Journal of Computational Physics 229 (2010) 2914–2931

Contents lists available at ScienceDirect

Journal of Computational Physics

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

An angular multigrid method for computing mono-energetic particle beams in Flatland

Christoph Börgers *, Scott MacLachlan

Department of Mathematics, Tufts University, Medford, MA 02155, United States

ARTICLE INFO

Article history:
Received 13 March 2009
Received in revised form 17 December 2009
Accepted 20 December 2009
Available online 11 January 2010

Keywords:
Multigrid methods
Charged-particle transport
Radiation dose planning

ABSTRACT

Beams of microscopic particles penetrating scattering background matter play an important role in several applications. The parameter choices made here are motivated by the problem of electron-beam cancer therapy planning. Mathematically, a steady particle beam penetrating matter, or a configuration of several such beams, is modeled by a boundary value problem for a Boltzmann equation. Grid-based discretization of such a problem leads to a system of algebraic equations. This system is typically very large because of the large number of independent variables in the Boltzmann equation—six if no dimension-reducing assumptions other than time independence are made. If grid-based methods are to be practical for these problems, it is therefore necessary to develop very fast solvers for the discretized problems. For beams of mono-energetic particles interacting with a passive background, but not with each other, in two space dimensions, the first author proposed such a solver, based on angular domain decomposition, some time ago. Here, we propose and test an angular multigrid algorithm for the same model problem. Our numerical experiments show rapid, grid-independent convergence. For high-resolution calculations, our method is substantially more efficient than the angular domain decomposition method. In addition, unlike angular domain decomposition, the angular multigrid method works well even when the angular diffusion coefficient is fairly large.

1. Introduction

Charged-particle transport plays an important role in many fields; examples include electron microscopy [20], cancer therapy using electrons [12,13], protons, or heavy ions [22], and various other applications of ion beams [21,26]. The work presented here aims to contribute to the development of accurate and efficient simulation methods for charged-particle transport. The parameter choices in this paper are motivated by the electron-beam cancer therapy dose-calculation problem [12,13]. Procedures for electron-beam cancer treatment plan optimization require the solution of many electron transport problems; the efficiency of the algorithms used for these transport problems is therefore important.

Mathematically, a particle beam, or a configuration of several such beams, is modeled by a Boltzmann equation. This equation may be linear or nonlinear, depending on whether or not the beam particles interact with each other. Here, we will assume linearity, a common and accurate approximation in electron-beam cancer therapy planning.

Thus, our investigation belongs to the vast subject of numerical methods for the linear Boltzmann equation. One important source of difficulty in the computational solution of the linear Boltzmann equation is the sheer size of the problems: There are, in general, seven independent variables (position and velocity in three dimensions, and time), and still six when considering time-independent boundary value problems, as we do here. Of course, this is the number of independent

* Corresponding author. Tel.: +1 617 627 2366; fax: +1 617 627 3966.
E-mail address: christoph.borgers@tufts.edu (C. Börgers).

0021-9991/$ - see front matter © 2010 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2009.12.023

variables in any kinetic problem (unless the geometry is special), not just in charged-particle transport. However, there are additional difficulties associated specifically with charged-particle transport: The mean free path tends to be small, scattering tends to be very *forward-peaked* (*i.e.*, particles are typically deflected only very slightly by a single interaction with the background), and particles typically lose very little energy in a single interaction. These properties of charged-particle transport cause difficulties with the accuracy of discretizations and with the efficiency of solution algorithms for the discretized problems [16, Section 3.2], which have lead many in the Medical Physics community to believe that the most efficient way of modeling electron beams may be Monte Carlo simulation. However, based on a rough theoretical complexity estimate presented in [4], we believe that deterministic, grid-based methods could eventually prove to be a very attractive alternative to Monte Carlo simulation, provided that all available tools of numerical computing are brought to bear to develop highly accurate discretizations as well as optimally efficient solution algorithms for the discretized problems. Some algorithm and code development efforts in this direction are in fact underway; see, for instance, [2,9].

In this paper, we focus on the problem of designing highly efficient solvers for a grid-based discretization of the model equation of [3] (reviewed in Section 2). This equation describes physics in "Flatland" [1], *i.e.*, in a fictitious two-dimensional world. It is arguably the simplest possible caricature of charged-particle transport in more than one space dimensions. We propose and test an angular multigrid method for this problem. The idea of angular multigrid methods for particle transport with forward-peaked scattering was first proposed, for a one-dimensional problem, by Morel and Manteuffel [17]; extensions of the idea to higher dimensions have had limited success so far [18]. However, for our two-dimensional model problem, the convergence of the angular multigrid method turns out to be rapid, and the speed of convergence appears to be independent of the grid size. It is not entirely clear at this point why our approach, for the simpler problem discussed here, does not encounter the obstacles described in [18]; see Section 10 for some thoughts on this point.

2. The model problem

To make this paper as self-contained as possible, we will review the model equation of [3] and its properties here, closely following but abbreviating the exposition of [3]. We will mix physical and mathematical terminology, writing, for instance, about "particles" that move "in a domain $\Omega \subseteq \mathbb{R}^2$".

2.1. Model equation

We consider mono-energetic particle transport in two space dimensions. It must be emphasized that this is *not* the same as (and, indeed, is simpler than) the projection of three-dimensional particle transport into a plane. We consider the motion of particles in a domain, $\Omega \subseteq \mathbb{R}^2$, assuming that all particles move at the same constant speed, $c > 0$. Each particle experiences collisions at random times, causing random direction changes. The inter-collision distances, $\lambda > 0$, are exponentially distributed and independent of each other; their expectation, $\bar{\lambda} > 0$, is called the *mean free path*. The deflection angles, η, (see Fig. 1) are independent of each other and of the inter-collision distances.

The probability density of η is $p : (-\pi, \pi) \to \mathbb{R}_+$. We assume that p is an even function, *i.e.*, that particles have no preference for scattering to the right over scattering to the left or vice versa. The graph of p qualitatively looks like that shown in Fig. 2, where the forward-peakedness of the scattering is reflected by the peak in the graph of p near $\eta = 0$. For realistic models of the scattering of electrons, however, this peak would be much more pronounced than in Fig. 2.

The *phase space density*, $f = f(x, y, \theta, t)$, is the number of particles per unit (x, y, θ)-volume, where $(x, y) \in \Omega$ denotes the particle position, $(\cos\theta, \sin\theta)$ is the particle direction, and $t \geqslant 0$ is time. The function f is 2π-periodic in θ. The time evolution of f is governed by the *linear Boltzmann equation*, the mathematical statement of the law of conservation of particles,

$$f_t + c\cos\theta f_x + c\sin\theta f_y = cQf. \tag{1}$$

Here, c denotes the particle speed (assumed constant in this model problem), and the *collision operator* Q is defined by

$$Qf = \frac{p * f - f}{\bar{\lambda}},$$

where $*$ denotes convolution with respect to θ:

$$(p * f)(\theta) = \int_{-\pi}^{\pi} p(\eta) f(\theta - \eta)\, d\eta.$$

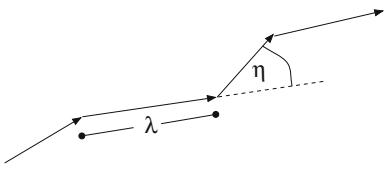

Fig. 1. An example of a particle path.