naima: a Python package for inference of particle distribution properties from nonthermal spectra

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The ultimate goal of the observation of nonthermal emission from astrophysical sources is to understand the underlying particle acceleration and evolution processes, and few tools are publicly available to infer the particle distribution properties from the observed photon spectra from X-ray to VHE gamma rays. naima is an open source Python package that provides models for non-thermal radiative emission from homogeneous distribution of relativistic electrons and protons. Contributions from synchrotron, inverse Compton, nonthermal bremsstrahlung, and neutral-pion decay can be computed for a series of functional shapes of the particle energy distributions, with the possibility of using user-defined particle distribution functions. In addition, naima provides a set of functions that allow to use these models to fit observed nonthermal spectra through an MCMC procedure, obtaining probability distribution functions for the particle distribution parameters. In this contribution I will present the models and methods available in naima and an example of their application to the understanding of a galactic nonthermal source.

naima’s documentation, including how to install the package, is available at http://naima.readthedocs.org.
1. Introduction

Over the past few years, there has been a wealth of facilities that allow for an unprecedented level of sensitivity in the high-energy and very-high-energy gamma-ray bands, most notably Fermi-LAT and the Cherenkov telescope arrays H.E.S.S., MAGIC, and VERITAS. These energy bands probe the highest energies at which particles are known to be accelerated, and provide valuable insight into the acceleration and energy loss processes of a growing population of galactic and extragalactic sources.

A first step in understanding the mechanisms through which a given source has accelerated the particles that are responsible for the emission we detect is to characterize the present age particle energy distribution. For many sources, such as pulsar wind nebulae emitting gamma-rays through inverse Compton scattering on the Cosmic Microwave Background (CMB), the derivation of the particle distribution can be done in a model-independent way. To date, there are few public codes that allow this sort of analysis, and most calculations are done with models coded ad-hoc for the discussion of a given observation.

Here we present naima, an open source Python package developed with the aim of providing proven methods for computing the nonthermal radiative output of relativistic particle distributions. There are two main components of the package: a set of nonthermal radiative models, and a set of utility functions that make it easier to fit a given model to observed spectral data.

2. Features

The radiative models are implemented in a modular way that allows to select a functional shape for the particle distribution. There are several functions included for this purpose, and the user can as well define their own following the instructions in the documentation, therefore allowing to implement any type of particle cooling, escape, or acceleration physics before computing its radiative output with naima. The radiative models currently available in naima are synchrotron, inverse Compton, nonthermal bremsstrahlung, and neutral pion decay. See Section 3 for details on the implementation. In addition, naima includes a set of wrappers around these models that allow them to be used within the sherpa spectral analysis package [1] in the module naima.sherpa_models.

A set of fitting utilities are provided in naima with the goal of inferring the properties of the parent particle distribution that gives rise to an observed nonthermal spectrum. These use Markov Chain Monte Carlo (MCMC) sampling to obtain both the maximum likelihood parameters as well as their uncertainties in a single run. Details on the implementation can be found in Section 4. Several plotting functions are available as well to analyse the results of the MCMC run.

naima uses the astropy package [2] extensively, most notably through the use of its physical unit module astropy.units. This allows users to define the input spectra and parameters in their preferred units, and naima will be able to convert them as needed in its internal calculations, with the added benefit of ensuring that the algorithms in naima are dimensionally correct.
3. Implementation of radiation models

3.1 Synchrotron

Synchrotron radiation is produced by all charged particles in the presence of magnetic fields, and is ubiquitous in the emitted spectrum of leptonic sources. A full description and derivation of its properties can be found in [3]. The derivation of the spectrum is usually done considering a uniform magnetic field direction, but that is rarely thought to be the case in astrophysical sources. Considering random magnetic fields results in a shift of the maximum emissivity from \( E_{\text{peak}} = 0.29E_c \) to \( 0.23E_c \), where \( E_c \) is the synchrotron characteristic energy [4]. The \texttt{naima.models.Synchrotron} class implements the parametrization of the emissivity function of synchrotron radiation in random magnetic fields presented by [4, appendix D]. This parametrization is particularly useful as it avoids using special functions, and achieves an accuracy of 0.2\% over the entire range of emission energy.

3.2 Inverse Compton

The inverse Compton (IC) scattering of soft photons by relativistic electrons is the main gamma-ray production channel for electron populations [3]. Often, the seed photon field will be a blackbody or a diluted blackbody, and the calculation of IC must be done taking this into account. \texttt{naima} implements the analytical approximations to IC upscattering of blackbody radiation developed by [5]. These have the advantage of being computationally cheap compared to a numerical integration over the spectrum of the blackbody, and remain accurate within one percent over a wide range of energies. Both the isotropic IC and anisotropic IC approximations are available in \texttt{naima}.

The implementation in \texttt{naima} allows to specify which blackbody seed photon fields to use in the calculation, and provides the three dominant galactic photon fields at the location of the Solar System through the CMB (Cosmic Microwave Background), FIR (far-infrared dust emission), and NIR (near-infrared stellar emission) keywords.

3.3 Nonthermal Bremsstrahlung

Nonthermal bremsstrahlung radiation arises when a population of relativistic particles interact with a thermal particle population. For the computation of the bremsstrahlung emission spectrum, the \texttt{Bremsstrahlung} class implements the approximation of [6] to the original cross-section presented by [7]. Electron-electron bremsstrahlung is implemented for the complete energy range, whereas electron-ion bremsstrahlung is at the moment only available for photon energies above 10 MeV. The normalization of the emission, and importance of the electron-electron versus the electron-ion channels, can be selected in the class, with the default values assuming a fully ionised target medium with solar abundances.

3.4 Pion Decay

The main gamma-ray production for relativistic protons are p-p interactions followed by pion decay, which results in a photon with \( E_\gamma > 100\text{MeV} \). Until recently, the only parametrizations available for the integral cross-section and photon emission spectra were either only applicable to limited energy ranges, or were given as extensive numerical tables [8, 9]. By considering Monte Carlo results and a compilation of accelerator data on p-p interactions, [10] were able to develop
analytic parametrizations to the energy spectra and production rates of gamma rays from p-p interactions. The \texttt{PionDecay} class uses an implementation of the formulae presented in their paper, and gives the choice of which high-energy model to use (from the parametrization to the different Monte Carlo results) through the \texttt{hiEmodel} parameter.

4. MCMC sampling

The following will briefly describe the implementation of spectral fitting in \texttt{naima}, and a full explanation of MCMC and the sampling algorithm can be found in \cite{11}, and in the documentation of \texttt{emcee}\footnote{http://dan.iel.fm/emcee/current/}, the package used for MCMC sampling \cite{12}.

The measurements and uncertainties in the observed spectrum are assumed to be correct, Gaussian, and independent (note that this is unlikely to be the case, see Section 6 on how this might be tackled in the future). Under this assumption, the likelihood of observed data given the spectral model \( S(\vec{p}; E) \), for a parameter vector \( \vec{p} \), is

\[
L = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left( -\frac{(S(\vec{p}; E_i) - F_i)^2}{2\sigma_i^2} \right),
\]

where \((F_i, \sigma_i)\) are the flux measurement and uncertainty at an energy \( E_i \) over \( N \) spectral measurements. Taking the logarithm,

\[
\ln L = K - \sum_{i=1}^{N} \frac{(S(\vec{p}; E_i) - F_i)^2}{2\sigma_i^2}.
\]

Given that the MCMC procedure will sample the areas of the distribution with maximum value of the objective function, it is useful to define the objective function as the log-likelihood disregarding constant factors:

\[
\ln L \propto \sum_{i=1}^{N} \frac{(S(\vec{p}; E_i) - F_i)^2}{\sigma_i^2}.
\]

The \( \ln L \) function in this assumption can be related to the \( \chi^2 \) parameter as \( \chi^2 = -2\ln L \), so that maximization of the log-likelihood is equivalent to a minimization of \( \chi^2 \).

In addition to the likelihood from the observed spectral points, a prior likelihood factor should be considered for all parameters. This prior likelihood encodes our prior knowledge of the probability distribution of a given model parameter. The combination of the prior and data likelihood functions is passed onto the \texttt{emcee} sampler function, and the MCMC run is started. \texttt{emcee} uses an affine-invariant MCMC sampler that has the advantage of being able to sample complex parameter spaces without any tuning required. In addition, having multiple simultaneous \textit{walkers} improves the efficiency of the sampling and reduces the number of computationally-expensive likelihood calls required.
Figure 1: Diagnostic plot produced by \texttt{naima.plot\_chain} for the sampling of the cutoff energy in the particle distribution. The top-left panel shows the traces for the 32 walkers in gray, with one of them highlighted in red, that can be used to estimate whether the sampling has stabilized around the maximum likelihood parameters. The right panel shows the posterior distribution of the parameter, along with the median (dashed line) and an estimate of the 1\sigma confidence interval (gray band). On the bottom-left, statistics of the parameter distribution, including a median with uncertainties based on the 16th and 84th percentiles, is shown. Note that the parameter is sampled in logarithmic space in this example, and given the label \texttt{log10(cutoff)} \texttt{naima} can identify this and convert it to its value and uncertainty in TeV, resulting in the estimate $E_{cutoff} = 113^{+28}_{-23}$ TeV.

5. Example analysis: hadronic emission from RX J1713–3946

As an example of nonthermal spectral analysis with \texttt{naima}, here we will show the results of inferring the particle distribution parameters of a hadronic population from a spectrum of the shell-type supernova remnant RX J1713–3946 obtained with the H.E.S.S. Cherenkov telescope array \cite{13}. The photon spectrum in the 0.3–100 TeV energy range is well characterized by a power-law with an exponential cutoff, so we will use a similar function for the particle distribution. Even though the leptonic or hadronic origin of the gamma-ray emission from RX J1713–3946 is still under debate \cite{14}, for the sake of example here we will assume an neutral pion decay origin of the VHE gamma-ray emission. Several other examples, with the full source code needed to reproduce them, are available in the \texttt{naima} documentation http://naima.readthedocs.org.

The first step is the definition of the radiative model to be fit, and in this case we will use the \texttt{ExponentialCutoffPowerLaw} particle distribution function and \texttt{PionDecay} radiative model. The spectrum from \cite{13} can be read as a table with \texttt{astropy.io.ascii}, and passed
Figure 2: Distribution of the free model parameters (norm is the particle distribution normalization at 5 TeV in units of TeV$^{-1}$, index is the power law index, and log10(cutoff) is the decimal logarithm of the cutoff energy in units of TeV during the MCMC sampling run.

onto the naima MCMC sampling functions along with the defined model function. We run the sampling with 32 simultaneous walkers (or sampling chains), for 100 steps of burn-in, and 400 steps of run that are saved for later analysis. The resulting sampled chains can be analysed with a set of naima functions that plot diagnostic and results plots. Such a chain diagnostic produced with naima.plot_chain can be seen for the energy of the exponential cutoff in the particle distribution model in Figure 1. Figure 2 shows a corner plot, which plots the distribution for all parameters against each other. It can be seen that there is a strong correlation between the distributions of the particle index and cutoff parameters. Finally, Figure 3 shows a comparison between the observed spectrum and the computed model, including the spread of the spectrum derived from 100 random parameter vectors taken from the MCMC chain, and an inset with the inferred particle energy distribution.

The result of the MCMC run provides estimates of the parameters of the particle distribution function. For this spectrum and radiative model, the particle index is constrained to $s = 1.92 \pm 0.07$, and the cutoff energy is $E_c = 120 \pm 30$ TeV. The MCMC parameter chain can also be used to compute the distribution of quantities derived from the particle spectrum, such as total energy content in protons, which for RX J1713–3946 is constrained to $W_p(E_p > 1.22 GeV) = (1.2^{+0.3}_{-0.17}) \times 10^{50} n_H^{-1} d_{1kpc}^{-2}$ erg, where $n_H$ is the target density and $d_{1kpc}$ is the distance to the source in kpc.

6. Limitations and future development

The main limitation of the approach used by naima for spectral fitting is the assumption of uncorrelated, gaussian errors. Even though this may be incorrect for many spectra, mostly
Figure 3: H.E.S.S. spectrum of RX J1713–3946 [13], computed spectrum from a hadronic model, and residuals of the maximum likelihood model (bottom panel). The thick black line indicates the maximum likelihood spectrum, and the gray lines are 100 samplings of the posterior distribution of the model parameter vector. The inset shows the energy distribution of the proton population in erg versus the proton energy in TeV.

when considering fine structure, it is often the only approach possible when simultaneously fitting published spectra from radio to VHE gamma-rays. When instrument response functions are available, a way to avoid this assumption is to use the sherpa models in naima.sherpa_models.

Future development of the package will focus on:

- Addition of simple particle cooling functions (more complex physics, such as time-dependent particle evolution, should be done on a case-by-case basis).
- Use of naima radiative models in gammapy\(^2\), a Python package for gamma-ray data analysis.

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\(^2\)http://github.com/gammapy/gammapy
References

[1] P. Freeman, S. Doe, and A. Siemiginowska, *Sherpa: a mission-independent data analysis application*, in *Astronomical Data Analysis* (J.-L. Starck and F. D. Murtagh, eds.), vol. 4477 of Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series, pp. 76–87, Nov., 2001. astro-ph/0108426.

[2] Astropy Collaboration et al., *Astropy: A community Python package for astronomy*, A&A 558 (Oct., 2013) A33, [arXiv:1307.6212].

[3] G. R. Blumenthal and R. J. Gould, *Bremsstrahlung, Synchrotron Radiation, and Compton Scattering of High-Energy Electrons Traversing Dilute Gases*, Reviews of Modern Physics 42 (1970) 237–271.

[4] F. A. Aharonian, S. R. Kelner, and A. Y. Prosekin, *Angular, spectral, and time distributions of highest energy protons and associated secondary gamma rays and neutrinos propagating through extragalactic magnetic and radiation fields*, Phys. Rev. D 82 (Aug., 2010) 043002, [arXiv:1006.1045].

[5] D. Khangulyan, F. A. Aharonian, and S. R. Kelner, *Simple Analytical Approximations for Treatment of Inverse Compton Scattering of Relativistic Electrons in the Blackbody Radiation Field*, ApJ 783 (Mar., 2014) 100, [arXiv:1310.7971].

[6] M. G. Baring, D. C. Ellison, S. P. Reynolds, I. A. Grenier, and P. Goret, *Radio to Gamma-Ray Emission from Shell-Type Supernova Remnants: Predictions from Nonlinear Shock Acceleration Models*, ApJ 513 (Mar., 1999) 311–338, [astro-ph/9810158].

[7] E. Haug, *Bremsstrahlung and pair production in the field of free electrons*, Zeitschrift Naturforschung Teil A 30 (Sept., 1975) 1099–1113.

[8] S. R. Kelner, F. A. Aharonian, and V. V. Bugayov, *Energy spectra of gamma rays, electrons, and neutrinos produced at proton-proton interactions in the very high energy regime*, Phys. Rev. D 74 (Aug., 2006) 034018, [astro-ph/0606058].

[9] T. Kamae, N. Karlsson, T. Mizuno, T. Abe, and T. Koi, *Parameterization of γ, e+−, and Neutrino Spectra Produced by p-p Interaction in Astronomical Environments*, ApJ 647 (Aug., 2006) 692–708, [astro-ph/0605581].

[10] E. Kafexhiu, F. Aharonian, A. M. Taylor, and G. S. Vila, *Parametrization of gamma-ray production cross sections for p p interactions in a broad proton energy range from the kinematic threshold to PeV energies*, Phys. Rev. D 90 (Dec., 2014) 123014, [arXiv:1406.7369].

[11] D. J. C. Mackay, *Information Theory, Inference and Learning Algorithms*. Oct., 2003.

[12] D. Foreman-Mackey, D. W. Hogg, D. Lang, and J. Goodman, *emcee: The MCMC Hammer*, PASP 125 (Mar., 2013) 306–312, [arXiv:1202.3665].

[13] F. Aharonian et al., *Primary particle acceleration above 100 TeV in the shell-type supernova remnant RX J1713.7-3946 with deep HESS observations*, A&A 464 (Mar., 2007) 235–243, [astro-ph/0611813].

[14] S. Gabici and F. A. Aharonian, *Hadronic gamma-rays from RX J1713.7-3946?*, MNRAS 445 (Nov., 2014) L70–L73, [arXiv:1406.2322].

[15] J. D. Hunter, *Matplotlib: A 2d graphics environment*, Computing In Science & Engineering 9 (2007), no. 3 90–95.