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Solving Parker's transport equation with stochastic differential equations on GPUs

P. Dunzlaff, R.D. Strauss *, M.S. Potgieter

Centre for Space Research, North-West University, 2520 Potchefstroom, South Africa

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ABSTRACT

The numerical solution of transport equations for energetic charged particles in space is generally very costly in terms of time. Besides the use of multi-core CPUs and computer clusters in order to decrease the computation times, high performance calculations on graphics processing units (GPUs) have become available during the last years. In this work we introduce and describe a GPU-accelerated implementation of Parker's equation using Stochastic Differential Equations (SDEs) for the simulation of the transport of energetic charged particles with the CUDA toolkit, which is the focus of this work. We briefly discuss the set of SDEs arising from Parker's transport equation and their application to boundary value problems such as that of the Jovian magnetosphere. We compare the runtimes of the GPU code with a CPU version of the same algorithm. Compared to the CPU implementation (using OpenMP and eight threads) we find a performance increase of about a factor of 10–60, depending on the assumed set of parameters. Furthermore, we benchmark our simulation using the results of an existing SDE implementation of Parker's transport equation.

1. Introduction

The propagation of charged particles in the heliosphere, i.e. the region influenced by the solar wind and the interplanetary magnetic field (IMF), is generally described by the transport equation derived by Parker [1] and is a special case of the general Fokker–Planck equation. Parker's equation describes the pitch–angle averaged diffusion of particles in the heliosphere, including adiabatic energy changes, convection with the solar wind, as well as drifts arising from gradients and curvatures in the IMF and reads

$$\frac{\partial f}{\partial t} + \underbrace{(\mathbf{v}_{sw} + \langle \mathbf{v}_d \rangle) \cdot \nabla f}_{\text{convection \& drifts}} - \underbrace{\frac{1}{3}(\nabla \cdot \mathbf{v}_{sw}) \frac{\partial}{\partial E}(\Gamma E f)}_{\text{ad. energy changes}} = \underbrace{\nabla \cdot (\mathbf{K} \cdot \nabla f)}_{\text{diffusion}} + Q. \quad (1)$$

Here, $f = f(\mathbf{x}, E, t)$ is the phase space density, proportional to the cosmic ray intensity, and is a function of position, energy and time. The solar wind velocity and the averaged drift velocities are given by $\mathbf{v}_{sw}$ and $\mathbf{v}_d$, respectively. Adiabatic energy changes are described by the third term on the left side where

$$\Gamma = \frac{E + 2E_r}{E + E_r}, \quad (2)$$

with E_r being the rest energy of the particles and E the kinetic energy. In the expanding solar wind plasma, i.e. $(\nabla \cdot \mathbf{v}_{sw}) > 0$, particles lose energy with time. The diffusion tensor $\mathbf{K}$, arising from fluctuations in the interplanetary magnetic field [2], contains the diffusion coefficient parallel to the mean magnetic field $\kappa_\parallel$ and in the two perpendicular directions, $\kappa_{\perp,1}$ and $\kappa_{\perp,2}$. These diffusion coefficients generally depend on position and time as well as on the energy of the particles. Q represents any particle sources in the heliosphere and can also be a function of position, energy and time. For the simulation presented here, $Q = 0$.

For the examples shown in this work we make use of the expression

$$\lambda(r)_\parallel = \frac{\lambda_0}{2}\left(1 + \frac{r}{r_0}\right), \quad (3)$$

for the particle's parallel mean free path. Here, λ_0 is the mean free path at a point of reference (r_0), e.g. Earth and r is the radial distance from the Sun. The parallel diffusion coefficient follows as

$$\kappa(r)_\parallel = \frac{v\lambda(r)_\parallel}{3}, \quad (4)$$

* Corresponding author.
E-mail address: dutoit.strauss@nwu.ac.za (R.D. Strauss).

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where v is the particle's speed. The relation between the parallel and perpendicular diffusion coefficients is assumed to be

$$\kappa(r)_{\perp 1,2} = \chi \kappa(r)_{\parallel}, \quad (5)$$

with $\chi = 0.01$ a constant. Consequently, the diffusion coefficients used here increase with radial distance from the Sun, i.e. the center of the coordinate system.

There are four primary sources of charged particles that can be observed in the heliosphere: galactic cosmic rays (GCRs) entering the heliosphere from the outside [3], solar energetic particle (SEPs) accelerated during so-called solar flare events [4], the anomalous cosmic ray component thought to be accelerated in the outer regions of the heliosphere [5] and particles that originate from planetary magnetospheres. Well-known amongst the latter sources is the Jovian magnetosphere, a quasi-constant source of electrons [6], so-called Jovian electrons (JEs) of energies $\leq$ 20 MeV that can be observed in wide regions of the heliosphere and are the dominant contribution to the electron fluxes observed at these energies.

Parker's transport equation can be applied to a wide field of heliospheric and astrophysical particle transport problems, e.g. the propagation of Jovian electrons [7,8] and galactic cosmic rays [9,10, 3] in the heliosphere and, in a more general form, also for particle propagation in the galaxy [11,12] and, for the case of very small diffusion coefficients, for the propagation of SEPs.

2. SDE representation of the transport equation

Parker's transport equation is traditionally solved using finite-difference methods. However, in recent years a different approach using Stochastic Differential Equations (SDEs) was pursued by several authors, amongst others, [13–20]. The foundations of SDEs and their solution were derived in 1944 by K. Itō (cf. [21]); a comprehensive theoretical discussion is for example given by Øksendal [22] while Iacus [23] gives a more practical introduction to the numerical solution of SDEs.

A general expression for a set of SDEs can be written as

$$dx_i = a_i dt + \sum_i^k \sum_j^k b_{i,j} dW_i, \quad (6)$$

where x_i represents a spatial (or energy) coordinate, a_i drift terms (referring to first order, deterministic terms; not to be confused with the physical process of particle drifts), $b_{i,j}$ diffusion terms and k corresponds to the dimensions of the problem. In the last term $b_{i,j}$ is frequently called the volatility matrix (or tensor), especially in the field of financial mathematics [24] since $b_{i,j}$ is not identical (but related) to the diffusion tensor that appears in the equivalent Fokker–Planck formulation of the diffusion equation. The differential dW_i is a Wiener process [23] and is given by

$$dW = \sqrt{dt} N(0, 1), \quad (7)$$

where $N(0, 1)$ is a random number drawn from a normal (Gaussian) distribution with zero mean and unit variance.

There are two ways to solve Fokker–Planck equations in terms of SDEs: a time-forward and a time-backward approach. For each of these approaches, the set of SDEs that are equivalent to the Fokker–Planck equation changes. For the case of solar modulation in the heliosphere (the main topic of study in this work), the particle intensity is usually only calculated at a small number of phase-space positions, e.g. an energy spectrum or intensities along a spacecraft trajectory. For these applications, the time-backward approach is the most effective, while, if global particle intensities are calculated, the time-forward approach could be more effective. In order to find a time-backward SDE expression for Parker's transport equation, Eq. (1) must be cast into the corresponding time-backward Kolmogorov equation (see [25] for a detailed discussion regarding the time-forward and time-backward equations)

$$\frac{\partial f(\mathbf{x}, E, t)}{\partial t} = \underbrace{\sum_{i=1}^k a(\mathbf{x}, E, t)_i \frac{\partial f(\mathbf{x}, E, t)}{\partial x_i}}_{\text{drift terms}} + \underbrace{\frac{1}{2} \sum_{i=1}^k \sum_{j=1}^k C(\mathbf{x}, E, t)_{i,j} \frac{\partial^2 f(\mathbf{x}, E, t)}{\partial x_i \partial x_j}}_{\text{diffusion}}, \quad (8)$$

where $a(\mathbf{x}, E, t)_i$ represents drift (again, referring to first-order terms) and $C(\mathbf{x}, E, t)_{i,j}$ the diffusion tensor. Note the factor 1/2 in front of the diffusion terms. This factor arises in the formal derivation of the diffusion equation [26] but is frequently found to be included in the diffusion tensor. It can be shown that the diffusion tensor $\mathbf{C}$ and the volatility $\mathbf{b}$ are related as

$$\mathbf{C} = \mathbf{b}\mathbf{b}^T, \quad (9)$$

where T indicates the transpose of $\mathbf{b}$.

Applying the transformations to Eq. (1) using spherical coordinates one obtains a set of three stochastic differential equations and one ordinary differential equation which is equivalent to the original Fokker–Planck equation:

$$d_r = a_r ds + b_{rr} \cdot dW_r + b_{r\vartheta} \cdot dW_\vartheta + b_{r\phi} \cdot dW_\phi \quad (10)$$

$$d_\vartheta = a_\vartheta ds + b_{\vartheta\vartheta} \cdot dW_\vartheta + b_{\vartheta\phi} \cdot dW_\phi \quad (11)$$

$$d_\phi = a_\phi ds + b_{\phi\phi} \cdot dW_\phi \quad (12)$$

$$dE = a_E ds. \quad (13)$$

Note that the change in the particle's energy does not explicitly contain a random process, but could if momentum diffusion, for example, was included into the Parker equation. The derivation of the coefficients above is discussed in detail by [27] and references therein.

The most straightforward way to solve SDEs on a computer is to apply the Euler–Maruyama scheme [23] to a discretized version of the relevant set of SDEs, which, for the one-dimensional case reads

$$x_{t+1} = x_t + a_t \Delta t + b_t \Delta W_t, \quad (14)$$

where Δt is the time increment and $\Delta W_t = \sqrt{\Delta t} N(0, 1) \approx dW_t$. This numerical scheme is first-order accurate in time [28].

The solution of Eq. (14), therefore constitutes a trajectory in phase-space following the temporal evolution of a phase-space density element (an ensemble of *real* particles)—referred to as a pseudo-particle. Because of the statistical properties of the Wiener process, a large number of these pseudo-particle paths must be integrated and averaged in order to obtain a probability distribution and thereby also the actual particle intensity (see the next section). A graphical illustration showing the differences between the time-forward and time-backward integration is shown in Fig. 1. The left panel shows the model boundaries (discussed in more detail in the next section): Galactic particles originate uniformly from the heliopause, while the inner boundary is reflective. We are interested in calculating the intensity at an *observational* point (the black square), e.g. at Earth's position. The middle panel shows how time-forward integration could be implemented: a large number of pseudo-particles (weighted with the boundary condition) are released uniformly at the heliopause and then propagate throughout the model domain until a temporal integration boundary is reached. In the time-backward formulation (the right panel), the pseudo-particles are released from the observational