**κmonty: a Monte Carlo Compton scattering code including non-thermal electrons**

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**ABSTRACT**

Low-luminosity active galactic nuclei are strong sources of X-ray emission produced by Compton scattering originating from the accretion flows surrounding their supermassive black holes. The shape and energy of the resulting spectrum depend on the shape of the underlying electron distribution function (DF). In this work, we present an extended version of the GRMONTY code, called κMONTY. The GRMONTY code previously only included a thermal Maxwell–Jüttner electron DF. We extend the GRMONTY code with non-thermal electron DFs, namely the κ and power-law DFs, implement Cartesian Kerr–Schild coordinates, accelerate the code with MPI, and couple the code to the non-uniform adaptive mesh refinement grid data from the general relativistic magnetohydrodynamics code BHAC. For the Compton scattering process, we derive two sampling kernels for both DFs. Finally, we present a series of code tests to verify the accuracy of our schemes. The implementation of non-thermal DFs opens the possibility of studying the effect of non-thermal emission on previously developed black hole accretion models.

**Key words:** plasmas – radiation mechanisms: non-thermal – radiative transfer – software: development – software: public release

**1 INTRODUCTION**

Active Galactic Nuclei (AGN) are strong sources of radiation over the full range of the electromagnetic spectrum, from radio up to γ-rays. The emission is expected to originate from a relativistic plasma flow close to these galaxies’ central supermassive black holes. Low-luminosity AGN (LLAGN) are well-known sources of X-ray emission. Sagittarius A* (SgrA*), the black hole in the centre of the Milky Way, shows X-ray variability on the time-scales of hours (Baganoff et al. 2003; Eckart et al. 2004). Messier 87 (M87), now famous for the first picture of a black hole shadow by the Event Horizon Telescope Collaboration (EHT Collaboration 2019a), is also active in X-ray emissions (Wilson & Yang 2001; Marshall et al. 2002; Perlman & Wilson 2005; Prieto et al. 2016), and shows X-ray variability on time-scales of days (Harris et al. 2009). One channel to generate the X-ray emission is via inverse Compton (IC) scattering.

To compute synthetic spectra of LLAGN, a variety of Monte Carlo (MC) codes have been developed (see e.g. Stern et al. 1995; Laurent & Titarchuk 1999; Böttcher & Liang 2001; Böttcher, Jackson & Liang 2003; Yao et al. 2005; Schnittman, Krolik & Hawley 2006; Schnittman & Krolik 2009; Dolence et al. 2009; Ryan, Dolence & Gammie 2015; Narayan et al. 2016; Zhang, Dowčiak & Bursa 2019; Mościbrodzka 2020). A large subset of the code uses the input from general relativistic magnetohydrodynamics (GRMHD) global simulations of weakly radiating accretion flows. In these simulations, the electron energy distribution function (DF) is not explicitly computed. GRMHD codes use a fluid approximation that only contains information on the bulk properties of the plasma and no information on the DF. A fluid approach also does not intrinsically contain collisionless effects. However, accretion flows in LLAGN like M87* and SgrA* have a mean free path for the electrons that is much larger than the actual system size, making them effectively collisionless, and deviations from thermality are, therefore, to be expected. Magnetic reconnection, dissipation of turbulent energy, shocks, and/or other plasma instabilities that influence the shape of the electron DF are, in general, poorly resolved, and sub-grid models for electron heating and acceleration have to be invoked. Successful attempts to resolve magnetic reconnection in global two-dimensional GRMHD simulation have been performed by Ripperda, Bacchini & Philippov (2020), Nathaniel et al. (2020) and, more recently, in three-dimensional simulations by Ripperda et al. (2022).

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These models further strengthen the need for non-thermal electron DFs. 

One of the first attempts to model non-thermal emission from SgrA* with radiatively inefficient accretion flows (RIAF) models were made by Özel, Psaltis & Narayan (2000). Later works using RIAF models include Yuan, Quataert & Narayan (2003), among others. Semi-analytical models of RIAFs, including jets, were developed by Broderick et al. (2015), who included electron acceleration via gap acceleration. Works by Quataert (2004) and Chan et al. (2015b, a) showed that for Sgr A* X-ray bremsstrahlung emission is non-negligible. More recently, dynamical models based on GRMHD simulations were published by Chan et al. (2009), Ball et al. (2016), Mao, Dexter & Quataert (2017), Chael, Narayan & Sadowski (2017), Davelaar et al. (2018b, 2019), Chatterjee et al. (2020), Cruz-Osorio et al. (2022), and Fromm et al. (2022). A common conclusion in all these works is that non-thermal electrons enhance the amount of near-infrared (NIR) and radio emission. However, most of these works rely on general relativistic ray tracing (GRTT) methods, so X-ray emission generated via IC is neither included nor approximated.

The importance of including X-ray emission in the current models used within the EHT community was shown by Mościbrodzka, Falcke & Shiokawa (2016). For M87, the X-ray emission is a clear discriminator between models. If the electron temperature in the accretion disc is too high, the model easily overproduces the observed X-ray flux. However, the electron DF was assumed to be a thermal Maxwell–Jüttner (MJ) distribution.

The X-ray emission is expected to be produced by synchrotron self-Comptonization. This process starts with electrons in the accretion flow that gyrate around magnetic field lines and produce emission via synchrotron emission. The emitted photons are then upscattered by the hot relativistic electrons inside the flow to X-ray and γ-ray energies via Compton scattering. Since the amount of energy that is transferred from the electron to the photon (∆E) depends on the Lorentz factor of the electron (γ) as ∆E ∝ γ^2, the resulting spectra of the upscattered photons depend on the choice of the DF. It is expected that adding accelerated particles will increase the total X-ray luminosity of the source since electrons with large γ factors and photons with larger frequencies (NIR) are present. Observed X-ray flares in AGN, and other astrophysical sources, are indicators of ongoing particle acceleration to rule out potential acceleration mechanisms models that include the generation of X-ray emission based on non-thermal electrons are needed.

In this work, we present kMONTY, a new flavour of the MC code GROMONTY originally developed by Dolence et al. (2012). GROMONTY is a general relativistic MC radiative transport code developed to compute spectra of accreting black holes. A more recent version called RADMOL (Moscibrodzka 2020) also included polarization and was extended to include non-thermal electron DFs (Moscibrodzka 2022). We made three large adaptations to the original Dolence et al. (2012) code. First, we coupled our code to the non-uniform adaptive mesh refinement (AMR) grid data structure of the GRMHD code BHAC (Porth et al. 2017; Olivares et al. 2019, www.bhac.science), in a similar manner as we described in Davelaar et al. (2019). Secondly, we implemented the fit formula for the emission and absorption coefficients as obtained by Pandya et al. (2016) for the initial seed photons. Thirdly, we derived and implemented semi-analytical sampling algorithms for the κ- and power-law DF. The methods described in this work were used to compute the X-ray Spectral Energy Distributions (SEDs) of the κ-DF based models in the Event Horizon Telescope results of Sagittarius A* (Event Horizon Telescope Collaboration 2022).

In Section 2, we explain our sampling routine and describe the set-up used. In Section 3, we perform a variety of code tests. We discuss and summarize our results in Section 5.

2 METHODS

In this section, we present the additions we made to the original GROMONTY code (Dolence et al. 2009). Our new code kMONTY includes the κ distribution and power-law distribution to study accelerated particle emission and is MPI and OPENMP optimized. At first, the superphotons, a packet of photons with weight w, where the weight w is the number of real photons represented by the superphoton, are initialized by either thermal, κ, or power-law-based emission coefficients. As they propagate through the plasma, the total intensity decreases due to absorption. Scattering events are selected based on the mean free path length. If a photon is selected for scattering, the electron has to be drawn from the relevant DF. In this section, we summarize the new features of kMONTY, which are new sets of coordinates, new DFs, and the coupling to non-uniform data formats. For a complete explanation of the initialization, integration, and scattering of the superphotons, see the paper by Dolence et al. (2009). In this section, we will give a global summary of the different aspects of the code, and we will explain in detail our modifications.

2.1 Geodesic integration

The trajectory of the superphotons is computed by solving the geodesic equation,

\[ \frac{d^2 x^\mu}{d\lambda^2} = -\Gamma^\mu_{\nu\lambda} \frac{dx^\nu}{d\lambda} \frac{dx^\lambda}{d\lambda}, \]

(1)

where \( \Gamma^\mu_{\nu\lambda} \) are the Christoffel symbols, and \( \lambda \) the affine parameter. The Christoffel symbols depend on derivatives of the metric and are given by,

\[ \Gamma^\alpha_{\mu\nu} = \frac{1}{2} g^{\alpha\rho} \left[ \partial_\mu g_{\rho\nu} + \partial_\nu g_{\rho\mu} - \partial_\rho g_{\mu\nu} \right]. \]

The Christoffel symbols are either provided analytically or can be computed by computing the metric derivatives using a second-order finite difference method.

2.1.1 Kerr–Schild coordinates

A rotating black hole is described by the Kerr metric (Kerr 1963). In spherical Kerr–Schild (KS) horizon penetrating coordinates, the non-zero covariant components of the metric\(^2\) \( g_{\mu\nu} \) are given by

\[ g_{\phi\phi} = g_{\phi\phi} = \left( 1 - \frac{2r}{\Sigma} \right), \]

(3a)

\[ g_{t\phi} = g_{\phi t} = \frac{-2ra \sin^2 \theta}{\Sigma}, \]

(3b)

\[ g_{\phi\phi} = \frac{\Sigma}{\Delta}, \]

(3c)

\[ g_{t \phi} = \frac{\Sigma}{\Delta}, \]

(3d)

\[ g_{\phi\phi} = \left( r^2 + a^2 \sin^2 \theta \right) \sin^2 \theta. \]

(3e)

\(^2\)We use the metric signature (−, +, +, +).
for a black hole with unitary mass $M = 1$ and angular momentum $J$, where $a_\ast = J/(2Mr)$ is the dimensionless spin parameter, $\Sigma = r^2 + a_\ast^2 \cos^2 \theta$, and $\Delta = r^2 - 2r + a_\ast^2$.

The GRMHD code used in this work BHAC primarily uses for the EHT GRMHD library (EHT Collaboration 2019b) modified KS (MKS) coordinates where the $r$ and $\theta$ coordinates are modified. The coordinates $(t, X_1, X_2, X_3)$ are related to standard KS via

$$t = t,$$

$$r = \exp(X_1),$$

$$\theta = X_2 + \frac{\hbar}{2} \sin(2X_2),$$

$$\phi = X_3.$$

This results in a grid that is logarithmic spaced in radius and concentrated towards the mid-plane in $\theta$, set by the $h$ parameter. Transforming the metric to MKS is done via multiplication of the metric terms with the non-zero elements of the Jacobian,

$$\partial r/\partial x_1 = r,$$

$$\partial \theta/\partial X_2 = 1 + h \cos(2X_2).$$

### 2.1.2 Cartesian Kerr-Schild coordinates

We extended the code to include Cartesian KS (CKS) coordinates, which relate to spherical KS coordinates via

$$t = t,$$

$$x = r (\cos(\phi) + a_\ast \sin(\phi)) \sin(\theta),$$

$$y = r (\sin(\phi) - a_\ast \cos(\phi)) \sin(\theta),$$

$$z = r \cos(\theta).$$

The covariant CKS metric, $g_{\mu\nu}$, is given by (Kerr 1963)

$$g_{\mu\nu} = \eta_{\mu\nu} + f l_{\mu} l_{\nu},$$

where $\eta_{\mu\nu}$ is the Minkowski metric and is given by $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$, and

$$f = \frac{2r^3}{r^4 + a_\ast^2 z^2},$$

$$l_{\nu} = \left(1, \frac{r x + a_\ast y}{r^2 + a_\ast^2}, \frac{r y - a_\ast x}{r^2 + a_\ast^2}, \frac{z}{r} \right).$$

where $r$ is given by

$$r^2 = \frac{R^2 - a_\ast^2 + \sqrt{(R^2 - a_\ast^2)^2 + 4a_\ast^2 z^2}}{2},$$

and

$$R^2 = x^2 + y^2 + z^2.$$  

In the limit of $R \gg a_\ast$, the radius $r \rightarrow R$. The contravariant metric is defined as

$$g^{\mu\nu} = \eta^{\mu\nu} - f l^{\mu} l^{\nu},$$

where $l^{\nu}$ is given by

$$l^{\nu} = \left(-1, \frac{r x + a_\ast y}{r^2 + a_\ast^2}, \frac{r y - a_\ast x}{r^2 + a_\ast^2}, \frac{z}{r} \right).$$

### 2.2 Distribution functions

For the DF, we either use an MJ DF, a $\kappa$-DF, or a power-law DF. All three DFs are isotropic.

The MJ DF is given by

$$\frac{dn_e}{dy} = n_e \frac{\gamma^2 \beta}{\Theta_e \kappa(a_\ast)} \exp \left(-\frac{\gamma}{\Theta_e} \right),$$

where $\gamma$, $e$, and $\Theta_e$ are the Lorentz factor of the electrons, $\kappa$, and $\Theta_e$ is the dimensionless electron temperature, $N_\ast$ is the modified Bessel function of the second kind. For the thermal DF, the emission coefficients used in $\kappa$-Monty can be found in Leung, Gammie & Noble (2011).

The $\kappa$-DF is used to describe the particle population of a variety of space plasma, such as the solar wind (Decker & Krinigis 2003), coronal flares on the Sun (Livadiotis & McComas 2013), turbulent flows (Kunz, Stone & Quataert 2016), and jets (Davelaar et al. 2018b). X-ray spectra generated based on this DF could, therefore, be of interest to a broad range of astrophysical problems. The DF in relativistic form (Xiao 2006) is given by,

$$\frac{dn_e}{dy} = n_e N \sqrt{y^2 - 1} \left(1 + \frac{\gamma - 1}{\kappa w} \right)^{-(\kappa + 1)},$$

where the $\kappa$-parameter sets the power-law index via $\kappa = p + 1$, $w$ is the width of the DF, and $N$ is a normalization constant. In the $\kappa$ case, the normalization constant $N$ is not known analytically and is, therefore, when needed, computed during run time with a $g_{\ast 1}$ integrator by demanding that

$$\int_1^\infty \frac{dn_e}{dy} dy = 1.$$  

The emission coefficients for the $\kappa$-DF can be found in Pandya et al. (2016).

Finally, the power-law DF is given by

$$\frac{dn_e}{dy} = n_e \frac{(p - 1) \gamma^{p-1}}{\left(\gamma_{\text{min}}^{1-p} - \gamma_{\text{max}}^{1-p}\right)},$$

where $p$ is the power-law index. The DF function is non-zero only when $y$ is between $\gamma_{\text{min}}$ and $\gamma_{\text{max}}$. The emission coefficients for the power-law DF can be found in Pandya et al. (2016).

All three DFs are shown in Fig. 1. The dependence of the DF in the code can be found in three places; the emission coefficients, the cross-section for scattering, and the sampling of the DF if a scattering event takes place. In the remainder of this section, we will explain what changes we made to the code for each of these.

### 2.3 Emission coefficients

For the emission coefficients, the code uses fit formulas from Leung, Gammie & Noble (2011) for the thermal DF and $\kappa$ and power law from Pandya et al. (2016). The fit formulas for the $\kappa$ coefficients are only valid for $\kappa < 7.5$, they do not recover the thermal DF in the limit of $\kappa \rightarrow \infty$.

### 2.4 Cross-sections

The cross-section for an IC scattering is dependent on the local electron population, both the energy budget as well as the shape of the distribution. The cross-section is given by

$$\alpha_\nu = n_e \sigma_\nu,$$
where \( \sigma_h \) is defined as the ‘hot cross-section’,

\[
\sigma_h = \frac{1}{n_e} \int d^3p \frac{d\sigma}{dp}(1 - \mu \beta) \sigma, \tag{18}
\]

where \( n_e \) is the number density of electrons, \( \frac{d\sigma}{dp} \) is the electron DF, \( \mu \) is the cosine of the angle between the superphoton momentum and the electron momentum, and \( \beta \) is the electron speed in the plasma frame, and \( \sigma \) the Klein–Nishina total cross-section.

From the cross-section, the code computes the scattering opacity \( \tau_s \), via \( \tau_s = \alpha \epsilon \hbar |e| c^2 |\Delta\lambda| \), where \( \alpha \) is the extinction coefficient given by \( \alpha = n_e \sigma_h \). The total probability for a scattering event is then given by \( p = 1 - e^{-\beta \tau_s} \), where \( \beta \) is a bias factor that enhances the scattering probability, as introduced in Dolence et al. (2009). This bias is then counteracted by splitting the scattered superphoton into an unscattered superphoton with weight \( bw \) and an unscattered remnant superphoton with weight \( (1 - \beta)w \). In this work, \( \kappa_{\text{MONTY}} \) only exploits the original GRMONTY bias function given by \( b = \Theta_j / (\Theta_j) \), where \( (\Theta_j) \) is the volume-averaged dimensionless electron temperature. More fine-tuned bias functions, such as the one in \( \text{igrm} \) (Wong et al. 2022), are not explored since the main focus of this work is the numerical algorithms for non-thermal DF sampling.

### 2.5 Sampling routines

The outcome of a Compton scattering event between a superphoton, and an electron depends on the superphoton’s wavevector and the electron’s four velocity. The electrons are, in the case of GRMHD models, coupled to the plasma parameters of the protons, which are approximated by a fluid description. We therefore, only know ensemble averages. To be able to select a single electron, we need a sampling algorithm that, given a set of plasma variables, draws a \( \gamma \) factor based on the chosen DF, in the original GRMONTY, the procedure from Canfield, Howard & Liang (1987) is used for the MJ DFs. Therefore, only new samplers for the \( \kappa \)-DF and power-law DF are needed.

#### 2.5.1 A semi-analytical sampling routine for the \( \kappa \)-distribution function

For the \( \kappa \)-DF, we will generalize the procedure from Canfield et al. (1987) for the \( \kappa \)-DF. The relativistic \( \kappa \)-DF as function of velocity \( \beta = \frac{v}{c} \) is given by

\[
f(\beta, w) = N_w b^2 \gamma \left( 1 + \frac{\gamma - 1}{\kappa w} \right)^{-\kappa - 1}, \tag{19}
\]

with \( \gamma = (1 - \beta^2)^{-1/2} \).

To sample electrons based on this DF, we derive a MC-based scheme. We first introduce a random variable \( y \) that is coupled to \( \gamma \) and \( w \)

\[
y = \gamma - \frac{1}{w}, \tag{20}
\]

and transform our probability density function (pdf) accordingly

\[
f(y, w) = f(\beta, w) \frac{\partial y}{\partial \beta}, \tag{21}
\]

\[
f(y, w) = N \frac{w}{\sqrt{2\pi w^2}} \sqrt{1 + 0.5w^2(1 + w^2)} \left( 1 + \frac{\gamma}{\kappa w} \right)^{-\kappa - 1}. \tag{22}
\]

Following the procedure by Canfield et al. (1987), we can split our pdf into a series of pdfs after multiplying with

\[
1 = 1 + \frac{w}{0.5w^2} \frac{1}{1 + \sqrt{0.5w^2}}, \tag{23}
\]

\[\text{Figure 1. The MJ, } \kappa, \text{ and power-law DFs. The MJ DF is shown for a dimensionless electron temperature of } \Theta_e = 10 \text{, the } \kappa \text{ DF is shown with } \kappa = 4.0, \text{ and } w = 2.5 \text{, and the power-law DF is shown with } \rho = 3, \gamma_{\text{max}} = 25, \text{ and } \gamma_{\text{max}} = 10^3.\]

to obtain

\[
f(\gamma, w) = \frac{\sqrt{w}y^2}{2} \left( 1 + \sqrt{0.5w}y \right) \left( 1 - 0.5w^2 \right) \left( 1 + wy \right) ^{-\kappa - 1} \times \left( 1 + \frac{\gamma}{\kappa w} \right)^{-\kappa - 1} N \frac{w}{2\sqrt{2\pi w^2}} \sqrt{1 + 0.5w^2} \frac{1}{1 + \sqrt{0.5w^2}}. \tag{24}
\]

this can be rewritten as

\[
f(\gamma, w) = \left( y^2 + \sqrt{0.5w}y^3 + wy^4 + w\sqrt{0.5w}y^4 \right) \times \left( 1 + \frac{\gamma}{\kappa w} \right)^{-\kappa - 1} N \frac{w}{2\sqrt{2\pi w^2}} \sqrt{1 + 0.5w^2} \frac{1}{1 + \sqrt{0.5w^2}}. \tag{25}
\]

We can now identify two different functions that are the core of the sampling routine, a rejection function \( H_j(w, y) \) and a sampling function \( G_j(w, y) \) such that

\[
f(\gamma, w) = G_j(w, y)H_j(w, y). \tag{26}
\]

The sampling function is given by

\[
G_j(w, y) = \sum_{j=3}^{6} \pi_j(w)g_j y, \tag{27}
\]

and consists of a series of sample coefficients \( g_j(y) \) and probability coefficients \( \pi_j(w) \). The sampling coefficients are given by

\[
g_j(y) \equiv \frac{y^{j-1}}{n_j} \left( 1 + \frac{\gamma}{\kappa w} \right)^{-\kappa - 1}, \tag{28}
\]

where \( n_j \) is a normalization constant obtained by integrating

\[
\int_0^\infty n_j g_j(y) dy = n_j. \tag{29}
\]

Performing these four integrals, we get

\[
n_3 = \sqrt{\kappa} \sqrt{\Gamma \left( -\frac{1}{2} + \kappa \right)}, \tag{30}
\]

\[
n_4 = \frac{\kappa}{2(-1 + \kappa)}, \tag{31}
\]

\[
n_5 = \frac{3\sqrt{\kappa} \Gamma \left( -\frac{1}{2} + \kappa \right)}{8\Gamma(\kappa)}, \tag{32}
\]

\[
n_6 = \frac{\kappa^2}{2 - 3\kappa + \kappa^2}. \tag{33}
\]
where $\Gamma(\kappa)$ is the Gamma function. The analytical solutions for the normalizations are only valid in the case that $\kappa > 2$. The probability coefficients are given by

\begin{align}
\pi_3(w) &= \frac{n_3}{S_3(w)}, \\
\pi_4(w) &= \frac{n_4 \sqrt{0.5w}}{S_4(w)}, \\
\pi_5(w) &= \frac{n_5 \sqrt{w}}{S_5(w)}, \\
\pi_6(w) &= \frac{n_6 \sqrt{0.5w}}{S_6(w)},
\end{align}

with

\[ S_i(w) = n_3 + n_4 \sqrt{0.5w} + n_5 w + n_6 w \sqrt{0.5w}. \]

The rejection function $H_3(w, y)$ is then defined as

\[ H_3(w, y) = \frac{N_1 \sqrt{2w} \sqrt{1 + 0.5wy^2}}{S_3(w)} \frac{\sqrt{1 + 0.5wy^2}}{1 + \sqrt{0.5wy}}. \]

The rejection criterion is then, similarly to Canfield et al. (1987),

\[ h(w, y) = \frac{\sqrt{1 + 0.5wy^2}}{1 + \sqrt{0.5wy}}. \]

The rejection criterion can be generalized even more when one also wants to add an exponential cut-off to the $\kappa$-DF:

\[ f_{x_i\sim\text{const}}(y) = f_x(y) e^{-\frac{y^2}{\text{const}}}. \]

We can contract the exponential cut-off into the rejection criterion. Since if we encounter a large value of $y$, it will decrease the likelihood of being accepted by the sampling routine,

\[ h(w, y) = \frac{\sqrt{1 + 0.5wy^2}}{1 + \sqrt{0.5wy}} e^{-\frac{y^2}{\text{const}}}. \]

The procedure for sampling the $\kappa$-DF is therefore

1. Draw a random number $x_1$.
2. If $x_1 < \pi_f$,
3. Find $y$ according to $g_f(y)$.
4. Draw a random number $x_2$.
5. Accept $y$ when $x_2 < h(w, y)$.

This rejection constraint is, as mentioned in Canfield et al. (1987), very efficient because for large values of $w$ or small values of $w$, $h(w, y)$ asymptotes to one.

The last step in this derivation of the sampling routine is to find a procedure for the third step, find $y$ according to $g_f(y)$. In the case of a thermal DF, the $g_f(y)$ are $\chi^2$ functions that can be sampled with standard $\chi^2$ library functions. In the case of the $\kappa$-DF, this is less straightforward. To sample $g_f(y)$, we make use of the fact that the cumulative distribution functions (CDFs) belonging to the pdfs $g_f(y)$ are monotonically increasing functions between zero and one. These CDFs can be obtained by integrating $g_f(y)$ from zero to $y$.

\[ F_f(y) = \int_0^y g_f(y) \, dy. \]

Performing these four integrals result in

\[ F_{12}(y) = 1 - \left( y^2 + \frac{\kappa}{\kappa} \right)^{-\frac{\kappa}{\kappa}} \Gamma(\kappa) \times \left[ -\kappa F_1 \left( 1, -\kappa - 1/2; 1/2; -y^2/\kappa \right) + y^2 (2\kappa + 1) + k \right], \]

\[ F_{13}(y) = \frac{\left( \frac{\kappa}{\kappa} \right)^{-\frac{\kappa}{\kappa}} \Gamma(\kappa)}{3\sqrt{\pi} y \sqrt{\kappa}} \left( \frac{y}{\kappa} + \frac{3}{2} \right) \times \left[ 3\kappa \left( F_1 (1, -\kappa - 1/2; 1/2; -y^2/\kappa) - 1 \right) + (1 - 4\kappa^2)^{\frac{\kappa}{2}} - 3\kappa (2\kappa + 1) y^2 \right], \]

\[ F_{14}(y) = \frac{\left( y^2 + y^2 + 2y^2 + 2 \kappa \right)^{-\frac{\kappa}{\kappa}}}{2\kappa^2}, \]

where $F_1$ is the second-order hypergeometrical function of the first kind. We can then find a $y$ by using an inverse transform sampling method.

(i) draw a number $u$ from a uniform distribution $[0, 1]$. (ii) solve such that $F_f(y) = u$, where $F_f(y)$ is the CDF of $g_f(y)$. (iii) $y$ is sampled according to $g_f(y)$.

To solve step two, we implemented a Brent root-finding algorithm. For the implementation of the algorithm, special attention has to be paid to the hypergeometrical functions encountered in the CDFs. For negative integer values of the arguments of the hypergeometrical function, it is impossible to use the series expansion form, as implemented in the $\chi^2$ library. We, therefore, pre-computed a table of the hypergeometrical function as a function of $\kappa$ and $y$ with MATHEMATICA, which is read in by $\kappa$-MONTY. The resulting table is then interpolated with a first-order interpolation scheme.

2.5.2 The $\kappa \to \infty$ limit

In the case that $\kappa \to \infty$, we expect our derived sampler to recover the original sampler by Canfield et al. (1987).

First, we check that equation 28 recovers the pdfs in Canfield et al. (1987) by taking $\lim_{\kappa \to \infty} g_f(y)$, resulting in

\[ g_f(y) = \lim_{\kappa \to \infty} \frac{\kappa}{y^2} \left( 1 + \frac{y^2}{\kappa} \right)^{-\frac{\kappa}{2}} = \frac{\kappa}{y^2} \frac{n_3}{n_2}. \]

\[ g_f(y) = \lim_{\kappa \to \infty} \frac{\kappa}{y^2} \left( 1 + \frac{y^2}{\kappa} \right)^{-\frac{\kappa}{2}} = \frac{\kappa}{y^2} \frac{n_3}{n_2}. \]

\[ g_f(y) = \lim_{\kappa \to \infty} \frac{\kappa}{y^2} \left( 1 + \frac{y^2}{\kappa} \right)^{-\frac{\kappa}{2}} = \frac{\kappa}{y^2} \frac{n_3}{n_2}. \]

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Here, we used that $\lim_{\kappa \to \infty} (1 + y/\kappa)^{-\kappa/2} = e^y$. The resulting $g_f(y)$ in this limit are consistent with Canfield et al. (1987).

Secondly, we check $\lim_{\kappa \to \infty} n_j(y)$, which are given by

\[ n_3 = \lim_{\kappa \to \infty} \sqrt{\kappa} \sqrt{\pi} \Gamma \left( \frac{3}{2} + \kappa \right) = \sqrt{\pi}/4, \]

\[ n_4 = \lim_{\kappa \to \infty} \frac{\kappa}{2(1 - 1/\kappa)} = 1/2, \]

\[ n_5 = \lim_{\kappa \to \infty} 3\sqrt{\pi} \Gamma \left( \frac{3}{2} + \kappa \right) = 3\sqrt{\pi}/8, \]

\[ n_6 = \lim_{\kappa \to \infty} 2 - 3\kappa + \kappa^2 = 1. \]

Here, we use that $\lim_{\kappa \to \infty} \kappa^{n/2} \Gamma(-n/2 + \kappa)/\Gamma(\kappa) = 1$. The resulting formulas are consistent with Canfield et al. (1987). Our last test is to check the rejection criterion, which is already in the same
form and is equal to the one by Canfield et al. (1987) in the case that \( \lim_{k \to -\infty} w = \Theta_c \), which is the case if \( w = \frac{1}{k} \Theta_c \).

2.5.3 A numerical sampling routine for the \( \kappa \)-distribution function

We also implemented a more mundane rejection sampling method for drawing electrons from the \( \kappa \)-distribution. This implementation can be found in the public code IGRMonty\(^3\) as well as in kMonty. The expression \( \partial \gamma / \partial \gamma = 0 \) is solved for \( \gamma \), hereafter \( \gamma_{\text{max}} \). Fiducial \( \gamma \) are then drawn uniformly in logspace between

\[
\begin{align*}
\gamma_{\text{min}} &= \text{MAX}(1, 0.01 \times \Theta_c), \\
\gamma_{\text{max}} &= \text{MAX}(100, 1000 \times \Theta_c),
\end{align*}
\]

where these parameters are chosen to ensure both accuracy and computational efficiency for all \( \Theta_c \). New \( \gamma \) are drawn until the condition \( \gamma f_k(\gamma) \gamma_{\text{max}} f_k(\gamma_{\text{max}}) > \text{rand} \), where rand is a uniformly distributed random number in the range \([0, 1]\) and the extra factors of \( \gamma \) arise from drawing fiducial \( \gamma \) uniformly in logspace.

This procedure generalizes to any realistic electron DF, including the MJ distribution, but also, e.g. anisotropic DFs, DF based on charged test particles in MHD, or DFs based on first-principle Particle-in-Cell (PIC) simulations. Compared to the Canfield et al. (1987) prescription for sampling MJ, this rejection sampling approach leads to only modestly \((-20\%\) percent) slower calculation wallclock times.

2.5.4 Power-law distribution

For the power-law DF, the procedure is much more trivial. The CDF is, in this case, given by

\[
F(\gamma) = \int_{\gamma_{\text{min}}}^{\gamma} \frac{(p - 1)\gamma^{-p}}{\gamma_{\text{min}}^{1-p} - \gamma_{\text{max}}^{1-p}} \, d\gamma = \frac{\gamma_{\text{min}}^{1-p} - \gamma^{1-p}}{\gamma_{\text{min}}^{1-p} - \gamma_{\text{max}}^{1-p}}. \tag{58}
\]

Since this CDF can be inverted analytically, we can use an inverse sampling method. We first pick a random number \( x \) between zero and one, and \( \gamma \) can then be found by computing the inverse of equation (58) and setting \( F(\gamma) = x \),

\[
\gamma = ((1 - x)\gamma_{\text{min}}^{1-p} + x\gamma_{\text{max}}^{1-p})^{1/(1-p)}. \tag{59}
\]

2.6 Interface with BHAC

The Black Hole Accretion Code (BHAC; Porth et al. 2017; Olivares et al. 2019) is a finite-volume code that solves the covariant GRMHD equation using a \( 3+1 \) split. The code is capable of using AMR grids that, during runtime, based on user-defined criteria, can refine or derefine the grid. BHAC outputs the GRMHD data in an octree structure. We fully interfaced kMonty to this data format similarly to Davelaar et al. (2019), and made kMonty capable of initializing superphotons and performing IC in a non-uniform grid.

3 CODE VERIFICATION

To verify our implementation of the described methods, we performed extensive code tests. In this section, we describe the performed tests and discuss the results.

\[^{3}\text{https://github.com/AFD-Illinois/igrmonty}\]

\[^{4}\text{https://github.com/jordydavelaar/raptor}\]
Figure 3. Output of the power-law sampler compared to the analytical form, $p = 4.0, p = 3.0, \text{ and } p = 2.0$. For all three cases, we set $\gamma_{\text{min}} = 1.0$ and $\gamma_{\text{max}} = 10^3$. The deviation between the sampler and the exact form is for almost the entire range less than 1 per cent, except for large $\gamma$ values, due to the steep power law populating the high end of the DF is affected by MC noise.

\begin{align}
  g_{\phi\phi} &= r^2, \\
  g_{\phi\phi} &= r^2 \sin^2(\theta). \\
  \rho &= \rho_0, \\
  \Theta_\gamma = \Theta_{\gamma,0}, \\
  B' &= 0. \\
  B'' &= B_0 \cos \theta, \\
  B'' &= -B_0 \sin \theta/r, \\
  B^\theta &= 0.
\end{align}

The solution is specified by constants $\rho_0, R_0, \Theta_{\gamma,0}$, and $B_0$, along with an outer boundary to the domain $R_{\text{out}}$. $\rho_0$ is given in terms of a characteristic Thomson depth $r_0$:

$$
\rho_0 = \frac{r_0}{\sigma_T R_0 L N},
$$

where $L$ is the code length unit conversion and $N$ is the electron number density unit conversion. $B_0$ is expressed in terms of the plasma $\beta$ at $r = 0, \beta_0$:

$$
B_0 = \sqrt{\frac{2 P_e}{\rho_0}},
$$

where $P_e$ is the gas pressure. We set the adiabatic index to $\gamma_{\text{adiab}} = 13/9$, and the ratio between the proton and electron temperature is set to be $T_{\text{rel}} = 3.0$.

3.2.1 Comparison with RAPTOR

To check whether the implementation of the emission coefficients is correct, we compute the SED without Compton scattering of the uniform sphere with $\kappa$ MONTY and RAPTOR. RAPTOR (Bronzwaer et al. 2018; Davelaar et al. 2018a; Bronzwaer et al. 2020) is a GRRT code that solves the covariant radiation transport equation in curved space-time. GRRT methods are intrinsically different from MC methods since they use bundles of rays. This makes them ideal for computing synthetic images since only a small portion of the sky is covered by a camera. The camera consists of pixels, and every pixel is assigned an initial wavevector used to solve the geodesic equation backwards in time. Along these geodesics, the unpolarized radiation transport equation is solved.

The set-up and code-specific parameters for both $\kappa$ MONTY as well as RAPTOR are shown in Table 1. The results of this test can be seen in Fig. 4. All three cases show minor discrepancies between the two codes except for the low-frequency part of the spectrum, which is dominated by MC noise. The thermal case shows deviations at the highest frequencies as well. The source becomes optically thin at these frequencies, and the emission region shrinks. The electrons responsible for this emission are at the exponential tail of the DFs, affecting the sampling.

<table>
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3.2.2 Comparison with IPOLE-IL

As an additional independent test to validate both $\kappa$ MONTY as well as RAPTOR, we also cross-compared the output of $\kappa$ MONTY with the IPOLE-IL ray tracing code (Mościbrodzka & Gammie 2018; Wong et al. 2022). This test is identical to the test with RAPTOR presented in the previous subsection. The result can be seen in Fig. 5, and the agreement between the two codes is identical to the test with RAPTOR.

3.2.3 Compton scattering test

To test the implementation of the non-thermal DFs within the Compton scattering module, we cross-compared a semi-analytical implementation with a numerical one in IGRMONTY. The camera is positioned at a distance of $10^2\mathcal{L}$, and we compute spectra for three inclinations $30^\circ, 60^\circ, 90^\circ$. The full set of parameters is similar to the ones shown in Table 1, except that $N_\rho = 3, N_\phi = 1$. And we use folding around the equator, meaning bins in the half-sphere above and below the equator are averaged to increase statistics.

The results of this comparison can be seen in Fig. 6. There is clear consistency between the two methods, with a relative difference of less than 1 per cent for most of the SED. The MC noise grows at high frequencies due to the low probability of double-scattering events. To test the convergence of this test, we performed multiple runs with different amounts of initial superphotons. The convergence can be seen in the right panel of Fig. 6. There is a clear $\sqrt{N}$ convergence visible, as would be expected of an MC code.

3.3 GRMHD test

A more challenging test is performed by comparing the synchrotron part of the SED between $\kappa$ MONTY and RAPTOR computed from a snapshot of a GRMHD simulation. The simulation, in CKS coordinates, is the same as that presented in Davelaar et al. (2019) and Olives et al. (2019). The initial condition of this simulation is a Fishbone & Moncrief (1976) torus with black hole spin parameter $a_\ast = 15/16$, inner radius $6GM/c^2$, pressure maximum at $12GM/c^2$, and adiabatic index $\gamma = 4/3$. The initial magnetic field profile is a single poloidal loop that follows isocontours of the density profile. The initial torus is weakly magnetized and set by the ratio between the maximum magnetic pressure $P_{\text{mag,max}}$ and maximum gas pressure $P_{\text{max}}$ and is set to be $P_{\text{max}}/P_{\text{mag,max}} = 100$.

Since the GRMHD simulation used does not include electron thermodynamics, we use a parametrization for the electron temperature

$$\Theta_e = \frac{U(\gamma - 1)m_p}{\rho m_e(T_{\text{ext}} + 1)},$$

where $U$ is the internal energy, $m_p$ the proton mass, $m_e$ the electron mass, and $T_{\text{ext}}$ the ratio between the proton to electron temperature which we set to $T_{\text{ext}} = 3.0$. To impose charge neutrality of the plasma, we set the electron number density equal to the proton number density.

The GRMHD simulation is scale-free from code to c.g.s. units. Besides the aforementioned length and time unit, also a mass unit $\mathcal{M}$ is needed. The length and time units are given by the black hole length and gravitational time-scales, $r_g = GM_{\text{BH}}/c^2$ and $t_g = r_g/c$, while the mass unit sets the energy content of the simulation and is tightly related to the mass accretion rate via $M = M_{\text{inj}}\mathcal{M}/T$. To convert the plasma variable to c.g.s. units, the following conversion factors are used: $\rho_0 = \mathcal{M}/L^3$, $u_0 = \rho_0 c^2$, and $B_0 = c\sqrt{4\pi\rho_0}$.

The test-specific parameters for the camera, DF, and GRMHD parameters can be seen in Table 1. Only the inner 40$r_g$ of the GRMHD domain is used to limit the field of view needed and speed up the convergence of the MC solution.

The results of this test can be seen in Fig. 7. For all three DFs, the error is close to 1 per cent in most frequency bins. For the thermal case at high frequency, the error grows at high frequencies, similar to the uniform sphere test. All three DFs show less agreement at lower frequencies (around $10^{10}$ Hz), due to opacity effects.

4 CODE PERFORMANCE AND AVAILABILITY

Since the convergence of an MC simulation scales with $\sqrt{N}$, with $N$ the amount of superphotons, it is computationally demanding to
acquire a fully converged solution. To accelerate the convergence, GRMONTY was parallelized with OPENMP, allowing it to run on multiple cores on a single node. To improve our code performance even further, we parallelized GRMONTY with MPI, which allows us to run over many nodes. We identified two potential ways to MPI parallelize our computations. One could either distribute the GRMHD domain over all the available MPI processes and trace superphotons through the domain, this could lead to substantial communication overhead when superphotons leave/enter the domain of a processor, or would require a very labour intensive implementation where batched superphotons are sent and received with non-blocking MPI.

Alternatively, one could launch independent MPI instances that all have the full domain in memory and at termination, sum all the resulting spectra. The first option has the benefit that it is memory efficient. However, scaling is limited to the IO overhead as the domain per MPI instance gets smaller. The second option is more memory demanding but is trivial to implement and is easily scalable to large numbers of nodes as long as the domain fits within the memory per MPI task. A typical 256\(^3\) simulations takes about five Gigabytes of memory, which allows for this implementation strategy, for high-resolution simulations either the first method or a hydro OPENMP + MPI implementation should be explored. For \(k\)MONTY, we opted for the second parallelization strategy. In the remainder of this section, we test our implementation for scalability and performance.

The code is publicly available on GitHub.\(^5\) To test the performance of \(k\)MONTY, we ran a BHAC MKS GRMHD snapshot with scattering for the \(k\)-DF and thermal-DF. First, we varied the number of initial superphotons to test for the solution’s self-convergence. The resulting spectra for \(N = (10^6, 10^7, 10^8, 10^9)\) can be seen in the left panel of Fig. 8. The right panel shows the convergence rate, which shows a \(\sqrt{N}\) scaling. Secondly, we ran the code on varying amounts of nodes to test our code’s scalability. For this test, we used nodes with 128 AMD Rome cores with a total processing power per node of 4.6 teraflops. We compiled the code with the intel compiler and standard intel optimization flags. We varied the number of nodes from 1 to 40 nodes. Again, we use the GRMHD set-up with scattering and start the code with \(N = 10^8\) superphotons per core. The scaling is shown in Fig. 9, and shows an evident linear scaling. Overall we achieve a speed of a few thousand superphotons per second per core, although note that this highly depends on the problem, stepsize, and

\(^5\)https://github.com/jordydavelaar/kmonty

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**Figure 6.** Comparison between the semi-analytical (\(k\)MONTY) and numerical sampler (IGRMONTY) at three inclinations, top left: spectra at inclinations of 30\(^\circ\), 60\(^\circ\), and 90\(^\circ\). All three cases show consistent spectra with order 1 percent differences (bottom left). The MC noise grows at high frequencies due to the low probability of double-scattering events. Right: \(L_1\) convergence of the comparison between the semi-analytical and numerical samplers. As expected of MC methods, a clear \(\sqrt{N}\) trend is visible.

**Figure 7.** Comparison between RAPTOR and \(k\)MONTY for the GRMHD test, left: Thermal DF, middle: \(k\)-DF, right: power-law DF. Consistent with the uniform sphere test, the deviations are of the order of 1 percent except for the high- or low-frequency part of the spectrum.
scattering opacity. The 40 nodes run achieves a speed of ten million superphotons per second. The difference between the thermal, power law, and $\kappa$-DFs is negligible since the computational bottleneck is the handling of the non-uniform data structure and geodesic integration.

We also tested the performance of the semi-analytical samplers. We provide a standalone OpenMP accelerated code of the sampling routines on GitHub. We ran the samplers on the same architecture as for the $\kappa$Monty performance test. The $\kappa$-DF samples a few hundred thousand electrons per second per core, while the power-law and thermal DF samples around ten million electrons per second per core. Although the $\kappa$-DF is orders of magnitude slower, since it does not make use of heavily optimized gsl samplers, the routine is only called at most one or two times per superphoton, meaning the computational cost is negligible when used by $\kappa$Monty.

\footnote{https://github.com/jordydaalder/edf-samplers}

**5 CONCLUSION**

We presented our new $\kappa$Monty code. The code is an extension of GRMONTY and now includes $\kappa$- and power-law DFs for both the radiative transfer coefficients and sampling routines. The code can also post-process the AMR data format of BHAC. We tested our sampling routines by comparing the numerical output to the analytical DFs. We used a uniform isothermal sphere to test the implementations of the emission coefficients by comparing them with the ray tracing code RAPTOR. We tested the full emission and scattering kernels by comparing them to an implementation of the kappa distribution in IGRMONTY that uses the numerical sampling routine. And finally, test the coupling to BHAC by comparing the synchrotron emission with RAPTOR by using a snapshot of a black hole simulation in Cartesian coordinates which uses AMR.

**Software:** PYTHON (Oliphant 2007; Millman & Aivazis 2011), SCIPY (Jones et al. 2001), NUMPY (van der Walt, Colbert & Varoquaux 2011), MATPLOTLIB (Hunter 2007), RAPTOR (Bronzwaer et al. 2018, 2020).

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DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding author.

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