly clustered in grains. Therefore, low-energy photons that hit a dust grain will be absorbed in the front part of the grain, and will never "see" the atoms on the other side of the grain . The effect of shielding is to decrease the photo-ionization absorption cross-sections at low energies; at higher energies, for the dust grain sizes considered here, shielding is minimal. Shielding is implemented in the cross-sections of Draine (2003a) that are used in REFLEX.

Fluorescence resulting from X-ray photo-ionization is implemented exactly as for the gas phase. In particular, it was verified in [22] that, with the grin sizes considered here, the self-opacity of grains to their own fluorescence emission can be neglected (see [22] for details).

5.6 Polarization

In the context of reflection of X-rays on cold matter, photon polarization essentially impacts the direction in which incoming photons are scattered in Compton scattering. The formalism is presented in [17]. While there are not many observational constraints on polarization in the X-rays, this could change in the future with the advent of X-ray polarimeters (e.g., [23]). Polarization-dependent Compton scattering in the Klein-Nishina regime is implemented as an option in REFLEX. By default, it is ignored.

5.7 Normalization of spectra

In the former case, the production of spectra in physical units of flux, either in counts s^{-1} cm^{-2} keV^{-1} or in keV s^{-1} cm^{-2} keV^{-1}, requires a normalization factor. This is calculated by setting the luminosity of the unabsorbed source in a given energy range and its redshift; the redshift is in addition applied to all photons escaping to `WORLD`. This translates into a flux for each photon. Since the number of photons is fixed, an "observation time" is thus defined. It is important to note that only the intrinsic, unabsorbed luminosity of the primary source of X-ray photons integrated over 4π can be determined, since an observed luminosity would depend on the details not only of the simulation, but also of the viewing direction.

5.8 Domain of validity

The physical processes implemented in REFLEX are "exact", i.e. no simplifying assumption is made on their calculations. However, the accuracy of REFLEX simulations is limited by a number of factors. Implemented physical processes depend on parameters which are usually only known with some limited precision and accuracy. As an example, the photoelectric cross-sections used in REFLEX, while commonly used in astronomy, are not unique; in addition to the cross-sections used in REFLEX (`vern`), XSPEC can also use the cross-sections from [4] with either the new H and He cross-sections from [28] (`bcmc`) or the original cross-sections (`obcm`).

Similarly, while the Klein-Nishina cross-section is computed using the exact formula, corrections for bound electrons and Rayleigh scattering cross-sections are computed using approximations, which are interpolated using the tables from [12].

Many of the fluorescence lines (and all the most prominent ones) have been measured in the laboratory by [5]; however, the energy levels of many minor lines have been calculated. More importantly, all probability transitions are also calculated.

The main limitations of REFLEX come however from the physical processes that are not implemented, in particular the following:

- Pair production contributes to opacity at energies above 1 MeV, and even starts to dominate around 10 MeV. Likewise, photon-photon opacity is not included.
- Matter velocities, thermal broadening and turbulence are not included, although we plan to include these processes at a later stage; this may induce unrealistically sharp features in the REFLEX spectra. This is mitigated by the limited spectral resolution of X-ray telescopes.
- Coster-Kronig process is a special case of an Auger effect where the vacancy is filled by an electron from the same shell. In this case, a secondary recombination may occur, which could be in the form of a fluorescence line. Since Coster-Kronig process cannot affect the K shell,

only L-shell fluorescence and above can occur. Because L-shell fluorescence is already weak and because Coster-Kronig process is a second-order effect, it has not been implemented in ReflеX. Likewise, M-shell (and above) fluorescence is neglected.

- Raman scattering, which is an inelastic scattering of a photon with an atom or a molecule, is not included, since it has much lower probability than Rayleigh scattering.

6 Output

When run, ReflеX outputs its log through `stderr`; it contains all the information relative to the processing which is contained in the parameter file. This is used to provide metadata and to ensure that the parameter file has been interpreted correctly. ReflеX has four different ways to output the result of the simulations; all of them can be used simultaneously.

6.1 Text output

Each event affecting the simulated photon can be output. The user can select which of these events is displayed. The text output is normally sent to `stdout`, but it can be output to a file instead. This is the only output type where the full information on the trajectory of the photon and on the history of interactions is preserved. It is however not very easy to read and is generally used for debugging or educational purpose. The following event types can be selected:

- Photon is created
- Photon hits `WORLD`
- Photon is destroyed
- Photon enters an object
- Photon exits an object
- Photon is absorbed by photo-ionization
- Photon makes a fluorescence
- Photon makes a Compton scattering
- Photon makes a Rayleigh scattering
- Photon is absorbed by dust
- Photon is scattered by dust

6.2 FITS binary table output

FITS binary table: The properties of photons hitting `WORLD` can be output in FITS binary table format. The user can select which of the fields are output. The binary output must be written to a file. Any selection of the photon fields can be specified. These fields are:

- Number of fluorescence emissions

- Number of Compton scatterings
- Number of Rayleigh scatterings
- Number of scatterings on dust
- Number of scatterings (sum of Compton, Rayleigh and dust scatterings)
- Number of interactions (sum of the number of scatterings and of the number of photo-electric absorptions)
- Number of hit objects
- Time when the photon hits World
- Photon energy
- Integrated path length across objects
- Integrated column density across objects
- Photon direction (X, Y, Z) coordinates, each coordinate individually
- Photon location (X, Y, Z) coordinates, each coordinate individually
- Photon polarization (X, Y, Z) coordinates, each coordinate individually

A selection can be performed on any of these parameters. When several selection criteria are provided, they are combined with AND.

6.3 FITS image output

The user can place a virtual imaging detector anywhere in `WORLD`. An arbitrary number of images can be created in each run of ReflеX. Image outputs must be written to a file. The principle of the imager is that of a pinhole camera. Photons are collected inside a circular aperture defined by the user. The aperture also limits the resolution, as photons emitted at a distance D will be seen by the detector at angles A/D, where A is the diameter of the aperture. The aperture size is thus a trade-off between the need to collect as many photons as possible and the loss of resolution. In order to alleviate the problem, the user can place many detectors, taking advantage of possible symmetries in the simulated system. It is even possible to define a completely axisymmetric camera, which makes probably sense only if the object has such symmetry; it must be noted however that the image resolution in the azimuthal direction is practically infinite, so that the PSF looks like a vertical segment. Photons can be selected according to the following properties:

- Number of fluorescence emissions
- Number of Compton scatterings
- Number of Rayleigh scatterings
- Number of scatterings on dust
- Number of scatterings (sum of Compton, Rayleigh and dust scatterings)

- Number of interactions (sum of the number of scatterings and of the number of photo-electric absorptions)
- Number of hit objects
- Time when the photon hits World
- Integrated path length across objects
- Integrated column density across objects
- Photon energy
- Photon direction (X, Y, Z) coordinates, each coordinate individually
- Photon location (X, Y, Z) coordinates, each coordinate individually
- Photon polarization (X, Y, Z) coordinates, each coordinate individually

A selection can be performed on any of these parameters. When several selection criteria are provided, they are combined with AND.

6.4 Spectrum output

Photons hitting `WORLD` or exiting from another object can be binned into spectra with user-defined arbitrary bins (linear or logarithmic). Any number of spectra can be created in each run of REFLEX. Spectra are written to a file in ascii format. The file has three columns: bin minimum energy, bin maximum energy and counts or flux in the bin. Photons can be selected according to the following properties:

- Number of fluorescence emissions
- Number of Compton scatterings
- Number of Rayleigh scatterings
- Number of scatterings on dust
- Number of scatterings (sum of Compton, Rayleigh and dust scatterings)
- Number of interactions (sum of the number of scatterings and of the number of photo-electric absorptions)
- Number of hit objects
- Time when the photon hits World
- Integrated path length across objects
- Integrated column density across objects
- Photon energy
- Photon direction (X, Y, Z) coordinates, each coordinate individually

- Photon location (X, Y, Z) coordinates, each coordinate individually
- Photon polarization (X, Y, Z) coordinates, each coordinate individually

A selection can be performed on any of these parameters simultaneously. When several selection criteria are provided, they are combined with AND.

6.5 Histogram output

Photons hitting `WORLD` or exiting from another object can be binned into histograms of any of the photon properties with user-defined bins (linear or logarithmic). Any number of histograms can be created in each run of REFLEX. Histograms are written to a file in ascii format. The file has three columns: bin minimum value, bin maximum value and counts. Histograms of any of the following properties can be built. Photons can be selected according to the same properties:

- Number of fluorescence emissions
- Number of Compton scatterings
- Number of Rayleigh scatterings
- Number of scatterings on dust
- Number of scatterings (sum of Compton, Rayleigh and dust scatterings)
- Number of interactions (sum of the number of scatterings and of the number of photo-electric absorptions)
- Number of hit objects
- Time when the photon hits World
- Photon energy
- Integrated path length across objects
- Integrated column density across objects
- Photon energy
- Photon direction (X, Y, Z) coordinates, each coordinate individually
- Photon location (X, Y, Z) coordinates, each coordinate individually
- Photon polarization (X, Y, Z) coordinates, each coordinate individually

A selection can be performed on any of these parameters simultaneously. When several selection criteria are provided, they are combined with AND.

7 Commands

The parameter file is a series of ASCII commands. The commands are grouped into several categories: general setup commands, object setup commands, physics commands, output commands. Commands marked with a star (*) can be repeated several times. Although it is not always needed, a good practice is to write the commands in the order of the subsections below.

In the following, `text` is a command that must be typed as is, while X[type] refers to parameter X, whose type is provided in parenthesis (Int, Float, String, or Bool). Underlined commands are mandatory, as they have no sensible default values.

7.1 Control commands

These commands define how the simulation is run.

- `RANDOM` N[Int]

  When specified, `RANDOM` sets the seed of the random number generator to N. This allows to reproduce the results between different runs. If not specified, a random seed is used, so the results are not reproducible. In multi-threading, the M generators are initialized with seeds N,$N+1$,...,$N+M-1$.

- `NPHOTS` N[Int]

  Sets the number of photons to be run in the simulation to N. If N=0, the number of photons is infinite and the simulation must be stopped by a time limit or by sending `SIGINT` (Ctrl+C) or `SIGTERM`.

- `TIME` N[Int]

  Sets the duration of the simulation in seconds. If it is 0 (the default value), the duration is infinite the simulation must be stopped by a limit in the number of photons or by sending `SIGINT` (Ctrl+C) or `SIGTERM`.

- `RESUME` B[Bool]

  If B is `ON`, RefleX attempts to resume an existing simulation in order to increase the number of photons. Currently, the functionality only works with spectral outputs. It requires that RefleX is called with exactly the same parameter file (with the possible exception of the number of photons) and the previous log file is available in the directory where RefleX is run. The log file can have any name, and the resume functionality can be run any number of times, provided a new log file is created each time. RefleX will refuse to use a log file more than once. In order to create the log file, a redirection of `stderr` is usually necessary (See Section 2).

  The functionality has two main uses:

  - Increase the number of photons: A short simulations has been run; after checking the results, the user may want to increase the number of photons, without discarding the existing spectra. It might be necessary to change the parameter `NPHOTS`.
  - When running on a cluster, jobs typically have a time limit; alternatively, setting a lower time limit may increase the priority of the jobs. With the `RESUME`, the user can set a time

limit to the REFLEX simulations using the `TIME` command slightly below the maximum duration of the jobs (say, about one minute to be on the safe side). The user can then relaunch new jobs until the requested number of photons is reached.

When resuming a simulation, REFLEX does not try to be extremely smart. It merely identifies the last log file, and retrieves the number of photons already simulated. It is important not to modify the parameter file (with the possible exception of the number of photons), otherwise the results might be inconsistent in an unpredictable way (including segmentation faults if the size of spectra is modified).

- `THREAD` N[Int]

  Runs REFLEX using N threads. There is no checks that the processor can handle these threads, and the optimal number of threads depends a lot on the machine on which it runs, so N should be adapted to the hardware used for the computations by the user. The maximum of threads is 256 in any case. Note that verbosity should be set to zero when using multi-threading, because the outputs of the different threads are merged without any locking of the other threads, as such locking would essentially results in having only one running thread at a time. All other outputs (events, images, spectra) are thread-safe.

- `MAXINT` N[Int]

  Sets the maximum number of interactions that a photon can undergo until it is declared lost to N. The default is 10000. Normally, N should practically never be reached, and reaching N interactions for a single photon would indicate a problem. `MAXINT` is able to kill such photons, in order not to block the simulations. This should be very rare, so it is harmless. The number of killed photons is reported by REFLEX.

- `STEP` F[Float]

  Defines F, the energy resolution of the cross-section pre-computations below 10 keV. It is expressed in eV and the default value is 1 eV. Above 10 keV, since there is no atomic transition anymore, the step is increased by a factor 100. Computation time does not depend dramatically on the value of STEP, except when creating the grid (it takes however only a few seconds per grid). However, in simulations with many objects with different compositions or physical conditions, the grids might occupy a lot of memory. With the default resolution of 1 eV, each grid takes about 10 MB.

- *`LENGTH` *Unit*[String]

  Sets the unit of all length (and derived, such as densities) directives in the parameter file to *Unit*. The value can be:

  - `Meter` (default)
  - `Centimeter`
  - `Millimeter`
  - `Micrometer`
  - `Lightyear`
  - `Lightsecond`

- `Parsec`

Setting `LENGTH` affects all subsequent commands until a new `LENGTH` command is issued. It can be changed any number of times.

- `FRESET` B[Bool]

  If B =ON, resets the number of scatterings (Compton and Rayleigh) to 0 after a fluorescence event. This allows to determine the scattering order of photons generated with fluorescence, erasing their previous history. Default is OFF.

7.2 Physics setup commands

These commands allow the user to select the physical conditions of the simulation. A single set of physical conditions need to be selected before the objects are created, otherwise results might be unpredictable. In principle, the default physics (with all physical processes except polarization) should be used, unless for educational purposes, or in case the user wants to reproduce "legacy" models. Note also that the `TEMPERATURE` command, which can be changed for all objects, does affect the physics.

- *`PHYSICS` *Process*[String] B[Bool]

  Turns on (B =ON) or off (B =OFF) the physical process *Process*. There can be several `PHYSICS` commands, one for each physical process. *Process* can be:

  - `COMPTON` : Turns on Compton scattering. This is ON by default.
  - `RAYLEIGH` : Turns on Rayleigh scattering. This is ON by default.
  - `PHOTO` : Turns on photo-ionization. This is ON by default.
  - `FLUOR` : Turns on fluorescence after photo-ionization. This is ON by default. Photo-ionization needs to be ON for this physical process to play any role.
  - `KN` : Uses the Klein-Nishina cross-sections for free electrons. This is ON by default. If OFF, the Thomson cross-section is used at all energies. This is ON by default.
  - `DUST_PHOTO` :Turns on photo-ionization on dust grains. This is ON by default.
  - `DUST_SCAT` :Turns on scattering on dust grains. This is ON by default.
  - `THOMSON` : Uses Thomson cross-sections at all energies and treat all Compton scatterings as elastic. This is OFF by default.
  - `FIRON` : Discards fluorescence from elements other than Iron and Nickel. This is OFF by default.
  - `POLAR` : Turns on polarization effects in the ray tracing. This is OFF by default.

- `COSMOLOGY` H_0[Float] Ω_M[Float] Ω_Λ[Float]

  Sets the cosmological parameters to H_0 km s^{-1} Mpc^{-1}, Ω_M and Ω_Λ This is used only if the `LUMINOSITY` command is used. The default is the Planck 2018 cosmology [21]: $H_0 = 67.4$ km s−1 Mpc−1, $\Omega_M = 0.315$ and $\Omega_\Lambda = 0.685$.

7.3 Emission setup commands

- EMSPEC *Shape*[String] ...

  Sets the emission spectrum of the source. This command is mandatory. The *Shape* parameter and additional parameters can be:

  - MONO P_1[Float]
    Generates mono-energetic photons at energy P_1 eV.
  - GAUSS P_1[Float] P_2[Float]
    Generates photons following a Gaussian distribution centered on P_1 eV, with a standard deviation of P_2 eV.
  - PWRLAW P_1[Float]
    Generates photons following a power law distribution with photon index P_1.
  - CUTOFF P_1[Float] P_2[Float]
    Generates photons following a cut-off power law distribution with photon index P_1 and exponential cut-off at energy P_2 eV.
  - BLACKBODY *P1*[Float]
    Generates photons following a blackbody distribution with temperature P_1 eV.
  - WIEN P_1[Float]
    Generates photons following a Wien distribution with temperature P_1 eV.
  - REFLEXINO
    Generates RefleXinos, i.e. virtual particles that have no interaction with matter. RefleXinos keep nevertheless track of all crossed objects and column densities.

- EMGEOM *Geom*[String] ...

  Sets the geometry of the source. This command is mandatory. The *Geom* parameter and additional parameters can be:

  - POINT X[Float] Y[Float] Z[Float] ϑ[Float] φ[Float] α[Float]
    The source is a point source centered on (X, Y, Z), and photons are emitted in a cone around (ϑ, φ) deg, with an opening angle of α deg. If $\alpha = 0$, all photons have the direction (ϑ, φ). $\vartheta = 0$ corresponds to the Z axis.
  - SPHERE X[Float] Y[Float] Z[Float] R[Float] ϑ[Float] φ[Float] α[Float]
    The source is a sphere centered on (X, Y, Z) with a radius R, and photons are emitted in all directions on a cone around (ϑ, φ) deg on the surface of a sphere, with an opening angle of α deg. If $\alpha = 0$, all photons are emitted from the point $R(\vartheta, \varphi)$. α cannot be larger than 90 deg. $\vartheta = 0$ corresponds to the Z axis.
  - DISC X[Float] Y[Float] Z[Float] R[Float] ϑ[Float] φ[Float] α[Float]
    The source is a disc in the (X, Y) plane centered on (X, Y, Z) and radius R, and photons are emitted in a cone around (ϑ, φ) deg, with an opening angle of α deg. If $\alpha = 0$, all photons have the direction (ϑ, φ). $\vartheta = 0$ corresponds to the Z axis.

- `ANNULUS` X[Float] Y[Float] Z[Float] R_{OUT}[Float] R_{IN}[Float] ϑ[Float] φ[Float] α[Float]
  The source is annulus in the (X, Y) plane centered on (X, Y, Z) and with inner radius R_{IN} and outer radius R_{OUT}, and photons are emitted in a cone around (ϑ, φ) deg, with an opening angle of α deg. If $\alpha = 0$, all photons have the direction (ϑ, φ). $\vartheta = 0$ corresponds to the Z axis.

- `ECUT` E[Float]

  Sets the photon termination energy to E eV, i.e., the photon is destroyed if its energy falls below this value.

- `EGEN` E_1[Float] E_2[Float]

  Generates photons in the range $[E_1, E_2]$ eV only.

- `LUMINOSITY` E_1[Float] E_2[Float] L[Float]

  Sets the source intrinsic luminosity in the range $[E_1, E_2]$ eV to 10^L erg s^{-1}.

- `REDSHIFT` F[Float]

  Sets the source's redshift to F. This is used (and required) only if the source luminosity is set.

7.4 Composition setup commands

Composition setup commands define the gas and dust content of the objects that will be defined later. Each object can have its own composition, so each of the following commands can be repeated any number of times. However, the composition definition is persistent: Once it is defined, it stays the same for all subsequent objects, until composition is changed.

- *`DENSITY` n[Float]

  Sets the density of Hydrogen atoms (either in atomic or molecular form) to n per cubic unit length. Thus the user needs to make sure the length unit is set correctly using the `LENGTH` command.

- *`COLDENS` N_{H}[Float]

  Sets the column density of Hydrogen atoms (either in atomic or molecular form) to N_{H} per squared unit length. Thus the user needs to make sure the length unit is set correctly using the `LENGTH` command. The column density is measured at different places in the different objects. See Figure fig:objects and Section 7.5.

- *`MATTER` *COMPOSITION*[String]

  Loads a predefined composition, which is defined as the number ratio of the first 30 elements compared to Hydrogen. *COMPOSITION* can be:

  - `lodd` or `lodders03`: Abundances from [14].
  - `angr`: Abundances from [2].
  - `aspl` or `asplund`: Abundances from [3].
  - `feld` or `feldman`: Abundances from [9].

- `aneb`: Abundances from [1].
- `grsa`: Abundances from [11].
- `wilm` or `wilms`: Abundances from [27].
- `lpgp` or `loddersp`: Photospheric abundances from [15].
- `lpgs` or `lodderss`: Proto-solar abundances from [15].
- `cosm` or `cosmic`: This composition mimics the primordial (cosmological) gas abundance and has the He abundance from [14] and all other elements set to 0.
- `void`: pure Hydrogen.

If no composition is set, the cosmological gas abundance is used. Only elements with atomic number smaller or equal to 30 (Zinc) are considered.

- *`ELEMENT` Z[Int] F[Float]

  Sets the abundance of element Z relative to H to F. Z must be between 2 and 30 included.

- *`METALLICITY` F[Float] Sets the metallicity to F, i.e., the abundance of all elements with atomic number between 3 and 30 is multiplied by F. Note that this is relative to the base composition, so to go back to a metallicity of 1 after having issued `METALLICITY 2`, a command `METALLICITY 1` should be issued, and not `METALLICITY 0.5`. To avoid confusion, `METALLICITY` should be set after the `MATTER` and/or `ELEMENT` command(s).

- *`TEMPERATURE` T[Int]

  Sets the ionization in the subsequent objects. If $T = 0$, the medium is cold, and all atoms are considered neutral, so Compton and Rayleigh scattering happens on bound electrons only. If $T = 1$, the medium is warm and Hydrogen and Helium are considered to be fully ionized; all electrons on elements heavier than He are ignored. This is consistent with the assumption in `pexrav`, `pexmon`, `MYTorus`, etc.

- *`H2FRACTION` F[Float]

  Sets the fraction of Hydrogen in molecular form to F. One must have $0 \leq F \leq 1$. Note that this is relative to the base composition, so to go back to a molecular Hydrogen fraction of 1 after having issued `H2FRACTION 0.5`, a command `H2FRACTION 1` should be issued, and not `H2FRACTION 2` (which would be illegal anyway). If the medium is warm ("`TEMPERATURE 1`"), F is set to 0. Attempts to change it results in an error.

- *`DUST` F[Float]

  Sets the fraction of Iron captured in dust grains to F. One must have $0 \leq F \leq 1$. Note that this is relative to the base composition, so to go back to a dust fraction of 1 after having issued `DUST 0.5`, a command `DUST 1` should be issued, and not `DUST 2` (which would be illegal anyway). However, the maximum values for the `wilm` and `angr` are 0.691 and 0.758, respectively, due to their lower relative Silicon abundance (Silicon is fully depleted before Iron).

- `RESTORE` *NAME*[String]

Reads the cross-sections from the FITS file *NAME*, which can be created by the `DUMP` command. This can be useful in particular in the case of very short simulations, in order to avoid wasting time recalculating the cross-sections. The details of the format are described under the `DUMP` command.

7.5 Object setup commands

- `OBJECT WORLD` R[Float]

  `WORLD` is a special object that defines the domain where simulations are run. It is a sphere centered on (0,0,0) and of radius R. The `WORLD` object is mandatory.

- *`OBJECT` *TYPE*[String] *NAME*[String] X[Float] Y[Float] Z[Float] ...

  Add an object. All objects (except `WORLD`)have the same first five parameters. The object geometry is given by *TYPE*. The different geometries are shown on Figure 1. Objects can be attributed a name using the *NAME* parameter in order to be able to select photons coming from a specific object. If the user does not need this functionality, it is more efficient to set *NAME* to `NULL`. The next three parameters X, Y, Z give the center of the object. Depending on the value of *TYPE*, additional parameters need to be set:

  - `SPHERE`: R[Float]
    Creates a sphere of radius R. The column density is measured along the diameter of the sphere (length $2R$).
  - `SHELL`: R_{OUT}[Float] R_{IN}[Float]
    Creates a shell of outer radius R_{OUT} and inner radius R_{IN}. The column density is measured along the diameter of the sphere (length $2(R_{OUT} - R_{IN})$).
  - `DISC`: R[Float] H[Float]
    Creates a disc of radius R and total height H. The plane of the disc is parallel to the ((1,0,0),(0.1,0)) plane (XY plane) if no rotation is applied. The column density is measured along the Z axis (length H).
  - `ANNULUS`: R_{OUT}[Float] R_{IN}[Float] H[Float]
    Creates an annulus of outer radius R_{OUT}, inner radius R_{IN} and total height H. The plane of the disc is parallel to the ((1,0,0),(0.1,0)) plane (XY plane) if no rotation is applied. The column density is measured along the Z axis (length H).
  - `TORUS`: R_{OUT}[Float] R_{IN}[Float]
    The object is a torus of center $(0, 0, 0)$, outer radius R_{OUT} and inner radius R_{IN}. The column density is measured when crossing the torus once along in the XY plane (length $2R_{IN}$).
  - `CONE`: B[Float] T[Float] R_B[Float] R_T[Float]
    The object is a cone of center $(0, 0, 0)$, which starts at height B up to height T. The bottom radius is R_B, while the top radius is R_T. The cone is around the Z axis (0,0,1). The column density is measured along the edge of the cone (length $\sqrt{(T-B)^2 + (R_T - R_B)^2}$).
  - `HCONE`: B[Float] T[Float] $R_{B,OUT}$[Float] $R_{T,OUT}$[Float] $R_{B,IN}$[Float] $R_{T,IN}$[Float]
    The object is a hollow cone of center $(0, 0, 0)$, which starts at height B up to height T. The outer bottom radius is $R_{B,OUT}$, while the outer top radius is $R_{T,OUT}$. The inner

bottom radius is $R_{B,IN}$, while the inner top radius is $R_{T,IN}$. The hollow cone is around the Z axis (0,0,1). The column density is measured along the edge of the hollow cone (length $\sqrt{(T-B)^2+(R_{T,OUT}-R_{B,OUT})^2}$).

- `ROTATION` ϑ[Float] φ[Float] α[Float]

  The `DISC`, `ANNULUS`, `TORUS`, `CONE` and `HCONE` objects are oriented by default with an axis of symmetry parallel to the Z axis. Before creating the objects, a rotation can be applied using the `ROTATION` command, which defines the new orientation by performing a rotation of α deg around the direction around (ϑ, φ) deg. The rotation is always defined as a rotation from the original orientation, so a 90-deg rotation around the Z axis (`ROTATION 0 0 90`) followed by another identical rotation transforms again the X axis into the Y axis, and not into the -X axis. `ROTATION x y 0` returns to the Z axis, whatever the value of x and y.

7.6 Monitoring commands

- *`VERBOSE` *Event*[String] ...

  Define the verbosity of the text output. *Event* defines which event is printed:

  - `NEW`: Photon is created
  - `WORLD`: Photon hits WORLD
  - `KILLED`: Photon is killed, either because of an Auger effect, or because its energy is too low
  - `ENTER`: Photon enters an object
  - `EXIT`: Photon exits an object
  - `PHOTO`: A photoelectric absorption takes place
  - `FLUOR`: A fluorescence photon is created
  - `COMPTON`: Photon is Compton-scattered
  - `RAYLEIGH`: Photon is Rayleigh-scattered
  - `DUSTABS`: Photon is absorbed by dust
  - `DUSTSCAT`: Photon is scattered by dust
  - `ALL`: All events are printed
  - `NONE` or `0`: Verbosity is suppressed

  Multiple `VERBOSE` commands can be issued to control which events are printed. Default is none. Multiple *Event* can be set at the same time, for instance:

  ```
  VERBOSE NEW ENTER EXIT WORLD
  ```

  is valid. Note that this option does not work well in multi-threading, because the outputs of the different threads are merged without any locking of the other threads, as such locking would essentially results in having only one running thread at a time. All other outputs (events, images, spectra) are thread-safe.

- `OUTNAME` *Name*[String]

  Sets the text controlled with the `VERBOSE` command to be saved in the file *NAME*. If not set, all output goes to `stdout`.

- `PERCENT` *B*[Bool]

  Prints out the percentage of processed photons along the way if *B* is ON. Default is OFF.

- `DUMP` *NAME*[String]

  Dumps the full current cross-sections for the specified processes into the file *Name*. The format is a FITS file with the following float columns:

  - `PHOTO`: Total photoionization cross-section
  - `RAYLEIGH`: Total Rayleigh scattering cross-section
  - `COMPTON`: Total Compton cross-section
  - `DUST`: Dust extinction cross-section
  - `ALBEDO`: Dust albedo
  - `THETA`: Dust median scattering angle
  - `PHOTO_ELEM`: Element-by-element photoionization cross-section (array of 31 floats)
  - `RAYLEIGH_ELEM`: Element-by-element Rayleigh scattering cross-section (array of 31 floats)

  Keywords are also specified in order to uniquely identify the composition: `METALLIC`, `TEMPERAT`, `H2FRAC`, and `DUST`. Elemental abundances are indicated by the `ELEM`N keywords, with $N = 0, \ldots, 30$; element 0 refers to H_2. The extension name is `CROSSSECTIONS`.

  Energies are derived from the `STEP` keyword: The energy at row N is $N \cdot$`STEP` for energies below 10 keV. Above 10 keV, the step is increased by a factor 100, since there are no atomic transitions anymore.

  Cross-sections stored in a FTS file with the same format can be read in REFLEX with the `RESTORE` command.

7.7 Output commands

- `EVENTS` *Name*[String]

  Create a FITS output event file with name *Name*. Each event reaching `WORLD` is recorded, subject to event selection (see Sect. 7.8).

- `FIELDS` *Bitfield*[String]

  Defines which photon fields are written in the Binary output file. *Bitfield* must be a sequence of 15 "0" and "1", "1" indicating that the field is output. The fields are :

  - Digit 1: Number of Compton scatterings
  - Digit 2: Number of Rayleigh scatterings
  - Digit 3: Number of fluorescence emissions
  - Digit 4: Number of dust scatterings

- Digit 5: Numbers of hit objects
- Digit 6: Time when the photon hits World
- Digit 7: Photon energy
- Digit 8: Path length through objects
- Digit 9: Column density through objects
- Digit 10: Photon direction X coordinate
- Digit 11: Photon direction Y coordinate
- Digit 12: Photon direction Z coordinate
- Digit 13: Photon location X coordinate
- Digit 14: Photon location Y coordinate
- Digit 15: Photon location Z coordinate
- Digit 16: Photon polarization X coordinate
- Digit 17: Photon polarization Y coordinate
- Digit 18: Photon polarization Z coordinate

- *`SPECTRUM BINNING` E_1[Float] E_2[Float] ΔE `[LOG]`

  Defines a new binning for all subsequent spectra from E_1 eV to E_2 eV with constant step ΔE eV. If `LOG` is specified, E_1 and E_2 are expressed in (decimal) logarithm and $10^{\Delta E}$ is a multiplicative constant.

- *`SPECTRUM NEW` *Name*[String]

  Create a new spectrum with filename *Name*.

- *`SPECTRUM MODE` *Mode*[String]

  Set the format of the current spectrum according to *Mode*, which can be:

  - `COUNTS`: The spectrum consists in integer photon counts (no normalization)
  - `PHOTON`: The spectrum is expressed in $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}\ \mathrm{keV}^{-1}$
  - `FLUX`: The spectrum is expressed in $\mathrm{keV}\ \mathrm{cm}^{-2}\ \mathrm{s}^{-1}\ \mathrm{keV}^{-1}$

  Note that the flux spectra (either `PHOTON` or `FLUX`) require that the luminosity and redshift of the source are set. It also assumes that the spectrum is collected over 4π. If this is not the case, e.g., because the user has selected specific photon directions, it is up to the user to correct the flux for this factor, as REFLEX cannot be aware of that.

- *`HISTOGRAM BINNING` P_1[Float] P_2[Float] ΔP `[LOG]`

  Defines a new binning for all subsequent histograms from P_1 to P_2 with constant step ΔP. If `LOG` is specified, P_1 and P_2 are expressed in (decimal) logarithm and $10^{\Delta P}$ is a multiplicative constant.

- *`HISTOGRAM NEW` *Parameter*[String] *Name*[String]

  Create a new histogram for the parameter *Parameter* with filename *Name*. *Parameter* can be any of the parameters listed in Sect.7.8.

- *`IMAGE NEW` *String* X[Float] Y[Float] Z[Float] A[Float] F[Float] N[Int]

  Create a new FITS image with filename *String*. The detector is placed at (X, Y, Z) and is oriented towards the center $(0, 0, 0)$ of the simulation. All photons passing at a distance smaller than A from (X, Y, Z) are recorded. Hence A is the aperture of the "camera"; a larger aperture will increase fluxes at the expense of image resolution. The image is a square of NxN pixels, and has a total field-of-view of F degrees. See Sect. 6.3 for some remarks on how images are constructed, and in particular on their resolutions.

  *`IMAGE NEW` *String* X[Float] `AXIS` Z[Float] A[Float] F[Float] N[Int] If `AXIS` is specified instead of Y, the detector is placed at coordinates $(X, 0, Z)$, and then rotated 360 deg around the Z axis. This is equivalent to placing an infinite amount of repeated detectors (see `IMAGE REPEAT` below) at all possible coordinates (x,$\sqrt{X^2 - x^2}$,Z), without the need of adding numerous detectors. Using this feature makes sense only if the system is axisymmetric. Note that this gives a quite asymmetric PSF, with a much better horizontal resolution than the vertical one.

  *`IMAGE REPEAT` X[Float] Y[Float] Z[Float]

  Add a detector at (X, Y, Z), identical to the one that has been previously defined. Any number of `IMAGE REPEAT` can be added. This functionality is used to increase the signal in cases where the system has a symmetry.

- `SOURCE` *RA*[Float] *Dec*[Float] *PosAngle*[Float]

  Sets the source coordinates to RA=*RA* and Dec=*Dec* and the position angle to *PosAngle* (all angles in degrees). This allows the REFLEX image to be superimposed directly on a real sky image using (for instance) DS9.

7.8 Event selection

- *`EVENTS` *Par*[String] *Cond*[String] *Val*[Float]
  *`SPECTRUM` *Par*[String] *Cond*[String] *Val*[Float]
  *`IMAGE` *Par*[String] *Cond*[String] *Val*[Float]

  Adds a new selection for the event output, the current spectrum, or the current image. If other selections have already been made for the same output, they are combined with an AND operation. *Par* can be:

  - `COMPTON`: Number of Compton scatterings
  - `FLUOR`: Number of fluorescence emissions
  - `RAYLEIGH`: Number of Rayleigh scatterings
  - `DUSTSCAT`: Total number of scatterings on dust
  - `SCATTER`: Total number of scatterings (Compton+Rayleigh+dust)
  - `INT`: Total number of "interactions" (Compton+Rayleigh+dust+Fluorescence)
  - `OBJECT`: Number of objects hit
  - `TIME`: Time when reaching `World` or camera
  - `ENERGY`: Energy when reaching `World` or camera
  - `LENGTH`: Integrated path length across objects

- `NH`: Integrated column density across objects
- `DIR_X`: X-axis direction when reaching `World` or camera
- `DIR_Y`: Y-axis direction when reaching `World` or camera
- `DIR_Z`: Z-axis direction when reaching `World` or camera
- `LOC_X`: X-axis position when reaching `World` or camera
- `LOC_Y`: Y-axis position when reaching `World` or camera
- `LOC_Z`: Z-axis position when reaching `World` or camera
- `POL_X`: X-axis polarization when reaching `World` or camera
- `POL_Y`: Y-axis polarization when reaching `World` or camera
- `POL_Z`: Z-axis polarization when reaching `World` or camera

The condition *Cond* can be any of $<$, $<=$, $==$, $!=$, $>=$, $>$. The parameter *Par* is compared to the value *Val* using the condition *Cond*.

8 Obsolete commands

- `OUTDATA` *String*

  This command is replaced by the `EVENTS` command, and is going to be removed in the future. A warning is issued.

- `MARGIN` F[Float]

  This command is not needed anymore (a warning is issued), since the boundary detection scheme in REFLEX has been improved. `MARGIN` used to define the minimum distance that a photon has to cross at each iteration relative to the size of the object.

- `ABUNDMIN` F[Float]

  This command is now obsolete (a warning is issued), as it does not lead to any significant gain in computation time with the new implementation of the selection of interactions introduced in REFLEX 2.0. `ABUNDMIN` was used ot restrict the calculation of photo-ionization cross-sections to sufficiently abundant elements.

9 Useful tools

9.1 `reflex2pha`

`reflex2pha` is a very simple shell script that transforms an output spectrum file from REFLEX into a PHA file with associated response, so that the PHA file can be used with tools such as `xspec`. `reflex2pha` requires that HEASoft is installed. See: `https://heasarc.gsfc.nasa.gov/lheasoft/`. Usage is very simple:

```
reflex2pha specfile.ext
```

This command creates a PHA file from a REFLEX spectral output file `specfile.ext`. `reflex2pha`

creates the files `specfile.pha` and the associated response `specfile.rsp`. The spectrum must be in counts, so that Poisson errors can be computed. The PHA file is grouped to have at least 5 counts per bin. The `specfile.pha` can be read directly, for instance in `xspec`:

```
data specfile.pha
```

9.2 `merge_spectra`

`merge_spectra` is a Python script that collects a liste of ascii spectrum files from RefleX and sums them or average them, as requested by the user. This is particularly useful to gather the results from multiple runs of RefleX on a cluster. The script requires `numpy`. `merge_spectra` can be called in two different ways:

```
merge_spectra File1 File2 ...  FileN OutputFile [sum|avg]
```

or

```
merge_spectra FileList OutputFile [sum|avg]
```

The behavior is selected based on the number of parameters. In the first instance (with 4 or more parameters), the spectral output files `File1` `File2` up to `FileN` are read and summed or averaged, depending on the last parameter, and the result is written in the file `OutputFile`. In the second instance (with 3 parameters), `FileList` is the name of a text file that contains the list of spectral output files to be read and summed or averaged, depending on the last parameter; again, the result is written in the file `OutputFile`

A Changelog history

RefleX 2.1

This is a minor release, with no significant effect on the results. Users who perform simulations with many objects need however to upgrade to RefleX 2.1 for computation efficiency (see last bullet point below).

Physics

- H_2 fraction is treated more consistently.

Control

- RefleX can now output the computed cross-sections.
- Fixed a bug which forced recomputing cross-sections for all objects, even if the properties are unchanged.

RefleX 2.0

Optimization

- Major speed improvements thanks to precomputation of all cross-sections, with user-defined accuracy, and a more clever selection of the interactions
- Many bug fixes (not affecting the physics)

Physics

- A Wien input spectrum has been added.
- Setting H_2 fraction is forbidden for warm media.

Geometry

- All objects can now be placed at any position.
- A cone and a hollow-cone geometry have been added.

Images

- Many bug fixes in the creation of images.
- Images of axisymmetric geometries can now make use of this symmetry for increased efficiency.

Units

- Length unit light-seconds has been added.

Control

- RefleX can now use multi-threading, with some caveat.
- RefleX can be stopped after a user-specified number of seconds.
- RefleX can be interrupted by SIGINT or SIGTERM while preserving the computations already achieved.
- Control of stuck photons, which occur sometimes because of rounding errors for complex geometries.

RefleX 1.0

First released version

B K-shell (1s1/2) Fluorescence lines implemented in RefleX

List of K-shell (1s1/2) fluorescence lines implemented in REFLEX. The transition name is provided using Siegbahn notation. Energy is as determined in [5], or, when absent, from the LBNL X-ray Data Booklet [24]. Yields (transition probabilities) are always taken from the LBNL X-ray Data Booklet.

Element	Transition	Energy eV	Yield
C	$\alpha_2 KL_{II}$	277	0.000561488
	$\alpha_1 KL_{III}$	277	0.0011206
N	$\alpha_2 KL_{II}$	392.4	0.0010942
	$\alpha_1 KL_{III}$	392.4	0.00218181
O	$\alpha_2 KL_{II}$	524.9	0.00190768
	$\alpha_1 KL_{III}$	524.9	0.00380027
F	$\alpha_2 KL_{II}$	676.8	0.00306841
	$\alpha_1 KL_{III}$	676.8	0.00610743
Ne	$\alpha_2 KL_{II}$	848.6	0.00464329
	$\alpha_1 KL_{III}$	848.6	0.00922967
Na	$\alpha_2 KL_{II}$	1041.0	0.00668996
	$\alpha_1 KL_{III}$	1041.0	0.0132959
Mg	$\alpha_2 KL_{II}$	1253.60	0.00927327
	$\alpha_1 KL_{III}$	1253.60	0.0184189
Al	$\alpha_2 KL_{II}$	1486.27	0.0123699
	$\alpha_1 KL_{III}$	1486.70	0.0245528
	$\beta_3 KM_{II}$	1557.4	0.0000755854
	$\beta_K M_{III}$	1557.4	0.000150039
Si	$\alpha_2 KL_{II}$	1739.38	0.0159791
	$\alpha_1 KL_{III}$	1739.98	0.0317052
	$\beta_3 KM_{II}$	1835.9	0.000272402
	$\beta_K M_{III}$	1835.9	0.000540444
P	$\alpha_2 KL_{II}$	2012.7	0.020122
	$\alpha_1 KL_{III}$	2013.7	0.0398749
	$\beta_3 KM_{II}$	2139.0	0.000621469
	$\beta_K M_{III}$	2139.0	0.0012321
S	$\alpha_2 KL_{II}$	2306.64	0.0247822
	$\alpha_1 KL_{III}$	2307.84	0.0490644
	$\beta_3 KM_{II}$	2468.1	0.00115591
	$\beta_K M_{III}$	2464.0	0.00228902

Element	Transition	Energy eV	Yield
Cl	$\alpha_2 KL_{II}$	2620.78	0.0299473
	$\alpha_1 KL_{III}$	2622.39	0.0592357
	$\beta_3 KM_{II}$	2792.48	0.00190852
	$\beta_K M_{III}$	2792.61	0.00377764
Ar	$\alpha_2 KL_{II}$	2955.63	0.0355868
	$\alpha_1 KL_{III}$	2957.70	0.0703336
	$\beta_3 KM_{II}$	3190.5	0.00291258
	$\beta_K M_{III}$	3190.5	0.00575646
K	$\alpha_2 KL_{II}$	3311.1	0.0418599
	$\alpha_1 KL_{III}$	3313.8	0.0826518
	$\beta_3 KM_{II}$	3589.6	0.00399739
	$\beta_K M_{III}$	3589.6	0.00791008
Ca	$\alpha_2 KL_{II}$	3688.09	0.0487196
	$\alpha_1 KL_{III}$	3691.68	0.0961323
	$\beta_3 KM_{II}$	4012.7	0.00517776
	$\beta_K M_{III}$	4012.7	0.0102489
Sc	$\alpha_2 KL_{II}$	4086.1	0.0563841
	$\alpha_1 KL_{III}$	4090.6	0.11113
	$\beta_3 KM_{II}$	4460.5	0.00622301
	$\beta_K M_{III}$	4460.5	0.012304
	$\beta_2 KN_{II}$	4486.5	0.00000019612
	$\beta_2 KN_{III}$	4486.5	0.000000289041
Ti	$\alpha_2 KL_{II}$	4504.86	0.0645982
	$\alpha_1 KL_{III}$	4510.84	0.12714
	$\beta_3 KM_{II}$	4931.81	0.00732672
	$\beta_K M_{III}$	4931.81	0.014475
	$\beta_2 KN_{II}$	4962.3	0.000000590112
	$\beta_2 KN_{III}$	4962.3	0.000000868503
V	$\alpha_2 KL_{II}$	4944.64	0.0732827
	$\alpha_1 KL_{III}$	4952.20	0.144051
	$\beta_3 KM_{II}$	5427.29	0.00848408
	$\beta_K M_{III}$	5427.29	0.0167441
	$\beta_2 KN_{II}$	5462.9	0.00000126461
	$\beta_2 KN_{III}$	5462.9	0.00000185722
Cr	$\alpha_2 KL_{II}$	5405.51	0.0825759
	$\alpha_1 KL_{III}$	5414.72	0.16209
	$\beta_3 KM_{II}$	5946.71	0.00949389
	$\beta_K M_{III}$	5946.71	0.018701
	$\beta_2 KN_{II}$	5986.9	2.5254e-06

Element	Transition	Energy eV	Yield
	$\beta_2 KN_{III}$	5986.9	3.6955e-06
Mn	$\alpha_2 KL_{II}$	5887.65	0.0917726
	$\alpha_1 KL_{III}$	5898.75	0.179949
	$\beta_3 KM_{II}$	6490.45	0.010936
	$\beta_K M_{III}$	6490.45	0.0215229
	$\beta_2 KN_{II}$	6535.2	0.00000385518
	$\beta_2 KN_{III}$	6535.2	0.00000564148
Fe	$\alpha_2 KL_{II}$	6390.84	0.101391
	$\alpha_1 KL_{III}$	6403.84	0.198621
	$\beta_3 KM_{II}$	7057.98	0.0122111
	$\beta_K M_{III}$	7057.98	0.0240042
	$\beta_2 KN_{II}$	7108.1	0.00000600794
	$\beta_2 KN_{III}$	7108.1	0.00000877226
Co	$\alpha_2 KL_{II}$	6915.30	0.11122
	$\alpha_1 KL_{III}$	6930.32	0.21747
	$\beta_3 KM_{II}$	7649.43	0.013502
	$\beta_K M_{III}$	7649.43	0.026513
	$\beta_2 KN_{II}$	7705.9	0.00000890651
	$\beta_2 KN_{III}$	7705.9	0.000012974
Ni	$\alpha_2 KL_{II}$	7460.89	0.12106
	$\alpha_1 KL_{III}$	7478.15	0.236419
	$\beta_3 KM_{II}$	8264.66	0.014805
	$\beta_K M_{III}$	8264.66	0.0290299
	$\beta_2 KN_{II}$	8328.6	0.000012691
	$\beta_2 KN_{III}$	8328.6	0.000018445
Cu	$\alpha_2 KL_{II}$	8027.83	0.131119
	$\alpha_1 KL_{III}$	8047.78	0.255668
	$\beta_3 KM_{II}$	8902.9	0.0158899
	$\beta_K M_{III}$	8905.29	0.0310908
	$\beta_2 KN_{II}$	8977.0	0.0000179389
	$\beta_2 KN_{III}$	8977.0	0.0000259348
Zn	$\alpha_2 KL_{II}$	8615.78	0.14062
	$\alpha_1 KL_{III}$	8638.86	0.273809
	$\beta_3 KM_{II}$	9572.0	0.017389
	$\beta_K M_{III}$	9572.0	0.0339969
	$\beta_2 KN_{II}$	9650.1	0.0000235079
	$\beta_2 KN_{III}$	9650.1	0.0000339889

C Examples of parameter files

Example 1: Absorbed power law spectrum

Creates a pure transmission spectrum with $10^{23}\,\mathrm{cm}^{-2}$.

```
# No verbosity
VERBOSE 0
# 1 billion photons
NPHOTS 1000000000
# Show progress
PERCENT ON
# Drop any photon below 100 eV
ECUT   100.0
# Generate photons between 100 eV and 100 keV
EGEN   100.0 1000000
# Generate photons following a power law with an index 0
EMSPEC PWRLAW 0
# Select proto-solar abundances from Lodders et al. (2009)
MATTER lpgp
# Define all lengths to be in centimeter
LENGTH Centimeter
# Set the column density to be 10^23 cm-2 across the shell
COLDENS 1e23
# Metallicity is Solar
METALLICITY 1.0
# Use cold physics
TEMPERATURE 0
# Set molecular hydrogen fraction to 20%
H2FRACTION 0.2
# Create an isotropic point source at (0,0,0)
EMGEOM POINT  0.0 0.0 0.0 0 0 180
# WORLD is 10^5 cm in radius
OBJECT WORLD  1e5
# Create an unnamed shell with a 1cm thickness
OBJECT SHELL NULL 0.0 0.0 0.0 2.0 1.0
# Define a logarithmic energy binning between 100 eV and 100 keV
SPECTRUM BINNING 2 5 0.001 LOG
# Create a spectrum
SPECTRUM NEW transmitted.dat
# Add constraint: only photons that did not make any interaction
SPECTRUM INT == 0
```

Example 2: RXTorus configuration

Create one simulation used in the RXTorus model with Γ=1.9, $N_{\mathrm{H,eq}} = 10^{24}\,\mathrm{cm}^{-2}$ and Solar metallicity. The spectral output is simplified, as it is very long. Here we pass the inner radius parameter.

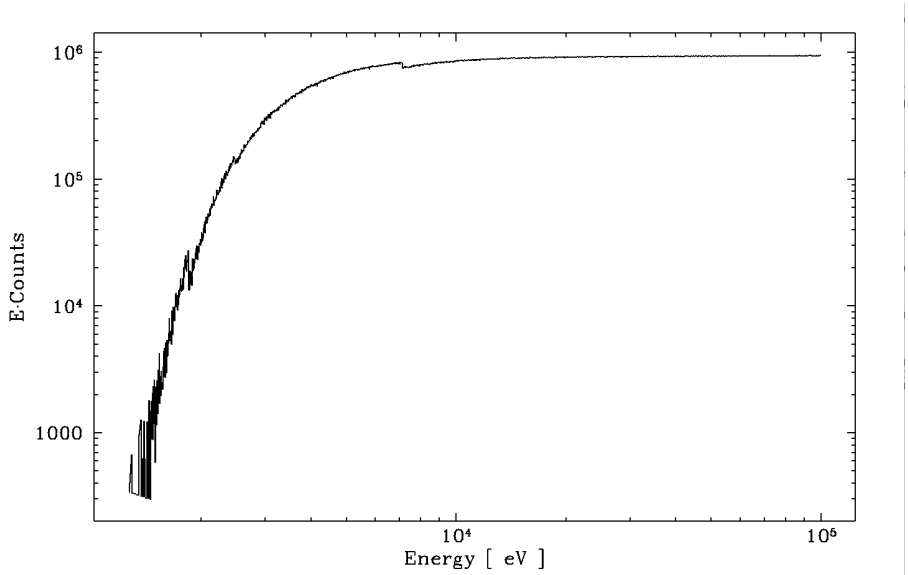

Figure 2: Results from Example 1: `transmitted.dat`

For a MYTorus geometrical configuration, REFLEX should be called like this:
`reflex %R=0.5 example_2.par`

```
# No verbosity
VERBOSE 0
# 1 billion photons
NPHOTS 1000000000
# Drop any photon below 300 eV
ECUT   300.0
# Generate photons between 300 eV and 1 MeV
EGEN   300.0 10000000
# Generate photons following a power law with an index 1.9 and a cut-off at 200 keV
EMSPEC CUTOFF 1.9 200000
# Select proto-solar abundances from Lodders et al. (2009)
MATTER lpgp
# Define all lengths to be in centimeter
LENGTH Centimeter
# Set the density to be 1 H atom per cubic centimeter
DENSITY 1e24
# Metallicity is Solar
METALLICITY 1.0
# Use cold physics
TEMPERATURE 0
# Set molecular hydrogen fraction to 20%
H2FRACTION 0.2
# Create an isotropic point source at (0,0,0)
```

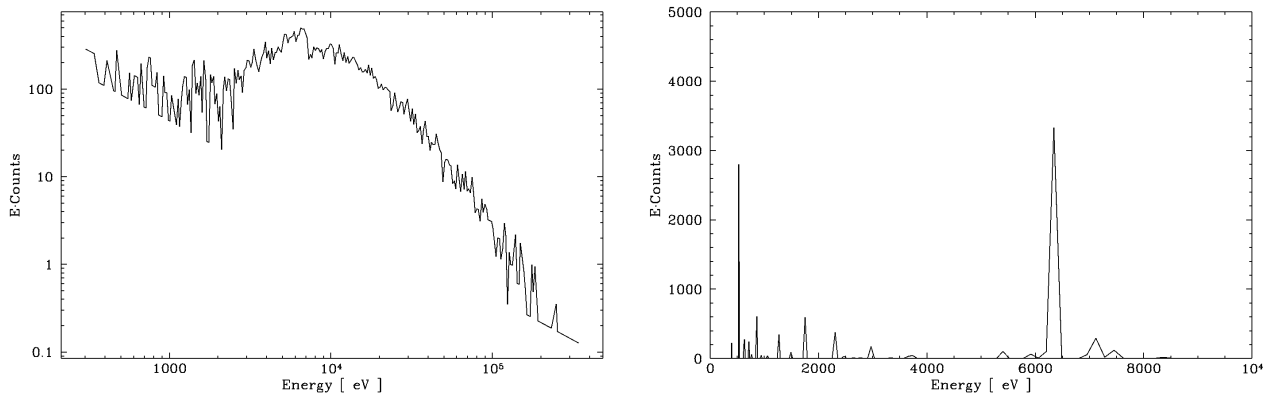

Figure 3: Results from Example 2: (Left) `scat_00_high.txt`. (Right) `fluo_00_high.txt`

```
EMGEOM POINT  0.0 0.0 0.0 0 0 180
# WORLD is 10^5 cm in radius
OBJECT WORLD  1e5
# Create an unnamed torus with a 1cm outer radius and Rcm inner radius
OBJECT TORUS NULL 0.0 0.0 0.0 1.0 %R
# Logarithic binning between 300 eV and 1 MeV
SPECTRUM BINNING 2.477121255 6.0 0.001 LOG
#  Create a new spectrum for scattered emission at low inclination (0-3 deg)
SPECTRUM NEW     scat_00_high.txt
# cos(0 deg)
SPECTRUM DIR_Z   <=  1.0
# cos(3 deg)
SPECTRUM DIR_Z   >   0.998629534755
# Scattered component is interaction without fluorescence
SPECTRUM INT >  0
SPECTRUM FLUOR   == 0
#  Create a new spectrum for fluorescence emission at low inclination (0-3 deg)
SPECTRUM NEW     fluo_00_high.txt
# arccos(0 deg)
SPECTRUM DIR_Z   <=  1.0
# arccos(3 deg)
SPECTRUM DIR_Z   >   0.998629534755
# Only fluorescence photons (and their descendance)
SPECTRUM FLUOR   > 0
```

Example 3: Images of a cone

Create three images of a double hollow con structure.

```
# Suppress printed output
```

```
VERBOSE 0
# Set a time limit to 1 hour
TIME 3600
# Set a seed
RANDOM 31415926535
# Turn on multi-threading
THREAD 4
# Length unit is centimeter
LENGTH Centimeter
# Stop propagating photons with less than 300 eV
ECUT 300.0
# Generate spectra between 0.3 and 100 keV
EGEN 300.0 100e3
# Emitted spectrum is a cutoff power law with photon index of 1.9 and cutoff at 200 keV
EMSPEC CUTOFF 1.9 200e3
# Objects composition is from Anders & Grevesse
MATTER angr
# Set up object column density
COLDENS 1e22
# Set molecular hydrogen fraction to 20%
H2FRACTION 0.2
# Solar metallicity
METALLICITY 1
# Medium is cold
TEMPERATURE 0
# Create an isotropic point source at (0,0,0)
EMGEOM POINT  0.0 0.0 0.0 0 0 180
# Set up WORL with radius 500 m
OBJECT WORLD 50000
# Set up two hollow cones, one is oriented along +Z and the other along -Z
OBJECT HCONE NULL 0.0 0.0 0.0 50 800 400 800 300 300
OBJECT HCONE NULL 0.0 0.0 0.0 -50 -800 400 800 300 300
# Create a face-on image taken 5000 cm above the XY plane.
# Aperture is 100 cm in diameter. FOV is 30 deg. Image is 300x300 pixels
IMAGE NEW cone.fits 0 0 5000 100 30 500
# Only select photons having interacted with the cones
IMAGE INT > 0
# Create an edge-on image. Here we use axisymmetry
IMAGE NEW cone2.fits 5000 AXIS 0 100 30 500
IMAGE INT > 0
# Create an image with the detector at 45 deg. Here we use axisymmetry
IMAGE NEW cone3.fits 2500 AXIS 2500 100 30 500
IMAGE INT > 0
```

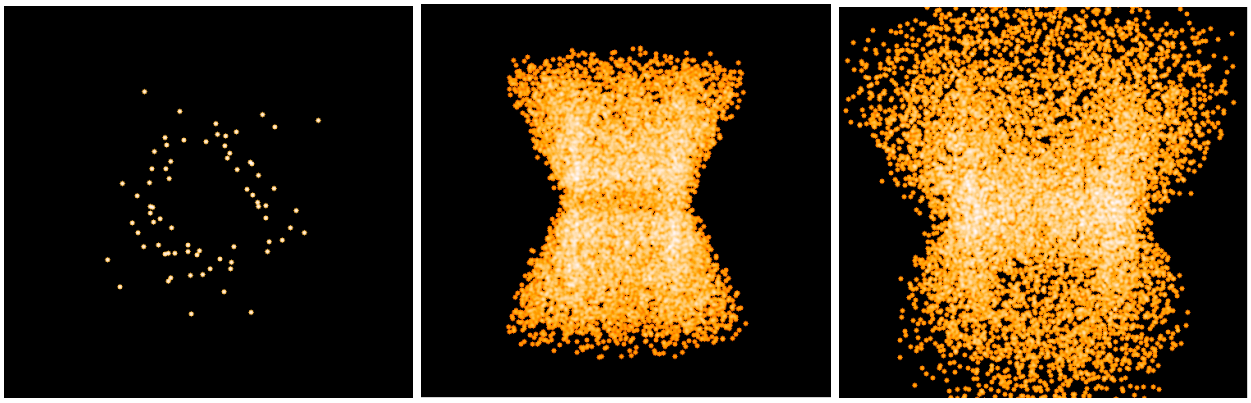

Figure 4: Results from Example 3: (Left) `cone.fits`. (Center) `cone2.fits` (Right) `cone3.fits.txt`

References

[1] E. Anders and M. Ebihara. Solar-system abundances of the elements. *Geochimica et Cosmochimica Acta*, 46(11):2363–2380, Nov. 1982.

[2] E. Anders and N. Grevesse. Abundances of the elements: Meteoritic and solar. *Geochimica et Cosmochimica Acta*, 53(1):197–214, Jan. 1989.

[3] M. Asplund, N. Grevesse, A. J. Sauval, and P. Scott. The Chemical Composition of the Sun. *Annual Reviews of Astronomy & Astrophysics*, 47(1):481–522, Sept. 2009.

[4] M. Balucinska-Church and D. McCammon. Photoelectric Absorption Cross Sections with Variable Abundances. *The Astrophysical Journal*, 400:699, Dec. 1992.

[5] J. A. Bearden. X-Ray Wavelengths. *Reviews of Modern Physics*, 39(1):78–124, Jan. 1967.

[6] D. E. Cullen, M. H. Chen, J. H. Hubbell, S. T. Perkins, E. F. Plechaty, J. A. Rathkopf, and J. H. Scofield. *Tables And Graphs Of Photon Interaction Cross Sections From 10 eV To 100 GeV Derived From The LLNL Evaluated Photon Data Library (EPDL), UCRL-50400*, volume 6, Rev. 4. Lawrence Livermore National Laboratory, 1989.

[7] B. T. Draine. Scattering by Interstellar Dust Grains. II. X-Rays. *The Astrophysical Journal*, 598(2):1026–1037, Dec. 2003.

[8] A. C. Fabian, A. Zoghbi, R. R. Ross, P. Uttley, L. C. Gallo, W. N. Brandt, A. J. Blustin, T. Boller, M. D. Caballero-Garcia, J. Larsson, J. M. Miller, G. Miniutti, G. Ponti, R. C. Reis, C. S. Reynolds, Y. Tanaka, and A. J. Young. Broad line emission from iron K- and L-shell transitions in the active galaxy 1H0707-495. *Nature*, 459(7246):540–542, May 2009.

[9] U. Feldman. Elemental abundances in the upper solar atmosphere. *Physica Scripta*, 46(3):202–220, Sept. 1992.

[10] S. Furui, Y. Fukazawa, H. Odaka, T. Kawaguchi, M. Ohno, and K. Hayashi. X-Ray Spectral Model of Reprocess by Smooth and Clumpy Molecular Tori in Active Galactic Nuclei with the Framework MONACO. *The Astrophysical Journal*, 818(2):164, Feb. 2016.

[11] N. Grevesse and A. J. Sauval. Standard Solar Composition. *Space Science reviews*, 85:161–174, May 1998.

[12] J. H. Hubbell, W. J. Veigele, E. A. Briggs, R. T. Brown, D. T. Cromer, and R. J. Howerton. Atomic form factors, incoherent scattering functions, and photon scattering cross sections. *Journal of Physical and Chemical Reference Data*, 4(3):471–538, July 1975.

[13] Y. Liu and X. Li. An X-Ray Spectral Model for Clumpy Tori in Active Galactic Nuclei. *The Astrophysical Journal*, 787(1):52, May 2014.

[14] K. Lodders. Solar System Abundances and Condensation Temperatures of the Elements. *The Astrophysical Journal*, 591(2):1220–1247, July 2003.

[15] K. Lodders, H. Palme, and H. P. Gail. Abundances of the Elements in the Solar System. *Landolt Börnstein*, 4B:712, Jan. 2009.

[16] P. Magdziarz and A. A. Zdziarski. Angle-dependent Compton reflection of X-rays and gamma-rays. *Monthly Notices of the Royal Astronomical Society*, 273(3):837–848, Apr. 1995.

[17] G. Matt, G. C. Perola, E. Costa, and L. Piro. X-ray polarization of the reprocessed emission from accretion disk in Seyfert galaxies. In J. Hunt and B. Battrick, editors, *Two Topics in X-Ray Astronomy, Volume 1: X Ray Binaries. Volume 2: AGN and the X Ray Background*, volume 296 of *ESA Special Publication*, pages 991–993, Nov. 1989.

[18] K. D. Murphy and T. Yaqoob. An X-ray spectral model for Compton-thick toroidal reprocessors. *Monthly Notices of the Royal Astronomical Society*, 397(3):1549–1562, Aug. 2009.

[19] K. Nandra, P. M. O'Neill, I. M. George, and J. N. Reeves. An XMM-Newton survey of broad iron lines in Seyfert galaxies. *Monthly Notices of the Royal Astronomical Society*, 382(1):194–228, Nov. 2007.

[20] S. Paltani and C. Ricci. RefleX: X-ray absorption and reflection in active galactic nuclei for arbitrary geometries. *Astronomy & Astrophysics*, 607:A31, Nov. 2017.

[21] Planck Collaboration, N. Aghanim, Y. Akrami, M. Ashdown, J. Aumont, C. Baccigalupi, M. Ballardini, A. J. Banday, R. B. Barreiro, N. Bartolo, S. Basak, R. Battye, K. Benabed, J. P. Bernard, M. Bersanelli, P. Bielewicz, J. J. Bock, J. R. Bond, J. Borrill, F. R. Bouchet, F. Boulanger, M. Bucher, C. Burigana, R. C. Butler, E. Calabrese, J. F. Cardoso, J. Carron, A. Challinor, H. C. Chiang, J. Chluba, L. P. L. Colombo, C. Combet, D. Contreras, B. P. Crill, F. Cuttaia, P. de Bernardis, G. de Zotti, J. Delabrouille, J. M. Delouis, E. Di Valentino, J. M. Diego, O. Doré, M. Douspis, A. Ducout, X. Dupac, S. Dusini, G. Efstathiou, F. Elsner, T. A. Enßlin, H. K. Eriksen, Y. Fantaye, M. Farhang, J. Fergusson, R. Fernandez-Cobos, F. Finelli, F. Forastieri, M. Frailis, A. A. Fraisse, E. Franceschi, A. Frolov, S. Galeotta, S. Galli, K. Ganga, R. T. Génova-Santos, M. Gerbino, T. Ghosh, J. González-Nuevo, K. M. Górski, S. Gratton, A. Gruppuso, J. E. Gudmundsson, J. Hamann, W. Handley, F. K. Hansen, D. Herranz, S. R.

Hildebrandt, E. Hivon, Z. Huang, A. H. Jaffe, W. C. Jones, A. Karakci, E. Keihänen, R. Keskitalo, K. Kiiveri, J. Kim, T. S. Kisner, L. Knox, N. Krachmalnicoff, M. Kunz, H. Kurki-Suonio, G. Lagache, J. M. Lamarre, A. Lasenby, M. Lattanzi, C. R. Lawrence, M. Le Jeune, P. Lemos, J. Lesgourgues, F. Levrier, A. Lewis, M. Liguori, P. B. Lilje, M. Lilley, V. Lindholm, M. López-Caniego, P. M. Lubin, Y. Z. Ma, J. F. Macías-Pérez, G. Maggio, D. Maino, N. Mandolesi, A. Mangilli, A. Marcos-Caballero, M. Maris, P. G. Martin, M. Martinelli, E. Martínez-González, S. Matarrese, N. Mauri, J. D. McEwen, P. R. Meinhold, A. Melchiorri, A. Mennella, M. Migliaccio, M. Millea, S. Mitra, M. A. Miville-Deschênes, D. Molinari, L. Montier, G. Morgante, A. Moss, P. Natoli, H. U. Nørgaard-Nielsen, L. Pagano, D. Paoletti, B. Partridge, G. Patanchon, H. V. Peiris, F. Perrotta, V. Pettorino, F. Piacentini, L. Polastri, G. Polenta, J. L. Puget, J. P. Rachen, M. Reinecke, M. Remazeilles, A. Renzi, G. Rocha, C. Rosset, G. Roudier, J. A. Rubiño-Martín, B. Ruiz-Granados, L. Salvati, M. Sandri, M. Savelainen, D. Scott, E. P. S. Shellard, C. Sirignano, G. Sirri, L. D. Spencer, R. Sunyaev, A. S. Suur-Uski, J. A. Tauber, D. Tavagnacco, M. Tenti, L. Toffolatti, M. Tomasi, T. Trombetti, L. Valenziano, J. Valiviita, B. Van Tent, L. Vibert, P. Vielva, F. Villa, N. Vittorio, B. D. Wandelt, I. K. Wehus, M. White, S. D. M. White, A. Zacchei, and A. Zonca. Planck 2018 results. VI. Cosmological parameters. *Astronomy & Astrophysics*, 641:A6, Sept. 2020.

[22] C. Ricci and S. Paltani. Ray-tracing simulations and spectral models of x-ray radiation in dusty media. *The Astrophysical Journal*, in press, 2023.

[23] P. Soffitta, X. Barcons, R. Bellazzini, J. Braga, E. Costa, G. W. Fraser, S. Gburek, J. Huovelin, G. Matt, M. Pearce, J. Poutanen, V. Reglero, A. Santangelo, R. A. Sunyaev, G. Tagliaferri, M. Weisskopf, R. Aloisio, E. Amato, P. Attiná, M. Axelsson, L. Baldini, S. Basso, S. Bianchi, P. Blasi, J. Bregeon, A. Brez, N. Bucciantini, L. Burderi, V. Burwitz, P. Casella, E. Churazov, M. Civitani, S. Covino, R. M. Curado da Silva, G. Cusumano, M. Dadina, F. D'Amico, A. De Rosa, S. Di Cosimo, G. Di Persio, T. Di Salvo, M. Dovciak, R. Elsner, C. J. Eyles, A. C. Fabian, S. Fabiani, H. Feng, S. Giarrusso, R. W. Goosmann, P. Grandi, N. Grosso, G. Israel, M. Jackson, P. Kaaret, V. Karas, M. Kuss, D. Lai, G. La Rosa, J. Larsson, S. Larsson, L. Latronico, A. Maggio, J. Maia, F. Marin, M. M. Massai, T. Mineo, M. Minuti, E. Moretti, F. Muleri, S. L. O'Dell, G. Pareschi, G. Peres, M. Pesce, P.-O. Petrucci, M. Pinchera, D. Porquet, B. Ramsey, N. Rea, F. Reale, J. M. Rodrigo, A. Różańska, A. Rubini, P. Rudawy, F. Ryde, M. Salvati, V. A. de Santiago, S. Sazonov, C. Sgró, E. Silver, G. Spandre, D. Spiga, L. Stella, T. Tamagawa, F. Tamborra, F. Tavecchio, T. Teixeira Dias, M. van Adelsberg, K. Wu, and S. Zane. XIPE: the X-ray imaging polarimetry explorer. *Experimental Astronomy*, 36(3):523–567, Dec. 2013.

[24] A. C. Thompson, A. Kirz, D. T. Attwood, E. M. Gullikson, M. R. Howells, J. B. Kortright, Y. Liu, A. L. Robinson, J. H. Underwood, K.-J. Kim, i. Lindau, P. Pianetta, H. Winick, G. P. Williams, and J. H. Scofield. *X-ray data booklet, third revision, LBNL-PUB490, Rev. 3.* Lawrence Berkeley National Laboratory, 2009.

[25] D. A. Verner, G. J. Ferland, K. T. Korista, and D. G. Yakovlev. Atomic Data for Astrophysics. II. New Analytic FITS for Photoionization Cross Sections of Atoms and Ions. *The Astrophysical Journal*, 465:487, July 1996.

[26] D. A. Verner and D. G. Yakovlev. Analytic FITS for partial photoionization cross sections. *Astronomy & Astrophysics Supplement Series*, 109:125–133, Jan. 1995.

[27] J. Wilms, A. Allen, and R. McCray. On the Absorption of X-Rays in the Interstellar Medium. *The Astrophysical Journal*, 542(2):914–924, Oct. 2000.

[28] M. Yan, H. R. Sadeghpour, and A. Dalgarno. Photoionization Cross Sections of He and H_2. *The Astrophysical Journal*, 496(2):1044–1050, Mar. 1998.