Kinetic Modeling of Radiation Belt Electrons with GEANT4 to Study Energetic Particle Precipitation in Earth's Atmosphere

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Abstract

We present a new model designed to simulate the process of energetic particle precipitation, a vital coupling mechanism from Earth's magnetosphere to its atmosphere. The atmospheric response, namely excess ionization in the upper and middle atmosphere, together with bremsstrahlung X-ray production, is calculated with kinetic particle simulations using the GEANT4 Monte Carlo framework. Mono-energy and mono-pitch angle electron beams are simulated and combined using a Green's function approach to represent realistic electron spectra and pitch angle distributions. Results from this model include more accurate ionization profiles than previous analytical models, deeper photon penetration into the atmosphere than previous Monte Carlo model predictions, and predictions of backscatter fractions of loss cone electrons up to 40%. The model results are verified by comparison with previous precipitation modeling results, and validated using balloon X-ray measurements from the BARREL mission and backscattered electron energy and pitch angle measurements from the ELFIN CubeSat mission. The model results and solution techniques are developed into a Python package for public use.







300

180

Increasing E₀

150

120 150 Pitch Angle [deg]

0 Me\

10⁴

10³

10¹

10⁰

90



















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Key Points:

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• A GEANT4-based model has been developed to simulate radiation belt energetic particle precipitation (EPP) q

- A range of mono-energy and mono-pitch angle beams are simulated to be com-10 bined using the Green's function method to represent realistic EPP quantities of 11 interest 12
- Model results and the Green's function method are validated using balloon X-ray 13 and in-situ electron spectra measurements that compare favorably to modeled ob-14 servations 15

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16 Abstract

We present a new model designed to simulate the process of energetic particle pre-17 cipitation, a vital coupling mechanism from Earth's magnetosphere to its atmosphere. 18 The atmospheric response, namely excess ionization in the upper and middle atmosphere, 19 together with bremsstrahlung X-ray production, is calculated with kinetic particle sim-20 ulations using the GEANT4 Monte Carlo framework. Mono-energy and mono-pitch an-21 gle electron beams are simulated and combined using a Green's function approach to rep-22 resent realistic electron spectra and pitch angle distributions. Results from this model 23 include more accurate ionization profiles than previous analytical models, deeper pho-24 ton penetration into the atmosphere than previous Monte Carlo model predictions, and 25 predictions of backscatter fractions of loss cone electrons up to 40%. The model results 26 are verified by comparison with previous precipitation modeling results, and validated 27 using balloon X-ray measurements from the BARREL mission and backscattered elec-28 tron energy and pitch angle measurements from the ELFIN CubeSat mission. The model 29 results and solution techniques are developed into a Python package for public use. 30

³¹ Plain Language Summary

The upper atmosphere and near-Earth space interact with each other through charged 32 particle (electrons, e.g.) transport from space into the atmosphere in a process called en-33 ergetic particle precipitation. This process disturbs the atmosphere and causes X-rays 34 to be generated, among other direct and indirect effects to the atmosphere, including ozone 35 destruction. This work describes a physics-based model that simulates this process across 36 realistic input values for energy and electron velocity direction. Results of this work in-37 clude an estimate of the number of excess ion-electron pairs generated in the atmosphere 38 from precipitation, how many electrons are lost to the atmosphere versus those that re-39 bound and return to space, and the energy and amount of X-rays generated by precip-40 itation. The model outputs are checked using balloon-based measurements of X-rays in 41 the middle atmosphere and by a low Earth orbiting satellite that spins to measure elec-42 trons heading towards and away from Earth. 43

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44 1 Introduction

Energetic particle precipitation (EPP) is a coupling mechanism between Earth's 45 magnetosphere and atmosphere wherein charged particles are lost from the magnetosphere 46 and are subsequently deposition into the atmosphere. At Earth, this process for ener-47 getic electrons is sourced by the outer radiation belt which is comprised of high inten-48 sities of energetic and relativistic electrons and is located approximately 3-7 Earth radii 49 from the equator at the Earth's surface (Akasofu & Chapman, 1961; Shprits et al., 2008). 50 Within the radiation belts, plasma waves generate these relativistic populations by ac-51 celerating electrons from low energies (eV - keV) to relativistic and ultra-relativistic en-52 ergies (100s keV – MeV electron kinetic energies) (R. B. Horne et al., 2005; Chen et al., 53 2007; Millan & Baker, 2012). 54

Plasma waves can also alter an electron's momentum direction relative to the mag-55 netic field line (i.e. pitch angle) to be redirected into the "loss cone," which is the re-56 gion of electron phase space that allows electrons to reach altitudes lower than 100 km. 57 At these altitudes the electrons can interact with the neutral molecules in Earth's at-58 mosphere and thus these electrons can be lost from the radiation belt population (Lyons 59 et al., 1972; Sergeev et al., 1983; Summers & Thorne, 2003). Electrons spanning 10s keV 60 to MeV kinetic energies precipitate from the radiation belts due to magnetospheric plasma 61 waves from a variety of natural and anthropogenic sources, including solar activity which 62 drives geomagnetic storms and wave activity, atmospheric lightning, and Earth-based 63 radio transmitters (R. Horne & Thorne, 2003; R. Horne et al., 2003; Lam et al., 2010). 64

Electrons within the loss cone lose energy by scattering with neutral particles in 65 the atmosphere, and when charged particles can no longer leave Earth's atmosphere the 66 electron is considered lost or precipitated to the atmosphere. An additional consequence 67 of this process is bremsstrahlung X-ray production, which occurs when a high energy elec-68 tron scatters through the Coulomb field of an atomic nucleus and results in a fraction 69 of the electron's kinetic energy being converted into an energetic photon (Koch & Motz, 70 1959; Bunkin & Fedorov, 1966). These photons are typically in the X-ray to gamma-ray 71 energies (10s keV – GeV) and can be used as a remote sensing proxy measurement for 72 EPP (Imhof et al., 1974, 1985). 73

The model used in this work is built from the GEANT4 (GEometry ANd Track-ing) framework, a validated radiation and particle transport code originally developed

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at CERN (Agostinelli et al., 2003; Allison et al., 2006). Initial conditions are chosen that 76 cover a realistic range of energies and pitch angles, and the model then propagates and 77 tracks the 3D trajectory and energy of a large number of electrons and generated pho-78 tons as they interact with atmospheric neutral particles using the Monte Carlo method. 79 The results from this model are used to compute derived products, such as atmospheric 80 ionization rates, that are vital to atmospheric modeling (Sinnhuber et al., 2012; Mironova 81 et al., 2015; Funke et al., 2016). Model results are verified by comparison with previous 82 models, and validated with spacecraft and balloon data in case studies. 83

Further, this work expands on and updates previous models that perform similar calculations with improved cross section implementations, and includes photon and secondary ionization peaks. Finally, a Python software package is described that allows user access to these model outputs, as well as a multitude of the analysis and inversion techniques described in Sections 5 and 6.

⁸⁹ 2 Background

The radiation belt driving mechanisms of EPP, namely wave-particle interactions, 90 occur in the entire magnetized region around Earth on short time scales, which makes 91 it difficult to provide comprehensive measurements of waves and particles to constrain 92 when and where EPP is occurring (R. Anderson et al., 1982; LaBelle & Treumann, 1988; 93 Ni et al., 2016). In addition to the high spatial and temporal coverage that is needed to 94 characterize EPP, high energy and angular resolution measurements are also required 95 to determine the effects of plasma wave drivers on precipitating electron spectra and 96 pitch angle distributions (Frank & Ackerson, 1971). For these reasons, EPP is difficult 97 to observe directly and as a consequence, the drivers of EPP in the radiation belts and 98 the relative importance of EPP in the atmosphere are known only indirectly. 99

One of the primary drivers of EPP are wave-particle interactions from plasma waves Earth's magnetosphere, which include electromagnetic ion cyclotron (EMIC), whistlermode chorus, hiss, lightning-generated whistlers (LGWs), and other very-low frequency (VLF) waves from Earth-based transmitters (Asikainen & Ruopsa, 2016; Pytte et al., 1976; McPherron, 1979; Inan et al., 1988; Rodger et al., 2007; Glauert et al., 2014). Some of these wave modes are generated by geomagnetic storm activity and space weather events, which lead to anistropies in the energetic plasma, and are ultimately driven by solar ac-

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tivity (Schwenn, 2006; Engebretson et al., 2008; Baker et al., 2018). In general, electrons
at 100s keV kinetic energies are typically resonant with whistler mode chorus waves, and
at MeV energies with EMIC waves, two types of plasma waves that are detected in the
inner magnetosphere and have been shown to be drivers of EPP (R. Horne & Thorne,
2003; R. Horne et al., 2003; Lam et al., 2010).

Once electrons have entered the atmosphere, EPP has important effects on the up-112 per and middle atmosphere. The primary mode of energy loss of high energy electrons 113 is through radiative collisions, such as ones that generate X-ray photons. At lower en-114 ergies, the electron energy loss begins to favor collisional interactions, such as impact ion-115 ization (Kim et al., 1997). The impact ionization process yields excess electron-ion pairs 116 generated from neutral species which enhance the ionospheric plasma population. The 117 bulk effect is that EPP alters the chemistry balance which causes NO_x and HO_x 118 production, the former of which goes on to be transported to lower altitudes near the 119 poles where it catalytically destroys ozone (Thorne, 1980; Codrescu et al., 1997; Seppälä 120 et al., 2007; Sinnhuber et al., 2012; Andersson et al., 2014; Mironova et al., 2015). Ad-121 ditionally, excess ionization alters the conductivity of the ionosphere and further alters 122 the geomagnetic current systems that couple the atmosphere and magnetosphere (Ridley 123 et al., 2004; G. Khazanov et al., 2018) 124

In atmospheric models, EPP is typically addressed via parameterized input in or-125 der to save on computation speed in exchange for event specificity. Typical quantities 126 that are used to characterize precipitation are some measure of flux (e.g. number flux, 127 energy flux) and energy spectrum, or parameter(s) that describe the spectrum, such as 128 a folding energy for an exponential distribution. The early work of R. G. Roble and Ri-129 dley (1987) used an analytical approach using the electron stopping power formulation 130 to characterize auroral precipitation inputs for the thermospheric global atmosphere model 131 TGCM. The work of Frahm et al. (1997) calculates atmospheric ionization rates by in-132 cluding electrons and secondary photons using a Boltzmann transport equation multi-133 stream model, based off the model of Lorence Jr and Morel (1992). The improved an-134 alytical model of Fang et al. (2008, 2010) was created for convenient use in "high top" 135 whole atmosphere models such as WACCM-X that extend to the mesosphere and above 136 (Liu et al., 2018). This analytical model forward-models mono-energy beams with isotropic 137 pitch angle distributions that an end user can combine to represent an arbitrary contin-138 uous and smooth spectrum. Finally, the work of Xu et al. (2020) uses a full Monte Carlo 139

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manuscript submitted to Earth and Space Science

model with forward-modeled mono-energy and mono-pitch angle electron beams that more
realistically represents high energy processes, but does not include bremsstrahlung transport to lower altitudes. Bremsstrahlung tranpsort is shown for three energies in Xu et
al. (2021): the last two of these previous works are directly compared to this work in Section 6. Other models exist that use similar Monte Carlo techniques for different purposes,
such as the auroral model of Solomon (2001).

Radar remote sensing of excess ionization in the ionospheric D- and E- regions is 146 difficult due to high atmospheric neutral density driving fast recombination, which causes 147 ionization enhancements to dissipate quickly. Atmospheric effects can be measured as 148 a proxy to precipitation inputs, but the complicated chemistry and transport dynam-149 ics makes the inversion to precipitation characteristics difficult and uncertain (Marshall 150 & Cully, 2020). On the other hand, direct in-situ measurements of charged particles from 151 spacecraft have difficulty obtaining the spatial and temporal coverage due to the afore-152 mentioned large spatial scales of EPP and the nature of low-Earth orbits. Additionally, 153 charged particle instruments are often angular resolution-limited and are therefore un-154 able to resolve the loss cone at various points in the orbit, which is necessary to provide 155 a global image of precipitation (L. W. Blum & Breneman, 2020; Capannolo et al., 2021). 156

In order to obtain global measurements of EPP, remote measurements of X- and 157 gamma- ray photons can instead be used to infer EPP over larger spatial scales. Brems-158 strahlung photon energy and emission direction is strongly dependent on the precipitat-159 ing electron energy, such that statistical relationships can be formed between the X-ray 160 and electron spectra. A component of this work is to prepare for future hard X-ray ob-161 servation missions of Earth to quantify the extent of radiation belt EPP, such as the up-162 coming AEPEX CubeSat mission (Marshall et al., 2020). A variety of information can 163 be garnered on EPP from inverting X-ray spectral measurements of Earth from low Earth 164 orbit or from balloon measurements, where a review of the former, X-ray observations 165 from space, is included in Berland et al. (2023) for Earth and Bhardwaj et al. (2007) for 166 other planets. 167

Open questions of magnetosphere-atmosphere coupling primarily relate to the wave particle interaction driving mechanism of EPP: how does EPP vary seasonally, temporally, and with magnetospheric conditions; and what are the spatial scales over which this process occurs? The answers to these questions will help constrain the total energy

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- ¹⁷² budget of the radiation belts and atmosphere, and lend a deeper understanding of the
 ¹⁷³ dynamic interactions between Earth's magnetosphere and atmosphere. For a review of
- EPP open questions, see Marshall et al. (2020).
- **3** Model Description

This work aims to explore an input space comprised of electron pitch angle and en-176 ergy distribution through various radiation belt magnetic latitudes using the EPP model 177 described in this section. The range of magnetic latitudes describe the atmospheric pro-178 files and magnetic dip angle, both of which change the linear distance that an electron 179 will travel through a given atmospheric density, effectively increasing the integrated col-180 umn density that an electron will traverse. In order to explore these continuous input 181 spaces, the approach of Fang et al. (2010) and Xu et al. (2020) is taken by simulating 182 a finite number of mono-energy and mono-pitch angle electrons beams through a refer-183 ence atmosphere at one magnetic dip angle. In order to convert model results to a dif-184 ferent atmospheric profile, a rescaling method similar to Xu et al. (2020) is described and 185 implemented in Section 4. 186

The mono-energy, mono-pitch angle beams can be weighted and linearly combined 187 using a Green's function approach. Green's functions are maps from Dirac delta func-188 tion in an input space to the subsequent impulse response in an output space that can 189 be used to solve boundary value problems in a variety of fields (Melnikov, 1977; Stak-190 gold & Holst, 2011). In this work, we use the Monte Carlo forward method to approx-191 imate the Green's functions instead of finding an analytical form, which is difficult due 192 to the rarefied and stochastic interactions that occur between high energy electrons and 193 neutral particles. This method is discussed and formalized in Section 5. 194

The geometry of the model is a 500 km tall x 1000 km diameter 3D column that 195 is filled with the MSIS2.0 (Mass Spectrometer Incoherent Scatter Radar-Empirical) model 196 atmosphere, which includes the atmospheric state (temperature, pressure, density) and 197 constituent number densities, taken at 1 km intervals (Picone et al., 2002). MSIS takes 198 as inputs the F10.7 and A_p indices, which largely affect the scale height in the diffusive 199 region above 100 km altitude, and therefore the altitudinal distribution of constituents 200 and altitude of constant pressure surfaces in the atmosphere. The majority of scatter-201 ing and photon production occurs below 100 km, so these indices are not considered as 202

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Figure 1. (Left) Single particle pitch angle evolution with altitude, where α_0 is the pitch angle at 500 km altitude. The black dashed line marks 100 km, which is the altitude used to define the edge of the loss cone. (Right) Energy evolution with altitude from electrons injected at field-aligned pitch angles. Highlighted here is the relative depth of penetration into the atmosphere with initial particle energy.

- a strong influence on the resulting quantities of interest. The location for the reference
 atmosphere profile selected is over the Poker Flat Incoherent Scatter Radar (PFISR) station located in Alaska at 65° North latitude 147° West longitude, at midnight local time.
- A tilted dipole magnetic field is used to model the near-Earth magnetic field in-206 tensity vector since the field intensity only varies on the order of 2% at 500 km from a 207 higher fidelity magnetic model such as IGRF (Alken et al., 2021). An important aspect 208 of the geometry of EPP is the additional path length an electron must travel due to the 209 local magnetic inclination at a given latitude. The magnetic inclination I, defined as $\tan(I) =$ 210 B_r/B_{θ} , at PFISR is approximately 78°, or 12° away from zenith. Until the electron's 211 motion is dominated by collisions, the guiding center of the cyclotron motion will fol-212 low the magnetic field line, adding an additional factor of sec(I) to the path length the 213 electron travels through the atmosphere. The magnetic latitudes of 45° (L = 2) and 90° 214 $(B_{\theta} = 0)$ where the inclinations are 64° and 90°, respectively, are also simulated to an-215 alyze the effects of varying magnetic dip angle through all magnetic latitudes where pre-216 cipitation most often occurs. 217

In the simulation electrons are injected at 300 km altitude, where the loss cone edge 218 is approximately 73° , with pitch angles defined relative to the inclined magnetic field. 219 The resulting electron backscatter and zenith-propagating photons are tracked until 500 km 220 altitude, where they are sufficiently above the neutral atmosphere to be considered es-221 caped from the atmosphere. An example of the general pitch angle and energy dynam-222 ics of a single particle with various initial conditions is shown using analytical approx-223 imations in Figure 1. In this figure, the electrons are started at a higher altitude of 500 km 224 where the loss cone edge is at 66° , and the progression to lower pitch angles shows that-225 if not for the effects of atmospheric backscatter- electrons more than a few degrees away 226 from the edge of the loss cone must surely precipitate. The assumption that the entire 227 population of the loss cone precipitates is challenged by simulation results in Section 4 228 and by in-situ electron data in Section 6.3. 229

The forward model selected for this work is built from GEANT4, a radiation and 230 charged particle transport code originally developed at CERN for high energy physics 231 (Agostinelli et al., 2003; Allison et al., 2006). GEANT4 is a collection of C++ classes 232 and implementations that allow for modular creation of physics simulations with arbi-233 trary geometries and materials, types of charged particles and photons, and a list of phys-234 ical processes and cross sections to simulate. A variety of cross section implementations 235 and scattering models, called physics lists, have been developed for a variety of appli-236 cations including the space radiation environment (Truscott et al., 2000; Ersmark et al., 237 2007). For this simulation work, we choose the validated QBBC physics list, which it-238 self is a collection of previous validated scattering cross sections and model implemen-239 tations (Ivanchenko et al., 2010). 240

Included in this simulation are the effects of impact ionization including single, dou-241 ble, K-shell ionization, etc. that are ultimately determined via the Møller electron-electron 242 scattering cross sections (Mark, 1982). For the electron energies considered by this work, 243 GEANT4 implements the Livermore low-energy electromagnetic model, which includes 244 validated cross sections and implementations for electron ionization and bremsstrahlung. 245 the photoelectric effect, and Compton scattering from 250 eV – 100 GeV, and pair pro-246 duction from 1022 keV ($2 \times$ electron rest energy) – 100 GeV (Ivanchenko et al., 2011). 247 For electron multiple scattering effects through matter the Urban, Wentzel VI, and Coloumb 248 scattering models are implemented which include angular diffusion (Urban, 2002; Ivanchenko 249 et al., 2010)

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For electron angular diffusion, GEANT4 implements the Goudsmit-Saunderson model, 251 which parameterizes the multiple Coulomb scattering physics that primarily affect pre-252 cipitating electrons below 100 km altitude (Ivanchenko et al., 2010). For thin-target brems-253 strahlung photon production, the Seltzer-Berger model is implemented (Berger & Seltzer, 254 1972; Seltzer & Berger, 1986). A comparison between bremsstrahlung cross section im-255 plementations, including the cross section model used in Xu et al. (2020), is presented 256 in Köhn and Ebert (2014). The bremsstrahlung cross section becomes more dominant 257 at higher energies (MeV electron kinetic energies), so it is a rare process at lower ener-258 gies. For this reason, a statistical biasing method is implemented to better inspect pho-259 ton production via the bremsstrahlung interaction for simulation energies below 500 keV. 260 This method samples the bremsstrahlung cross section N times for every time a pho-261 ton would be generated and assigns a weight of 1/N to every subsequent photon and sec-262 ondary particle scoring quantity, such as energy deposition. In this study an N value of 263 100 is used to smooth the X-ray spectral distributions. Figure 2 shows the influence of 264 this method on the quality of the results, with particular benefit for X-ray propagation 265 at lower altitudes. 266

The energy range selected corresponds to realistic energies characteristic of the outer 267 radiation belt (Li & Temerin, 2001; Whittaker et al., 2013). The simulations implement 268 energy via a monoenergetic beam, with energies spaced approximately logarithmically 269 from 10 keV to 10 MeV. A variety of energy distributions can be evaluated using these 270 beam energies as control points and using the corresponding normalized function value 271 as a weight to apply to a linear summation. This same method can be performed with 272 mono-pitch angle beams to reproduce arbitrary pitch angle distributions. This method 273 is formalized via Green's function analysis in Section 5 for various quantities of inter-274 est, including atmospheric ionization rate. Additionally, in order to obtain various quan-275 tities of interest from this model, a series of conversion factors is needed to relate the model 276 outputs to physical quantities. These conversion factors relate energy deposition to ion-277 ization and number of particles run in the simulation to flux units, and are described be-278 279 low.

A conversion factor is needed to relate energy deposition rate in the atmosphere to atmospheric neutral ionization rate. In the work of Fang et al. (2008) and Xu et al. (2020) an average electron ionization is assumed to be a constant 35 eV/pair, however the average first ionization potential of a mixed gas is a function of gas mixing ratios and

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Figure 2. Profiles produced by simulating 10^5 electrons at energies of 10, 20, 50, 100, 200, and 500 keV (red to blue). Each profile is run with a 100x numerical bias towards brems-strahlung enabled. A comparison with and without the biasing method is shown here using an isotropic pitch angle distribution.

therefore of altitude in the atmosphere as well. An alternative to the constant ionization potential assumption are the simulation results of Krause (1998) where a relativistic electron beam is simulated through the atmosphere. It's found that an affine function of the following form provides a better estimate for ionization in the atmosphere:

$$I(h) = I_0 + \frac{\partial I}{\partial h} \cdot h \tag{1}$$

valid for altitudes h between 45 km and 240 km, with $I_0 = 39.78 \text{ eV/pair}$ and a slope parameter of $\partial I/\partial h = -0.03 \text{ eV/pair/km}$. This formulation yields ionization energies that vary up to 10% from the constant 35 eV/pair assumption, but more importantly the ionization rate conversion is now a function of altitude, so the shape of the altitudinal ionization profile is affected. For simplicity, the results shown herein use the constant 35 eV/pair conversion and the software package described in Section 7 enables the conversion factor described by Equation 1 for higher accuracy.

In order to translate the number of particles run in the simulation to a differential flux unit, a conversion factor is needed. If we simply want total flux, i.e. $\text{cm}^{-2} \text{ s}^{-1}$, we can choose an effective detection area ΔA_d and time interval Δt to be unity, that is to say 1 cm² and 1 second, respectively, such that the number of particles run in the simulation can be related to the number flux of electrons. However if we want to express our flux differentially in angle space, an additional conversion factor is needed given the initial input pitch angle. In this work, we take the equation

$$N = -dt \ d\Omega_d \ \left(f(\hat{k}_s) \ \hat{k}_s \right) \cdot \left(dA_d \ \hat{k}_d \right) \left[\hat{k}_s \cdot \hat{k}_d < 0 \right]$$
(2)

where $d\Omega_d$ is the differential solid angle that couples the simulation geometry and distribution momentum direction, $f(\hat{k}_s) \hat{k}_s$ is the electron distribution in phase space, with momentum space vector \hat{k}_s , dA_d describes the differential geometry of the simulation surface with outwards surface normal \hat{k}_d , dt is the time in which electrons pass through the surface dA_d , and the bracketed term is the indicator function. The negative sign and indicator function term enforce inwards directionality to particles on the surface of the simulation. We can express the dot product between the momentum direction of the beam and surface normal as a function of mono pitch angle α_0 : $\hat{k}_s \cdot \hat{k}_d = \cos(\alpha_0)$ in order to obtain the relationship between number of particles simulated and differential flux in terms of integral flux f_0 . Finally, the indicator function restricts the limits of integration to $\pi/2$ to remove the effect of anti-Earthward directed electrons:

$$\frac{N}{dt \ dA_d} = f_0 \ \int_0^{2\pi} \int_0^{\pi/2} \cos(\alpha_0) \ \sin(\alpha) \ d\alpha \ d\theta \tag{3}$$

The conversion factor from integrating over the hemisphere is then purely a function of the angle at which the beam is directed through the simulation surface normal:

$$f_0 = \frac{1}{2\pi \cos(\alpha_0)} \frac{N}{dt \ dA_d} \tag{4}$$

which represents the relationship between a desired differential flux in units of $cm^{-2} s^{-1} sr^{-1}$ 289 from N particles run in a simulation at mono-pitch angle α_0 . When the beam is field-290 aligned, the normalization factor is 2π and the conversion factor is also well behaved at 291 $\alpha_0 = 90^\circ$ since the number of particles passing through the simulation surface N van-292 ishes at that angle. Once properly normalized, the flux can be scaled multiplicatively 293 since we assume EPP is a linear process, i.e. electrons do not sufficiently interact with 294 each other. Further, this flux can be made differential in energy by multiplying with an 295 energy distribution function in units of keV^{-1} that integrates to unity. 296

The methods described in this section are a description of the treatments applied to the raw data output by the model, which include histograms of: 1) weighted energy deposition per altitude bin, 2) a particle's weighted energy passing through a 2D energyaltitude bin, and 3) pitch angle and energy recorded at 500 km. These outputs and their physical meanings are discussed in the next section.

302 4 Model Results

The GEANT4 model is run on a supercomputer across 5 nodes using 40 cores per 303 node, parallelized across one thread per core. In order to evaluate variation information 304 for a given simulation, 10^5 particles are split evenly between 40 simulation threads in 305 order to produce histograms from 2500 electrons/thread. The sample standard devia-306 tion is calculated across the 40 output histograms and we conclude a sufficient number 307 of particles have been simulated since the standard deviation varies less than 0.01%308 from the mean. The 40 histograms are then summed and divided by the number of par-309 ticles run, in addition to the conversion factor described in the previous section, to con-310 vert to differential flux units. The runtime for the full simulations are on the order of 311 3-4 days for a run with 19 energies \times 15 pitch angles, with the higher pitch angle sim-312 ulations taking significant more time than lower pitch angles due to the longer path length 313 traversed by those electrons. 314

The first primary outputs from the simulation are altitude distributions of energy deposition into the atmosphere, shown in Figure 3. This figure shows the results of a sin-

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Figure 3. Green's function ionization response to mono-energy mono-pitch angle inputs. Variation in pitch angle from field-aligned (0°, green) to near the edge of the loss cone (70°, blue) is shown, at pitch angle spacing $\Delta \alpha = 5^{\circ}$ and variation in pseudo-log-spaced energies denoted on the plot, with peaks descending in altitude. The deposited energy is normalized to integrate to unity.



Figure 4. (Left) Altitudes of maximum ionization with beam energy and pitch angle. (Right) The rate of change of altitude of peak ionization with beam energy with varying pitch angle. A 2^{nd} order polynomial fit is included to show the trend in $\partial h/\partial E_0$ with pitch angle, where α is in radians.

gle energy E_0 and pitch angle α_0 profile normalized by the input energy flux so that they 317 integrate to unity. These profiles can be directly converted into ionization rate using ei-318 ther a constant 35 eV/pair assumption or, for higher accuracy, the conversion factor de-319 scribed by Equation 1. The input energy is varied from 10 keV to 10 MeV using 19 pseudo-320 logarithmically spaced points and the input pitch angle at 300 km is varied from 0° to 321 70° with $\Delta \alpha = 5^{\circ}$ resolution, which extends near the edge of the loss cone at 300 km 322 of 73°. Theses profiles are the basis functions $G(E, E_i, \alpha, \alpha_i)$ of the Green's functions 323 method and can be combined to estimate ionization from an arbitrary input electron spec-324 trum and pitch angle distribution. 325

Two main features stand out in Figure 3. First, a small variation in peak ionization altitude with pitch angle is evident, with more field-aligned pitch angles depositing slightly lower in the atmosphere and with a sharper ionization peak. Secondly, the main source of variation is with beam energy, where the altitude of peak ionization descends about 20 km per decade of beam energy increase, with a slight pitch angle dependence. Both of these results are summarized in Figure 4.

The second set of primary outputs from the simulation is comprised of altitudeenergy histograms that are processed using the conversion factor in Equation 4 to produce number flux of electron and photon species at 1 km steps from $10^0 - 10^4$ keV in 100 logarithmically-spaced bins. Figure 5 shows beam energies of 500 keV and 5 MeV,

both of which are averaged with identical weights over pitch angle (i.e. an isotropic pitch 336 angle distribution). The transition region where the main electron beam flux is converted 337 into secondary electron and photon flux is a function of beam energy and is at approx-338 imately 65 km for 500 keV and 45 km for 5 MeV in Figure 5, which is reflected in the 339 energy deposition profiles as well. From that primary peak and below, the energy is trans-340 ported Earthwards via electromagnetic shower, where a primary electron creates a brems-341 strahlung photon which propagates and creates a free electron from Compton scatter-342 ing, which itself can be of substantial energy to create another bremsstrahlung photon, 343 until the energy from this cycle is absorbed into the atmosphere. At beam energies ap-344 proximately greater than 200 keV this phenomenon tends to create a coherent secondary 345 ionization peak at lower altitudes. The magnitude of the lower, secondary peak is pro-346 portional to the magnitude of the primary peak, as well as the initial beam energy. 347

In addition to observing the precipitation process through altitude and energy, these 348 histograms can be used to create secondary or derived simulation outputs. The first de-349 rived output is electron and photon backscatter, which can be inferred from the results 350 at the top of the model since 500 km is sufficiently above the neutral atmosphere for elec-351 trons to be considered reentering purely magnetized motion and ray-like propagation paths 352 for photons. The second derived output is electron and X-ray spectra at any specified 353 altitude, which can be obtained by integrating the histogram in altitude. The minimum 354 altitude resolution for this derived output is the 1 km bin size directly output by the sim-355 ulation. 356

The energy and pitch angle of atmospherically backscattered electrons at 500 km 357 altitude is recorded in order to evaluate the coupled energy-pitch angle distribution. This 358 work supports the conclusions of the previous modeling of Marshall and Bortnik (2018) 359 in an energy dependence to the loss cone, as well as likely provides a more accurate mea-360 sure of electron backscatter due to improved cross section and secondary electron pro-361 duction implementations. An interesting implication of Figure 6 is that a significant por-362 tion of the backscattered flux re-enters the trapped region and will not necessarily be 363 precipitated on subsequent bounces into the conjugate hemisphere. 945 309 4982 364

By integrating the photon altitude-energy spectrum, such as the histograms in Figure 5, we can obtain X-ray spectra at various altitudes. Figure 8 shows integrations over 25 - 35 km and over 250 - 300 km for a range of energies simulation. This derived prod-



Figure 5. Altitude-energy histogram plots of number flux from (top row) a 500 keV and (bottom row) 5 MeV electron beam at an isotropic pitch angle distribution, showing (left column) electron flux and (right column) photon flux. The input flux for both energies is $10^4 \text{ cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1} \text{ keV}^{-1}$.



Figure 6. (Top) An example of the coupled energy-pitch angle distribution recorded at 500 km that is output from the model. This distribution comes from an input energy of 200 keV and input pitch angle of 50°. (Bottom) One dimensional integrations of the backscattered electron energy-pitch angle spectrum recorded at 500 km altitude for the range of input energies, showing the characteristic rising-energy spectrum for low to medium energies.



Figure 7. Total backscatter from with an input beam energy E_0 and pitch angle α_0 at injection altitude 300 km. At low energies and high pitch angles, only 2/3 of the loss cone population is precipitating in one bounce interaction with the atmosphere.

uct is especially useful since X-rays can be used as an observable for precipitation inver-368 sion problems, such as the case study in Section 6.2. The characteristically peaked shape 369 of the bremsstrahlung X-ray distribution at 60 keV is a product of the composition of 370 Earth's atmosphere and the electron-neutral bremsstrahlung cross section, and is there-371 fore somewhat consistent across a wide range of energies and altitudes. The change in 372 the slope of the high-energy tail of the photon distribution is indicative of the driving 373 electron spectrum at all altitudes, in addition to the total number of photons produced 374 since bremsstrahlung efficiency is energy-dependent. Above the atmosphere, the slope 375 of both the high and low energy tails can be related to the driving electron spectrum. 376

Other notable features of Figure 8 include absorption of the lower energy portion 377 (< 20 keV) of the X-ray spectrum before that portion of the spectrum can propagate 378 to altitudes lower than ~ 40 km, which is supported by the work of Frahm et al. (1997) 379 and observations from BARREL and other balloon missions. This poses a difficulty to 380 balloon missions aiming to measure the X-ray spectrum as the < 20 keV portion of the 381 spectrum includes important information on the precipitating electrons. X-ray spectra 382 and electron pitch angle are not clearly related; the major effect seen in the X-ray spec-383 trum by varying pitch angle is bremsstrahlung conversion efficiency, which is likely due 384



Figure 8. X-ray spectra generated from GEANT4 model runs, (left) integrated from 25 – 35 km and (right) 250 – 300 km with isotropic pitch angle and mono energy beams with energy E_0 . The energy of peak flux and slope of the tail increase with increasing E_0 . Note that beam energies of 10 and 20 keV are absent from the left plot since those electron energies do not generate X-rays that reach 25 – 35 km altitude.

to higher backscatter rates and higher altitudes of maximum energy deposition at higherpitch angles.

Finally, we investigate the effect of the inclination of the magnetic field on ioniza-387 tion profile. The extra distance travelled by an electron through the atmosphere can be 388 found at a geomagnetic latitude λ with the expression sec $(\tan^{-1}(2\tan(\lambda)))$. At the lower 389 limit of the latitude investigated at 45° the extra distance traveled relative to a purely 390 zenith magnetic field is approximately 12%. It's found that the ionization profile in al-391 titude does not vary significantly based on magnetic inclination, and further the effect 392 of varying atmospheric density profile with latitude has a more significant impact on the 393 ionization profile. 394

In the atmospheric rescaling method, the abscissa altitude h is exchanged for atmospheric density as a function of altitude $\rho(h)$ and then a map $I(h) \rightarrow I(\rho(h))$ is created where performing operations on ρ will rescale I accordingly. This is possible since ρ is monotonic and the altitude resolution is chosen such that ρ is unique at every h. This method is akin to a pseudo-logarithmic transform due to the nature of the exponentially increasing mass density of the atmosphere with decreasing altitude. Operations on ρ to produce ρ' are translated to $I(\rho'(h))$ through linear interpolation in log-log space, which



Figure 9. Atmospheric ionization rate for the same initial conditions for three atmospheric density profiles and magnetic inclinations. The latitude of PFISR 65° is taken as the reference latitude for atmosphere and inclination angle.

can be explained simply as $I \circ \rho \to I' \circ \rho'$. An example of this method is shown in Figure 9 to highlight the variation in ionization rate profile from atmospheric profiles retrieved at different latitudes. This method differs from the method of Xu et al. (2020) only by a cumulative integration step, which is not necessary since ρ naturally meets the conditions that allows it to act as an abscissa.

5 Forward and Inverse Methods to Estimate Precipitation Characteristics

A key application for this model is in the generation of observable quantities for the largely unobservable geometry of EPP. Enhanced ionization rates (or indirect effects from these perturbations) and X-ray photons are two of the primary ways that EPP is measured directly. This section provides a framework to relate the results from this model to realistic electron energy and pitch angle distributions.

The simulation input space is a series of mono-energetic and mono-pitch angle beams $\delta(E-E_i, \alpha-\alpha_j)$ at electron beam energy E_i and input pitch angle at 300 km α_j , from which we can use a Green's function method to solve an inverse problem; that is to say, we want to estimate the initial condition at the top simulation boundary given observations (measured or simulated) from within the simulation volume. A similar approach is taken in Xu and Marshall (2019) and Patrick (2022). The formalism used here is similar to Omura et al. (2015): we take EPP to be a linear process, i.e. there is no self-interaction

within the electron beam and the neutral atmospheric state is not modified significantly with an impulse of precipitation. We then write the process of atmospheric response (e.g. X-ray production, ionization) as a linear differential operator \mathcal{L} that operates on a quantity of interest u(x, h) at altitude h in response to precipitation forcing spectrum $f(E, \alpha)$. For example, we can take the differential bremsstrahlung X-ray spectrum $u(\hbar\omega)$ at a given altitude as our quantity of interest, where $\hbar\omega$ is the photon energy:

$$\mathcal{L}[f(E, \alpha)] = u(\hbar\omega) \tag{5}$$

which by ansatz we assume has an integrable Green's function $G(E, E_i, \alpha, \alpha_j)$ relating an impulse in the electron energy and pitch angle to an output X-ray spectrum, from which we can formulate an inversion problem to estimate f given u:

$$\mathcal{L}^{-1}[\delta(E - E_0, \ \alpha - \alpha_0)] = G(E, E_0, \alpha, \alpha_0) \tag{6}$$

Since we now have the Green's functions from the GEANT4 simulation for a variety of input (E_i, α_j) , we can decompose our source spectrum $f(E, \alpha)$ as a summation of Dirac delta functions, each with differential intensity from the Green's function coefficient matrix S_{ij} :

$$f(E,\alpha) \approx \sum_{i=1}^{N} \sum_{j=1}^{M} S_{ij} \ \delta(E - E_i, \ \alpha - \alpha_j) \tag{7}$$

where the two sides are equal in the limit of $N, M \to \infty$. In this case, N and M are the total of the number of energy and pitch angle bins, respectively. We can form the beam intensities by evaluating a spectrum of interest, e.g. an exponential energy distribution with folding energy E_0 and sine pitch angle distribution, $S_{ij} \propto \exp(E_i/E_0) \sin(\alpha_j)$, that allows for coupling between energy and pitch angle. We can then write the quantity of interest solution using the set of intensities $S_{ij} \in \mathcal{R}^{N \times M}$:

$$u(\hbar\omega) = \sum_{i=1}^{N} \sum_{j=1}^{M} S_{ij} \ G(E, E_i, \alpha, \alpha_j)$$
(8)

The beam intensities S_{ij} , which are defined on $[0, \infty)$, can be found through a variety of fitting methods; for X-ray spectrum fitting a logarithmic least squares minimization works well in test cases. The formulation for this process to fit the maximum likelihood spectrum $u_{ML}(\hbar\omega)$ to data $g(\hbar\omega)$ with logarithmic least squares cost function is

$$S_{ij}^{ML} = \underset{S_{ij}}{\operatorname{arg\,min}} \sum_{k} \left(\log u(\hbar\omega_k) - \log g(\hbar\omega_k) \right)^2 = \underset{S_{ij}}{\operatorname{arg\,min}} \sum_{k} \log \left(\frac{u(\hbar\omega_k)}{g(\hbar\omega_k)} \right)^2$$
(9)

414

where $u(\hbar\omega)$ is generated iteratively through Equation 8 and is ultimately solved via the



Figure 10. (Left) Photon altitudinal spectra for a precipitation event with differential flux $10^5 \text{ cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1} \text{ keV}^{-1}$ and exponential energy distribution with folding energy $E_0 = 100 \text{ keV}$. Note the low flux bins in the lower left-hand corner are from noise. (Right) Altitude-integrated X-ray spectra averaged at altitudes 30, 60, and 150 km, averaged over a $\pm 5 \text{ km}$ altitude bin.

gorithm, which can be run on a personal laptop and allows for a large number of spectral Green's functions to be used (Dai, 2002). The logarithm cost function better emphasizes the smaller numbers in the high energy tail of the X-ray distribution than a linear least squares cost function. The high energy X-ray component is proportional to the high energy electron component, which is important since the highest energy electrons penetrate deepest into the atmosphere and cause X-ray production and ionization at the lowest altitudes.

An example of the latter portion of the Green's function method is shown in Figure 10 where an exponential energy distribution with folding energy $E_0 = 100$ keV and sine pitch angle distribution are recreated using the Green's function coefficient matrix S_{ij} . Slices of the normalized X-ray spectrum for three altitudes are also plotted, illustratingfor the same precipitation event- the range of photon spectra that are measurable. The inversion portion of this method is shown in the case studies in Section 6.

Using this same method, an ionization spectrum versus altitude can be generated from forward modeling loss cone data with linear combinations of the Green's function for ionization at a single energy and pitch angle. In theory, any observable generated by this model can be used to estimate precipitation parameters, however some observables contain less information than others. For instance, pitch angle is not particularly observable from X-ray observations. For a further analysis of precipitation inversion via X-ray

observations, see Patrick (2022). A 2D fitting process is performed in Section 6.3 using 435 spacecraft 2D electron-pitch angle data at 500 km altitude. 436

Since we are using a finite number of beams $N \times M$, a degree of uncertainty is in-437 troduced in the reconstruction of the forcing function $f(E, \alpha)$. Instead of Dirac delta func-438 tions, we can let our EPP forcing spectrum be an arbitrary smooth function, or com-439 bination of smooth functions, that we can use in the inversion problem. Xu and Mar-440 shall (2019) and Patrick (2022) show the extent of successful reproduction of various forc-441 ing distributions using mono-energetic beams. Various other choices of EPP forcing func-442 tion include a singular exponential distribution, or sum of exponential distributions char-443 acterized by folding energies, or power law distributions characterized by spectral coef-444 ficients. Studies of these distributions are left to future work since there is a dearth of 445 coincident X-ray and in-situ electron measurements that are needed to validate the use 446 of different spectral distributions. Interestingly, an example of a successful inversion us-447 ing X-ray and electron data has been performed at Jupiter in the work of Mori et al. (2022). 448

6 Model Validation through Case Studies 449

We aim to verify that the model results are quantitatively accurate and are not dis-450 similar from the previous model of Xu et al. (2020). The authors of Xu et al. (2020) com-451 pare their work with the previous model of Fang et al. (2008, 2010), which in turn com-452 pares to the older, purely analytical model of R. Roble and Ridley (1987) so the progres-453 sion of model accuracy can be discerned. 454

In addition to a comparison with previous work, we aim to validate the model ob-455 servables and inversion methods using electron and photon measurements, both in-situ 456 and remotely sensed. In this section we present two case studies. The first case study 457 analyzes X-ray spectra measured by the BARREL balloon campaigns while the FIRE-458 BIRD spacecraft was in magnetic conjunction to measure the electron spectrum in-situ. 459 The second case study uses electron energy-pitch angle measurements from the ELFIN 460 CubeSat missions to forward and inverse model atmospheric ionization. 461

462

6.1 Comparison with Previous Models

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Figure 11 shows the difference in ionization profile between this work and the results of Xu et al. (2020), which do not include photon and subsequent secondary elec-464

-24-


Figure 11. (Left) GEANT4 (solid lines) and EPMC (dashed lines) normalized energy deposition profiles with an isotropic pitch angle distribution at 6 energies up to 500 keV. (Right) Altitude of the maximum ionization peak with electron beam energy.

tron transport to lower altitudes. For this study, the same reference atmosphere and input space are used to compare the two models. GEANT4 predicts lower altitudes of maximum ionization than EPMC at beam energies less than 50 keV and higher peak altitudes at higher beam energies. Notably, the bremsstrahlung secondary peak extends much further downwards in altitude than the primary ionization peak but is generally 2 orders of magnitude lower in deposited energy, which may be an important effect in radiation dose at airline altitudes (Tobiska et al., 2016, 2022).

Figure 12 shows a comparison between EPMC simulation results from Xu et al. (2018), 472 where photon transport is handled by a separate model, and the GEANT4 simulations 473 across a larger range of energies at two discrete pitch angles. A peak that is both higher 474 and more narrow in altitude is seen in the GEANT4 results, in addition to more ioniza-475 tion below the main peak from photon and secondary electron transport. For higher en-476 ergy electrons beams, the EPMC and GEANT4 results match more closely in the sec-477 ondary peak. This matches with the prediction in Köhn and Ebert (2014) which states 478 the EPMC regime of bremsstrahlung cross section validity is $\hbar\omega \ll E_e$. This approx-479



Figure 12. Comparison between ionization profiles generated by Xu et al. (2018) (dashed lines) and the GEANT4 model presented in this work (solid lines), both of which include photon tracking to lower altitudes. (Left) Simulation run at 0° pitch angle, and (right) 45° pitch angle for energies 100 keV (black), 1 MeV (blue), and 10 MeV (red).

imation in the EPMC implementation should mainly affect the lower, secondary ionization peaks, and the specific ways in which the cross section deviates from a more accurate bremsstrahlung cross section is described Köhn and Ebert (2014).

483

6.2 X-ray Production in the Stratosphere

The goal of this case study is to analyze a time window in which X-ray data from 484 within the atmosphere and in-situ electron spectra from above the atmosphere are mea-485 sured during the same precipitation event, in this case the events studied in B. Ander-486 son et al. (2017). In this study, the EPP phenomenon is specifically microburst precip-487 itation, which is correlated with high energy precipitation on small spatial and tempo-488 ral scales which may have a significant impact on the atmosphere (Shumko et al., 2018; 489 Zhang et al., 2022; Seppälä et al., 2018). Additionally, microburst precipitation is asso-490 ciated with a slowly varying (5 - 15 second period) X-ray signal that has been measured 491 from balloon and rocket X-ray payloads (Tsurutani et al., 2013). In this study, balloon 492

⁴⁹³ X-ray measurements are made from the BARREL mission and in-situ electron measure ⁴⁹⁴ ments from the FIREBIRD II CubeSat mission.

The Balloon Array for RBSP Relativistic Electron Losses (BARREL) missions were 495 a series of stratospheric balloon flights in Antartica and Sweden that achieved altitudes 496 of >30 km for extended periods of time to study X-ray production from EPP with an 497 upwards (zenith) look direction (Millan et al., 2013). The balloon launches overlap with 498 the Van Allen Probes era, although conjunction data are not always available depend-499 ing on the location of the Van Allen Probes spacecraft along their orbits (Fox & Burch, 500 2014). The payloads were NaI scintillators with 256 energy channels ranging from 20 keV 501 -10 MeV with an energy-dependent geometric factor. Data from 13 August 2015 from 502 B. Anderson et al. (2017) is selected when the balloon is at approximately L = 6. 503

FIREBIRD II is a pair of 1.5 U ("unit," where $1 \text{ U} = 10^3 \text{ cm}^3$) CubeSats at a close 504 spatial separation which aimed to determine the scale sizes of precipitation regions. They 505 each have two detectors: a surface detector with a nearly 2π field-of-view and a collimated 506 detector with an approximately 45° field-of-view (Crew et al., 2016; Johnson et al., 2020). 507 The electron data reported in B. Anderson et al. (2017) is in counts per energy chan-508 nel, so the energy-dependent geometric factors from Johnson et al. (2020) are used to 509 convert counts to physical flux units, then an estimate of the electron flux and spectrum 510 at various times in the conjunction are made and are shown in Figure 14. The FIRE-511 BIRD satellite have a "wobble" period that is described in B. Anderson et al. (2017) that 512 implies the detectors are sampling portions of the trapped, loss cone, and anti-loss cone 513 populations. For this reason, we take the surface detector as the more consistent mea-514 surement of flux as the larger field-of-view measurement should vary less in coverage of 515 trapped versus non-trapped electrons than the collimated detector, given the spacecraft's 516 unknown look direction. Additionally, FIREBIRD is spatially separated from the mag-517 netic footprint where BARREL detected X-rays. For these reasons, we only attempt to 518 match the order of magnitude of measured electron flux and folding energy to the X-ray 519 inversion method. Using the Green's function inversion method, the electron spectrum 520 is inverted from the measured X-ray spectrum; the maximum likelihood electron spec-521 trum has flux 2.9×10^4 cm⁻² s⁻¹ sr⁻¹ keV⁻¹ with folding energy 145 keV and is shown 522 overplotted with FIREBIRD electron spectra in Figure 14. 523

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Figure 13. BARREL instrument counts per energy bin are shown in green and are adjusted down by the geometric factor to match the order of magnitude of the red line, which are an estimate of physical flux given some an estimate of NaI detection efficiency and is smoothed. The blue stairs plot is the linear combination of Green's function X-ray spectra (shown componentwise in dashed grey line) that is iterated upon until it matches the BARREL photon flux spectrum.

The inversion method described in Section 5 requires physical flux units in place 524 of instrument counts, so the following actions were taken to infer the BARREL instru-525 ment response to X-rays. An energy-agnostic geometric factor of 214 cm^2 sr was applied 526 to the spectrum and an estimate of the NaI efficiency as a function of energy is applied, 527 which primarily raises the flux in the high-energy tail of the spectrum (McCarthy, per-528 sonal communication, 2023, Akkurt, Gunoglu, & Arda, 2014). The lower energy portion 529 of the spectrum is more difficult to account for precisely in terms of energy response, and 530 the majority of the inversion information within the stratosphere is in the high energy 531 tail, so for those reasons the lower energy portion (< 30 keV) is excluded from this anal-532 vsis. Smoothing is also applied to remove channels with no X-ray counts after the BAR-533 REL background removal procedure implemented in SPEDAS is performed (Angelopoulos 534 et al., 2019). The results for the two events described in B. Anderson et al. (2017) are 535 shown in Figure 13. 536

From this result, we deem the X-ray inversion process validated since the inversion estimate falls within the interval of valid flux and folding energy estimates from the FIRE-

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BIRD surface detector electron measurements. A more in-depth investigation might suggest that the X-ray spectrum is generated by a two-component exponential or kappa distribution electron spectrum, since the high energy portion of the X-ray spectrum behaves more like a power law, which is not expected from a one-component exponential input spectrum.

544

6.3 Atmospheric Backscatter of Radiation Belt Electrons

In this case study, we consider the population of energetic electrons that are backscat-545 tered by the atmosphere, which is an observable quantity from this model. This popu-546 lation includes the case of electrons that have pitch angles within the loss cone but ul-547 timately are not lost to the atmosphere, as well as the case of secondary electron pro-548 duction in the upper atmosphere where those newly produced electrons rejoin the free 549 electrons in the radiation belts undergoing cyclotron motion. The former process can oc-550 cur through electron-neutral pitch angle scattering that reverses the field-aligned com-551 ponent of an electron's momentum vector, and the latter case can occur from impact ion-552 ization in which the secondary electron's momentum vector is anti-Earthwards. These 553 two populations are separate in origin, but to a LEO spacecraft may be indistinguish-554 able in measurement. This process has wide reaching implications for magnetosphere-555 ionosphere coupling and the generation of diffuse aurora, atmospheric electrodynamics, 556 and electron lifetime calculations (Selesnick et al., 2004; Marshall & Bortnik, 2018; G. V. Khaz-557 anov & Chen, 2021). 558

The GEANT4 model predicts a certain amount of electron backscatter per injected 559 electron beam for a given input energy and pitch angle. We seek to validate that these 560 model results accurately describe the electron backscatter phenomenon with in-situ elec-561 tron data. Selected for this study is the Electron Loss and Fields Investigation with a 562 Spatio-Temporal Ambiguity-Resolving (ELFIN) mission: a pair of CubeSats that spin 563 in order to measure the full pitch angle distribution of electrons from 50 keV - 5 MeV564 in a LEO orbit of 450 km altitude (Angelopoulos et al., 2020). These data are well suited 565 to estimate both precipitating electrons in the loss cone as well as backscattered elec-566 trons in the anti-loss cone. 567

In this section, we use the ability of ELFIN to directly measure backscattered electrons to validate the GEANT4 model. For this scope, we use the energy and pitch-angle

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Figure 14. Reanalysis of in-situ electron measurements from B. Anderson et al. (2017) showing (top) FIREBIRD 180°-FOV surface detector electron spectra and (bottom) 45°-FOV collimated detector electron spectra during the approximate conjunction between FIREBIRD and BARREL, where earlier spectra are in blue and progress to red. The possible exponential spectral distributions are shaded in grey for (top) fluxes of $8 \times 10^3 - 4 \times 10^4$ cm⁻² s⁻¹ sr⁻¹ keV and folding energies 140 – 170 keV for the surface detector, and (bottom) fluxes of $5 \times 10^2 - 6 \times 10^3$ cm⁻² s⁻¹ sr⁻¹ keV and folding energies 200 – 400 keV for the collimated detector. The GEANT4 inversion estimate (green line) yields a E_0 of 145 keV and an electron flux of 2.9×10^4 cm⁻² s⁻¹ sr⁻¹ keV⁻¹.

distributions in the public catalog of precipitation events likely associated with electro-570 magnetic ion cyclotron (EMIC) waves, provided by Capannolo et al. (under review 2023). 571 EMIC waves preferentially precipitate ~MeV energy electrons into the Earth's atmo-572 sphere and are also associated with strong proton precipitation (L. Blum et al., 2020; 573 Carson et al., 2013; Capannolo, Li, Ma, Chen, et al., 2019; Capannolo, Li, Ma, Shen, et 574 al., 2019). Within the scope of this work, the exact wave driver of the precipitation is 575 not essential; however, the Capannolo et al. (under review 2023) catalog is public and 576 events have been carefully selected to avoid possible instrumentation errors and are pro-577 cessed to remove noise (e.g. from low electron counts). More details on the analysis can 578 be found in Capannolo et al. (under review 2023). 579

For our validation case study, we select 8 ELFIN events. These 8 events have var-580 ious loss cone filling ratios, energy spectra, and pitch angle distributions, so these cases 581 are investigated in addition to the averaged behavior over many events. Figure 15 shows 582 three measurements from ELFIN: the measurement differential flux units are $cm^{-2} s^{-1} sr^{-1} MeV^{-1}$, 583 the bounce loss cone is between $0^{\circ} - 66^{\circ}$, $114^{\circ} - 180^{\circ}$ is the anti-bounce loss cone, and 584 between those regions are trapped electrons. Characteristic enhancements in the MeV 585 energy range are seen, such as the spectra shown in the center panel of Figure 15. ELFIN 586 data can also be seen with enhancements in flux in power law-like spectra, such as the 587 electron spectra in middle panel of Figure 15. These two spectral types, as well as ELFIN 588 data averaged over 144 EMIC-driven precipitation events in Figure 15, are analyzed to 589 validate the model results. 590

Two methods are employed in this analysis: the first involves inverting the ELFIN-591 measured anti-loss cone distribution and the second involves forward-modeling the ELFIN-592 measured loss cone distribution. The inversion method is performed by fitting a surface 593 to the electron backscatter spectrum and recording the coefficients used to generate that 594 surface. From there, a linear combination of the electron input space (E_0, α_0) is formed 595 with the coefficients acting as weights. The same weights are applied to the Green's func-596 tion ionization profiles and normalized by the loss cone input energy flux to ensure the 597 correct amount of ionization. This method is shown in blue in Figure 16. 598

The second method is a direct forward modeling of the ELFIN loss cone data where the data are evaluated at the input control points (E_0, α_0) to generate weights for the

-31-

601 602 linear combination method. The results of the forward modeling are used as a control or "truth" value for this analysis and are shown in red in Figure 16.

We find that the ionization profiles from these two methods match in general shape characteristics, i.e. altitude of maximum ionization, lowest ionization altitude, and so forth. The backscatter ratio is more difficult to validate as these measurements are averaged temporally and, due to satellite motion, spatially, so temporal and spatial dynamics may contribute to the amount of precipitation estimated from the data. Instead, we split the data into two parts: a downward and upward differential electron flux where one half is used as the initial conditions for the model and the other half is used as control data. We define two statistics, $R_{loss\ cone}$ and $R_{anti-loss\ cone}$ that denote the ratio of total energy flux that results from model processed-initial conditions versus the total energy flux of the control data, defined as:

$$R_i = \left(35 \ eV/pair * \int I_{model}(h) \ dh\right) \left(\int_{\Omega} \int_E f(E,\alpha) \cdot E \ dE \ d\Omega_i\right)^{-1}$$
(10)

where the numerator is the estimated energy flux input at the top of the atmosphere col-603 umn and the denominator is the energy flux from ELFIN data with i denoting the solid 604 angle fractions corresponding to the loss cone and anti-loss cone; the solid angle differ-605 ential unit is taken as $d\Omega = 2\pi \sin(\alpha) \ d\alpha$ to account for a full rotation in the electron 606 gyrophase at each pitch angle α , where the bounds of integration are taken as the loss 607 cone at 500 km of $\alpha < 66^{\circ}$. By multiplying by the energy bin center, we obtain energy 608 flux in units of $eV cm^{-2} s^{-1}$. We can then divide the energy flux by our assumed ion-609 ization energy of 35 eV/pair to match the integrated column ionization $\int I(h) dh$. This 610 is a two-sided statistic that encapsulates both measurement and physical process vari-611 ation. By computing the statistic for both the forward and inverse methods, any model 612 bias should average out. 613

The R_i statistic is plotted alongside $J_i/J_{trapped}$ for the 8 EMIC precipitation events 614 in Figure 17. Of note, when the $J_{anti-loss cone}/J_{trapped}$ ratio is small, the model and in-615 verse method more accurately reproduces the precipitating flux. Additionally, events 2, 616 3, and 6 show more differential electron flux in the anti-loss cone than in the loss cone, 617 which may be an artifact of temporal and spatial averaging or measurement errors as 618 it is unlikely to be true for a fixed point. Although 8 events are not sufficient for a sta-619 tistical study of this model's performance during EMIC precipitation, we find that for 620 cases where the model predicts more energy flux than the data shows $(R_i > 1)$, the cor-621

rection ratio R is less than 2, i.e. less than 50% error. For cases where the data shows more energy flux than modeled ($R_i < 1$) it is typically for the forward modeled loss cone data and implies that the evaluation method is missing some of the input energy flux. Since the forward and inverse methods used to evaluate the ELFIN data are deterministic, and the ELFIN data is bounded at 50% error, we conclude that the R values greater than 2 or less than 0.5 represent the true variation in the physical process of EPP.

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7 G4EPP Software Package

The Python package G4EPP has been developed to allow convenient user access to the data generated by this model, as well as a handful of analysis implementations that were used in this work. The software package is a class-based implementation that allows users to import an application programming interface (API) into their Python program and use the analysis methods directly in their code. Documentation for some implementations is included in Jupyter Notebooks which provide example usages of the methods, and direct access to the GEANT4 data products is offered as well.

Ionization profiles versus altitude can be generated from arbitrary initial energy and pitch angle distributions. Closed-form spectral distributions included in this package are exponential, power law, single and double Maxwellian, and relativistic Maxwellian distributions. These are used are commonly used for radiation belt electron spectral modeling and also have been applied to POES MEPED data. Additionally, the package offers the capability to convert from the reference atmosphere taken at PFISR to various atmospheric profiles via a scaling method implemented in Xu et al. (2020).

643 8 Conclusions

A new model of EPP has been developed based on the GEANT4 particle transport code. This code simulates EPP over a range of input parameters and simulation conditions to produce a lookup table from which measurement-based inversions can be performed to estimate precipitating electron parameters, including energy spectrum and flux. This model offers improvements over previous works, which are compared to these results to verify this work.

The results of this model are validated using balloon X-ray and satellite electron data. Through this analysis, the inversion techniques described are performed and re-



Figure 15. (Top row) EMIC-driven precipitation event observed by ELFIN-a on 2020-10-06/23:51 UT, showing (top row, left) the coupled energy-pitch angle spectrum (middle) the integrated energy spectrum per pitch angle bin from high (green) to low (blue) pitch angle, and (right) the pitch angle per energy bin from high (blue) to low (red) energy. (Middle row) EMIC-driven precipitation event observed by ELFIN-a on 2020-12-13/14:16 UT. This ionization profile shows a lower degree of agreement between the two ionization profile estimation techniques. (Bottom row) ELFIN data averaged over 144 events during EMIC wave-driven precipitation with energy and pitch angle-resolved measurements taken at 500 km altitude.



Figure 16. Predicted atmospheric ionization response from ELFIN data, performed with the methods described in Section 6.3: method 1 (blue) fits a surface to backscattered electron data and inverts to ionization profile, and method 2 (red) directly forward models loss cone data.



Figure 17. Loss cone and anti loss cone to trapped flux ratios (top) are presented above R_i (bottom), the ratio of the adjustment needed to match the model results with initial condition data. R_i equal to 1 notates no correction needed.

turn reasonable and realistic values for EPP parameters. Finally, a Python package is described that allows for user access to these data.

654 Open Research Section

The data generated by the model described in this work is incorporated into a Python package, G4EPP.py, which can be accessed at https://github.com/GrantBerland/G4EPP and includes documentation and notes on usage. BARREL data can be accessed at http:// barreldata.ucsc.edu/data_products/, and ELFIN data are available at https://plots .elfin.ucla.edu/.

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Figure 1.



Figure 2.



Figure 3.



Figure 4.



Figure 5.



Figure 6.



Figure.


Figure 7.



Figure 8.



Figure 9.



Figure 11.



Figure 12.





Figure 15.



60 90 120 150 180 Pitch Angle [deg]



Figure 15.



Figure 15.



60 90 120 150 180 Pitch Angle [deg]



Figure 16.



Figure 16.



Figure 16.



Figure 17.



Figure 10.



Figure 13.



Figure 14.

