

Chapter 4

Stochastic Differential Equations and the Stochastic Transport Model

4.1 Introduction

In this chapter, a brief introduction to stochastic differential equations (SDEs) will be given, after which the newly developed SDE based CR modulation model, used extensively in this thesis, will be discussed. The equivalence between SDEs and Fokker-Planck equations will be discussed and illustrated by an example; that of 1D Brownian motion. With this equivalence established, the TPE is transformed into an equivalent set of SDEs and the methodology employed to solve this set of SDEs numerically is also discussed. Details of this model were published by *Strauss et al.* [2011a]. Mainly because of numerical advantages, the SDE approach to CR modulation has become fashionable in recent times after *Zhang* [1999] successfully applied SDEs to the heliospheric CR modulation problem. Some historical and contemporary SDE models are discussed by e.g. *Krülls and Achterberg* [1994], *Fichtner et al.* [1996], *Yamada et al.* [1998], *Zhang* [1999], *Alanko-Huotari et al.* [2007], *Florinski and Pogorelov* [2009], *Pei et al.* [2010], *Kopp et al.* [2012] (who also discussed the mathematical and practical implementation of SDEs for a variety of general transport equations), *Bobik et al.* [2012] and *Luo et al.* [2013].

4.2 Stochastic Differential Equations

Several standard books deal with the mathematical formalism related to SDEs and their application in a variety of scientific fields [e.g. *Gardiner*, 1983; *Kloeden et al.*, 1994; *Kloeden and Platen*, 1999; *Øksendal*, 2003]. The discussion in this chapter is based on these sources. For the purpose of this thesis, it is sufficient to define an SDE as any equation that can be cast into the general form

$$\frac{\partial x(t)}{\partial t} = a(x, t) + b(x, t)\zeta(t) \quad (4.1)$$

for the 1D case where $a(x, t)$ and $b(x, t)$ are continuous functions, while $\zeta(t)$ represents a rapidly varying stochastic function, also referred to as the noise term. In SDE nomenclature, the first term on the right hand side of Eq. 4.1 is referred to as the *drift* term, while the second is referred to as the *diffusion* term (not to be confused with the physical drift and diffusive terms present in the TPE). Moreover, only SDEs of the Itô type are considered, where Eq. 4.1 can be rewritten as

$$dx(t) = a(x, t)dt + b(x, t)dW(t) \quad (4.2)$$

with $dW(t)$ representing the Wiener process; a time stationary stochastic Lévy process where the time increments have a Normal distribution with a mean of zero (i.e. a Gaussian distribution) and a variance of dt ; $dW(t) = W(t) - W(t - dt) \sim \mathcal{N}(0, dt)$. Essentially, Eq. 4.1 can be integrated rather straightforwardly as

$$x(t) = x_0 + \int_0^t a(x, t')dt' + \int_0^t b(x, t')dW(t') \quad (4.3)$$

where the first integral is a normal (Riemann or Lebesgue) integral, while the second is an Itô type stochastic integral. Analytical solutions for SDEs are however only available for a few scenarios, and as such, Eq. 4.3 is usually integrated numerically. In this thesis, the SDEs are integrated by using the Euler-Maruyama numerical scheme [Maruyama, 1955], where a finite time step Δt , is chosen and Eq. 4.2 is solved iteratively

$$x^{t+\Delta t} = x^t + a(x, t)\Delta t + b(x, t)\Delta W(\Delta t) \quad (4.4)$$

from an initial position $x = x_0$ at $t = 0$ and continued until either a boundary is reached at $x = x_e$ at $t = t^e$, or until a temporal integration limit is reached at $t = t^N$. Note that the Wiener process is discretized as

$$\Delta W(\Delta t) = \sqrt{\Delta t} \cdot \Lambda(t), \quad (4.5)$$

where $\Lambda(t)$ is a simulated Gaussian distributed pseudo-random number (PRN). The temporal evolution of x forms a trajectory through phase space, which is generally referred to as the trajectory of a pseudo-particle, discussed in detail in Section 4.4.4. Integrating Eq. 4.4 for a single pseudo-particle has no significance, as integration must be carried out over all possible trajectories (integrating over all possible Wiener processes; see Eq. 4.3), so that Eq. 4.4 is usually integrated $N \gg 1$ times and each time using a different series of simulated Wiener processes, i.e. starting the integration process with different seeds to the PRN generator (PRNG); also referred to as tracing N pseudo-particles. Numerically, the independence of the PRNs is very important to fulfil in the numerical model, as some PRNGs are not independent and have a quite short cycling period (meaning the same set of PRNs are repeated after a certain time).

To overcome these difficulties, the MT 19937 version of the Mersenne Twister PRNG [Matsumoto and Nishimura, 1988] is implemented in this thesis. This PRNG has a cycling period of $2^{19937} - 1$, while it is proven to produce independent normal deviates in 623 dimensions. In principle, any PRNG can be used to simulate a series of standard deviates, i.e. random numbers in the interval $(0, 1)$, where after the PRNs can be transformed to a Gaussian distribution by using e.g. the Box-Muller (also called the polar method) method [Box and Muller, 1958].

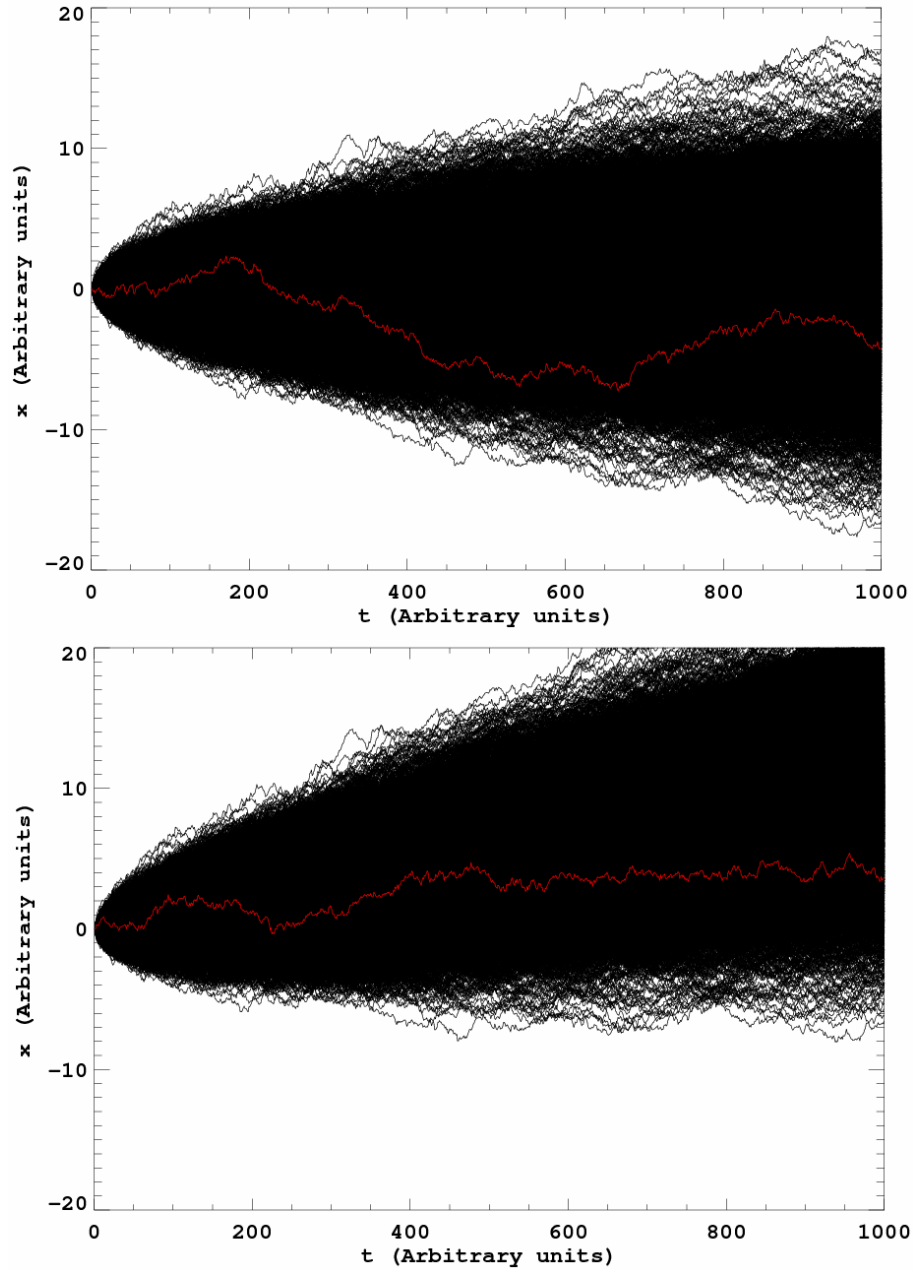


Figure 4.1: Solutions of Eq. 4.4 using $a(x, t) = 0$ and $b(x, t) = \sqrt{2}$ (top panel) and using $a(x, t) = 1$ and $b(x, t) = \sqrt{2}$ (bottom panel). The integration process is repeated for $N = 10000$ pseudo-particles, with the trajectory of the last pseudo-particle coloured red.

Fig. 4.1 shows the integration trajectories of $N = 10000$ pseudo-particles using Eq. 4.4 with

$a(x, t) = 0$ and $b(x, t) = \sqrt{2}$ (top panel) and for $a(x, t) = 1$ and $b(x, t) = \sqrt{2}$ (bottom panel). All trajectories start at $x_0 = 0$ and are continued until $t^N = 1000$. The trajectory of the last pseudo-particle is coloured red to illustrate the behaviour of a single pseudo-particle. An interpretation of the results are given in the next section. It is important to note that the pseudo-particles all start at the same position, while, on average, moving to larger values of $|x|$ with time.

A normalized (conditional) probability density $\rho'(x, t)$ can be calculated from the pseudo-particle trajectories, such that

$$\int_{\Omega} \rho'(x, t) d\Omega = 1, \quad (4.6)$$

where Ω denotes the entire integration space. Numerically this is done by dividing e.g. x into a series of bins, e.g. N' intervals, and calculating the number of pseudo-particles ending up in each bin, i.e. bin i has N_i particles, and dividing by N . The discretized version of Eq. 4.6 thus reads

$$\sum_{i=1}^{N'} \rho'_i(x, t) = \sum_{i=1}^{N'} \frac{N_i}{N} = 1. \quad (4.7)$$

The results of the top panel of Fig. 4.1 is binned at different times and the results presented in Fig. 4.2. The different pseudo-particle trajectories are again shown in the xt -plane, while the numerically calculated $\rho'(x, t)$ is shown in red at $t = 200, 400, 600, 800, 1000$. Note that at $t = 0$, $\rho'(x, t) = \delta(x - 0, t - 0)$, where δ represents a Dirac-delta function, while at later times, the distribution becomes Gaussian. See the next section for a discussion regarding the results of this figure.

4.3 Brownian Motion

Using Itô's lemma, it can be shown that every SDE (or set of SDEs) has an equivalent Fokker-Planck formulation. This is summarized by the so-called Kolmogorov equations, where the 1D time forwards Kolmogorov equation, given by

$$\frac{\partial \rho'(x, t)}{\partial t} = \frac{\partial}{\partial x} [a(x, t) \rho'(x, t)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [c(x, t) \rho'(x, t)] \quad (4.8)$$

with $c(x, t) = b^2(x, t)$ is equivalent to Eq. 4.2. Any partial differential equation can thus be transformed into an SDE (or set thereof) and vice versa. Using the case of 1D Brownian motion (the apparent irregular motion of particles in a medium), this section will illustrate this equivalence.

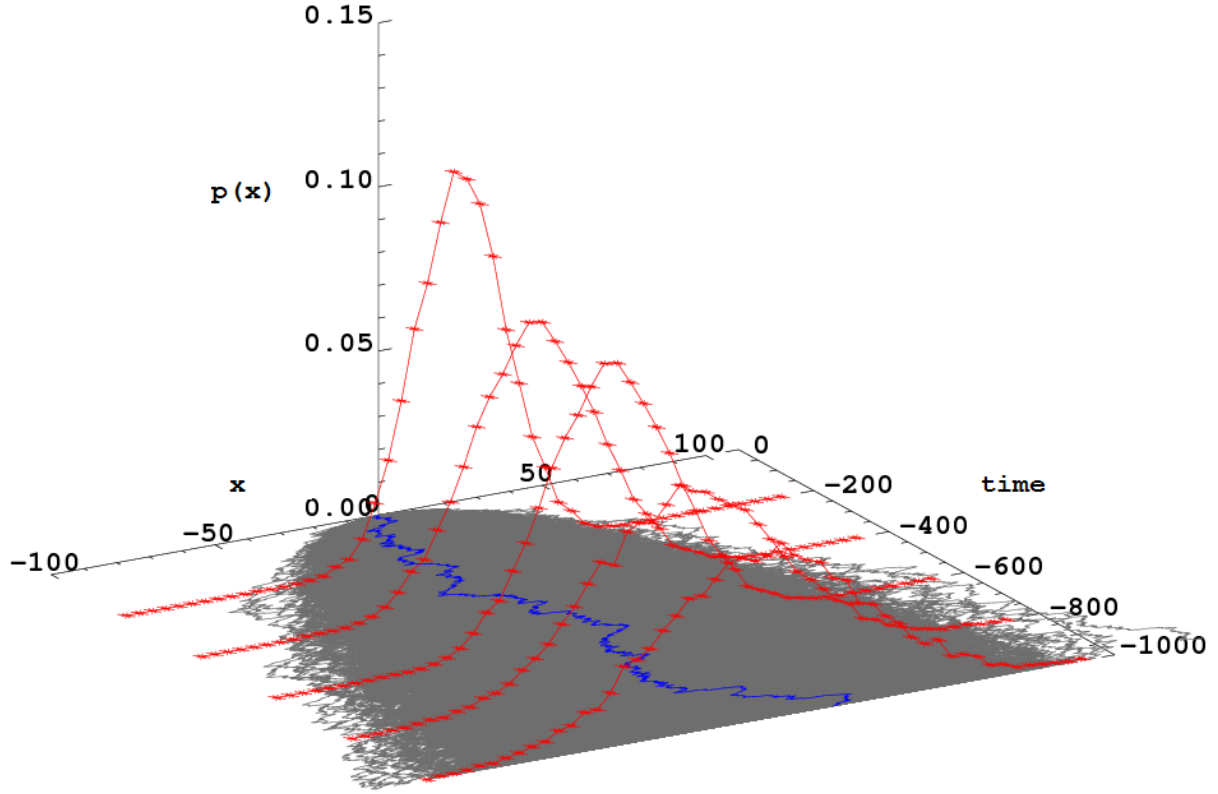


Figure 4.2: The xt -plane again shows the pseudo-particle traces originally shown in the top panel of Fig. 4.1, while the calculated $\rho'(x, t)$ is shown in red at different times. The trajectory of the last pseudo-particle is coloured blue.

Assuming Brownian motion due to collisions between e.g. pollen grains and water molecules, Einstein used thermodynamic principles to prove that the evolution of the pollen grains' probability distribution is given by Fick's law

$$\frac{\partial \rho'(x, t)}{\partial t} = -V \frac{\partial \rho'(x, t)}{\partial x} + \kappa \frac{\partial^2 \rho'(x, t)}{\partial x^2} \quad (4.9)$$

for constant values of V (the convective speed of the medium) and κ (the diffusion coefficient). Using the initial condition $\rho'(x, t) = \delta(x - 0, t - 0)$ and absorbing boundaries, $\rho'(x \rightarrow \infty, t) = 0$, this equation can be solved analytically to give

$$\rho'(x, t) = \frac{1}{\sqrt{4\pi\kappa t}} \exp \left[-\frac{(x - Vt)^2}{4\kappa t} \right]. \quad (4.10)$$

This analytical solution is shown in Fig. 4.3 for the parameters $\kappa = 1$, $V = 0$ (left panel) and $\kappa = 1$, $V = 1$ (right panel) at $t = 10, 500$ as the dashed lines. Starting from a delta function, $\rho'(x, t)$ becomes Gaussian, and with time, becomes increasingly broader. This is a well-known characteristic of normal diffusion (also referred to as Brownian diffusion). When convection

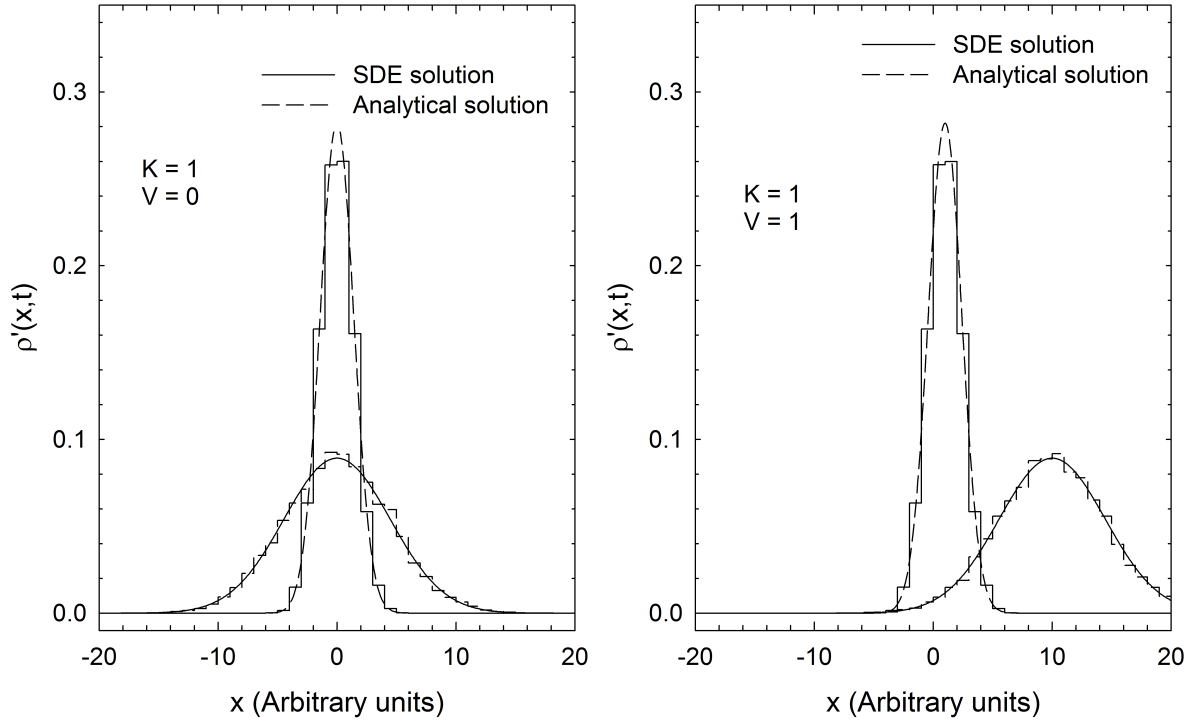


Figure 4.3: Solutions of E.g 4.10 for the parameters $\kappa = 1$, $V = 0$ (left panel) and $\kappa = 1$, $V = 1$ (right panel) for $t = 10, 500$, shown as the dashed lines. The solid lines show the calculated $\rho'(x, t)$ from the SDE approach in the previous section. In the left panel, $\rho'(x, t)$ is calculated from the results shown in the top panel of Fig. 4.1, while the results from the bottom panel of that figure are shown in the right panel of this figure.

is included in the diffusion process, the Gaussian distribution remains, while $\rho'(x, t)$ is simply convected along x .

Using Eq. 4.8, it is clear that Eq. 4.9 and Eq. 4.2 describe the same process, and therefore have the same $\rho'(x, t)$ when

$$\begin{aligned} a(x, t) &= V \\ b(x, t) &= \sqrt{2\kappa}. \end{aligned} \quad (4.11)$$

The SDE corresponding to Eq. 4.9 is generally referred to as the Langevin equation and gives an equivalent formulation of Brownian motion. The results from the SDE integration process discussed in the previous section are included in Fig. 4.3 and shown as the solid lines. It is clear that both approaches, the SDE and the more traditional partial differential equation (PDE) approach, yield the same $\rho'(x, t)$ when the boundary conditions and coefficients used in both approaches are equivalent. Moreover, making the connection between the results of the previous section and Brownian motion, the results of Fig. 4.1 can now be interpreted from a

physics point-of-view: The integration trajectories can be interpreted, for this specific case, as a possible trajectory of a neutral particle undergoing diffusion and convection in a medium, e.g., at $t = 0$ pollen grains are released at $x = 0$ in a standing pond (top panel) and in a moving stream (bottom panel). In the top panel they undergo diffusion, which leads to $\langle \Delta x^2 \rangle \propto \langle \Delta t \rangle$, so that the particles generally move away from one another (i.e. the particle density gradient becomes smaller with time). In the bottom panel, where the pollen grains also undergo convection, the medium simply convects the particle density towards larger values of x .

4.4 A Stochastic Transport Model

4.4.1 The Relevant Stochastic Differential Equations for Cosmic Ray Transport

In this work, the TPE is solved by means of SDEs in a so-called *time backwards* fashion. The time forwards and backwards approaches are equivalent, but for CR modulation, the latter approach is numerically easier to handle and also computationally much faster. An *observational point* point is chosen $(\vec{x}^0, s^0)$, i.e. the phase space position where the CR intensity will be calculated, and the trajectory of this pseudo-particle is then integrated time backwards until a modulation boundary is reached at $(\vec{x}^e, s^N)$. Here, s is a time (backwards) parameter, related to t by

$$s = t^N - t \quad (4.12)$$

i.e. in the normal time forwards scenario, integration is performed in the time domain $t = 0 \rightarrow t = t^N$, while in the time backwards case, this becomes $s = 0(t = t^N) \rightarrow s = s^N(t = 0)$. In both cases the temporal integration domain however remains constant, i.e. $t^N = s^N$. Furthermore, $\vec{x}$ represents any set of phase space coordinates. From Eq. 4.12 it follows that

$$\frac{\partial}{\partial t} = -\frac{\partial}{\partial s}. \quad (4.13)$$

For an n -dimensional set of SDEs, the general formulation becomes

$$dx_i = a_i(x_i, s)ds + \sum_{j=1}^n b_{ij}(x_i, s) \cdot dW_j(s), \quad (4.14)$$

where $\vec{a}$ is an n -dimensional vector and $\mathbf{b}$ is a $n \times n$ matrix. When time backwards integration is performed, Eq. 4.14 is equivalent to the following Fokker-Planck equation (also referred to as the time backwards Kolmogorov equation)

$$-\frac{\partial \rho'(x_i, s)}{\partial s} = \sum_{i=1}^n a_i(x_i, s) \frac{\partial \rho'(x_i, s)}{\partial x_i} + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n C_{ij}(x_i, s) \frac{\partial^2 \rho'(x_i, s)}{\partial x_i \partial x_j}. \quad (4.15)$$

Note that this equation is similar to Eq. 4.8, although the latter is in a conservative form. See *Kopp et al.* [2012] for a detailed discussion on how the time forwards and backwards SDE formulation is related to different Fokker-Planck equations. Here,

$$C_{ij}(x_i, s) \equiv (b_{ij}(x_i, s) \cdot b_{ij}(x_i, s)^T). \quad (4.16)$$

The TPE can therefore be cast into the form of Eq. 4.15, the quantities $\vec{a}$ and $\mathbf{b}$ obtained, and the equivalent SDE formulation for CR transport emerges naturally. The n -dimensional TPE is therefore transformed into a set of $n - 1$, 2D SDEs, with the latter being much easier to handle numerically.

In spherical coordinates, the TPE becomes

$$\begin{aligned} \frac{\partial f}{\partial t} = & \left[\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta r} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \kappa_{\phi r}}{\partial \phi} - V_r \right] \frac{\partial f}{\partial r} \\ & + \left[\frac{1}{r^2} \frac{\partial}{\partial r} (r \kappa_{r\theta}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta\theta} \sin \theta) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\phi\theta}}{\partial \phi} - \frac{V_\theta}{r} \right] \frac{\partial f}{\partial \theta} \\ & + \left[\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\theta\phi}}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial \kappa_{\phi\phi}}{\partial \phi} - \frac{V_\phi}{r \sin \theta} \right] \frac{\partial f}{\partial \phi} \\ & + \kappa_{rr} \frac{\partial^2 f}{\partial r^2} + \frac{\kappa_{\theta\theta}}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\kappa_{\phi\phi}}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} + \frac{2\kappa_{r\phi}}{r \sin \theta} \frac{\partial^2 f}{\partial r \partial \phi} + \frac{2\kappa_{r\theta}}{r} \frac{\partial^2 f}{\partial r \partial \theta} \\ & + \frac{2\kappa_{\theta\phi}}{r^2 \sin \theta} \frac{\partial^2 f}{\partial \theta \partial \phi} + \frac{p}{3} (\nabla \cdot \vec{V}_{sw}) \frac{\partial f}{\partial p}, \end{aligned} \quad (4.17)$$

where $\vec{V} = \vec{V}_{sw} + \vec{v}_d$ was introduced. Assuming that $f(\vec{x}, t) \propto \rho'(\vec{x}, t)$ and using Eq. 4.13, it follows that

$$\begin{aligned} a_r &= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta r} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \kappa_{\phi r}}{\partial \phi} - V_r \\ a_\theta &= \frac{1}{r^2} \frac{\partial}{\partial r} (r \kappa_{r\theta}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta\theta} \sin \theta) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\phi\theta}}{\partial \phi} - \frac{V_\theta}{r} \\ a_\phi &= \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\theta\phi}}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial \kappa_{\phi\phi}}{\partial \phi} - \frac{V_\phi}{r \sin \theta}, \\ a_p &= \frac{p}{3} (\nabla \cdot \vec{V}_{sw}) \end{aligned} \quad (4.18)$$

and

$$\mathbf{C} = \begin{bmatrix} \kappa_{rr} & \frac{\kappa_{r\theta}}{r} & \frac{\kappa_{r\phi}}{r \sin \theta} \\ \frac{\kappa_{r\theta}}{r} & \frac{\kappa_{\theta\theta}}{r^2} & \frac{\kappa_{\theta\phi}}{r^2 \sin \theta} \\ \frac{\kappa_{r\phi}}{r \sin \theta} & \frac{\kappa_{\theta\phi}}{r^2 \sin \theta} & \frac{\kappa_{\phi\phi}}{r^2 \sin^2 \theta} \end{bmatrix} \quad (4.19)$$

and the multidimensional Wiener process

$$d\vec{W} = [dW_r, dW_\theta, dW_\phi]. \quad (4.20)$$

Note that because only spatial diffusion is taken into account, $\mathbf{b}$ can be reduced from a 4×4 matrix to a 3×3 matrix (see also the discussion in *Kopp et al. [2012]*). To calculate $\mathbf{b}$, the square root of $\mathbf{C}$ must be calculated. As discussed by e.g. *Johnson et al. [2002]*, the magnitude and form of $\mathbf{b}$ may not be unique, but all of these $\mathbf{b}$'s will be mathematically equivalent. Here,

$$\mathbf{b} = \sqrt{2} \begin{bmatrix} \sqrt{\frac{\kappa_{\phi\phi}\kappa_{r\theta}^2 - 2\kappa_{r\phi}\kappa_{r\theta}\kappa_{\theta\phi} + \kappa_{rr}\kappa_{\theta\phi}^2 + \kappa_{\theta\theta}\kappa_{r\phi}^2 - \kappa_{rr}\kappa_{\theta\theta}\kappa_{\phi\phi}}{\kappa_{\theta\phi}^2 - \kappa_{\theta\theta}\kappa_{\phi\phi}}} & \frac{\kappa_{r\phi}\kappa_{\theta\phi} - \kappa_{r\theta}\kappa_{\phi\phi}}{\kappa_{\theta\phi}^2 - \kappa_{\theta\theta}\kappa_{\phi\phi}} \sqrt{\kappa_{\theta\theta} - \frac{\kappa_{\theta\phi}^2}{\kappa_{\phi\phi}}} & \frac{\kappa_{r\phi}}{\sqrt{\kappa_{\phi\phi}}} \\ 0 & \frac{1}{r} \sqrt{\kappa_{\theta\theta} - \frac{\kappa_{\theta\phi}^2}{\kappa_{\phi\phi}}} & \frac{\kappa_{\theta\phi}}{r\sqrt{\kappa_{\phi\phi}}} \\ 0 & 0 & \frac{\sqrt{\kappa_{\phi\phi}}}{r \sin \theta} \end{bmatrix}. \quad (4.21)$$

The set of SDEs governing CR transport therefore becomes

$$\begin{aligned} dr &= a_r \cdot ds + b_{rr} \cdot dW_r + b_{r\theta} \cdot dW_\theta + b_{r\phi} \cdot dW_\phi \\ d\theta &= a_\theta \cdot ds + b_{\theta\theta} \cdot dW_\theta + b_{\theta\phi} \cdot dW_\phi \\ d\phi &= a_\phi \cdot ds + b_{\phi\phi} \cdot dW_\phi \\ dp &= a_p \cdot ds, \end{aligned} \quad (4.22)$$

which can be integrated relatively easily by means of the Euler-Maruyama scheme mentioned earlier. Note that the momentum SDE can also be rewritten in terms of kinetic energy as

$$dE = \frac{1}{3} \left(\nabla \cdot \vec{V}_{sw} \right) \Gamma E \cdot ds, \quad (4.23)$$

with

$$\Gamma \equiv \frac{E + 2E_0}{E + E_0}, \quad (4.24)$$

where E_0 is the rest mass energy.

Advantages and Disadvantages of the SDE Modelling Approach

Numerically, there are many advantages to adopting an SDE based numerical model over more traditional finite difference numerical schemes: The SDE numerical model is unconditionally stable and much easier to implement than finite difference schemes. An SDE model can also be executed on parallel computing platforms, making use of a computer cluster to significantly speed up the calculations. From a physics point of view, the following chapters will emphasize that the SDE approach can lead to additional insight into the CR modulation process.

The only disadvantage of the SDE approach is the inherent difficulty of this approach to calculate global CR intensities. The model only calculates the CR intensity at a single phase space point each time integration is performed and the model must therefore be repeated for each position in phase space where the intensity is needed. This can however be overcome by implementing multiple instances of the modulation model on the different computational nodes of a computer cluster.

4.4.2 Boundary Conditions

Dirichlet (First Type) Boundary Conditions

This type of boundary condition is specified at the HP for GCR as the LIS (or for the Jovian electrons in the Jovian magnetosphere; see chapter 6). In general it can be handled by using the Green's function interpretation of the *conditional* probability density $\rho'(\vec{x}, t)$ [e.g. Webb and Gleeson, 1977],

$$f(\vec{x}^0, t^0) = \int_0^{t^0} \int_{\vec{x} \in \Omega_b} f_b(\vec{x}, t) \rho'(\vec{x}, t) d\Omega dt + \int_{\Omega} f_a(\vec{x}, 0) \rho'(\vec{x}, 0) d\Omega, \quad (4.25)$$

where $f_b(\vec{x}, t)$ represents the boundary condition (i.e. the LIS), $f_b(\vec{x}^0, t^0)$ the phase space position where the intensity is calculated, i.e. the *observational* point, $f_a(\vec{x}, 0)$ the initial condition, which, for CR modulation, is usually set to $f_a(\vec{x}, 0) = 0$ (a heliosphere empty of CRs), Ω_b the boundary of the integration domain and where $\vec{x} = \{r, \theta, \phi, p\}$. The focus in this thesis is on stationary (steady state) solutions of the TPE, where $t \rightarrow \infty$ (no temporal restriction on the time), reducing Eq. 4.25 to

$$f(\vec{x}^0) = \int_{\vec{x} \in \Omega_b} f_b(\vec{x}) \rho'(\vec{x}) d\Omega. \quad (4.26)$$

For CRs, the boundary values are only momentum dependent so that only integration over momentum space is performed, i.e. $d\Omega \rightarrow dp$,

$$f(\vec{x}^0) = \int_0^p f_b(p') \rho(\vec{x}) dp' \Big|_{\vec{x} \in \Omega_b}, \quad (4.27)$$

which is essentially a convolution of the boundary condition and the probability distribution. A similar form can be used when two disjointed boundaries are present, such that $\Omega'_b \cap \Omega_b = 0$,

$$f(\vec{x}^0) = \int_0^p f_b(p') \rho(\vec{x}) dp' \Big|_{\vec{x} \in \Omega_b} + \int_0^p f'_b(p') \rho(\vec{x}) dp' \Big|_{\vec{x} \in \Omega'_b}. \quad (4.28)$$

Two approaches can be used to incorporate these boundary conditions. Firstly, the set of SDEs can be solved to provide $\rho'(\vec{x})$, whereafter Eq. 4.27 is used to obtain the CR flux. A second,

and numerically easier approach is to calculate the weighted value of $f(\vec{x}^0)$ for each pseudo-particle individually, before normalizing this to the correct magnitude at the end of the integration process. The second approach is used in this thesis. For a single pseudo-particle, reaching a momentum dependent boundary with $p_i = p_i^e$ (where i labels the pseudo-particles),

$$\rho'_i(\vec{x}) = \delta(p_i - p_i^e)|_{\vec{x} \in \Omega_b}, \quad (4.29)$$

because of the normalization condition. This implies that

$$f_i(\vec{x}^0) = f_b(p_i^e), \quad (4.30)$$

so that each pseudo-particle traced to the boundary makes some (weighted; see Eq. 4.31) contribution to the total solution. Repeating for $N \gg 1$ pseudo-particles, the numerical solution of the TPE can be calculated as

$$f(\vec{x}^0) = \frac{1}{N} \sum_{i=1}^N f_b(p_i^e), \quad (4.31)$$

which follows from Eqs. 4.7 and 4.27.

Neumann (Second Type) Boundary Conditions

Generally, all modulation models assume a boundary condition at small values of r . This is mainly done because some of the heliospheric parameters, e.g. the HMF, is undefined at $r = 0$. Here, a reflecting inner boundary condition is assumed at $r_{\min} \ll 1\text{AU}$,

$$\left. \frac{\partial f(\vec{x})}{\partial r} \right|_{r=r_{\min}} = 0. \quad (4.32)$$

For SDEs, this means that a pseudo-particle penetrating this boundary is again placed into the computational domain by reflection at the boundary

$$r < r_{\min} : r \rightarrow 2r_{\min} - r. \quad (4.33)$$

Other Boundary Related Conditions

Although the SDE approach does not have to prescribe boundary conditions at the computational domains of the angular coordinates, the angular position of the pseudo-particles needs to be renormalized so that $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$. This is done by specifying the following conditions:

$$\begin{aligned}
\phi < 0 & : \phi \rightarrow \phi + 2\pi \\
\phi > 2\pi & : \phi \rightarrow \phi - 2\pi \\
\theta < 0 & : \theta \rightarrow |\theta|; \phi \rightarrow \phi \pm \pi \\
\theta > \pi & : \theta \rightarrow 2\pi - \theta; \phi \rightarrow \phi \pm \pi
\end{aligned} \tag{4.34}$$

which occur when the pseudo-particle either propagates around the ecliptic plane or cross the solar poles.

4.4.3 Benchmarks

This section shows and discusses two benchmark solutions of the SDE approach when solving the TPE numerically. Additional benchmarks are performed in Chapters 5 and 7.

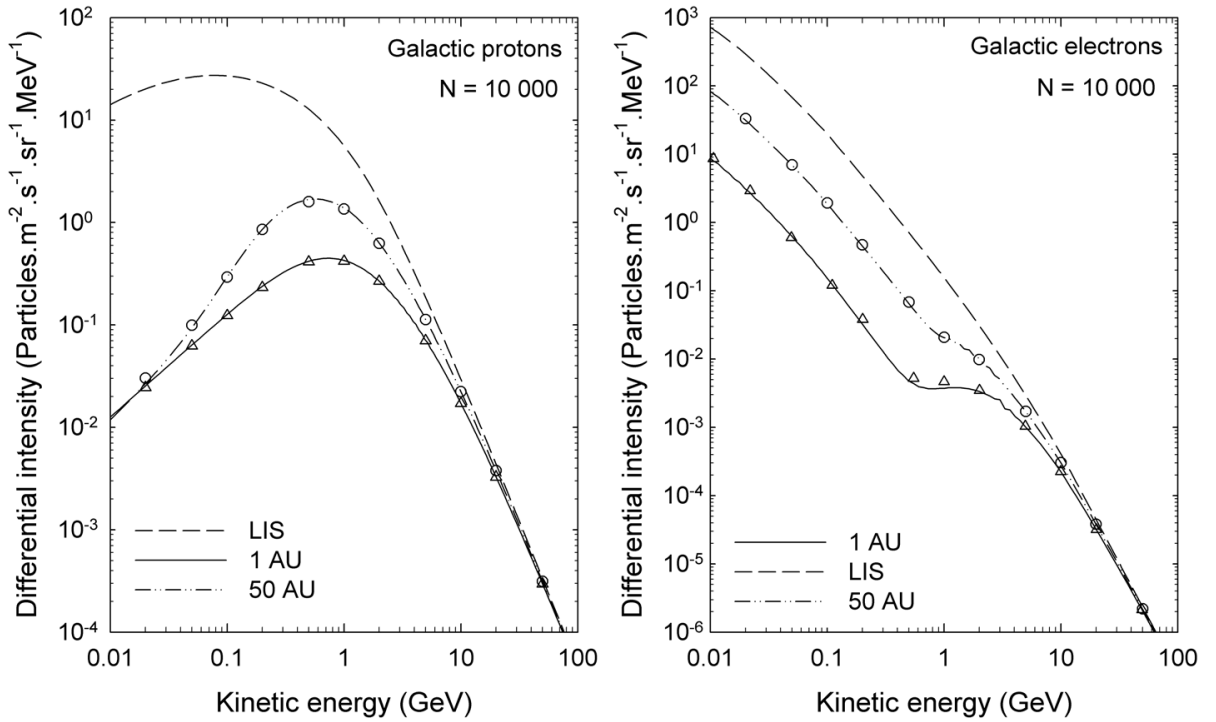


Figure 4.4: Benchmarking results from the SDE model (scatter points) with those of the Du Fort-Frankel finite differences numerical scheme (lines) for the modulation of GCS protons (left panel) and electrons (right panel) for a spatially 1D version of the TPE. See also *Strauss et al. [2011b]*. The energy spectra are shown at Earth (1 AU) and at 50 AU with respect to the LIS prescribed at 100 AU (i.e. the position of the HP).

Fig. 4.4 shows a benchmarking study which compares the solutions of the SDE model (scatter points) to that of a Du Fort-Frankel numerical scheme (lines) for a spatially 1D version of the TPE. Results are shown for GCR protons (left panel) and electrons (right panel) at radial positions of 1 AU, 50 AU and 100 AU (LIS). These results, as well as the modulation parameters

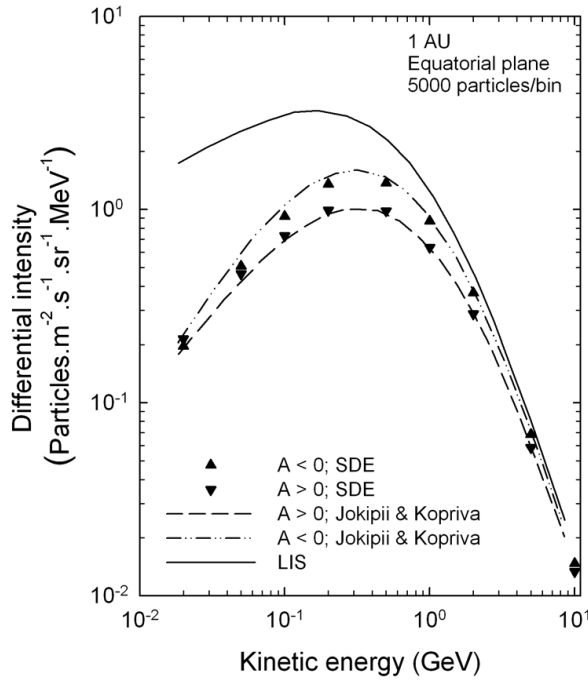


Figure 4.5: Similar to Fig. 4.4, but now for a 3D version of the TPE which includes drifts. See also *Strauss et al.* [2011a]. Results are compared to those of *Jokipii and Kopriva* [1979] at Earth for both HMF drift cycles. For each phase space position, $N = 5000$ pseudo-particles were integrated.

used, were reported by *Strauss et al.* [2011b]. Similar 1D benchmarks were performed by *Yamada et al.* [1998] and illustrates the applicability and validity of the SDE model in calculating CR intensities.

A similar benchmarking procedure is shown in Fig. 4.5. Here, results from a 3D (including drifts) version of the SDE modulation model is compared to earlier results from *Jokipii and Kopriva* [1979] for protons in both HMF drift cycles. All transport parameters are set identically to those used by *Jokipii and Kopriva* [1979]. Similar benchmarking studies were performed by *Zhang* [1999] and *Pei et al.* [2010] and emphasize the validity of these results based on the SDE numerical modulation model.

4.4.4 Pseudo-particle Traces

Although the terminology *pseudo-particles* and *trajectories/traces* of the pseudo-particles were used extensively in this chapter, the meaning thereof in the context of CR modulation will now be discussed. A pseudo-particle trace (or trajectory) is the temporal evolution of a pseudo-particle's phase space coordinates. Fig. 4.6 shows four such trajectories when solving the TPE for GCR electrons in the $A > 0$ (left panel) and $A < 0$ (right panel) HMF drift cycles [*Strauss et al.*, 2011a]. In the following chapter it will be shown how these traces may be used to highlight features of CR modulation and even give additional insight into the modulation processes.

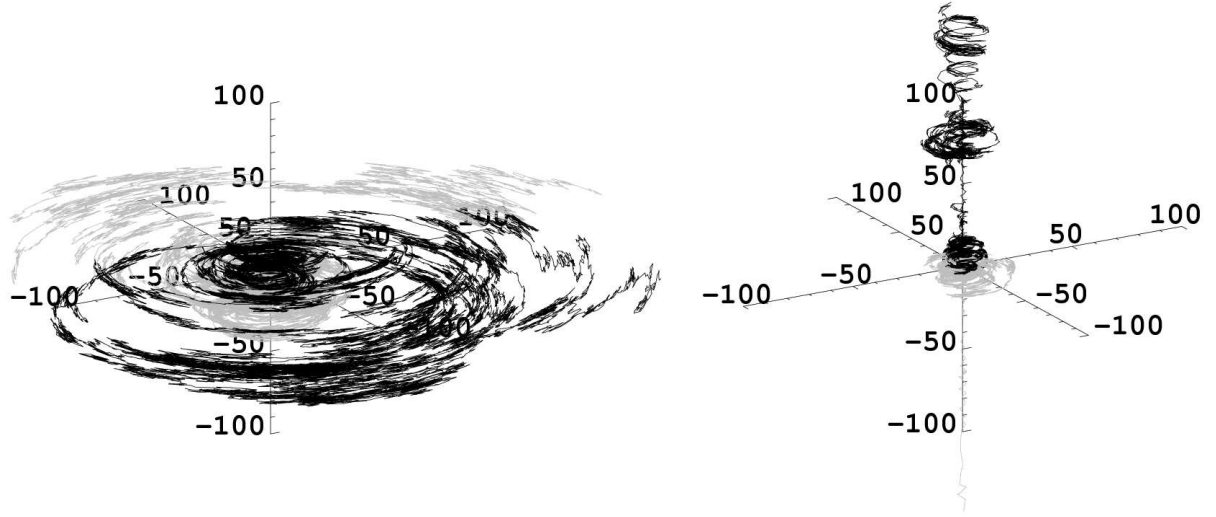


Figure 4.6: Pseudo-particle traces for GCR electrons in the $A > 0$ (left panel) and $A < 0$ (right panel) HMF drift cycles. All axes are labelled in AU with the Sun located at the origin and the HP at a radial distance of 100 AU. For each scenario, two pseudo-particle trajectories are shown, coloured in black and grey respectively. The vertical axis represents the polar axis of the heliosphere. See also *Strauss et al.* [2011a].

The question however remains: What is a pseudo-particle, or what does it physically represent?

The answer is surprisingly simple: Because the SDE model solves for $f(\vec{x}, t)$, a pseudo-particle represents a realization of $f(\vec{x}, t)$, so that, for the purposes of this thesis, a pseudo-particle is defined as an ensemble of CR particles, where the ensemble is constructed such that it results in a gyro- and isotropic collection of particles. A more accurate term for a pseudo-particle is that of a *phase space density element*. However, the nomenclature of a pseudo-particle is ingrained into the field of SDE based modulation models, and as such, will be used throughout this thesis. Many authors mistakenly assume that a pseudo-particle represents an actual CR particle, or the guiding centre of such a particle [e.g. *Kóta, 2012*], which is of course not the case, as a single CR particle would obey the Lorentz law. The way in which particle source and/or loss terms is treated in the SDE approach [e.g. *Kopp et al., 2012*] also shows that pseudo-particles are in fact not physical particles; pseudo may be assumed to refer to the fact that they are simply mathematical realizations of particle distribution functions.

The trajectory of a pseudo-particle also has an overlooked and very important physical significance. Along the trajectory of a single pseudo-particle (where $\mathcal{L}$ labels the set of phase space coordinates along this trajectory)

$$\rho'(\mathcal{L}) = 1, \quad (4.35)$$

which is an extension of Eq. 4.29, and occurs because of the normalization condition (see Eq. 4.6) of $\rho'(\vec{x}, t)$ as shown in Eq. 4.29. Because $f(\vec{x}, t) \propto \rho'(\vec{x}, t)$, it follows that

$$f(\mathcal{L}) = \text{constant}, \quad (4.36)$$

so that

$$\frac{Df(\mathcal{L})}{Dt} = 0, \quad (4.37)$$

which is a Lagrangian derivative along $\mathcal{L}$. Eq. 4.37 is simply a restatement of Liouville's theorem: Along the trajectory of a pseudo-particle through phase space, the CR distribution function remains constant. The trajectory of a pseudo-particle therefore also shows a graphical illustration of Liouville's theorem. Moreover, this proves that the SDE approach automatically satisfies this theorem, without the need to include additional boundary conditions, e.g. the so-called *matching condition* used in finite difference models to simulate shock acceleration.

4.5 Summary and Conclusions

It was shown that for any Fokker-Planck equation, an equivalent set of SDEs exist, so that CR modulation can be described and modelled by either of these formulations. The relevant set of SDEs describing CR transport (i.e. being equivalent to the TPE) was derived and the resulting SDE based CR modulation model's numerical implementation was discussed. Successful benchmarks of this model with previous models, adopting finite difference numerical schemes, were shown. In the following chapters, the advantages of the SDE modelling approach will be shown and discussed, including visualization of particle transport through pseudo-particle trajectories, as discussed in this chapter.