New Astronomy 45 (2016) 1–6

Contents lists available at ScienceDirect

New Astronomy

journal homepage: www.elsevier.com/locate/newast

A graphics-card implementation of Monte-Carlo simulations for cosmic-ray transport

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HIGHLIGHTS

- A graphics-card implementation of a Monte-Carlo simulation is presented.
- Major applications are the diffusion of cosmic rays and solar energetic particles.
- Due to the SIMD model and shared memory, the code runs faster than the CPU version.
- The code decreases the computational cost of such simulations.
- The comparison with an existing implementation shows good agreement.

ARTICLE INFO

Article history:
Received 3 July 2015
Revised 21 August 2015
Accepted 28 October 2015
Available online 3 November 2015

Communicated by J. Makino

Keywords:
Cosmic rays
Turbulence
Diffusion
CUDA

ABSTRACT

A graphics card implementation of a test-particle simulation code is presented that is based on the CUDA extension of the C/C++ programming language. The original CPU version has been developed for the calculation of cosmic-ray diffusion coefficients in artificial Kolmogorov-type turbulence. In the new implementation, the magnetic turbulence generation, which is the most time-consuming part, is separated from the particle transport and is performed on a graphics card. In this article, the modification of the basic approach of integrating test particle trajectories to employ the SIMD (single instruction, multiple data) model is presented and verified. The efficiency of the new code is tested and several language-specific accelerating factors are discussed. For the example of isotropic magnetostatic turbulence, sample results are shown and a comparison to the results of the CPU implementation is performed.

1. Introduction

Describing the stochastic motion of particles in a turbulent medium has been a long-standing problem. Early examples are diffusion (Fick, 1855), Brownian motion (Einstein, 1905), and random walks (Chandrasekhar, 1943), which are all related on the level of the individual particles. An important class of such problems is given by electrically charged particles moving in a tenuous magnetized plasma, which has the additional difficulty that the turbulence is typically anisotropic if a large-scale magnetic field is present. In addition, turbulent electric fields can lead to diffusion also in momentum space—the so-called stochastic acceleration. Prominent examples include the transport and acceleration of cosmic rays (Schlickeiser, 2002; Duffy and Blundell, 2005; Shalchi, 2009; Tautz, 2012), solar energetic particles causing the so-called space weather (Scherer et al., 2005; Bothmer and Daglis, 2006), and particle transport in fusion plasmas (Bourdelle, 2005; Angioni et al., 2009).

In many scenarios that involve turbulent transport, particularly in the astrophysical theater, an analytical solution is often too simple and misses important contributions from non-linear dynamics. Recently, therefore, self-consistent simulations have been favored that are based either on (magneto) hydrodynamics, smoothed particle hydrodynamics, the particle-in-cell approach, or a combination forming so-called hybrid simulations. The advantage is that the interaction of electromagnetic fields and plasma particles can be treated self-consistently. The analytical understanding, however, is severely impeded by the complexity of the covered dynamics. In addition, these simulations are computationally very demanding but are nevertheless limited with respect to the large scales, which poses a problem for example for extended astrophysical systems with curved mean magnetic fields.

Analytical theories thus remain in use, to treat either plasma instabilities (test-wave approach) or particle diffusion (test-particle ansatz). The latter is particularly applicable for the propagation of cosmic rays and solar energetic particles, which have a significantly lower number density than the ambient plasma. The back-reaction of the particles on the plasma can thus be neglected. To test the validity of the test-particle calculations, Monte-Carlo simulations have

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http://dx.doi.org/10.1016/j.newast.2015.10.012
1384-1076/

been widely used as a tool that operates under the exact same conditions and assumptions. By averaging over the trajectories of charged particles being scattered by turbulent electromagnetic fields, diffusion coefficients, intensity time profiles, and/or information about the anisotropy of a particle distribution can be obtained. While in some cases the integration of a thousand particles is sufficient, there are some problems that easily rfuire millions of particles (e. g., Tautz et al., 2013), thereby again making this approach computationally expensive.

Recently, the use of graphics cards for scientific computations has received considerable attention. The main reason is that the cost of a typical high-performance graphics card is much lower compared to that for a comparable amount of CPU processing cores. The programming effort, however, is increased. Here, the CUDA programming language by Nvidia (2011), which is an extension of C/C++, comes in handy. This ansatz allows the modification and extension of already existing programs so that only those parts have to be modified that will be executed on the graphics processors. Here, the adaptation of the Padian code (Tautz, 2010) for the use with graphics cards is presented. While the principal approach remains unchanged, there are some peculiarities that merit a detailed discussion.

The paper is organized as follows. In Section 2, the analytical and numerical aspects of describing cosmic-ray transport are briefly outlined. The CUDA implementation is presented in Section 3 together with a discussion of some optimization issues. Section 4 contains benchmark results in order to illustrate the computational speed-up, and sample results for isotropic magnetostatic turbulence, accompanied by a comparison with the previous CPU implementation of the transport code. A brief summary and a discussion of the results is given in Section 5.

2. Cosmic-ray transport

Test particle theory attempts to describe the particle motion in turbulent electromagnetic fields without taking into account the back-reaction of the particles on the fields. Analytically, the random walk of individual particles is identified with a diffusive expansion of a fluid by comparing the exponents in the random-walk probability distribution (Chandrasekhar, 1943) and the solution of the diffusion equation (Fick, 1855). However, no all-encompassing results have been found so far except for very simplified turbulence models. Usually, a diffusive behavior of the particle motion is assumed so that the formalism of diffusion can be applied to the scattering mean-free paths. In three dimensions, the resulting Einstein–Smoluchowski (cf. Islam, 2004) relation reads $\kappa = \lambda\langle v\rangle/3$, where κ and λ are the diffusion coefficient and the mean-free path, respectively.

2.1. Analytical transport theory

The standard theory of cosmic-ray diffusion, the "classic" quasilinear theory (QLT; see Jokipii, 1966) has been able to describe the diffusion coefficients successfully for simplified turbulence models such as slab turbulence, where the turbulent fields depend only on the spatial coordinate along the mean magnetic field (e. g., Michałek and Ostrowski, 1996). However, it has also been demonstrated (Tautz et al., 2006) that QLT often results in singularities for time-independent magnetic turbulence, because it cannot describe the so-called 90° scattering, where particles reverse their motion in the direction parallel to the ambient magnetic field (Tautz et al., 2006).

To solve this problem, a number of non-linear theories have been proposed (e. g., Shalchi, 2009; Tautz, 2012), some of which actually give an accurate description of the transport parameters. For the diffusion of high-energy particles in the directions parallel and perpendicular to the ambient mean magnetic field, these are the second-order quasi-linear theory (Shalchi, 2005; Tautz et al., 2008) and the unified non-linear theory (Shalchi, 2010; Shalchi et al., 2011), respectively. For the first, QLT is treated as a perturbation approach, which has been evaluated to the second order. For the second, the diffusion coefficients are derived based on the correlation function of the velocity components, which has been evaluated using the solution of the Fokker–Planck equation as the weighting function.

However, both theories could, so far, only be applied to magnetostatic turbulence and are presumably difficult to generalize for more realistic turbulence models. Therefore, heuristic approaches remain in use, including scaling laws (Reinecke et al., 1993) and simplified expressions for the ratio of perpendicular and parallel diffusion (see (Shalchi, 2015) and references therein).

2.2. Test-particle simulations

Analytical theories require rather strict assumptions as to the underlying electromagnetic turbulence (such as magnetostatic fields only; a homogeneous mean magnetic field; simplified turbulence models). It is therefore essential to test the validity of these calculations calculations by comparison with observations and/or numerical results. The latter has the advantage that the same assumptions and simplifications as in the analytical derivations can be employed. Observations, on the other hand, are the ultimate test for every theory but often involve a variety of additional effects so that it is hard to benchmark initial theoretical approaches.

For the numerical determination of diffusion coefficients, their direct connection to the trajectories of randomly scattered test particles is exploited. A diffusive particle motion can be expressed through the mean-square displacement, which should then increase linearly with time. Accordingly, from the second moment of the diffusion equation, one has

$$\kappa_i = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle(\Delta r_i)^2\right\rangle \approx \frac{\left\langle(\Delta r_i)^2\right\rangle}{2t}, \tag{1}$$

where the mean-square displacement, $\langle(\Delta x)^2\rangle$, is obtained from averaging over a sufficiently large number of particles with different initial positions and velocity directions.

Numerical simulation tools such as Padian (Tautz, 2010) and many previous or other codes (Giacalone and Jokipii, 1999; Dalla and Browning, 2005; see also Tautz and Dosch, 2013) solve the equation of motion—i. e., the Newton–Lorentz equation

$$\frac{\mathrm{d}}{\mathrm{d}t}(\gamma \boldsymbol{v}) = \frac{q}{m}\left[\delta\boldsymbol{E}(\boldsymbol{x},t) + \frac{1}{c}\,\boldsymbol{v}\times\left(\boldsymbol{B}_0 + \delta\boldsymbol{B}(\boldsymbol{x},t)\right)\right], \tag{2}$$

where $\boldsymbol{v}$ and $\boldsymbol{x}$ are the particle's velocity and position, respectively. Other parameters are: m the particle mass, c the speed of light, q the electric charge and $\gamma = (1+v^2/c^2)^{-1/2}$ the relativistic Lorentz factor. In what follows, a normalized time variable will be introduced as $\tau = \Omega t$, where $\Omega = qB/(mc)$ is the gyro frequency.

In addition to a homogeneous background field $\boldsymbol{B}_0$, a turbulent magnetic field $\delta\boldsymbol{B}$ is assumed and, in the case of dynamical plasma-wave turbulence, also an electric field $\delta\boldsymbol{E}$. For each of the typically 10^3–10^6 particles, this is a system of six coupled ordinary differential equations. The required accuracy for the solution is very high, because it directly translates to energy conservation of the particles, which has to be maintained over 10^3–10^7 gyration periods. For that reason, methods with adaptive integration step sizes are being used.

The turbulent magnetic fields, $\delta\boldsymbol{B}$, are obtained by superposing typically 10^2 to 10^4 Fourier modes with random orientations and directions of propagation (cf. Tautz and Dosch, 2013) according to

$$\begin{aligned}\delta\boldsymbol{B}(\boldsymbol{r},t) = &\sum_{n=1}^{N}\hat{\boldsymbol{e}}'_{\perp}\sqrt{G(k_n)\,\Delta k_n}\\ &\times\cos\left(k_n z' - \omega(k_n)t + \beta_n\right)\end{aligned} \tag{3}$$

where $G(k) = |\ell_0 k|^q\big/[1+(\ell_0 k)]^{(s+q)/2}$ is the turbulence power spectrum with q and s the spectral indices for the energy and inertial