First steps towards SimProp-Sirente

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Outline

Why SimProp Sirente?

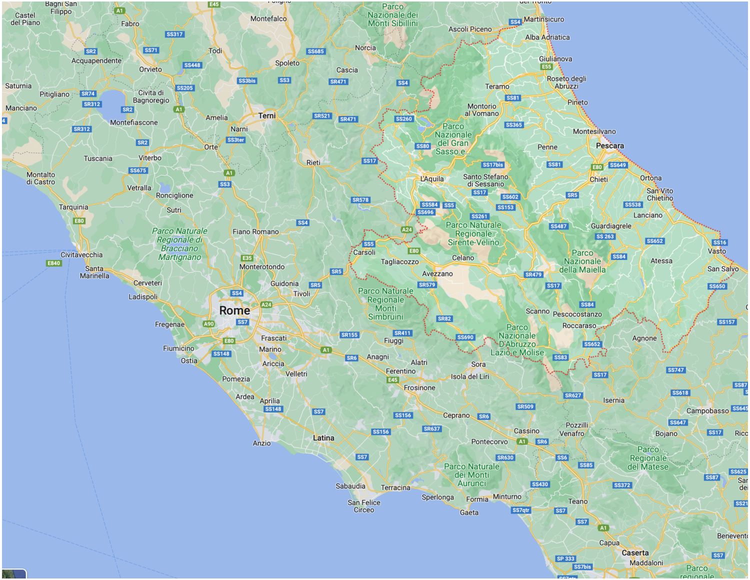
- SimProp is a public code to perform Monte Carlo simulations of ultra-high energy cosmic ray propagation
- Latest stable version available at https://augeraq.sites.lngs.infn.it/SimProp/
- Great legacy in PAO Collaboration [arXiv:2305.16693]
- Private versions extended to study in-source interactions [arXiv:2209.08593] and large-scale magnetic fields []
- At least two (public) codes to validate each other (see, e.g., CMS and ATLAS...)
- SimProp-Sirente is the next release, written in modern C++, and designed to take advantage of most of open-source best practices.
- My full gratitude to CRPropa developers (see our HERMES paper [arXiv:2105.13165])

Quentin Remy, Andy Strong, Luigi Tibaldo and Silvia Vernetto for useful conversations and insights. We further thank the CRPropa development team for providing a good role model for developing a high-quality C++ astrophysical code and making it available as free software, aside from the fact that HERMES borrows CRPropa's implementation of magnetic fields and abstract vector and grid classes. A.D. acknowledges the P.O.I.N.T. Association, Križevci, Croatia for providing computational resources needed for testing HERMES. This work was funded through Grants ASI/INAF No. 2017-14-H.O. D. Gaggero has received

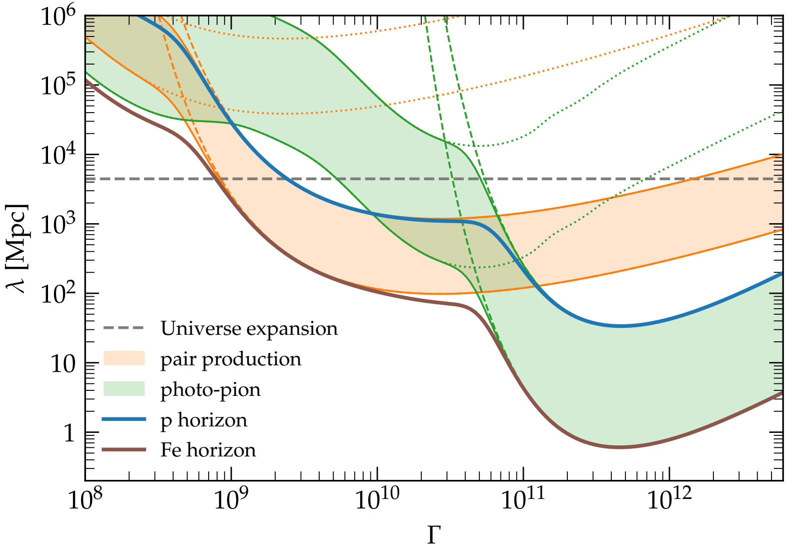
Why SimProp Sirente?

- Public repository: https://github.com/carmeloevoli/SimProp-Sirente
- CI: https://github.com/carmeloevoli/SimProp-beta/actions/workflows/ci.yml
- Issue tracking
- TDD: make test
- Modular structure (see later)
- Version tagging
- Documentation: https://simprop.github.io/
- Dependency manage
- Python wrapper (not in first priority)

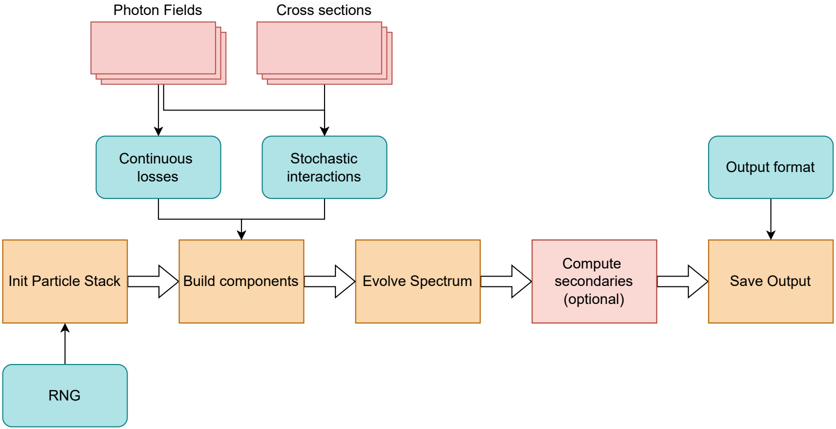
Why SimProp Sirente?



UHECR processes and horizons

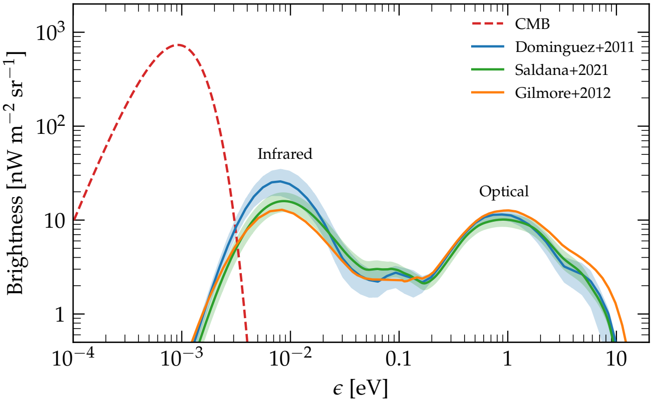


What is SimProp-Sirente?



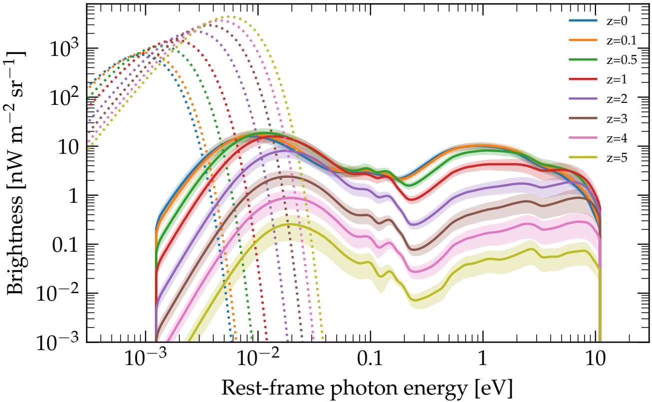
- Each module can be easily replaced (e.g., BSM extensions)
- Open and fully tested: https://github.com/carmeloevoli/SimProp-Sirente/

Photon-fields at $z = 0$ (local)



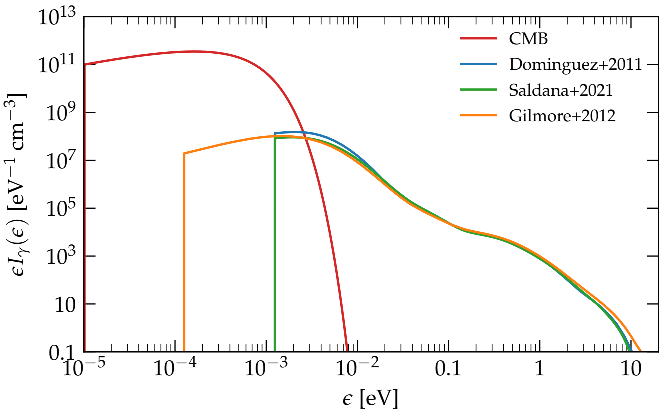
- EBL models implemented are
  1. Dominguez et al., 2011, ...
  2. Gilmore et al., 2012, ...
  3. Saldana-Lopez et al., 2021, ...
  4. For comparison, CMB at $z = 0$ is a black-body with $T \simeq 2.725$ K.

The EBL comoving energy density



- The EBL comoving photon density, defined as $n_\gamma(\epsilon)(1+z)^{-3}$, is shown at different redshifts according to the Saldana2012 model.

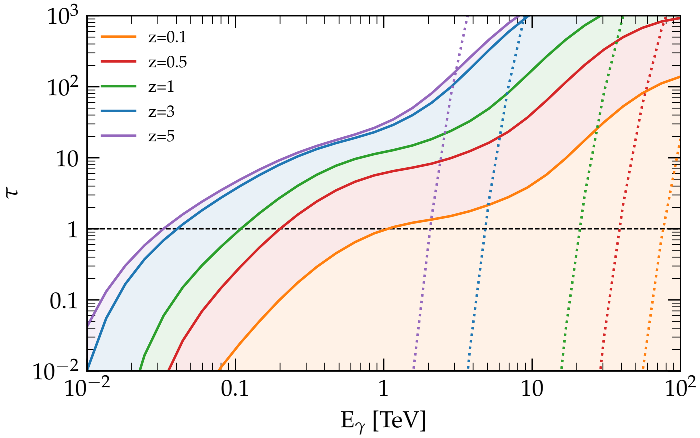
The photon integral



- A relevant integral, analytical for CMB and pre-computed for each EBL model, is

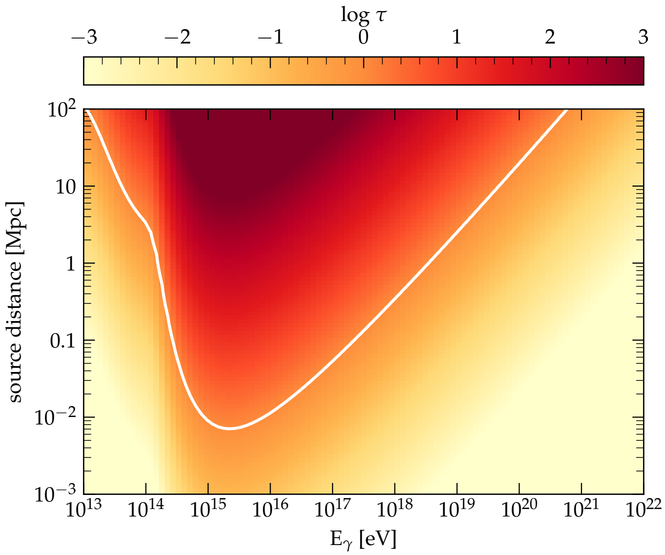
$$I_\gamma(\epsilon_{\rm min}) = \int_{\epsilon_{\rm min}}^{\infty} d\epsilon \frac{n_\gamma(\epsilon)}{\epsilon^2}$$

γ-rays Optical Depth in Sirente



The optical depth computed for the Saldana-Lopez EBL model (solid lines). Dotted lines show the absorption due to CMB photons.

γ-rays Optical Depth in Sirente



Continuous energy losses

- The equation of motion in redshift for a particle with Lorentz factor Γ is given by

$$-\frac{1}{\Gamma}\frac{d\Gamma}{dz} = \frac{1}{1+z} + \left|\frac{dt}{dz}\right| \sum_i \beta_i(\Gamma, z) \tag{1}$$

where $\beta_i(\Gamma, z)$ describes each energy loss rate which depends on the photon background and the factor $1/1+z$ is accounting for the adiabatic losses due to the Universe expansion.

- The generic loss rate β_i is given by

$$\beta_i(\Gamma, z) = \frac{c}{2\Gamma^2}\int_{\epsilon'_{\rm th}}^{\infty} d\epsilon' \epsilon' Y(\epsilon')\sigma_A(\epsilon') I_\gamma(\epsilon'/2\Gamma) \tag{2}$$

where

$$I_\gamma(\epsilon_{\rm min}) = \int_{\epsilon_{\rm min}} d\epsilon \frac{n_\gamma(\epsilon, z)}{\epsilon^2} \tag{3}$$

and Y is the inelasticity, σ_A is the cross-section on nuclei, ϵ is the photon energy in the interaction rest-frame, ϵ' is in the the nucleus rest frame (NRF), and n_γ is the proper photon density.

- The energy-loss length is defined as $c/\beta(\Gamma, z)$

Pair-production losses

- Following Chodorowski et al., 1992 ApJ, for pair-production the rate can be obtained as:

$$\beta_{pp}(\Gamma, z) = \left(\frac{Z^2}{A}\right) \frac{\alpha c r_0^2}{\Gamma} \frac{m_e}{m_p} (m_e c^2) \int_2^\infty d\kappa \, n_\gamma \left[\epsilon(\kappa), z\right] \frac{\phi(\kappa)}{\kappa^2} \quad (4)$$

where $\kappa \equiv 2\Gamma\epsilon/m_e c^2$ and $\phi(\kappa)$ is a parametrized function given by their Eq.s (3.14) and (3.18).

- The energy threshold for pair-production is

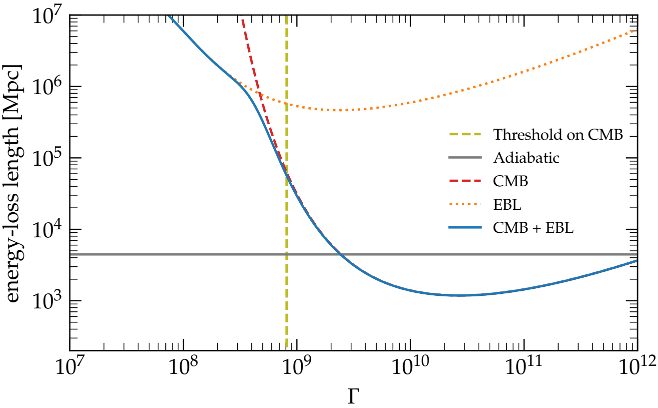
$$E_p \epsilon_{\rm th} = \frac{m_e^2 + 2 m_e m_p}{(1 - \cos\theta)} \to \frac{m_e^2 + 2 m_e m_p}{2} \quad (5)$$

following

$$\Gamma \epsilon_{\rm th} = \frac{m_e^2 + 2 m_e m_p}{2 m_p} = m_e \left(1 + \frac{m_e}{2 m_p}\right) \sim m_e \to \frac{\epsilon'_{\rm th}}{m_e} = 2 \quad (6)$$

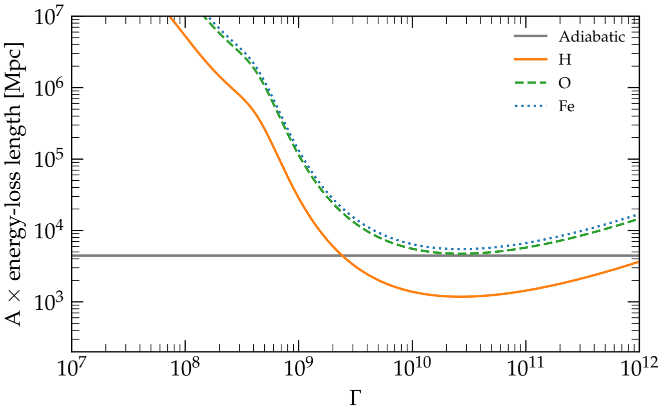
- Similar to CRPropa3 here.

Pair-production losses



- The energy-loss length $\lambda(\Gamma, z=0)$ for protons due to pair-production at $z=0$.
- The energy threshold for pair-production is $E_{\text{th}} = \frac{m_e^2 + 2 m_e m_p}{\epsilon(1 - \cos\theta)} \simeq \frac{m_e^2 + 2 m_e m_p}{\epsilon}$

Pair-production losses on nuclei



- The energy-loss length $\lambda(\Gamma, z = 0)$ for different nuclei due to pair-production, scales roughly with Z

Pion-production losses

- Pion production can be described either as a continuous loss or stochastic interaction (see later)
- The loss rate β_π is given by

$$\beta_\pi(\Gamma) = \frac{c}{2\Gamma^2} \int_{\epsilon'_{\rm th}}^{\infty} d\epsilon' \epsilon' Y(\epsilon') \sigma_A(\epsilon') I_\gamma(\epsilon'/2\Gamma) \tag{7}$$

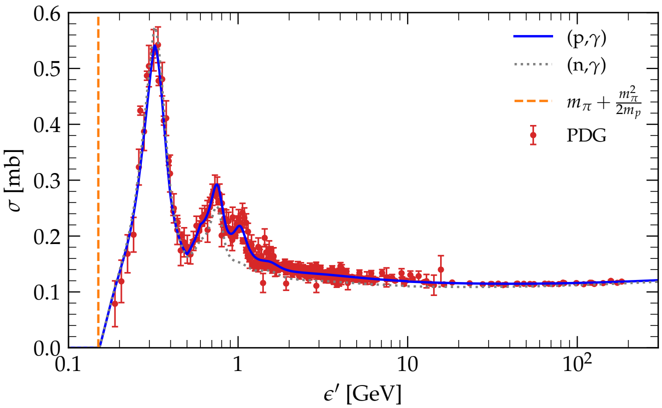
where Y is the inelasticity, σ_A is the pion-production cross-section for a nucleus of mass A

- We assume the superposition model thereby

$$\boxed{\sigma_A = Z\sigma_p + (A-Z)\sigma_n}$$

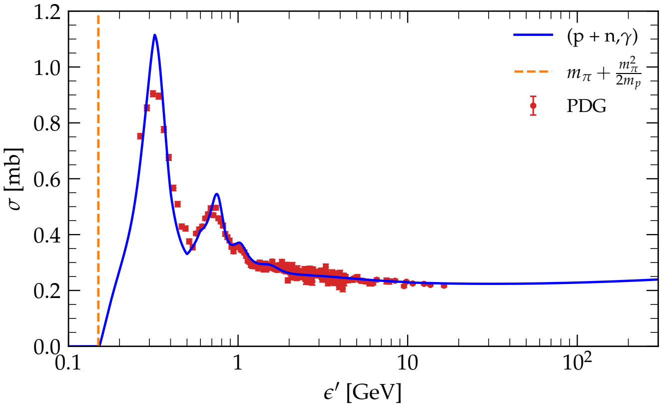
- The threshold energy is $\epsilon'_{\rm th} = m_\pi + \frac{m_\pi^2}{2m_p}$

Photo-pion production cross section



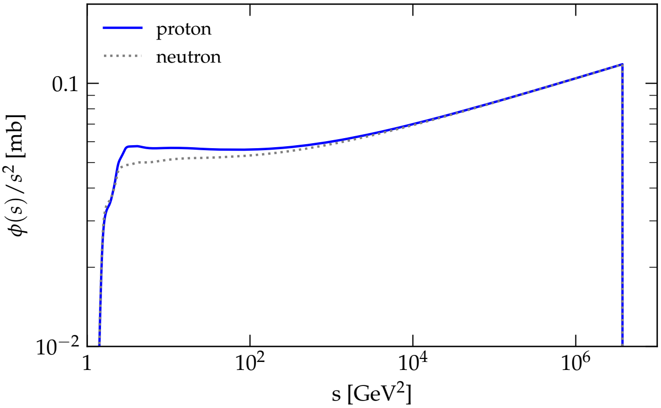
- Photo-pion cross-section for $p + \gamma$ and $n + \gamma$ as a function of ϵ' against PDG data on total pγ cross-section (elastic part is negligible)
- The relation between s and ϵ' is given by $s = m_p^2 + 2E_p\epsilon(1 - \cos\theta) = m_p^2 + 2m_p\epsilon'$
- Notice the difference with neutron, well explained in Morejon et al.

Photo-pion production cross section



- The superposition model: p + n cross-section against d data

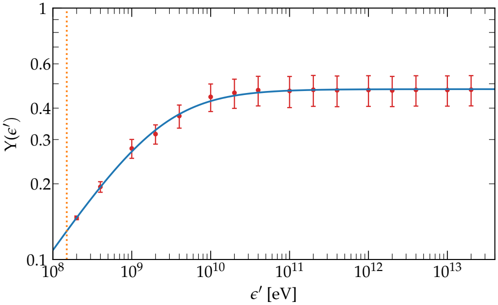
Photo-pion production cross section



Pre-computed for efficiency purpouses:

$$\phi(s) = \int_{s_{\text{th}}}^{s} (s' - m_p^2)\sigma(s')ds' \tag{8}$$

Pion-production losses



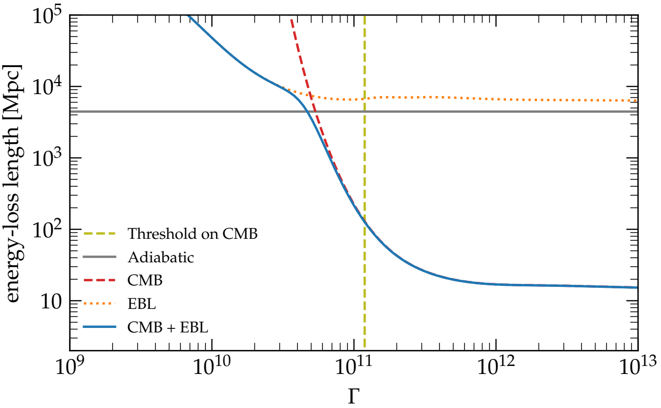
- the inelasticity is defined as the mean energy fraction lost per interaction

$$Y(\epsilon') = \left\langle \frac{E_{\mathrm{in}} - E_{\mathrm{out}}}{E_{\mathrm{in}}} \right\rangle$$

- here is simulated with Sophia and fitted with a broken power-law:

$$Y(x) = Y_\infty \frac{(x/x_{\mathrm{b}})^\delta}{\left[1 + (x/x_{\mathrm{b}})^{\delta/s}\right]^s}$$

Pion-production losses



- The energy-loss length $c/\beta(\Gamma, z=0)$ for protons due to pion-production at $z = 0$.
- The energy threshold for pair-production is $E_{\text{th}} = \frac{m_\pi^2 + 2m_\pi m_p}{2\epsilon(1-\cos\theta)} \simeq \frac{m_\pi^2 + 2m_\pi m_p}{4\epsilon}$

Pion-production energy losses

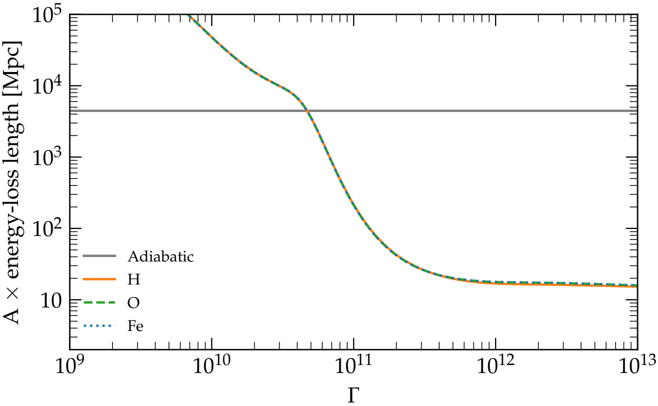


Figure: Pion-production losses for different species normalized to A.

- Differences due to p-n asymmetry are negligible at this level.

Photo-pion production

- Photo-pion production can be treated also stochastically.
- The total interaction rate is given by

$$\mathcal{R}_\pi = \mathcal{R}_{\pi,\text{CMB}} + \mathcal{R}_{\pi,\text{EBL}} \tag{9}$$

  where we consider separately the contribution by CMB and EBL to the total rate.
- In both cases the interaction rate is computed as

$$\boxed{\mathcal{R}_{\pi,i} = \frac{c}{2\Gamma^2} \int_{\epsilon'_{\text{th}}}^{\infty} d\epsilon' \epsilon' \sigma_A(\epsilon') I_{\gamma,i}(\epsilon_{\text{min}})}$$

  where $\epsilon_{\text{min}} = \epsilon'/2\Gamma$

Pion-production mean free path

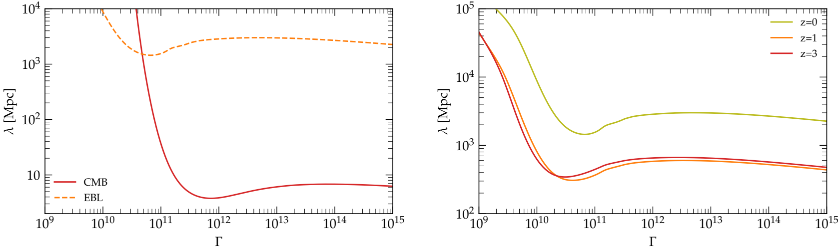
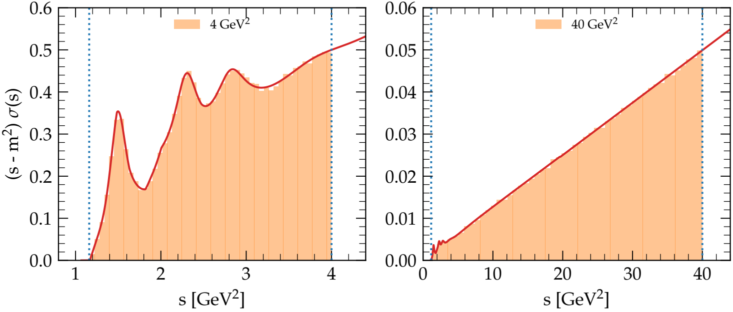


Figure: Pion-production interaction lenghts.

Photo-pion: sampling the invariant mass energy



- The generator function for s is:

$$P(s) \propto (s - m_p^2)\,\sigma(s) \quad \longrightarrow \quad r\phi(s_{\rm max}) = \phi(s) \tag{10}$$

with s lies in the range $s_{\rm th} = (m_p + m_\pi)^2$ and $s_{\rm max} = m_p^2 + 2(1 - \cos\theta_{\rm max})E_p\epsilon = m_p^2 + 4E_p\epsilon$

- Where we defined

$$\phi(s) = \int_{s_{\rm th}}^{s} (s' - m_p^2)\sigma(s')ds' \tag{11}$$

Optimization: $\phi(s)$ is pre-tabulated.

- We test here the cases with $s_{\rm max} = 4$ GeV^2 and $s_{\rm max} = 40$ GeV^2

Photo-pion: sampling the background photon energy

- We pick ϵ by using the distribution function:

$$P(\epsilon, z) \propto \epsilon^{-2} n_\gamma^p(\epsilon, z)\phi[s_{\text{max}}(\epsilon)] \tag{12}$$

  which becomes using comoving photon densities:

$$P(\epsilon, z) \propto \epsilon^{-2} n_\gamma^c\left(\frac{\epsilon}{1+z}, z\right)\phi[s_{\text{max}}(\epsilon)] \tag{13}$$

- The CDF method implies:

$$r\int_{\epsilon_{\text{min}}}^{\epsilon_{\text{max}}} d\epsilon' P(\epsilon') = \int_{\epsilon_{\text{min}}}^{\epsilon} d\epsilon' P(\epsilon') \tag{14}$$

- About ϵ_{min} : it is the minimum between $\epsilon_{\text{min}}^{\gamma}$ and $\epsilon_{\text{min}}^{\text{th}}$ where is derived by imposing $s_{\text{max}} = s_{\text{th}}$:

$$\epsilon_{\text{min}}^{\text{th}} = \frac{m_\pi^2 + 2m_p m_\pi}{4E_p} \tag{15}$$

Photo-pion: sampling the background photon energy

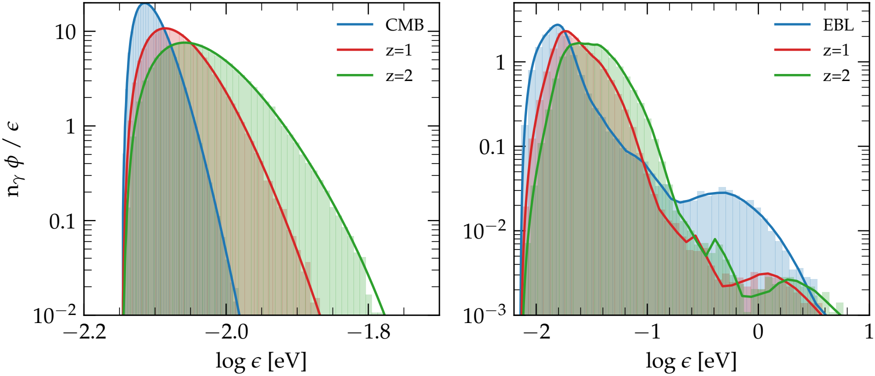


Photo-pion: sampling the pion energy

- Having generated s we can compute the outgoing pion energy E_π (LAB frame):

$$E_\pi = \frac{E_p}{\sqrt{s}} E^*_\pi (1 + \beta^*_\pi \mu^*_\pi) \quad (16)$$

where E^*_π, β^*_π, and μ^*_π are the pion energy, velocity and angle of emission in the CMF, respectively

$$\mu^*_\pi = \text{rand}[-1, 1] \quad (17)$$

$$E^*_\pi = \frac{s - m_p^2 + m_\pi^2}{2\sqrt{s}} \quad (18)$$

$$p^*_\pi = \frac{\sqrt{[s - (m_\pi + m_p)^2][s - (m_\pi - m_p)^2]}}{2\sqrt{s}} \quad (19)$$

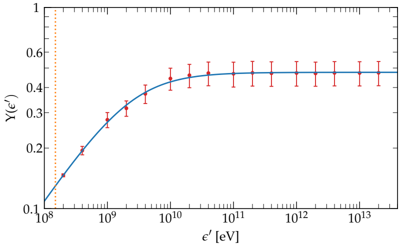
- In Sirente μ^*_π is extracted from $dP/dt(\mu)$
- Finally, a neutral pion π^0 is generated with probability $2/3$ and a charged pion $\pi^\pm$ with probability $1/3$:

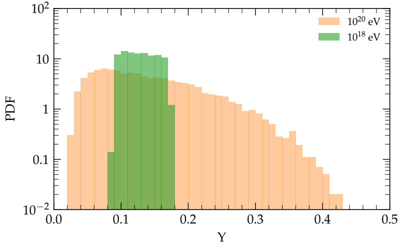
$$p(n) + \gamma \to p(n) + \pi^0 + \ldots \qquad \text{p} = 2/3 \quad (20)$$

$$p + \gamma \to n + \pi^+ + \ldots \qquad \text{p} = 1/3 \quad (21)$$

$$n + \gamma \to p + \pi^- + \ldots \quad (22)$$

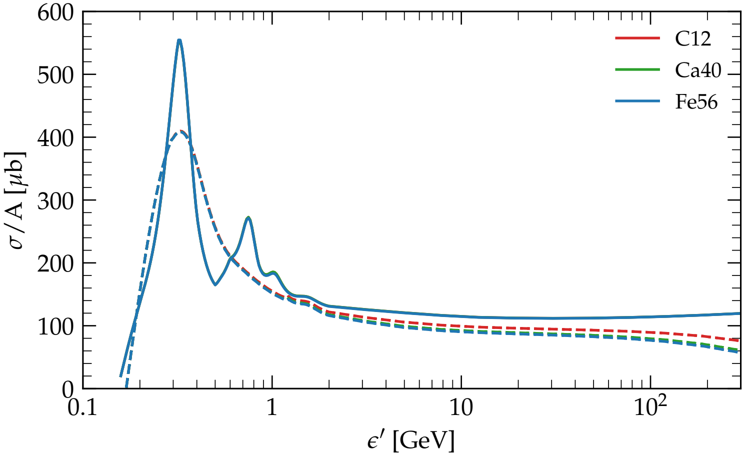
Photo-pion: sampling the pion energy



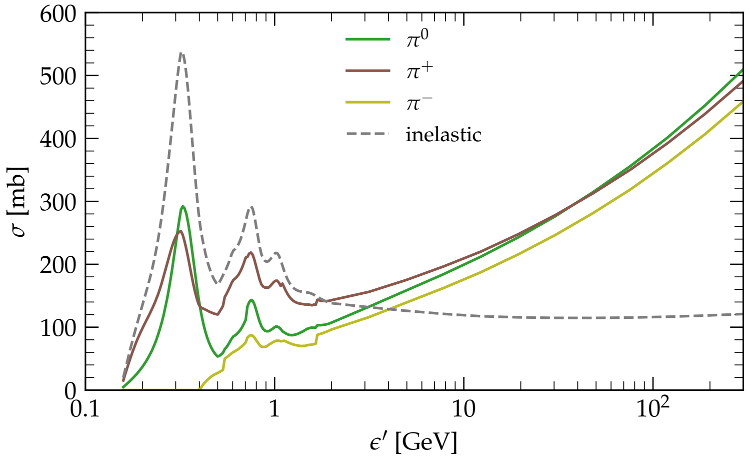


The inelasticity of the π-production process is $\sim$13% in the energy range of interest.

Pion-production in AstroPhoMes



Pion-production in AstroPhoMes



▷ Inclusive production cross-section: are they useful for multi-π production?

Initial particle distribution function

SimProp provides 3 different builders for the initial particle distribution:

- SingleParticleBuilder, same z and Γ for all the particles
- SingleSourceBuilder, same z and spectrum $\propto \Gamma^{-\alpha}$
- SourceEvolutionBuilder, see next slide

Initial particle distribution function

Assuming as injection source term:

$$Q(\Gamma, z) \propto \Gamma^{-\alpha} \mathrm{e}^{-\Gamma/\Gamma_c} (1+z)^m$$

Particle are generated with a distribution written as:

$$p(\Gamma, z) \propto \Gamma^{-1} \otimes (1+z)^{-1}$$

and with a weight

$$w(\Gamma, z) = Q/p = \Gamma^{1-\alpha} \mathrm{e}^{-\Gamma/\Gamma_c} \frac{(1+z)^{m+1}}{E(z)}$$

- Generate energies from Γ_{min} to Γ_{max}:

$$\frac{\Gamma}{\Gamma_{\mathrm{min}}} = \left(\frac{\Gamma_{\mathrm{max}}}{\Gamma_{\mathrm{min}}} \right)^r \quad (23)$$

- Generate positions from z_{min} to z_{max}:

$$\frac{1+z}{1+z_{\mathrm{min}}} = \left(\frac{1+z_{\mathrm{max}}}{1+z_{\mathrm{min}}} \right)^r \quad (24)$$

where r is a random variable uniformly distributed $\in [0, 1[$.

Initial particle distribution function

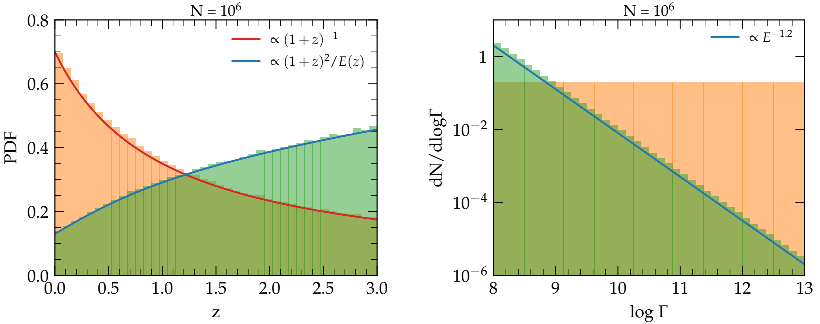


Figure: Histograms of $N = 10^6$ simulated particle assuming $z_{\text{min}} = 0$, $z_{\text{max}} = 3$, $m = 2$, $\alpha = 2.2$, and $\Gamma_c = \infty$. In orange the simulated particle distribution, in green after re-weighting.

Continuous evolution in redshift

- We first consider the case without stochastic interactions. Using the formalism before, the evolution equation can be written:

$$\frac{1}{\Gamma}\frac{d\Gamma}{dz} = -\sum_i \beta_i(\Gamma, z)\frac{dt}{dz} \tag{25}$$

- integrated in a redshift step $\Delta z = z_1 - z_0$:

$$\int_{z_0}^{z_1} dz \frac{1}{\Gamma}\frac{d\Gamma}{dz} = -\int_{z_0}^{z_1} dz \underbrace{\sum_i \beta_i(\Gamma, z)\frac{dt}{dz}}_{Y(z)} \tag{26}$$

- The LHS is integrated exactly while the RHS numerically with Simpson's rule (notice $z_1 < z_0$):

$$\ln\left(\frac{\Gamma_1}{\Gamma_0}\right) \simeq -\frac{\Delta z}{6}\left[Y(z_0) + 4Y(z_0 - \Delta z/2) + Y(z_0 - \Delta z)\right] \equiv -\delta(\Delta z) \tag{27}$$

- Finally we rewrite the latter as:

$$\Gamma_1 = \Gamma_0\left[1 - \Delta\Gamma(\Delta z)\right] \tag{28}$$

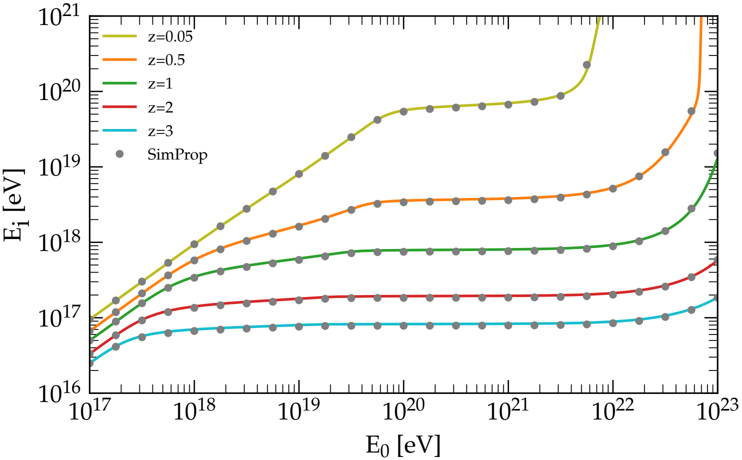
  which defines:

$$\Delta\Gamma(\Delta z) \equiv 1 - \exp\left[-\delta(\Delta z)\right] \tag{29}$$

- How to choose Δz? We decide a maximum allowed fractional change for Γ and we invert

$$\Delta\Gamma_c = \Delta\Gamma(\Delta z) \tag{30}$$

Continuous evolution in redshift



The algorithm

Basically the propagation algorithm must handle two kind of processes: a stochastic process and the continuous losses.

The proposed algorithm is similar to GEANT4 and it works as follows:

- A distance to the next reaction is selected according to an exponential distribution. This is realized by using a uniformly distributed random number $0 < r < 1$ via:

$$\Delta l_s = -\lambda_s \ln(1-r) \tag{31}$$

  where λ_s is obtained as the sum of all the stochastic processes $\lambda_s^{-1} = \sum_i \lambda_{s,i}^{-1}$.

- Another distance is given by imposing a maximum allowed fractional energy loss due to continuous losses:

$$\int_{z_0}^{z_0-\Delta z_c} dz \frac{d \ln \Gamma}{dz} = \delta \longrightarrow \int_{z_0}^{z_0-\Delta z_c} dz \beta(\Gamma, z) \frac{dt}{dz} = \delta \tag{32}$$

  where β is given by the sum of all losses and $\delta \simeq 10\%$ is the maximal allowed fractional energy loss.

- If $\Delta l_s \leq \Delta l_c$ the particle is propagated over the path length Δl_s. That means that first energy losses are computed over Δl_s and after that it performs an interaction.

- Otherwise, that is $\Delta l_s > \Delta l_c$, the particle is propagated over the distance Δl_c over which continuous losses are applied without interactions.

Comparison with the analytical solution

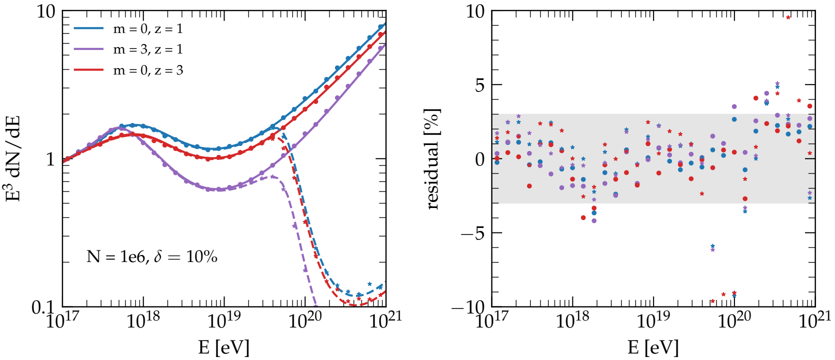


Figure: .

Performances

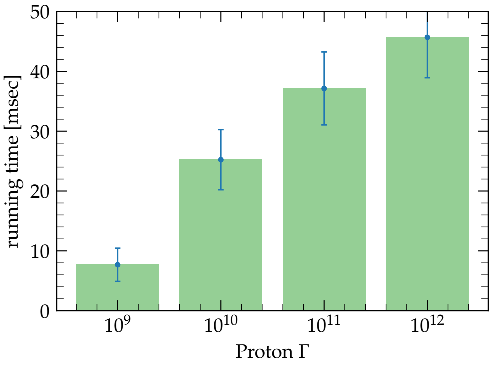


Figure: Particles injected at $z = 1$. My laptop.

Table of Contents

Main differences with v2r4 so far...

- Implemented new EBL model
- Added EBL to γ-pair production
- Improved sampling of incoming photon
- Improved γ-pion production: differentiate proton and neutron cross-section in the SPM
- Improved γ-pion production: implementing realistic angular distribution for outgoing pion
- A more efficient evolution algorithm

How to reach the Sirente peak?

- ☐ Implement cosmogenic neutrinos
- ☐ Test cosmogenic neutrinos against analytical solution
- ☐ Implement multi-π production (using AstroPhoMes?)
- ☐ Documentation, documentation, documentation. . .

Thank you!

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- slides available at: https://zenodo.org/communities/carmeloevoli_talks