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Ministero dell'Università e della Ricerca

Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA

ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Wind in the Ionised Nuclear Environment (WINE) Code optimisation and parallelisation

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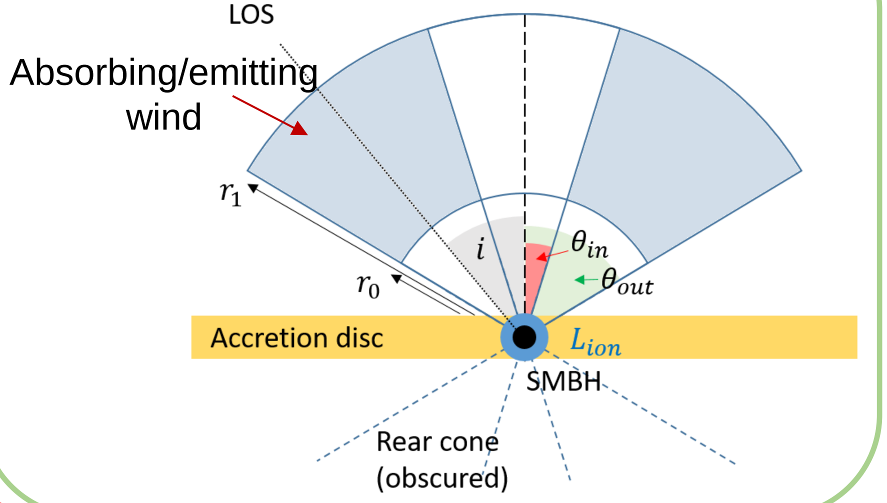
Scientific Rationale

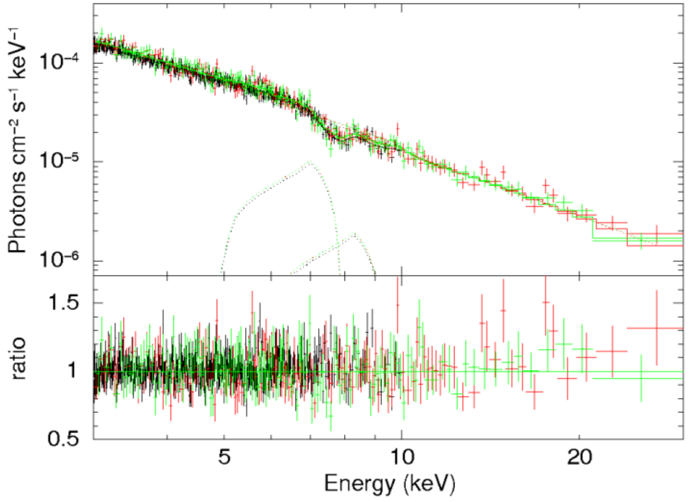
An UV/X-ray spectroscopic model tailored for disc winds in AGNs and compact sources.

WINE couples photoionisation and radiative transfer with special relativistic effects and a three-dimensional modellisation of the emission profiles

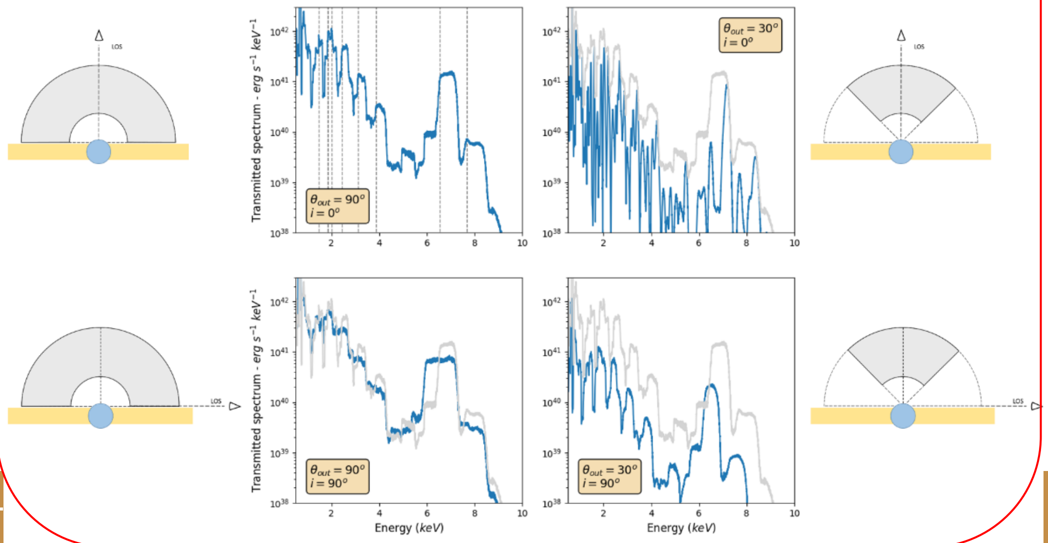
WINE wind structure:



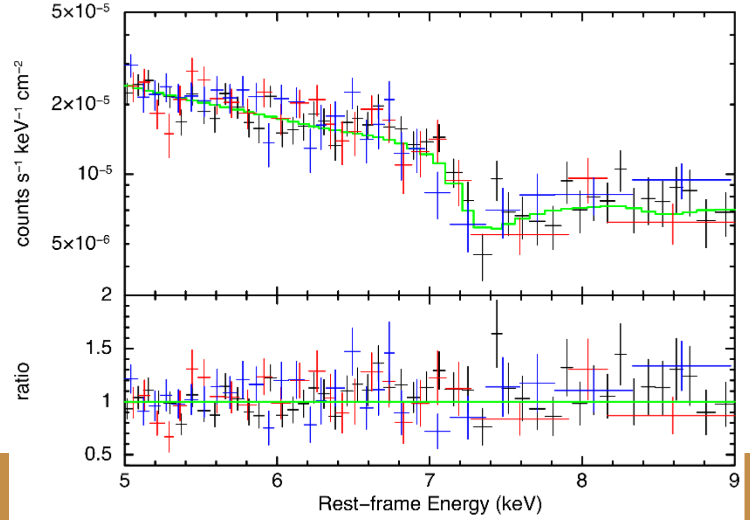
WINE fit of the disc wind in PDS 456; Luminari+18



Emission profiles as a function of the geometry; Luminari+24



WINE fit of the disc wind in PG 1448+273; Laurenti, AL+21



Technical Objectives, Methodologies and Solutions

WINE is hugely time-consuming, since it requires multiple calls to a public photoionisation code (XSTAR, Cloudy) + a Monte-Carlo modellisation of the emission profiles, which has to be convolved with the computed photoionisation spectrum

Three main lines of action:

- **parallelisation (scheduling) of the photoionisation computations**
- **porting to Python3 to benefit of public-available libraries and compatibility with similar codes**
- **replacement of Monte-Carlo modellisation with exact analytic profiles**

Main Results

- **Parallelisation:**

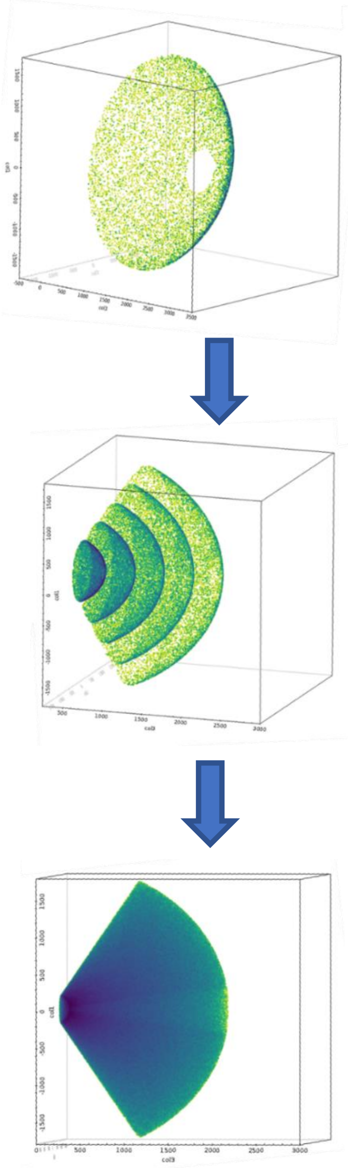
The code is now running with unified data structure, simpler configuration files and is called through *HTCondor/slurm* schedulers.

This allows to have unique configuration file for all the runs and simply scale the number of folders required for each run.

Scheduling allows a fast, traceable and clean simulation set, which can be also extended and run jointly on different clusters working on the same storage

- **Porting:**

The main code has been passed from *bash* to *python3*, enabling a smooth integration with the existing subroutines (already in Python) and benefitting from public, community-developed libraries, such as Astropy for the *fits* file format



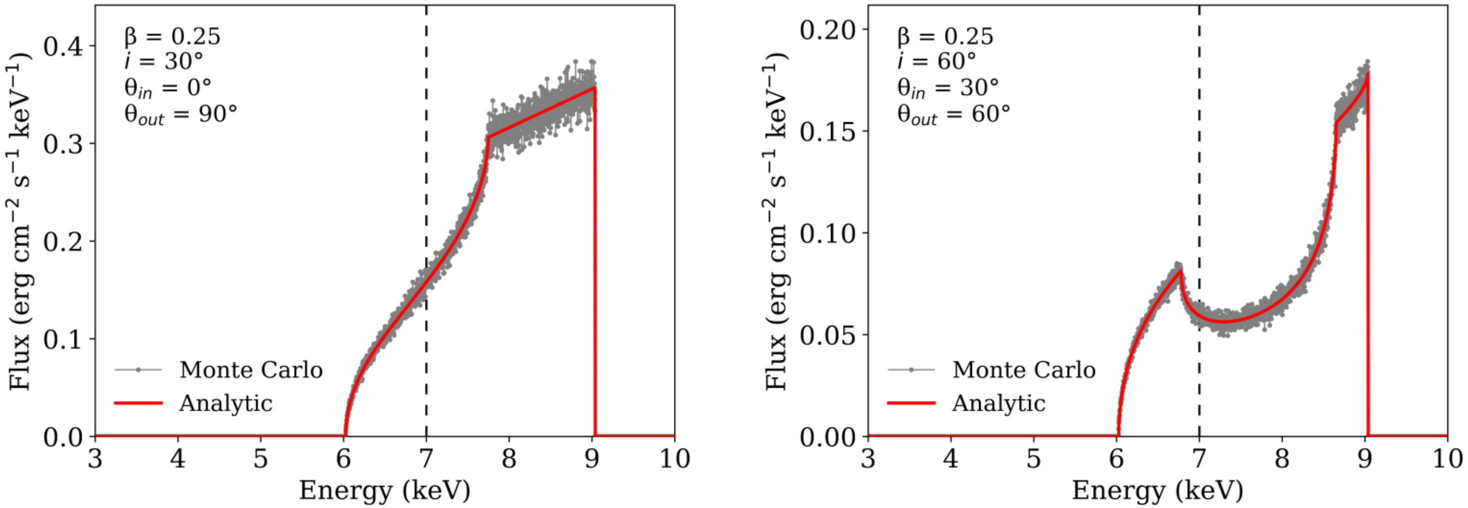
Main Results

- Analytic modelling:

Previous line profiles were computed through Monte-Carlo simulation of the emitting region: slow and needed to accumulate huge number of datapoints (10^5) for each geometric configuration to get sufficient statistic. Around 30 hours to span the geometry parameter space (just for one given ionisation and outflow velocity).

Replaced with exact analytic expression, taking around 5 minutes – a factor 360 less!

Monte Carlo (grey) vs. analytic profiles (red)



Final Steps

The code update is mostly done. Final actions are to:

- **Test and debug the new version**
- **Document the changes**
- **Compute new sets of simulations, to be used as table-models to fit observed UV and X-ray spectra**
- **Make computed tables publicly available on the code website: https://baltig.infn.it/ionisation/wine**