

X-ray radiative transfer in 3D with the SKIRT code

A quick start guide

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1 Introduction

This document collects some resources & advice to get started with the X-ray Monte Carlo radiative transfer code SKIRT (Vander Meulen et al. 2023). For more information feel free to get in touch.

2 The SKIRT website

Your first point of reference will be the SKIRT website: <https://skirt.ugent.be/>. On this website, you can find an installation guide, a user guide, a developer guide, and reference documentation for all simulation elements in SKIRT.

3 SKIRT installation

Most scientific users will want to install SKIRT using the command line (Unix or macOS). This (and other installation options) are explained in great detail on the SKIRT website. Finally, note that when downloading the SKIRT resource files (see the installation guide), only the `Core` and `AtomsMolecules` resource files are needed for X-ray simulations, (so no `BPASS`, `TODDLERS`, `ExtraDust`, or `ExtraBands`, which could take a long time to download).

4 SKIRT tutorials

Once the SKIRT code is installed, let's get started with some SKIRT tutorials.

Historically, the SKIRT code was developed to study dust reprocessing in galaxies, in the IR-to-UV wavelength regime. Therefore, most SKIRT tutorials focus on dust reprocessing, and not on X-rays. Yet, these first tutorials are important to get introduced to basic SKIRT concepts, such as sources, media, spatial grids, and wavelength grids. We highly recommend new X-ray users to:

- Have a look at the first few hand-on SKIRT tutorials (marked with a keyboard icon).

You can review them in the presented order (or simply skip to the topics of interest).

5 X-ray radiative transfer with SKIRT

We provided one SKIRT tutorial on X-ray radiative transfer. This should form a good starting point. Some important guidelines for X-ray simulations are highlighted below:

1. Select the 'energy' output style both for wavelengths and fluxes.
2. For X-ray simulations, the simulation mode should always be 'ExtinctionOnly': All X-ray physics in SKIRT are implemented in the ExtinctionOnly mode.

3. As X-ray interactions in cold material reduce the photon energy, you will need to also consider radiative transfer at higher photon energies than the range you are interested in. This means that the ‘minWavelength’ of the ‘SourceSystem’ must be a higher energy than the energies that you are interested in (note that the minWavelength corresponds to the highest energy). See the last paragraph of Sect. 3.2.4 of Vander Meulen et al. (2023) for some guidelines.
4. All X-ray physical processes are implemented in the XRayAtomicGasMix. You can configure custom gas mixes by specifying the abundance of each element, or choose to approximate bound-electron scattering by free-electron scattering. For more information on configuring this material type, see the XRayAtomicGasMix class documentation.
5. To get started with X-ray simulations, we recommend to not use any dust (so only gas, i.e., an XRayAtomicGasMix medium). In the XRISM range, the effect of dust is a higher order effect; while it will slow down the radiative transfer simulations significantly.
6. To observe weak fluorescent lines, it might be needed to set minWeightReduction to 1e10. See the Advanced section on low-intensity lines at the bottom of the X-ray torus tutorial.

Feel free to get in touch with any further questions.

6 X-ray polarisation in SKIRT

Currently, there is no SKIRT tutorial on our website to introduce X-ray polarisation simulations (Vander Meulen et al., 2024b). One could start from the X-ray (spectroscopy) tutorial, noting that:

1. There are two SKIRT media that support X-ray polarisation: XRayAtomicGasMix (i.e., cold gas; set `scatterBoundElectrons="FreeWithPolarization"`) and ElectronMix (i.e., free electrons; set `includePolarization="true"`). They implement the polarisation physics.
2. Record Stokes spectra by setting `recordPolarization="true"` in the SKIRT instruments.
3. We implemented some options to set the polarisation properties of the source emission (see `NoPolarizationProfile`, `SineSquarePolarizationProfile`, and `FilePolarizedPointSource`).

SKIRT calculates the Stokes spectra (I, Q, and U as a function of energy). The polarisation degree and polarisation angle can be calculated in Python. For more information feel free to get in touch.

7 Custom transfer media in SKIRT

SKIRT has many build-in geometrical building blocks to build your 3D transfer media (and sources). Furthermore, SKIRT has various interfaces to import tabulated transfer media from an ascii file:

1. The ImportedGeometry Class allows you to import a custom 3D density distribution in various coordinate formats: Cartesian, Cyllindrical, and Spherical, as well as various HD simulation formats such as Voronoi meshes, adaptive meshes (e.g., an Octree mesh) and particle data.
2. The ImportedMedium Class allows you to import a full medium including both densities and velocities, with the same level of flexibility as described above.

In particular, the Cyllindrical, and Spherical geometries have an ‘autorevolve’ function, which allow you to import a 2D (1D, respectively) density distribution from an ascii file, and ‘revolve’ it to obtain a 3D transfer medium. This is a good starting point to test simple, custom transfer geometries.

8 Reference

The main reference for the X-ray radiative transfer code SKIRT is **Vander Meulen et al. (2023)**. Intrinsic fluorescent line shapes were introduced to SKIRT in **Vander Meulen et al. (2024a)**. X-ray polarisation simulations with SKIRT are described in **Vander Meulen et al. (2024b)**.

The treatment of bound-electron scattering in SKIRT has been updated since Vander Meulen et al. (2023), and also the number of fluorescent lines has been extended, to also include all L-lines (Vander Meulen et al., in prep.). For more information feel free to get in touch.