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Review

Open-Source Radiative Modeling Tools for Extragalactic VHE Gamma-ray Sources

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Abstract: In this review, we discuss various open-source software for modeling the broadband emission of extragalactic sources from radio up to the highest gamma-ray energies. As we provide an overview of the different tools available, we discuss the physical processes that such tools implement and detail the computations they can perform. We also examine their conformity with modern good software practices. After considering the currently available software as a first generation of open-source modeling tools, we outline some desirable characteristics for the next generation.

Keywords: astrophysical jets; active galactic nuclei; gamma-ray bursts; radiative processes; open science; reproducibility

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1. Introduction

In the last two decades, the energy window in which active galactic nuclei (AGN) and gamma-ray bursts (GRBs) can be observed has been extended towards high ($E > 100$ MeV) and very-high ($E > 100$ GeV) energies [1–5]. The broadband emission of extragalactic sources, from radio to gamma rays, is commonly modeled with the radiative processes of non-thermal relativistic particles [6–8]. This modeling approach offers the promising prospect to study astrophysical acceleration mechanisms and, ultimately, identify the sources of cosmic rays [9]. Traditionally, once multi-wavelength (MWL) data are gathered and reduced, their interpretation is performed with closed-source software (i.e., software that cannot be publicly studied, changed, or distributed). Over the years, the growing amount and coverage of MWL data resulted in the production of several closed-source modeling software with increasing complexity, all inevitably engendering the issue of reproducibility of results. By reproducibility of results, we mean the possibility for a user to download the software and the scripts associated with a certain publication (and possibly the computational environment, e.g., in the form of a container) and reperform the calculations in autonomy. Moreover, despite often implementing the same physical processes, these software were never validated against each other, and only recently a systematic comparison of their results has been publicly presented [10]. While appreciating that these tools forged the current understanding of the emission of extragalactic sources, we observe that their validation and the reproducibility of their results remain inevitable limitations. In the context of the forthcoming era of high-energy astrophysics, the limited accessibility of these closed-source software represents another drawback. The next generation of gamma-ray observatories, such as the Cherenkov Telescope Array (CTA), will indeed provide open access to their data [11]. Preparing for this, astrophysicists have started to develop standardized data formats [12,13] and open-source analysis tools [14,15]. The amount of MWL data that the new observatories will make available in the future renders the old closed-source modeling approach simply not sustainable, urging for it to be opened to a wider number of astrophysicists. This introduces the necessity to provide modeling tools with open-source licenses and adopting modern good software practices. In this review, we

present the outset of this shift in the modeling paradigm. We describe several open-source software publicly available for interpreting the non-thermal emission of extragalactic jetted sources. We focus our attention on tools capable of describing the highest-energy emission of these sources. Our review has a strong bias towards AGN modeling since their emission up to TeV energies is long consolidated, while for GRBs this represents a more recent finding [4,5]. We also briefly examine the capability of the presented frameworks to model jetted sources of galactic origin (e.g., microquasars) characterized by the same radiative processes of their extragalactic counterparts.

This review is thus structured. In Section 2, we provide a quick overview of the major physical processes at play in extragalactic jetted sources, their knowledge being essential to understand what is being implemented by the different modeling tools. Section 3 presents the software publicly available, introducing the physical processes they model and their technical specifications (e.g., language in which they are implemented, resources available, etc.). For each tool, we also provide examples of its application. In Section 4, we critically review the available tools and suggest some desirable characteristics for a future generation of open-source modeling software. We close this review with some remarks on how to establish a more reproducible process of physical modeling and interpretation.

2. Physical Background

This section is meant to provide a brief physical background to the understanding of the astrophysical sources and physical processes modeled in each software.

2.1. Jetted Extragalactic Sources

The presence of relativistic jets is ubiquitous to radio-loud AGN and GRBs (and to some galactic sources). Jets are generated in the environments surrounding accreting black holes (BH), where collimated outflows of plasma can be launched with bulk velocities close to the speed of light c [16,17]. The main differences between these two categories of extragalactic sources reside in the velocity of the jet ($\Gamma_{\rm AGN}\sim 10$, $\Gamma_{\rm GRB}\sim 100$, with Γ bulk Lorentz factor of the outflow), in the dissipation of energy along the jet, and in the luminosity and duration of their emission.

AGN are galaxies characterized by strong nuclear activity, commonly associated with the accretion onto a supermassive BH with mass $M_{\rm BH} = 10^6$–$10^9\,M_\odot$ (with $M_\odot$ mass of the Sun). Accretion efficiently converts gravitational energy in thermal radiation, with a range of emission from infrared (IR) to X-rays, and a total luminosity reaching up to 10^{46}–$10^{47}\,{\rm erg\,s^{-1}}$ [18]. The emission in radio-loud AGN extends from radio to gamma rays (up to few TeV in some cases) and is dominated by the non-thermal radiation of the plasma flowing in the jet. As small plasmoids are observed streaming along the jet in the radio band [19], the non-thermal emission is commonly attributed to a small region of the outflow. The so-called *blazars* represent the class of jetted AGN most commonly observed at the highest energies. A small viewing angle between the jet axis and the observer [20] results in a strong relativistic boosting of their non-thermal radiation. Blazars show strong flux variability, with time scales ranging from minutes to decades [21,22], and high polarization in the optical band [23]. Blazars can be divided into two classes: BL Lacs, characterized by featureless optical spectra, and flat-spectrum radio quasars (FSRQs), showing significant line and thermal emission from hot gas orbiting the central BH. The photon fields produced by line and thermal emitters, located at sub-pc distances from the BH, should absorb via $\gamma\gamma$ pair production the gamma-ray spectra of FSRQs. Due to the rare observations of these absorption features (1 object out of 10) [24,25], it is inferred that the non-thermal emission region is located mostly at $\sim$pc scales.

GRBs are associated with the formation of a stellar-mass BH ($M_{\rm BH}\sim 10\,M_\odot$) following the merger of compact objects or a catastrophic star collapse. The ensuing outflow of plasma can be collimated in a jet [26], with particles accelerated in its progressive shocks. Non-thermal emission occurs at two characteristic distances, both well under the pc scale, characterizing two different phases of the emission (*prompt* and *afterglow*) [3]. The afterglow

phase is characterized by the interaction of the shocked material with the external (or circumstellar) medium, which results in the gradual decrease in the bulk Lorentz factor and in a fainting emission, in some cases detectable for days. GRB luminosities can achieve values of 10^{50}–10^{52} erg s^{-1}.

2.2. Physical Processes

The non-thermal emission spectrum of different types of extragalactic sources can be described by a power law (PL) over a broad range of photon energies. This PL of photons is the imprint of the PL energy distribution of the radiating particles, a result of first- and second-order Fermi acceleration processes [27]. It is commonly assumed that particles are accelerated and radiate in a finite region of the jet that we will refer to as emission region. The radiation, being emitted in a finite region moving at relativistic speeds, has its intensity relativistically boosted by a factor depending on Γ and on geometry. If a simple spherical plasmoid is considered, as in jetted AGN, the observed energy flux, νF_ν [erg cm^{-2} s^{-1}], is boosted by the fourth power of the Doppler factor $\delta_D = \frac{1}{\Gamma(1-\beta\cos\theta)}$, where β is the velocity of the outflow and θ the observer's viewing angle. For GRBs, with the emission region being extended to the whole jet section, the beaming pattern can be more complex ([26] see Section 2).

The spectral energy distribution (SED) of radio-loud AGN shows two main components: a low-energy one, peaking in the IR to X-ray band, commonly attributed to synchrotron radiation of relativistic electrons and positrons, and a high-energy component, peaking in gamma rays, that can be either *leptonic* or *hadronic* in origin. In leptonic models, the high-energy emission is due to inverse Compton (IC) scattering by $e^{\pm}$ [28] of target photon fields internal or external to the emission region. In what is commonly referred to as *synchrotron self-Compton* (SSC) scattering, the target photon field is internal to emission region and is provided by the synchrotron radiation of the very same accelerated $e^{\pm}$ [29]. In the so-called *external Compton* (EC) scenario, the photon fields target for Compton scattering can be provided either by the AGN line and thermal emitters: accretion disk, broad line region (BLR), or dust torus (DT) [30–32], or by the synchrotron emission of other components of the jet [33,34], or even by the cosmic microwave background (CMB) [35]. In hadronic models, on the other hand, the high-energy emission is explained with the radiative processes of the secondaries originated in pp or pγ interactions [10,36]. The soft photon fields target for IC or pγ interactions can also produce absorption of the high-energy radiation via $\gamma\gamma$ pair production. The same absorption can occur on the extragalactic background light (EBL) while the photons travel to Earth [37].

Given their very recent observations at the highest energies [4], the mechanisms of the broadband emission of GRBs are still under discussion. While some authors accommodate the whole MWL emission, up to TeV energies, with synchrotron radiation [38], others observed the presence of a second component at the highest energies, attributed, as in blazars, to SSC [39]. Hadronic models have also been suggested to accommodate the highest energy emission from GRBs [40].

Assuming a particular physical scenario and taking into account the corresponding radiative processes, one can fit the observed MWL SED (see, e.g., Figures 1–3) and hence infer the underlying particle energy distribution. The parameter space for these models is often degenarate, with changes in different parameters giving rise to similar patterns in the observed fluxes. Time-resolved SED modeling, properly taking into account the interplay between particles acceleration, cooling via radiative processes, and change of physical conditions in the emission region, constitutes a powerful tool to identify the physical mechanism or parameter responsible for a given observed emission. To obtain broadband spectra at different times (see, e.g., Figure 4), it is necessary to solve a differential equation regulating the time evolution of the underlying particle energy distribution (see, e.g., [8] Equation (7)).

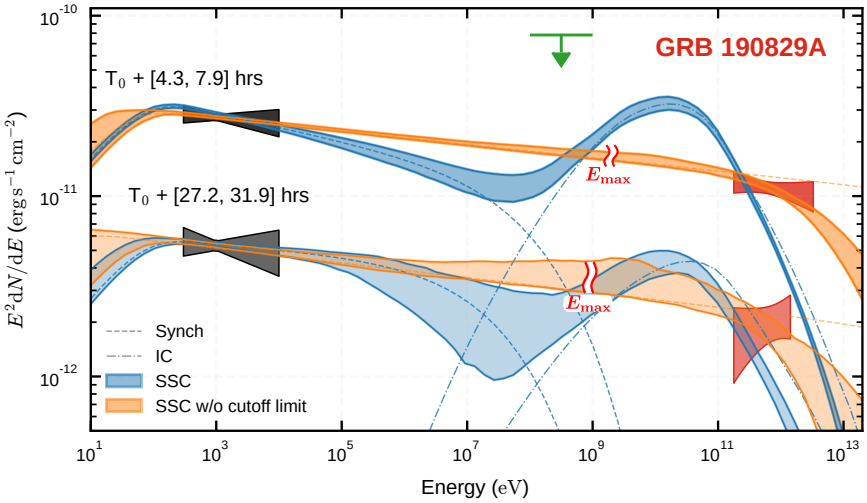

Figure 1. Synchrotron (orange) and SSC (blue) models for the emission GRB 190829A computed with naima. The shaded area represents the 68% confidence interval obtained from the MCMC fitting. Flux measurements from *Swift*−XRT (black band), *Fermi*−LAT (green upper limit), and H.E.S.S. (red band) are also displayed. Figure from [38], reproduced with permission of The American Association for the Advancement of Science.

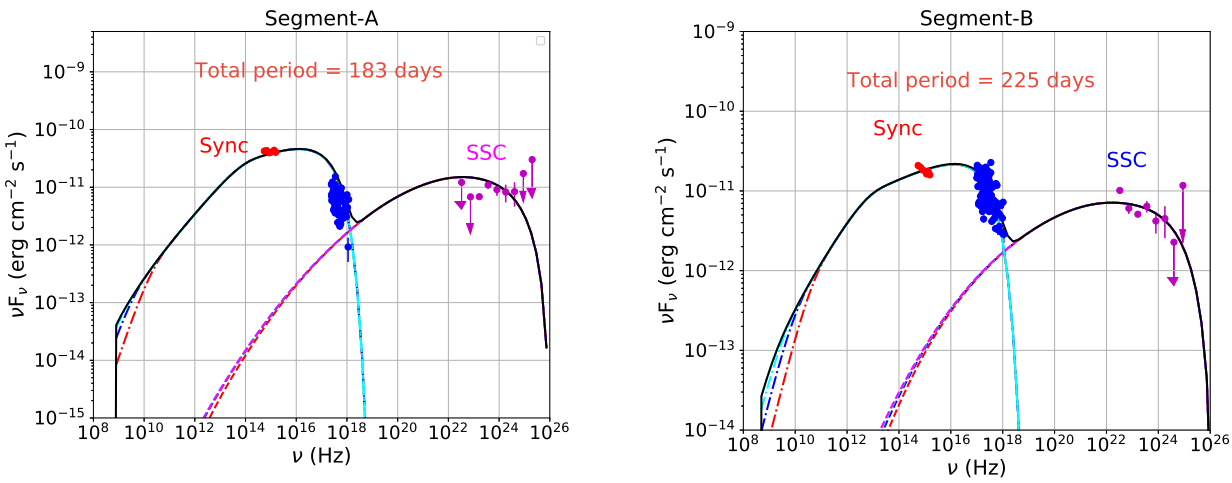

Figure 2. Models for the broadband emission from radio to gamma rays of OJ 287, for two datasets observed during the years 2017–2020. The dotted-dashed and dashed line represent synchrotron and SSC emission computed with GAMERA; the different colors represent different times of the electrons distribution evolution. Optical/UV, X-ray, and gamma-ray flux measurements are displayed with red, blue, and magenta markers, respectively. Figure from [41], reproduced with permission of Astronomy and Astrophysics.

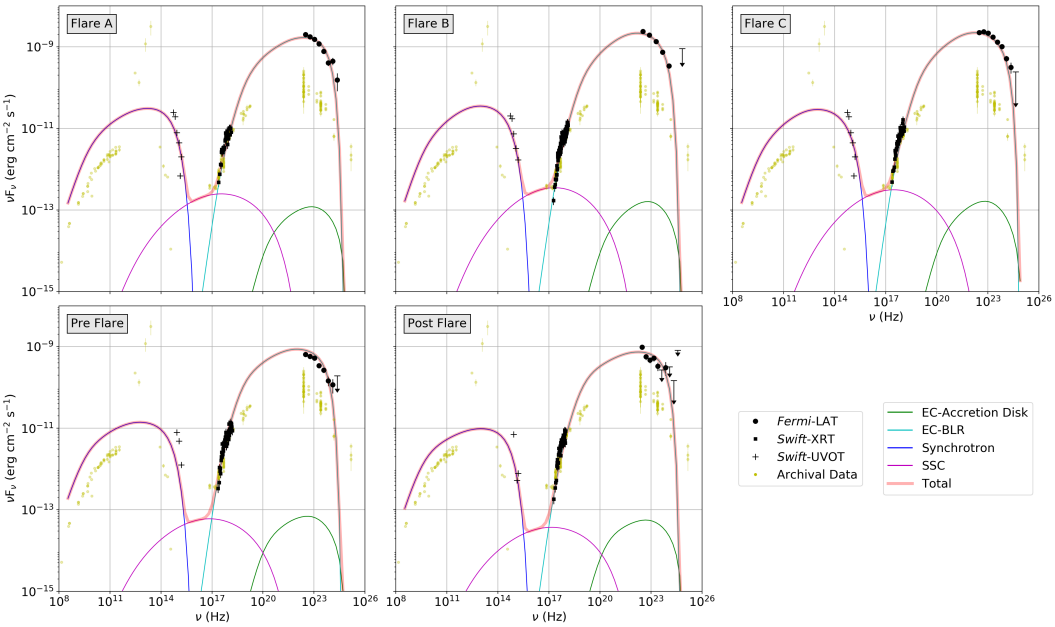

Figure 3. MWL emission of PKS 1830-211 in different flux states, modeled with GAMERA. The high-energy component of the FSRQ emission is described with a combination of SSC and EC scattering on anisotropic photon fields: disk (green line) and BLR (blue line), dominating. Figure from [42] reproduced with permission of the authors and IOPPublishing.

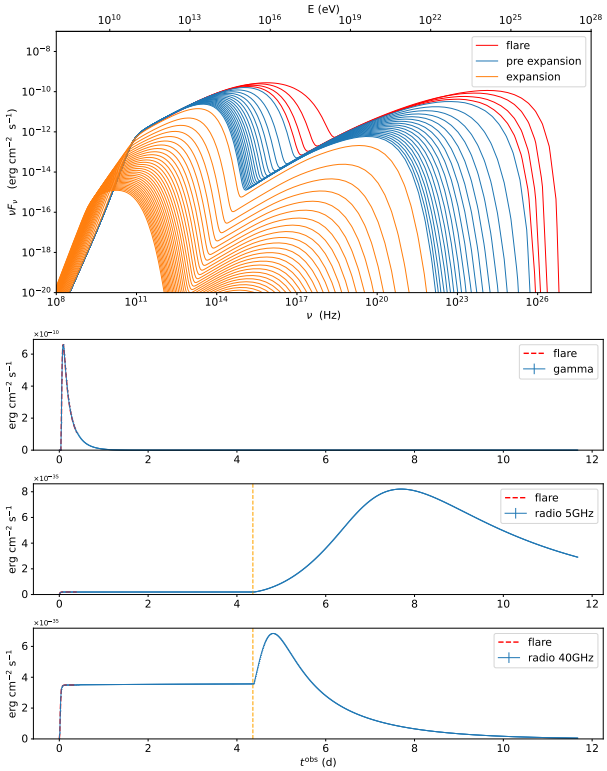

Figure 4. *Top panel*: time-resolved SEDs, computed with Jetset, for a flaring stage (red lines) followed by a pre-expanding stage (blue lines) and an adiabatic expansion stage (orange lines) with $\beta_{\rm exp} = 0.1$. The three *bottom panels* show the corresponding light curves at high energies, and in the radio at 5 and 40 GHz. The red dashed lines mark the light-curve segment belonging to the flaring stage, the orange vertical dashed lines mark the beginning of the expansion, and the orange line marks the expansion stage. Adapted from [43].

3. Open-Source Modeling Tools

In this section we provide an overview of the open-source software publicly available to model the broadband emission of extragalactic jetted sources. We detail their theoretical background, list the physical processes they model, and offer an overview of their resources and usage. In the following, we identify with the term *validation* the numerical comparison of the results produced by a given tool with the output of another software or the reproduction of results from the literature.

3.1. naima

naima [44] is a python package designed to infer the non-thermal particle distributions underlying an observed broadband photon spectrum. naima represented the first python package modeling non-thermal radiative processes made publicly available. It is built entirely in the ecosystem formed by NumPy [45], scipy [46], and astropy [47,48] and is one of the packages affiliated with the astropy project [49]. The packages forming this ecosystem provide the foundations on which an increasing number of tools for astrophysics are being built. For the calculation of the radiative processes, naima relies on a numerical approach: the observed emission is computed by integrating the analytical functions representing or approximating a given emission process with the particle energy distribution. Both non-thermal leptons and hadrons distributions can be considered. naima does not implement time evolution of the particle energy distributions, but can accept as input an arbitrary energy distribution (such that, for example, the result of a time evolution computed with another software can be considered). naima implements both leptonic and hadronic radiative processes. Synchrotron radiation, IC on isotropic photon fields, and non-thermal Bremsstrahlung radiation are available for electrons. For protons, the photon spectrum produced by the decay of the neutral pion result of pp interactions can be computed, though the spectrum of the secondary particles is not computed. The only $\gamma\gamma$ absorption considered is the one on the EBL, following the model of [50]. The code assumes co-moving densities of particles; therefore, it is inadequate to describe extragalactic jetted sources such as blazars or GRBs, in which the emission region typically moves at relativistic speed against a target (photon fields or other particles). The beaming pattern due to the relativistic motion of the emission region is also not computed and it has to be manually calculated by the user. There is no option to consider multiple emission regions. Being the inference of the particle distribution underlying one or more radiative processes the main objective of the package, routines for flux points handling, and SED fitting are provided. naima offers a wrapper to import its radiative models in sherpa [51,52], allowing the user to use sherpa's data handling and fitting capabilities. Gammapy [15], a python package for the analysis of gamma-ray data, includes a wrapper to the naima radiative models in its own source code. Alternatively, a Markov chain Monte Carlo (MCMC) fit can be performed interfacing naima with emcee [53], as illustrated in [44] and in other examples in the documentation. No validation of the radiative processes implemented in the package is provided in the documentation or in [44].

naima has mostly been used to model galactic sources, especially supernova remnants or pulsar wind nebulae (PWN). Nonetheless, for the simplest case of an emission region with a simple geometry and moving at relativistic speed, the package can be adapted to model jetted extragalactic sources (computing a flux and boosting it a posteriori). This approach was used for Mkr 421 in [54] and for GRB 190829A in [38]. The scripts using naima for the interpretation of GRB 190829A, illustrated in Figure 1, are also available online [55]. In this case, a spherical shell emission region is considered, with electrons accelerated by a forward shock swiping material from a stellar wind or from the interstellar medium (ISM). Since naima does not perform temporal evolution, a broken PL with an exponential cut-off is considered for the electron distribution.

naima's developement is hosted on GitHub [56], where eight contributors are listed. It follows modern good software practices adopted by other python packages: it provides a documentation hosted on read the Docs [57] and includes a test suite part of a continuous

integration (CI) system. naima can be installed via pip and conda. [44] constitutes the only reference publication for the package.

3.2. GAMERA

GAMERA [58] is a C++ library providing a modular approach to the modeling of the emission of different types of sources, along with some tools for population studies. GAMERA offers a python wrapper, gappa, returning the result of GAMERA's computations as NumPy arrays. Similar to naima, GAMERA relies on a numerical approach for the radiative processes computation. Non-thermal electron and proton distribution can be considered and can be evolved in time. It is possible to evolve the particle spectra considering cooling via all the radiative processes implemented in the package, which are the same as available in naima (synchrotron, IC, Bremmsstrahlung for $e^{\pm}$ and decay of π_0 from pp interactions). The numerical solution of the particle transport equation is based on an algorithm that interprets the transport as an advective flow in energy space and solves it using a donor-cell advection algorithm. For constant energy losses and no particle escape, GAMERA offers the possibility to use a semi-analytical method, providing a faster computation. For Compton scattering, the full angular dependency of the Compton cross section is considered, allowing to model the scattering of anisotropic photon fields by anisotropic electrons. The effect of $\gamma\gamma$ absorption on anisotropic photon fields is also modeled by the library. Several interacting emission regions can be considered. No validation for the radiative processes computation is provided in [58]; though the PWN model in [59] is reproduced, no numerical comparison of the SEDs is provided. GAMERA does not directly implement data handling, nor provides wrappers to other fitting packages. A python script for SED fitting is available in the documentation, but the model for fitting has to be manually modified by the user. GAMERA implements routines for flux point (the energy flux $[\mathrm{erg\,cm^{-2}\,s^{-1}}]$ measured by an instrument in a given energy bin) simulation: once an instrument response function (IRF) is provided, the observed flux corresponding to a specific radiative model can be obtained. Utilities representing the first steps in population studies are provided with the library. In [58], it is shown how to generate a population of young PWN in the galaxy, though it is left to the user to compute their total emission.

GAMERA has been mostly employed for AGN modeling [41,42,60]. In Figure 2, we show the model obtained with GAMERA fitting the MWL emission of the BL Lac OJ 287 observed during 2017–2020 [41]. The emission corresponds to an electron distribution with an injected log-parabolic spectrum cooling via synchrotron and IC radiation. In Figure 3, we instead show the application of GAMERA to model the highest energy component of the FSRQ PKS 1830-211 with EC scattering on photons produced by the BLR (anisotropic target photon field).

GAMERA's development is hosted on GitHub [61], where five contributors are listed; its documentation is hosted online [62]. No unit tests and no CI are set up. The C++ library is not distributed with any package system and has to be manually downloaded from GitHub and built with make. The python wrapper is not available via a standard package manager (pip, conda); a static library has to be manually built by the user and appended to the search path for modules in each python script.

3.3. Jetset

Jetset [63–65] is an open-source C/python framework to reproduce radiative and acceleration processes acting in extragalactic jets and galactic objects (beamed and unbeamed). Both static and time-dependent modeling are implemented, allowing the user to fit the numerical models to observed data. Jetset allows defining several leptonic radiative scenarios: synchrotron, SSC, EC on disk, BLR and DT photon fields, EC on the CMB. It also computes the $\gamma\gamma$ absorption on the EBL models of [50,66,67]. Moreover, Jetset models hadronic pp emission, considering γ from π^0 decay, and also the radiation from the secondaries of charged pions (evolved to equilibrium). Neutrinos spectra, result of the decay of these secondaries, can also be estimated. Jetset incorporates template models,

e.g., for the host galaxy and the *big blue bump* (BBB) feature produced by the disk. The code implements a self-consistent temporal evolution of the plasma under the effect of radiative and adiabatic cooling, and both first- and second-order (stochastic) acceleration processes. Jetset provides tools to handle observed data such as grouping, definition of datasets, and handling of upper limits and time ranges. All the datasets, the output tables, and the produced SEDs can be returned as astropy tables with units. The model fitting can be assisted by a prefit stage in which a phenomenological characterization of the SED is fitted to the data (via power-law and log-polynomial fit). The derived parameters, such as spectral indices, curvatures, peak fluxes, and frequencies, are used to constrain the parameter space of the synchrotron and SSC/EC scenarios. These constraints are taken into account in the successive fit stage, with the proper physical radiative models. From an implementation point of view, Jetset is fully object-oriented, with both inheritance and composition, and provides a broad range of models, implemented inheriting from the BaseModel class. Models can be combined together, using the FitModel class from the model_manager module, and then plugged to a minimizer for fitting. The main type of models are as follows:

- *Numerical models*:
  - Jet class, handling both leptonic and hadronic (pp) emission for extragalactic jetted objects, and the JetTimeEvol to perform temporal evolution of a leptonic plasma;
  - GalacticBeamed class for galactic jetted objects;
  - GalacticUnbeamed class for galactic objects without jets, such as PWN and SNR.
- *Analytical models*: handling the phenomenological models (e.g., power-law or log-polynomial models) used for the prefit stage. They can be additionally used to define user-defined analytical models to plug, via the model manager, to the fitting routines.
- *Template models*: used to reproduce template of the galaxy emission or of the BBB, and also used for the computation of the absorption on the EBL (with a dependency on redshift and energy).

The parameters of the models are handled by a dedicated class which implements, via composition and inheritance, complex and flexible features. The parameters wrap astropy `quantities`, for easy interface with other astropy-based packages. Parameters can be linked via mathematical expression, both within the same model or among different models. For example, one can define the magnetic field as function of the blob size and position across the jet; the BLR size as a function of the disk luminosity; or set an analytical dependency between the low- and high-energy indexes of a broken PL particle distribution. Dedicated classes handle both frequentist and Bayesian model fitting (see Figure 5, top panel). The frequentist model fitting class implements plugin to `iminuit` [68] and to the scipy least square bound implementation. The bayesian model fitting can instead be performed using a MCMC sampler with a plugin to emcee [53]. Best-fit SEDs and parameters, including MCMC results, can be stored to file. A plugin to use sherpa and Gammapy is also implemented. The temporal evolution of the leptonic plasma is implemented in the JetTimeEvol class. To follow the evolution of the particle distribution, Jetset proceeds through the numerical solution of a kinetic equation based on the the quasi-linear approximation with the inclusion of a momentum diffusion term in [69,70]. The numerical solution of the Fokker–Planck equation is obtained using the same approach as [64], which is based on the method proposed by [71,72]. The temporal evolution can connect together more than one region, allowing to simulate the acceleration and radiative regions separately, injecting the particles from the acceleration to the radiative region. The code allows to store particle distributions, SEDs, and light curves (with a user-specified sampling) and to convolve the light curves with the light crossing time through the emission region. Each defined model, including the models with temporal evolution, can be saved using python's pickling mechanism.

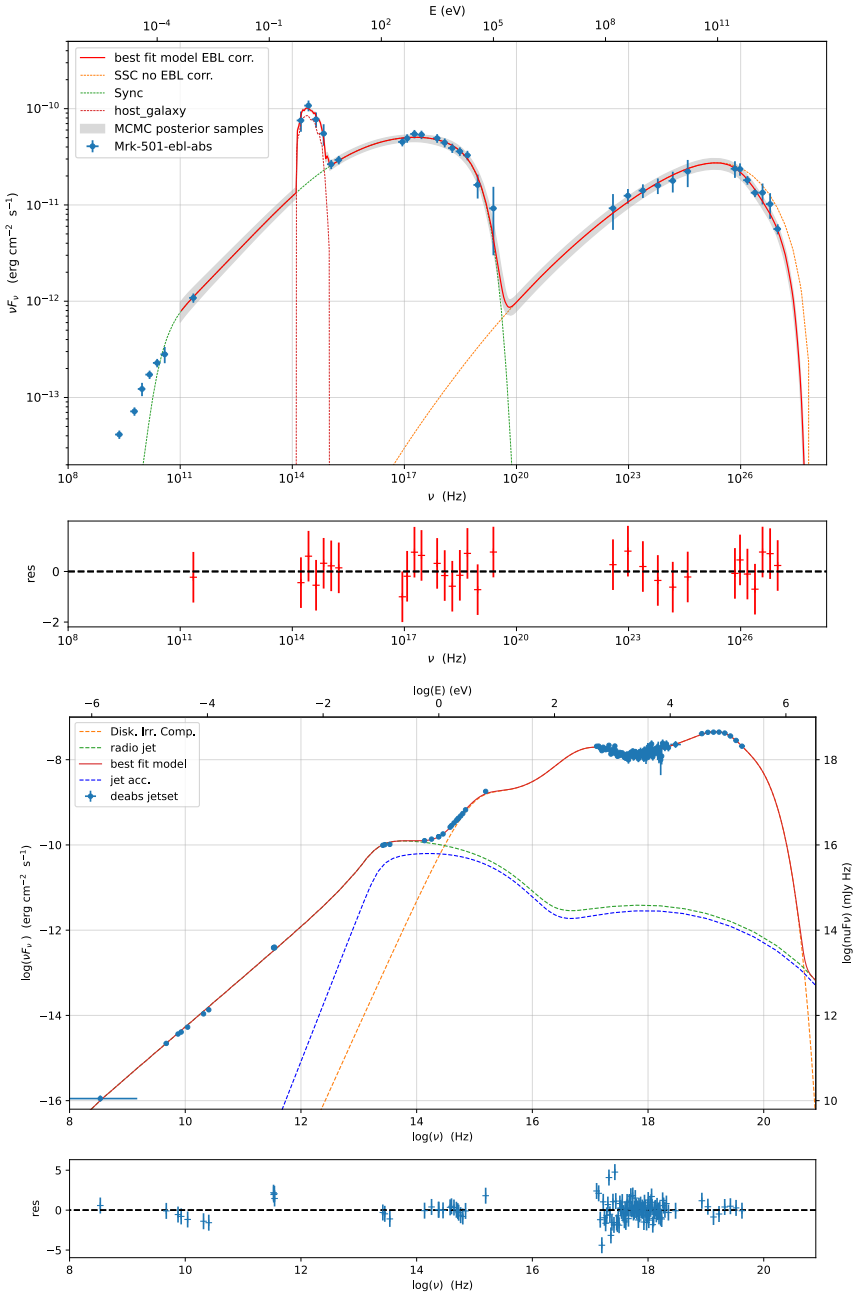

Figure 5. Fitting MWL SEDs with Jetset. *Top panel*: Best fit of the Mrk 501 SED considering synchrotron and SSC emission, the galaxy template, and the absorption on the EBL. The gray band illustrates the MCMC model posterior samples. Figure adapted from the Jetset documentation. *Bottom panel*: Best-fit model of the MWL emission of the microquasars MAXI J1820+070. The dashed lines represent the individual components; the red line, their sum. Figure from [73].

Jetset has been extensively used for modeling and fitting radiative emission in blazars both for BL Lacs and FSRQs. Temporal evolution capabilities have been used in recent work [43] to simulate the impact of the adiabatic expansion on radio to gamma-ray delays. In the model in Figure 4, particles are initially injected and accelerated in an acceleration region, where they undergo both acceleration and cooling. They then diffuse towards a radiative region, where only radiative losses and adiabatic expansion take place. The effect of the expansion, leading to a decrease in the magnetic field, can be observed both in the SEDs (top panel), showing a shift of the synchrotron self-absorption frequency, and in the light curves (three bottom panels), showing the delays observed between gamma-ray and

radio flares. The flexibility of the code allows building complex and flexible user-defined models, or plugins, as demonstrated for the microquasars MAXI J1820+070 during the 2018 outburst [73]. The model is composed of an irradiated disk with a Compton hump and a leptonic jet with an acceleration region and a synchrotron-dominated cooling region. Figure 5 (bottom panel) illustrates the best-fit SED for this scenario obtained with Jetset with the MWL data in [73].

Jetset is hosted on GitHub [74] and the documentation is hosted on read the Docs [75]. Continuous integration (CI) and continuous deployment (CD) are performed by GitHub Actions. Test suites are performed for each new release, available via conda and pip. Pre-releases, for source conda and pip, are hosted on GitHub [76], and documented on GitHub. Pre-releases can be easily installed using the script in the jetset-installer [77] repository.

3.4. agnpy

agnpy [78] is a python package modeling the radiative processes in jetted AGN. Similar to naima, agnpy is entirely built in the python scientific ecosystem and is one of the packages affiliated with the astropy project. As for the other packages, agnpy relies on a numerical approach to compute the radiative processes of non-thermal electron distributions. Routines for time evolution are not included in the package, though a module for the constraint of the spectral parameters according to a simple parametrization of the acceleration and radiation processes is available. agnpy implements synchrotron radiation, SSC, and EC on anisotropic (accretion disk, BLR, DT) and isotropic (CMB) photon fields. Similarly to GAMERA, the full angular dependency of the Compton cross section is taken into account, though only isotropic electron distributions can be considered. $\gamma\gamma$ absorption on all the photon fields target for Compton scattering can be computed (see, e.g., Figure 6). Values for the opacity due to different EBL models [50,66,67] are also included. The viewing angle θ_s of the observer to the jet axis is included among the parameters of all the physical processes implemented, such that agnpy can be adopted to describe radio-loud AGN, beside blazars. In its current state it is not possible to consider multiple or complex emission regions beside the simple homogeneous sphere (blob). Utilities for data handling and fitting are not included in the package; a Gammapy wrapper is provided instead. Living in the python scientific ecosystem, agnpy is seamlessly interfaceable with the fitting routines included in other tools such as sherpa, as shown in several examples in the documentation and in [78]. In Figure 7, as an illustrative example, we show a fit of the MWL emission of Mrk421 obtained by wrapping agnpy with Gammapy. agnpy is thoroughly validated by numerically checking the output of each radiative process against results from the main reference used for its implementation [7,31,79–81] and against Jetset ([78]; see Section 4). Examples of validation are illustrated in Figure 6 (left panel) and in Figure 8. Additional internal consistency checks are implemented: for example, EC spectra and $\gamma\gamma$ opacities are compared against an approximation considering the target photon fields as a monochromatic point source (see, e.g., Figure 6, right panel). Deviations well within 30% are achieved when comparing against the literature and against Jetset, when the same physical assumptions are considered. Differences within a factor of 2 are instead obtained when comparing against processes implemented with different assumptions (e.g., when comparing against the EC implemented in Jetset). agnpy is the first non-thermal modeling tool openly presenting such detailed numerical comparisons and integrating them in its test system. agnpy has been used for modeling blazars, especially FSRQs, thanks to its solutions for EC scattering and $\gamma\gamma$ absorption [82–84].

agnpy is hosted on GitHub [85], where six contributors are listed; its documentation is hosted on read the Docs [86]. The package includes a test suite part of its CI system. Numerical comparisons against literature reference and Jetset results are embedded in these tests. CD is also implemented, with each tagged version of the software made immediately available via pip and conda. Ref. [78] constitutes the release paper of the software.

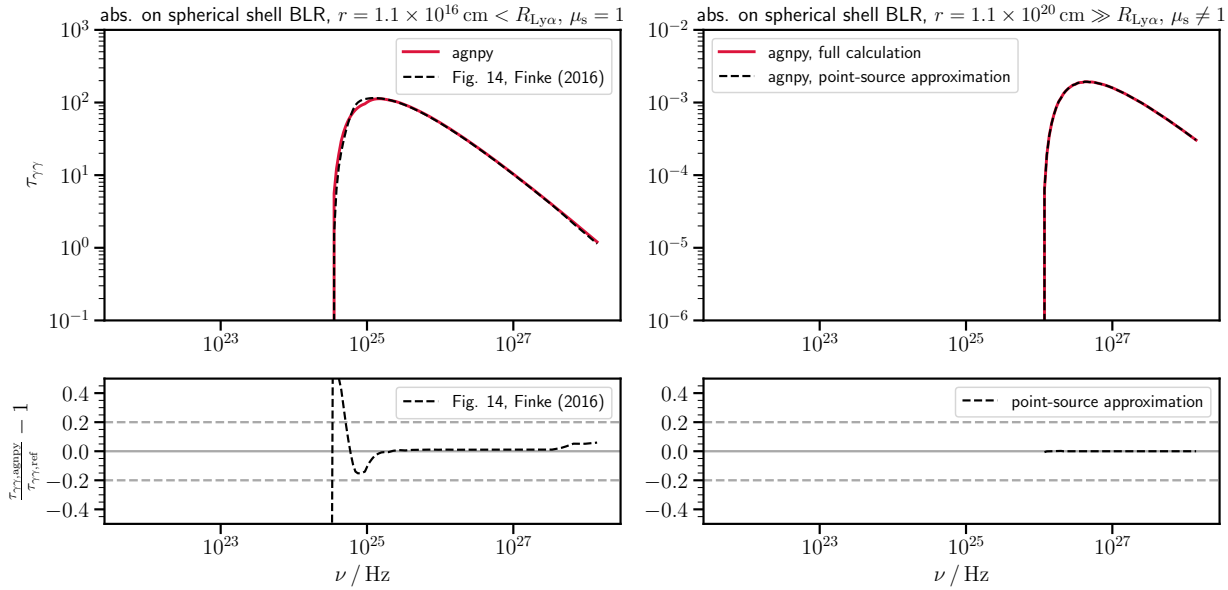

Figure 6. $\gamma\gamma$ opacity for absorption on the BLR photon field computed with agnpy. *Left panel*: Validation of agnpy result against the literature for a small viewing angle ($\theta_s = 0°$, blazar case). *Right panel*: Internal cross-check approximating, for large distances from the BH, the BLR as a monochromatic point source at the BH position. A non-null viewing angle is considered in this case ($\theta_s = 20°$, radio-loud AGN case). Figure from [78], reproduced with permission of Astronomy and Astrophysics.

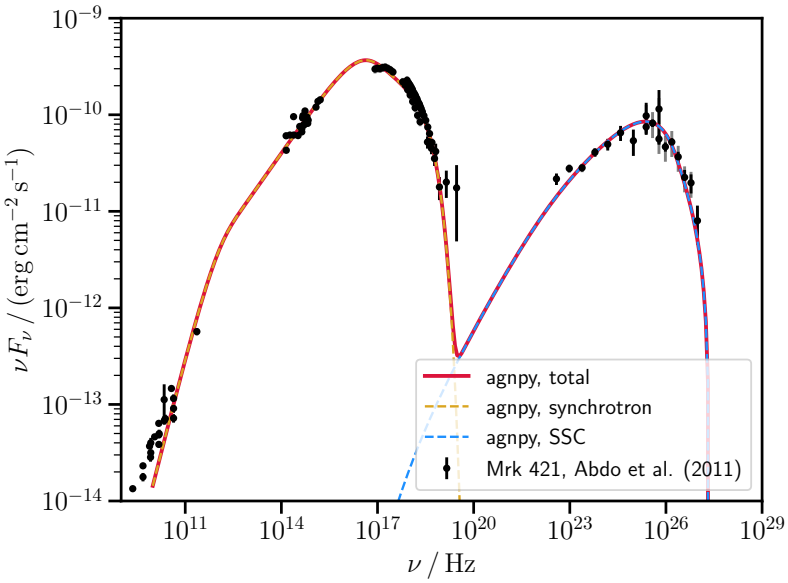

Figure 7. Fit of the MWL SED of Mrk 421 observed in [87], obtained wrapping the radiative provided by agnpy within the classes for flux points handling and model fitting in Gammapy. Figure from [78], reproduced with permission of Astronomy and Astrophysics.

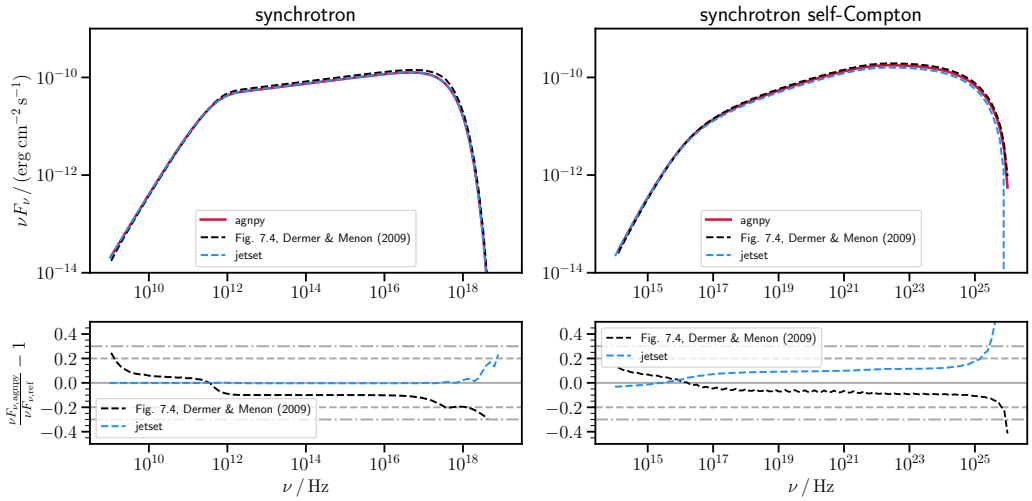

Figure 8. An example of validation: synchrotron and SSC SEDs generated with the same model parameters using agnpy and Jetset. Both spectra are compared against a result from the literature [7]. Figure from [78], reproduced with permission of Astronomy and Astrophysics.

3.5. BHJet

BHJet [88–90] is a set of C++ libraries modeling the emission of accretion/ejection systems of different scales: from black hole X-ray binaries (BHXB) to radio-loud AGN. It comprises the following libraries: Kariba, describing the radiative processes and their underlying particle distributions, and the AgnJetand BIJet libraries, modeling jets with different physical properties. AgnJetdescribes a mildly relativistic, pressure-driven jet [91–93], while BIJet describes a Blandford-Königl [28] magnetic-driven jet. A numerical approach is used for the radiative processes computations and a semi-analytical approach for the jet modeling calculations. As the library aims to also describe accretion systems, both thermal and non-thermal electron distributions can be considered. No time evolution is implemented, but a steady-state solution of the differential equation regulating the particle cooling can be evaluated, accounting for adiabatic, synchrotron, and IC losses only in the Thomson regime. The radiative processes modeled by Kariba are black-body radiation, cyclotron radiation due to thermal electrons, synchrotron radiation due to non-thermal electrons, and inverse Compton (SSC and EC on the AGN components). Successive scattering orders can be considered for the IC (i.e., the IC radiation can be target for further IC scattering). For both jet classes, a fluidodynamic equation representing the velocity profile can be solved, allowing to obtain the particle density and the magnetic field at each height of the jet, and hence for the steady-state solution of the cooling calculated. BHJet can therefore be used to evaluate the MWL emission from the entire outflow. No routines for SED fitting are provided, but the array returned by the radiative processes computations is compatible with `XSPEC` [94]. Some validation is provided for the radiative processes and the jet modeling in [90]. The Compton spectra are benchmarked against calculations of the compPS [95] included in XSPEC. The results of the semi-analytical modeling of the jet evolution (e.g., magnetic field, electron density) are instead compared against general-relativistic magnetohydrodynamics (GRMHD) simulations and it is observed that BHJet can approximately reproduce the magnetic field value and the particle density in the case of a mildly-relativistic pressure-driven jet or in the case of a highly-relativistic magnetized jet. Before its public release, previous versions of the software were extensively used for binaries and AGN modeling (see [90] and references therein). To illustrate an application of BHJet to compute the spectrum of a VHE source, we show, in Figure 9, the electron distribution and the MWL SED of an FSRQ computed for several distances along the jet axis.

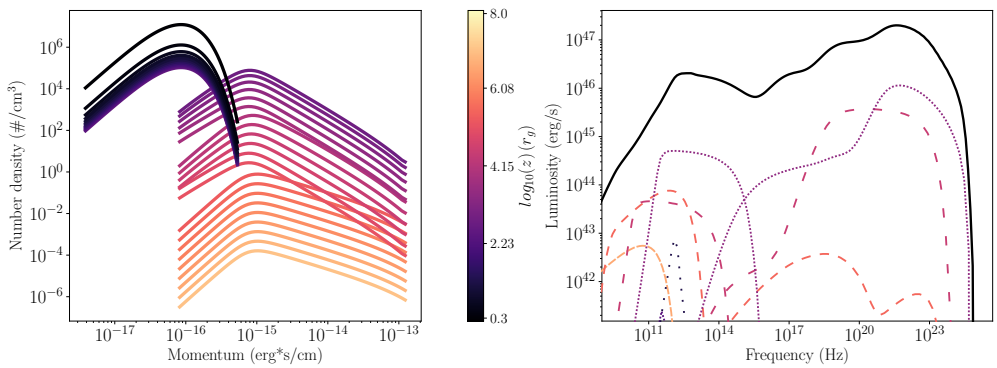

Figure 9. Electron distributions (left panel) and corresponding MWL SED (right panel) computed with BHJet at several distances along the jet axis of a FSRQ. The colored lines represent particles distributions or SEDs at different heights. The black line in the right plot represents the sum of the emission at all heights. Figure from [90], reproduced with permission of the authors.

BHJet is available on GitHub [96], where four contributors are listed. No documentation is provided, but a few example scripts to reproduce the results in [90] are available. The library is not distributed with any package system and has to be manually downloaded from GitHub and built with make, along with the example scripts. Ref. [90] constitutes the release paper of the software.

3.6. FLAREMODEL

FLAREMODEL [97] is a python package modeling astrophysical synchrotron sources. Contrary to the uniform (spherical) emission regions considered in the other packages, FLAREMODEL allows to consider inhomogenous spherical emission regions. The basic routines are written in C with options for multi-threading and wrapped with a python interface integrated with NumPy, but not with astropy. Differently to the other codes, FLAREMODEL employs ray-tracing, i.e., the propagation of imaginary rays is followed through a region with changing physical conditions, hence allowing to consider non-isotropic particle distributions in the emission region. Both thermal and non-thermal electron distributions can be employed. Their time evolution is modeled considering adiabatic and synchrotron losses, while IC cooling is not included. In addition to synchrotron radiation, SSC emission can also be computed. Multiple emission regions cannot be considered. A SED fitting routine built on lmfit [98] is made available. Validation is provided in [97] for the computations implemented in the package. The synchrotron emissivity and absorption coefficients are compared against those computed with the symphony code [99]. The synchrotron emission obtained by [100] for a sphere with power-law radial density and magnetic field is reproduced. A consistency check, illustrated in Figure 10, is performed for the SSC from a uniform sphere, comparing the solution obtained with ray-tracing against the numerical simplification that assumes a uniform particle distribution. Examples of time evolution under synchrotron and adiabatic cooling are provided in [97]. The software was used in [101] to model the synchrotron emission of Sgr A*.

FLAREMODEL is hosted on GitHub [102], where one contributor is listed. The documentation [103] includes basic notebook tutorials, reproducing the figures in the release paper [97]. FLAREMODEL is distributed via pip.

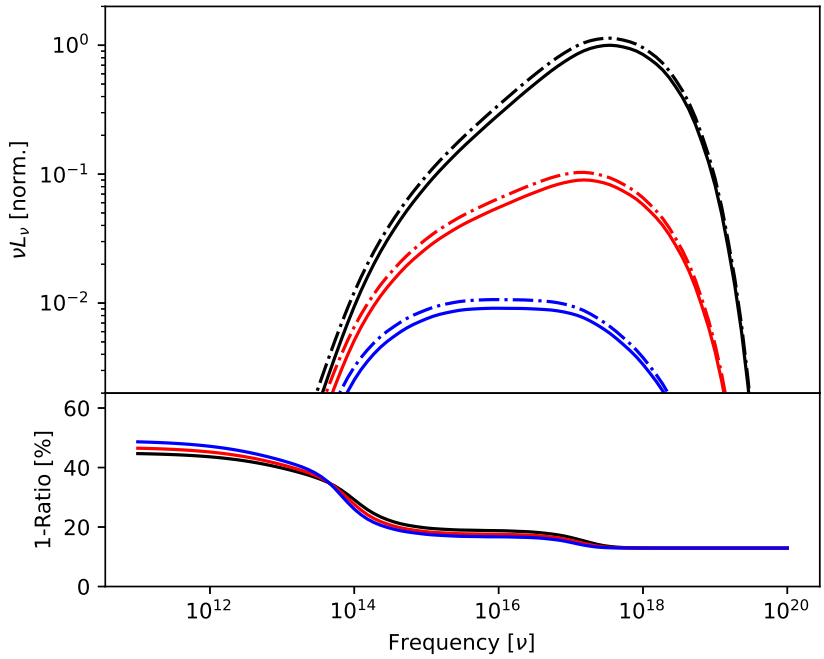

Figure 10. SSC emission computed with FLAREMODEL from a uniform emission region. SEDs with dashed line are obtained using the numerical ray-tracing approach, and solid ones are obtained with the numerical integration considering a uniform particle distribution. Figure from [97].

4. Discussion and Conclusions

4.1. Review of the Current Packages

We have examined in our review six packages modeling the non-thermal broadband emission of jetted extragalactic sources from radio to gamma rays. We briefly also consider their capability to describe galactic sources characterized by the same emission mechanisms. In Table 1, we present a global overview of the physical processes implemented by each software. All the tools provide leptonic synchrotron and SSC emission models. BHJet and FLAREMODEL provide the most sophisticated calculations for these radiative processes, with the first taking into account the emission from the whole plasma outflow and several orders of IC scattering, and the latter employing ray-tracing to consider a non-uniform emission region. Having being used to model low-energy sources, BHJet and FLAREMODEL are also the only libraries including thermal electron distributions. By considering the full angular dependency of the Compton cross section, GAMERA can compute IC scattering with anisotropic electrons and anisotropic target radiation fields. Similarly, agnpy provides IC scattering on anisotropic radiation field (with isotropic electrons though). Both GAMERA and agnpy can compute $\gamma\gamma$ absorption on anisotropic photon fields, while naima and Jetset provide only absorption on the EBL. Regarding hadronic radiative processes, a description of the pp interaction is implemented in naima, GAMERA, and Jetset, while none of the tools include photo-hadronic (pγ) emission models [10]. In naima and GAMERA, only the π_0 decay in gamma rays is modeled, while Jetset models the decay of charged pions, computing the equilibrium distributions of secondary $e^{\pm}$ pairs and their radiation (synchrotron, IC, and Bremsstrahlung). Jetset also computes the spectrum of ν produced in pion decays. For hadronic interactions, both GAMERA and naima follow the parametrization of [104], while Jetset implements that of [105]. GAMERA, Jetset, and FLAREMODEL can numerically solve the differential equation describing the particles temporal evolution. In addition, while FLAREMODEL and GAMERA take into account only the radiative cooling processes, Jetset also provides first- and second-order acceleration process, adiabatic expansion, and the possibility to have decoupled radiative and acceleration regions. The remaining packages offer simplified alternatives: naima allows for a custom particle distribution in input, agnpy offers a constraint of the model parameters

based on a simple parametrization of the acceleration and radiation processes, and BHJet provides the analytical solution of the differential equation at equilibrium. Concerning the type of sources that can be modeled, except for naima, all the tools reviewed can be directly applied to describe the emission of jetted AGN. naima, originally designed to model galactic high-energy sources, can be used to model jetted sources only through the manual implementation of the beaming pattern of the radiation. Incidentally, naima was the only package used to model GRB emission. BHJet and Jetset (through its plugins describing a microquasar or the blob expansion) are the only software considering the extended jet emission. The fit of an MWL SED with a tool ascribing the whole emission to a finite jet region underestimates the emission below a certain frequency in the radio band, as this is typically measured with a large integration region. As an example, one can see how the points below 10^{11} Hz in Figure 7 cannot be reproduced assuming synchrotron radiation from a blob, while these points are properly modeled in the microquasar model of Jetset, in Figure 5. We notice that the problem of integrating the non-thermal emission over a simple geometrical model of the jet has already been treated in the literature [43,106–109], and it would be an important implementation in the tools. Among the software considered, BHJet is the only one suited to describe non-jetted low-power AGN (see the M81* example in [90]). None of the tools considered can be applied to describe other classes of extragalactic gamma-ray emitters, such as starburst galaxies [110].

In Table 2, we instead examine the compliance of individual tools with good modern software practices. We notice that naima, Jetset, agnpy, and FLAREMODEL are the ones simultaneously providing test suites, proper documentation, and distribution via package managers. Though all the packages provide some degree of interface to fitting routines, naima, Jetset, agnpy, and FLAREMODEL, due to their interface with the python scientific ecosystem, are also the ones better usable in combination with modern python data-analysis tools and indeed provide wrappers to other data-analysis packages. We observe that in many of the software release papers, some degree of validation is provided, the most complete example being the cross-validation performed for agnpy and Jetset in the release paper of the former [78]. Starting from the same set of model parameters, the SEDs obtained with the different software are compared against each other and against a reference SED from the literature (see Figure 8). The other packages also showed a significant commitment to validation, with BHJet benchmarking the Compton computation against the compPS code and the quantities obtained from the semi-analytical description of the jet evolution against GRMHD results. FLAREMODEL instead validated the synchrotron computations against the symphony software and against the literature. Additionally, the SSC was internally checked, comparing the ray-tracing and the numerical solutions (see Figure 10). Among the tools examined, FLAREMODEL is the only one providing options for multi-threading (at C level). Jetset is instead the only framework with a specific class representing the model parameters. Having this object-oriented description of the parameters of the physical model allows one to impose physical limits and link them, and ultimately facilitates their wrapping with external packages (implementing their own parameters handling).

Table 1. Physical processes implemented in the software reviewed.

Software	Sources	Approach	Particles			Processes						Temp. ev.	Emission Region
			Thermal	Non-Thermal		Leptonic				Hadronic	Absorption		
				$e^{\pm}$	p	Synch.	SSC	EC	Brems.	pp	$\gamma\gamma$		
naima	PWN, SNR, GRB	numerical	✗	✓	✓	✓	✓	✓(CMB)	✓	✓ †	✓(EBL)	✗	not specified
GAMERA	PWN, SNR, AGN microquasars	numerical	✗	✓	✓	✓	✓	✓ ⊙	✓	✓ †	✓ ⋆	✓ (only cool.)	multiple uniform
Jetset	jetted AGN, PWN microquasars, SNR	numerical	✗	✓	✓	✓	✓	✓	✓	✓ ‡	✓(EBL)	✓ (acc. + cool.)	multiple uniform acc. + rad.
agnpy	jetted AGN	numerical	✗	✓	✗	✓	✓	✓ ⋆	✗	✗	✓ ⋆	✗	single uniform
BHJet	binaries, AGN	numerical semi-analytical	✓	✓	✗	✓	✓	✓	✗	✗	✗	✗	whole jet
FLAREMODEL	synch. sources	numerical ray-tracing	✓	✓	✗	✓	✓	✗	✗	✗	✗	✓ (only cool.)	single radial dep.

† pp interaction: computing only gammas from π_0 decay. ‡ pp interaction: computation of radiation from secondaries of charged pions (pairs evolved in time to equilibrium) and of ν spectra. ⊙ Full angular dependency of the Compton cross section: anisotropic electrons and anisotropic photon fields. ⋆ Full angular dependency of the Compton or $\gamma\gamma$ cross sections: anisotropic photon fields.

Table 2. Compliance of software reviewed with modern good software practices.

Software	Language	License	Documentation	Installation	CI or Test Units	CD
naima	python	BSD-3 [1]	Read the Docs	pip, conda	yes	no
GAMERA	C++, python	not specified	GitHub Pages	make file	minimal	no
Jetset	C, python	BSD-3	Read the Docs	pip, conda	yes	yes
agnpy	python	BSD-3	Read the Docs	pip, conda	yes	yes
BHJet	C++	MIT [2]	no	make file	no	no
FLAREMODEL	C, python	BSD-3	Read The Docs	pip	yes	no

[1] https://opensource.org/licenses/BSD-3-Clause (accessed 29 July 2022). [2] https://opensource.org/licenses/MIT (accessed 29 July 2022).

4.2. Desiderata for Future Modeling Packages

The number and quality of software reviewed illustrates that the shift in paradigm towards an open-source modeling approach, described in the introduction, is already taking place. We might consider the tools covered by this review as a *first generation* of open-source modeling tools. Therefore, after having reviewed the available software, we outline in this section what would be the *desiderata* for the future generation of radiative modeling tools.

- *Testing*: For such complex numerical models, test suites are mandatory.
- *Validation*: This constitutes the most fundamental point. If a software has to be provided to a large community of astrophysicists, it is essential to provide a numerical validation against other software, or against reference templates. For example, benchmark SEDs, corresponding to a given physical scenario and a given set of model parameters, can be generated and shared as validation templates. This has already been proposed in [78].
- *Interfaceability*: As proposed by [111], instead of several different packages, one could envision a library of interfaceable *fundamental solvers*, specialized, interconnectable, and respecting the single-responsibility principle. An example of combined workflow could be obtaining the particle energy distribution as a result of the time evolution performed with one of these solvers, and then obtaining the corresponding broadband SED using the radiative processes of another solver. This would imply for the tools to be developed on a more fine-grained level, delegating the high-level interface to separate modules. Additionally, these basic blocks should have a minimal data/model interface, to facilitate the exchange of products. For example, particles distributions or radiative fields could use standardized specifications to interface with the classes handling them in the different solvers. Similarly, final products, such as broadband SEDs, could be provided in the form of standardized (e.g., FITS [112] or astropy) tables with quantities (allowing units conversion). Table metadata could be used to store the model parameters (e.g., parameters of the particle distribution, radius of the emission region, magnetic field intensity, etc.). Using standardized inputs and outputs, with a proper interface between the fundamental solvers, will make the validation process smooth and secure. High-level interfaces should finally orchestrate the fundamental solvers, linking the parameters of the basic blocks and facilitating the interface to other frameworks.
- *Data access*: as already demonstrated by the tools in this review, by living in the same computational ecosystem, modeling and data-analysis tools can be easily interfaced. The interface to specific analysis software, and eventually to online services providing astrophysical data, broadens the horizon of model fitting, allowing, for example, combination of data from different experiments, or from current and future generations of instruments. Moreover, having access to the instrument-reduced data through the data-analysis packages would allow to perform a more accurate fit of the physical model, for example, folding it with the instrument IRF and computing a Poissonian likelihood of the observed and expected counts (as commonly performed in X-ray and gamma-ray astronomy [113] with simple analytical models, PL, log-parabola,

etc.). Due to the current limitations, a χ^2 fit is commonly performed to flux points that are often computed making assumption on the underlying shape of the photon spectrum and never provided with a matrix quantifying their correlations. naima, agnpy, and Jetset already demonstrate the possibility of forward-fold fit of high-energy astrophysical data through their sherpa and Gammapy wrappers (both sherpa and Gammapy can read the PHA OGIP standard adopted to represent counts and IRF of X-ray [114] and gamma-ray [115] instruments).

- *Accessibility*: We remark that making the code available online with a license is not sufficient to make it properly accessible. Care has to be taken by developers to write a proper documentation. The latter does not only serve didactic purposes; for example, it can be easily used in hands-on tutorials, but plays the fundamental role of forming future users or developers.

4.3. Conclusions

In this review, we presented the state-of-the-art of open-source, reproducible, frameworks modeling the radiative processes in extragalactic VHE gamma-ray sources. We highlighted the main features of the presented packages in terms of the physical processes they implement, and in terms of the good software practices they comply with. We consider these packages as a first generation of software paving the road for a future generation of frameworks realizing a fully-reproducible modeling of high-energy astrophysical sources. Before concluding, broadening the scope of our review, we would like to remark the following points concerning physical interpretation:

1. The current packages represent mostly single- or few-developer projects, with a strong commitment and effort from few individuals, who are offering a scientific product to the community, fulfilling the full chain from coding, to documentation and distribution.
2. Despite the aforementioned efforts, the attitude to publish scientific articles based on accessible and reproducible models is not yet standard. Closed-source software, if used in scientific publications, should at minimum be accessible in the form of binaries, to allow the astrophysical community to reproduce and validate what has been published.
3. Even though the presented products reach high-quality standards, none of them cover the entire panoply of physical processes, and a large overlap of features among the products is present. In this sense, the most desirable solution would be an effort to produce a library of interfaceable fundamental solvers, with a strong support from the community, the large collaborations, and the editorial boards.

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Conflicts of Interest: The authors are the main developers of the agnpy (C. Nigro) and Jetset (A. Tramacere) packages described in the review.

Abbreviations

The following abbreviations are used in this manuscript:

AGN	Active galactic nuclei
GRB	Gamma-ray burst

MWL	Multi-wavelength
CTA	Cherenkov Telescope Array
BH	Black hole
IR	Infrared
FSRQ	Flat-spectrum radio quasars
PL	Power law
SED	Spectral energy distribution
IC	Inverse Compton
SSC	Synchrotron self-Compton
EC	External Compton
BLR	Broad line region
DT	Dust torus
CMB	Cosmic microwave background
EBL	Extragalactic background light
MCMC	Markov chain Monte Carlo
PWN	Pulsar wind nebula
ISM	Interstellar medium
IRF	Instrument response function
BBB	Big blue bump
CI	Continuous integration
CD	Continuous deployment
BHXB	Black hole X-ray binary
GRMHD	General-relativistic magnetohydrodynamics

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