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Big Data and Quantum Computing

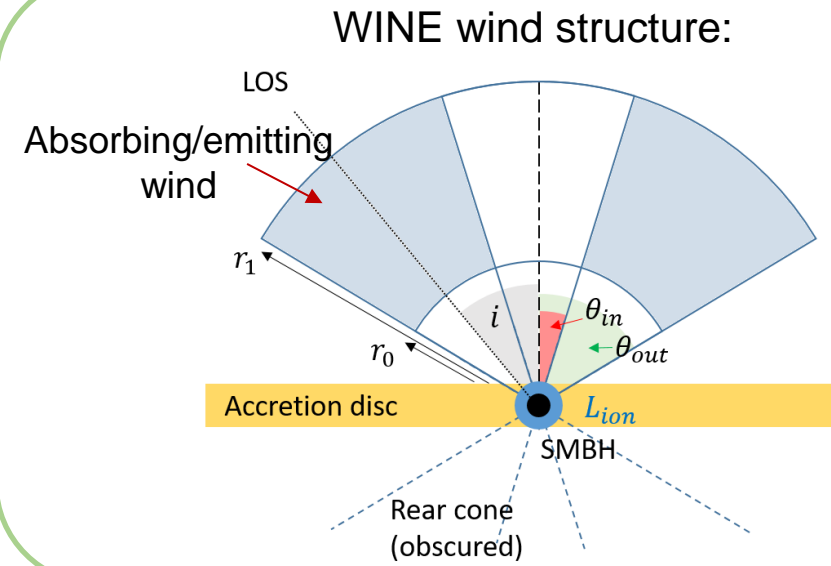
*Wind in the Ionised Nuclear Environment (WINE)
Code optimisation and parallelisation
Ferretti S., De Luca F., Condò P., Luminari A.*

Spoke 3 II Technical Workshop, Bologna Dec 17 -19, 2024

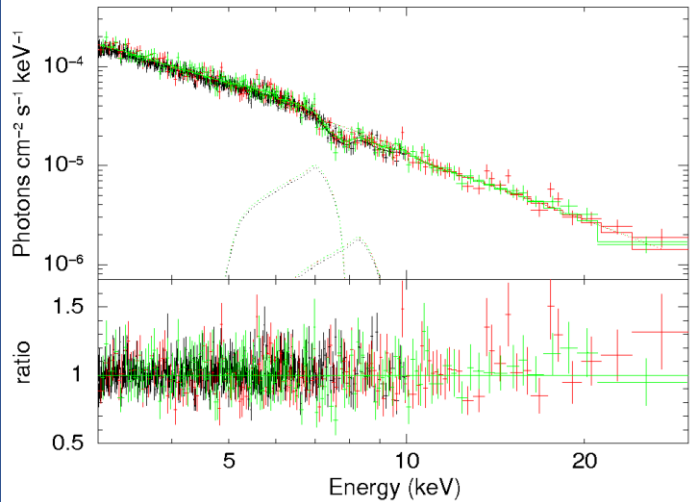
Scientific Rationale

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

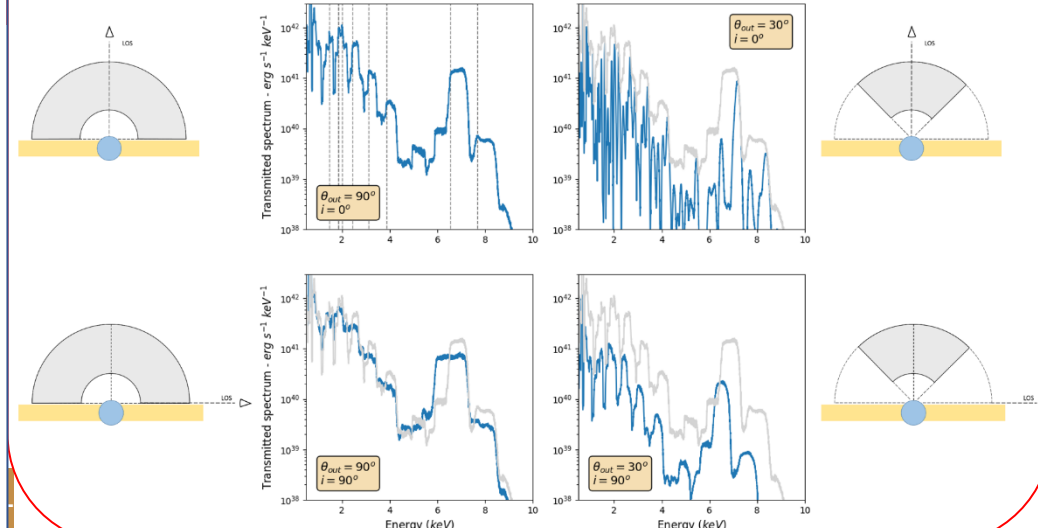
WINE couples photoionisation and radiative transfer with special relativistic effects and a three-dimensional modellisation of the emission profiles



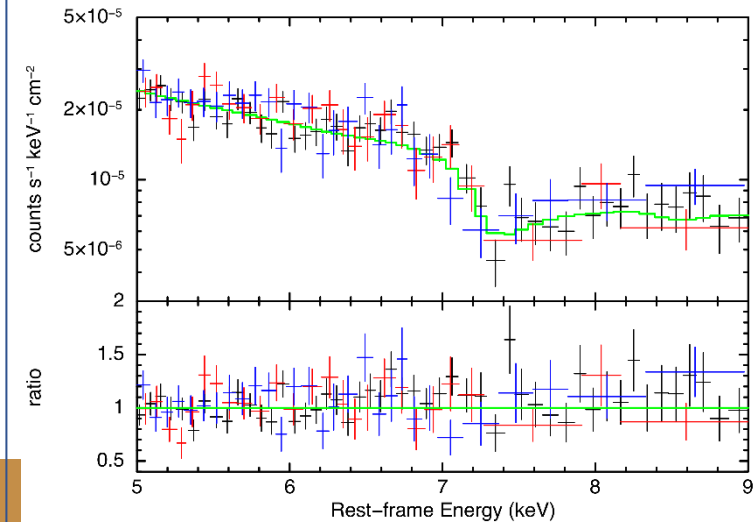
WINE fit of the disc wind in PDS 456; Luminari+18



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:

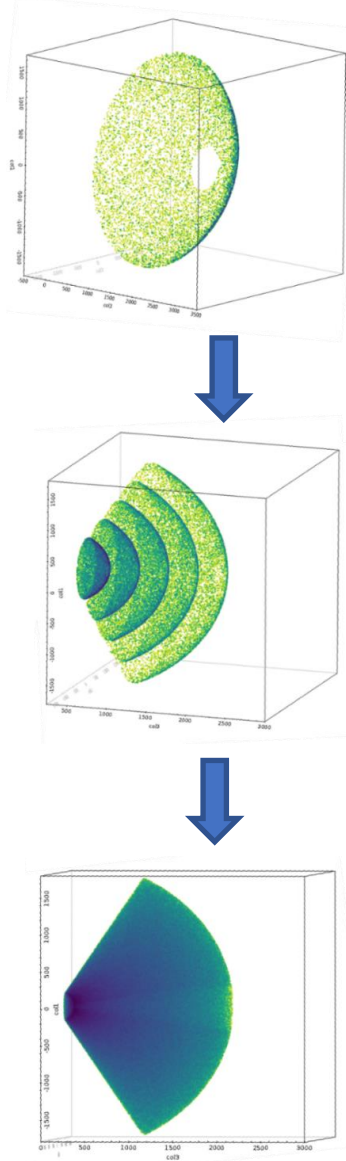
The main code has been passed from *bash* to *python3*, enabling a smooth integration with the existing subroutines (already in Python) and benefitting from public, community-developed libraries, such as *Astropy* for the *fits* file format

Main Results

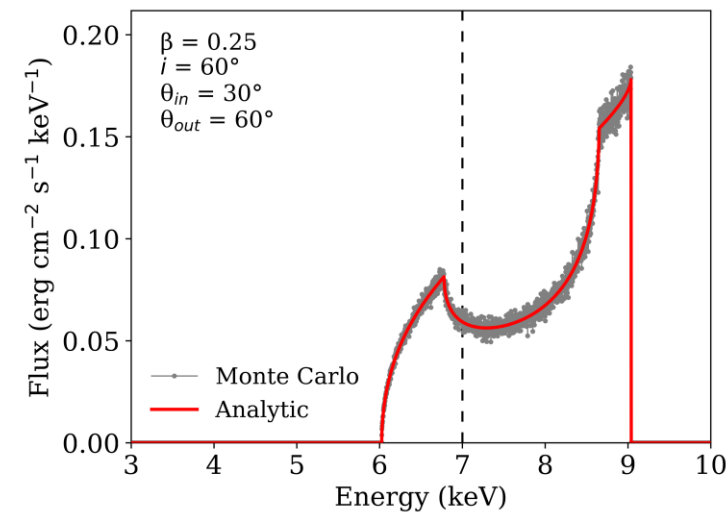
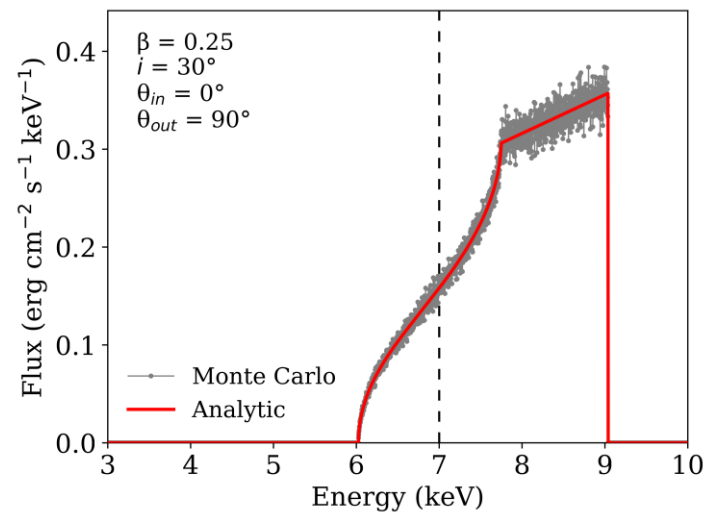
- Analytic modelling:

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>

WINE - Wind in the Ionised Nuclear Environment

main wine

Update file WINE_description.md
Alfredo Luminari authored 6 days ago

Name	Last commit	Last update
documents	Update file WINE_description.md	6 days ago
figures	Update 2 files	1 year ago
models	Update file WINE_table_models.md	5 months ago
.gitlab-ci.yml	Configure SAST in '.gitlab-ci.yml', creat...	1 year ago
README.md	Update 2 files	6 days ago

Project information

- 103 Commits
- 1 Branch
- 0 Tags
- 11 KiB Project Storage
- README
- CI/CD configuration
- Add LICENSE
- Add CHANGELOG
- Add CONTRIBUTING
- Add Kubernetes cluster
- Add Wiki
- Configure Integrations

Created on December 04, 2023

WINE - Wind in the Ionised Nuclear Environment

Welcome

This is the website of the Wind in the Ionised Nuclear Environment (WINE) code. Here you will find the documentation and the table models to get started with WINE and use it within popular spectral fitting models, such as xspec.

WINE is a spectroscopic model for disc winds in Active Galactic Nuclei and compact sources. Current energy resolution of the

List of available WINE table models

At the following links you can find the WINE table models presented in Luminari et. (2024), with different Spectral Energy Distributions (SEDs) and volume filling factors C_v .

Narrow-Line Seyfert 1 SED

Tables built with the typical SED of a Narrow-Line Sy1:

- Absorption component
- Emission component for volume filling factor $C_v = 0$
- Emission component for volume filling factor $C_v = 1$

The parameter space is as follows:

- Ionisation parameter $\log(\xi/erg\ cm\ s^{-1}) \in [3.0, 6.0]$, steps of 0.25
- Outflow velocity $v_{out} \in [0.0, 0.4]c$, steps of 0.025 c
- Column density $N_H \in [0, 2 \cdot 10^{24}]cm^{-2}$, steps of $2 \cdot 10^{23}cm^{-2}$
- Opening angle of the cone $\theta_{out} \in [0, 90]deg$, steps of 10deg
- Line-of-sight inclination $inc \in [0, 90]deg$, steps of 30deg

The intrinsic turbulent velocity is 3000 km/s (corresponding to 1σ).

A further table for absorption, with parameter space as above but with $\log(\xi/erg\ cm\ s^{-1}) \in [3.0, 5.5]$, steps of 0.5 and turbulent velocity of 15000 km/s can be found [here](#).

Powerlaw SED

Tables with Power-law SED with photon index $\Gamma = 1.8$:

- Absorption component
- Emission component for volume filling factor $C_v = 0$
- Emission component for volume filling factor $C_v = 1$