Numerical Solutions of Boltzmann Equations
A Research Plan for RIPS 2002

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April 23, 2002

1 The governing equation

The Boltzmann equation is an integro-differential equation modeling the statistical evolution of a moderately rarefied gas. We consider the Cauchy or initial-boundary value problem for the Boltzmann equation of the form:

$$f_t + \xi \cdot \nabla_x f = \frac{1}{\epsilon} Q(f, f), \tag{1}$$

where

$$f : (0, \infty) \times \mathbb{R}^n \times \mathbb{R}^n \mapsto [0, \infty),$$

represents the density of molecules at the x with velocity ξ at time t, and Q is the collision operator describing the interaction between particles. Let $\phi \in \mathcal{D}(\mathbb{R}^n)$, $Q(\phi, \phi)$ is a function of ξ, taking the form

$$Q(\phi, \phi) = \int_{\mathbb{R}^n} \int_{S^{N-1}} (\phi(\xi')\phi(\xi'_*) - \phi(\xi)\phi(\xi_*)) B(|\xi - \xi_*|, \omega) d\omega d\xi_*.$$

$B \geq 0$ is the collision kernel. $\xi' = \xi - (\xi - \xi_*) \cdot \omega\, \omega$ and $\xi'_* = \xi_* - (\xi - \xi_*) \cdot \omega\, \omega$ are the velocities immediately after collision of two particles, which had velocities ξ and ξ_* immediately before collision. This was first derived by Boltzmann and Maxwell, see e.g. [1]. The positive number ϵ is proportional to the mean free path between collision and is called the Knudsen number.

If there is no interaction between particles, e.g. the gas is very rarefied, the density will be constant along the path of each particle, and equation (1) is reduced to linear transport equation:

$$f_t + \xi \cdot \nabla_x f = 0.$$

1.1 Mathematical and computational challenges

In general, the mathematical challenges lies in the lack of estimates. The theory of existence and uniqueness of solution to (1) in various settings can be found in, e.g. [2, 3][5].

Looking at equation (1), one may immediately identify that one of the difficulties in the computation of solutions to Boltzmann's equation is the complexity due to both the dimensionality; i.e. the large number of independent variables $(2n)$, x for space, ξ for velocity , and at each point (x, ξ) in phase space the evaluation of the $2n - 1$ dimensional integral.

In addition, solutions generally have steep gradients such that extra attention is needed in order to devise a proper numerical scheme.

A common practice in deriving numerical schemes for (1) is to perform a splitting in time of the transport on the left hand side and the relaxation on the right hand side :

$$\frac{\partial f}{\partial t} = \frac{1}{\epsilon} Q(f, f) \tag{2}$$

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla_x f = 0. \tag{3}$$

Equation (2) is called the space homogeneous Boltzmann equation. It can be solved by Monte-Carlo methods, e.g. [8], or spectral method, e.g. [9].

Equation (3) is a simple transport equation in phase space that can be solved by a variety of methods, including finite difference, finite element, and finite volume methods.

We will base our work on this view point and we propose the following plan for the RIPS program.

2 Proposed plan of study

We will mainly concentrate on the numerical schemes for the transport part of the Boltzmann equation.

We will start by a brief review of numerical quadrature, followed by a more detailed review of finite difference and finite element method for linear PDEs with emphasis on method of lines and upwind/Godunov type schemes. The concept of consistency and stability is introduced. Some ODE solvers are also introduced. The materials will be based on [6]. This is stage one. Students are expected to have programs solving initial boundary value problems for 1D linear, time-dependent PDEs. They are expected to program also the Total Variation Diminishing Runge-Kutta scheme of [10].

In stage two, students will work on basic numerical methods for conservation laws. TVD methods and methods with limiters such as MUSCL, Superbee will be introduced. A nice introductory reference will be [7]. They will also work on the Discontinuous Galerkin (DG) method based on [4]. The emphasis will be on the concept of preventing oscillations at cell boundaries. Simultaneously, they will be expected to work on solving simple 1D Boltzmann equation.

Finally, if time allows, we will work on the ENO method, higher dimensional DG method, and other methods for solving the Boltzmann equation.

By the end of this workshop, the team is expected to have a running finite difference/TVD-DG code for 1D Boltzmann Equation.

Stage one:

- review of numerical quadratures.
- review of numerical methods for linear PDEs, including FDM, FEM, and FVM.

Stage two:

- introduction to numerical conservation laws, TVD methods, and limiters.
- introduction to discrete Galerkin method in 1D based on [4].

Stage three (if time allows)

- ENO interpolation and ENO method for conservation laws.
- Discrete Galerkin method in high dimensions.
- Methods for solving (2).

References

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