UCLA
COMPUTATIONAL AND APPLIED MATHEMATICS

Numerical Methods for Rarefied Gas Dynamics and Related Problems

Russel E. Caflisch
William J. Morokoff

June 1991

CAM Report 91-10

Department of Mathematics
University of California, Los Angeles
Los Angeles, CA. 90024-1555

Numerical Methods for Rarefied Gas Dynamics and Related Problems

Russel E. Caflisch and William J. Morokoff*
Mathematics Department, UCLA

June 12, 1991

Abstract

This article presents a survey of recent results on numerical methods for rarefied gas dynamics, including grid-based methods and particle methods,both random and deterministic. Numerical analytic convergence results for particle methods are discussed. Some recent results on quasi-random (well-distributed) sequences and their applications to integration and transport problems are described. A set of methods from linear transport theory are discussed, in which the numerical difference scheme has the correct diffusion limit.

1 Introduction

The kinetic theory of gases describes the behavior of a gas in which the density is not too large, so that the only interactions between gas particles are binary collisions. The resulting nonlinear Boltzmann equation,

$$\frac{\partial}{\partial t}F + \xi \cdot \frac{\partial}{\partial .}F = Q(F,F) \tag{1.1}$$

for the molecular distribution function $F(x,\xi,t)$, is a basic equation of nonequilibrium statistical mechanics. The collision operator is

$$Q(F,F)(\xi) = \int (F(\xi_1')F(\xi') - F(\xi_1)F(\xi))B(\omega,|\xi_1 - \xi|)d\omega d\xi_1 \tag{1.2}$$

*Research of both authors supported in part by the Air Force Office of Scientific Research under grant number AFOSR 90-0003.

in which ξ, ξ_1 represent velocities before a collision, ξ', ξ_1' represent velocities after a collision, and $\omega \epsilon S^2$ represents the collisions parameters.

Rarefied gas dynamics is of increasing technological importance with applications to re-entry vehicles, low-orbital aircraft design, particle beams, vacuum pumps and semi-conductors. Computational methods are necessary for quantitative results and for numerical experimentation in rarefied gas dynamics, as in any modern scientific theory. A particular difficulty of rarefied gas dynamics is that there are only almost no exact solutions (the main exception being the solution of Krook and Wu [39]) on which to build an understanding. Asymptotic methods can be used to produce approximate solutions in special regimes, such as the fluid dynamic limit [17]. For general flows however the only way to construct solutions is numerical.

Numerical solution of the Boltzmann equation is difficult mainly because of the complexity of the problem: The distribution function F depends on 7 variables $(t, x_1, x_2, x_3, \xi_1, \xi_2, \xi_3)$, or at least 4 variables $(t, x, \xi_x, \xi_\perp)$ for a time dependent problem with planar symmetry. The collision integral $Q(F, F)$ involves an integral over 5 dimensions (4 in the planar case) for every choice of the independent variables. To handle this complexity, random numerical methods are often used. While quite effective, the resulting random errors in F can be relatively large and difficult to analyze. On the other hand, the usual interest is only in moments of F and not in F itself, which reduces these random errors.

The focus of this article will be on numerical methods for the collisional process of the Boltzmann equation. Additional physical processes that can be important include chemical reactions, dissociation, ionization and even quantum effects. Realistic boundary conditions and internal degrees of freedom for non-monatomic gases are also important but will not be discussed here.

The methods to be discussed include grid-based methods (section 3) and particle methods (section 4), both deterministic and random. Mathematical convergence results for particle methods will be discussed in section 5. In section 6 some recent results on quasi-random (well-distributed) sequences and their applications to integration and transport problems will be discussed. Finally some numerical methods from linear transport theory, for which the finite difference scheme has the correct diffusion limit, are described in section 7.

The aim of this article is to provide a survey of some interesting recent and older results, rather than to provide a comprehensive review of all existing methods. The emphasis is on numerical analysis for the Boltzmann

equation, which we believe can play an important role in the design of new computational methods for rarefied gas dynamics, rather than on applications or computational studies.

2 The Boltzmann Equation

For a molecular distribution F, the macroscopic (or fluid dynamic) variables are the density ρ, velocity u and temperature T defined by

$$\begin{aligned} \rho &= \int F d\xi \\ u &= \rho^{-1} \int \xi F d\xi \\ T &= \rho^{-1} \int |\xi - u|^2 F d\xi. \end{aligned} \tag{2.1}$$

The importance of these moments of F is that they correspond to conserved quantities, i.e. mass, momentum and energy, for the collisional process, which is expressed as follows:

$$\int Q(F,F) d\xi = 0$$

$$\int \xi Q(F,F) d\xi = 0 \tag{2.2}$$

$$\int |\xi|^2 Q(F,F) d\xi = 0. \tag{2.3}$$

These also provide the degrees of freedom for the equilibrium distributions, the Maxwellian distributions

$$M(\xi,\ \rho,\ u,\ T) = (2\pi T)^{-3/2} e^{|\xi - u|^2/t}. \tag{2.4}$$

A dimensionless measure of the importance of collisions as opposed to the convective terms on the left side of the Boltzmann equation (1.1) is given by the Knudsen number ε, which is the ratio of the mean free collision time to a macroscopic time scale. As written in (1.1) the length and time scales for the Boltzmann equation are those of the collision process; if they are written instead in terms of macroscopic length and time scales, then (1.1) is replaced by

$$\frac{\partial}{\partial t} F + \xi \cdot \frac{\partial}{\partial x} F = \varepsilon^{-1} Q(F,F). \tag{2.5}$$

In the limit $\varepsilon \to \infty$, the Boltzmann equation goes to an equation for free molecular flow.

In the opposite limit $\varepsilon \to 0$, the solution F of (2.5) is given by the Hilbert or Chapman-Enskog expansion, in which the leading tern is a Maxwellian distribution of the form (2.4) in which ρ, u, T satisfy the compressible Euler or Navier-Stokes equations of fluid dynamics. This expansion is not valid in layers around shocks, boundaries and non-equilibrium initial data, where special boundary, shock or initial layer expansions can be constructed [17]. By varying this limit, taking the velocity u to be size ε as well, the compressible equations are replaced by the incompressible fluid equations [21,7].

A general mathematical existence theorem for the Boltzmann equation has been derived by DiPerna and Lions [23], although the solution they obtain is quite weak. For example, energy conservation is not proved for the solution, nor is uniqueness for given initial data. More specialized results for spatially homogeneous, near-equilibrium or near vacuum flows or flows near the fluid dynamic limit have been derived and are referenced in [23]. As usual in numerical analysis, we will assume the existence and regularity of solutions as needed.

3 Grid-Based Computational Methods

Numerical solution of the Boltzmann equation (1.1) consist of two parts: the convective part for the space-time derivatives on the left side of (1.1) and the collision part for the collision integral $Q(F,F)$. The first set of methods uses a fixed grid in physical space x, at each point of which the distribution function is represented in some way. Then the distribution is evolved by direct evaluation of the collision integral.

One of the earliest numerical methods for the nonlinear Boltzmann equation uses Monte Carlo evaluation of the collision integral at each point in phase space (x,ξ). First derived by Nordsieck and Hicks [53] and more recently discussed by Yen [64], this method represents the distribution function F by a set of values $F_{mn} = F(x_m,\xi_n)$ at a discrete set of points (x_m,ξ_n). The collision integral $Q_{mn} = Q(x_m,\xi_n)$ is evaluated at each point by pseudo-random sampling of the possible values of the collision partner $\xi_{n'}$ and the collision parameters ω. This method has been successfully applied to various problems such as planar shock profiles. The main errors of the method

come from random sampling errors and discretization errors in evaluating F. A similar method has been developed by Cheremisin [19].

The random errors of this method can be avoided by deterministic evaluation of the collision integral, as in the next set of methods. All of these methods require $O(N^2)$ steps for N velocity elements, since they require direct computation of all of the collision integrals. Chorin's method [20] represented the velocity dependence of the distribution function using a Hermite polynomial expansion around a Maxwellian distribution, with coefficients depending on x, t, i.e.

$$F(\xi, x, t) = M(\xi) \sum_{n=0}^{\infty} a_n(x, t) H_n(\xi). \tag{3.1}$$

Differential equations for the coefficients $a_n(x, t)$ were obtained using a Galerkin method, which requires computation of integrals of the form

$$\int H_l Q(H_m, H_n) d\xi. \tag{3.2}$$

(These integrals can be evaluated partly analytically using the formulas of [22].) The resulting equations were solved in x, t using finite differences. Various improvements on this method were implemented by Sod [58], and the method was used for computation of shock profiles in [20,58].

A related method using polynomial velocity elements was derived by Sugano and Sakurai [60]. They used a variational principle of Cercignani [18] to obtain the equations for the coefficients $a_n(x, t)$.

Aoki, Sone and Ohwada [2,59] have developed a deterministic method using finite difference in space and time, with finite elements to represent the velocity distribution. Again the collision integral is directly calculated at each node (x_m, ξ_n). They have applied their method to a wide range of flows involving evaporation, condensation and shear layers. A similar method has been formulated by Tan et al. [61].

For the interesting special problem of an infinitely strong shock, Narasimha and Das [49] derived a numerical method that decomposes the distribution into a background gas and a particle beam, as suggested earlier by Grad [29]. They then used Burnett polynomials as velocity elements for the background gas.

For the spatially homogeneous Boltzmann equation, an iteration scheme has been recently derived by Fujii, Barrachina and Garibotti [25].

4 Particle Methods

In particle methods for transport theory, the distribution $F(x,\xi,t)$ is represented as the sum

$$F_N(x,\xi,t) = \sum_{n=1}^{N} \delta(\xi - \xi_n(t))\delta(x - x_n(t)), \tag{4.1}$$

and the positions $x_n(t)$ and velocities $\xi_n(t)$ are evolved in time to simulate the effects of convection and collisions. The most common particle methods use random collisions between a reasonable number of particles (e.g. $10^3 - 10^6$) to simulate the dynamics of many particles (e.g. 10^{23}). Recently several deterministic methods have been introduced.

In the Direct Simulation Monte Carlo (DSMC) method pioneered by Bird [10,12,11,13,14], the numerical method is designed to simulate the physical processes as closely as possible. This makes it easy to understand and to insert new physics; it is also numerically robust. First, space and time are discretized into spatial cells of size Δx^3 and time steps of duration Δt. In each time step the evolution is divided into two steps: transport and collisions. For the transport step each particle is moved from position $x_n(t)$ to $x_n(t+\Delta t) = x_n(t)+\Delta t\xi_n(t)$. Boundary interactions may also be included.

In the collision step, random collisions are performed between particles. In each collision, particles ξ_n and ξ_m are chosen randomly from the full set of particles with probability p_{mn} given by

$$p_{mn} = \frac{S(|\xi_m - \xi_n|)}{\sum_{1\le i\le j\le N_0} S(|\xi_i - \xi_j|)}, \tag{4.2}$$

in which N_0 is the number of particles in the spatial bin, and

$$S(|\xi_i - \xi_j|) = \int_{S^2} B(\omega, |\xi_i - \xi_j|)d\omega \tag{4.3}$$

is the total collision rate between particles of velocity ξ_i and ξ_j. As written this choice requires $O(N^2)$ operations to evaluate the sum in the denominator in (4.2). By a standard acceptance-rejection scheme [37] however, each choice can be made in $O(1)$ steps, so that the total method requires only $O(N)$ steps. In all of the random particle methods, acceptance rejection methods must be used to reduce the operation count from $O(N)$ to $O(N^2)$.

Next the collision parameters ω are randomly chosen from a uniform distribution on S^2. The outcome of the collision is two new velocities ξ_n' and ξ_m' which replace the old velocities ξ_n and ξ_m.

The number of collisions performed in each time step has been determined by several methods. In the original "time-counter" (TC) method, a collision time Δt_c is determined. It is equal to one over the frequency for that collision type, i.e.

$$\Delta t_c = 2(nN_0 S(|\xi_m - \xi_n|))^{-1}, \tag{4.4}$$

in which n is the number density of particles. This collision time is added to the time-counter $t_c = \sum \Delta t_c$. In the time interval of length Δt beginning at t, collisions are continued until t_c exceeds the final time, i.e. until $t_c \geq t+\Delta t$. For N particles this method has operation count $O(N)$.

The DSMC method with the time-counter algorithm has been enormously successful. However the unlikely possibility of choosing a collision with very small frequency can results in a large collisional time step that may cause relatively large errors. To remove such errors, Bird [14] has developed a "no-time-counter" (NTC) method. The number of collisions to be performed in time step Δt is chosen as if the collision frequency were exactly S_{max}, a maximum collision probability, for all collision pairs. For each selection of a collision pair, the collision between ξ_m and ξ_n is then performed with probability $S(|\xi_m - \xi_n|)/S_{max}$, as in an acceptance-rejection scheme.

Several similar methods have been developed by other researchers. Koura [38] has developed a null-collision (NC) technique that also involves rejection of some collisions. Belotserkovskii, Erofeev and Yanitskii [9] have given an analysis of the convergence of Bird's method with the TC technique, using the theory of restoration processes, and have proposed an alternative method in which the collision time is chosen from an exponential distribution. As described their method (called the Bernoulli trials (BT) method) requires $O(N^2)$ steps, but a related method by Ivanov, Rogasinsky and Rudyak [35], called the majorant frequency (MF) scheme, is again $O(N)$.

The rather different method of Nanbu [48] follows a procedure that more closely resembles the mathematical form of the Boltzmann equation, rather than the physical collision process. For the collision step of Nanbu's method, first two identical copies $\{\xi_n\}$ and $\{\eta_n\}$ of the particles are made. For each n, a distinct index n' is chosen, so that $(\xi_n, \eta_{n'})$ is a possible collision pair. The collision between these two velocities is performed according to a random

decision based on the probability $nN_0\Delta t S(|\xi_n - \eta_{n'}|)/2$ that such a collision should occur in time step Δt. If the collision is performed then the collision parameters ω are randomly chosen and the velocity ξ_n is replaced by the new velocity ξ_n'. The velocity η_n is not used again, so it does not need to be replaced.

As formulated by Nanbu [48], this was an $O(N^2)$ method. However by use of an acceptance-rejection method [4], the Nanbu method, with this modification, also requires only $O(N)$ steps to compute.

This method has the mathematical advantage that no correlations between the particles will develop, since only one of the collision partners is retained. This seems to imply that propagation of chaos is automatic. The use of collision frequencies is also quite straightforward in Nanbu's method. On the other hand it has the severe disadvantage that energy and momentum are not conserved, except on average. In fact, Greengard and Reyna [30] have recently shown that in a spatially homogeneous computations, the total temperature for the distribution is decreasing at a rate proportional to N^{-1} for Nanbu's method.

Additional modification of Nanbu's method have been developed by Babovsky, Neunzert and co-workers [5,31]. The first modification is to make the method less random. They use deterministic, "quasi-random" sequences (described in section 6 below), rather than pseudo-random sequences for at least some of the random choices. Since quasi-random numbers have a smaller "discrepancy" (defined in section 6) than that of pseudo-random numbers, these methods have been named Low Discrepancy Methods. A second modification has been to effectively replace both velocities ξ_n and η_n by ξ_n' and η_n', so that momentum and energy are exactly conserved. This makes the method more like the DSMC method. Computational tests of this method have been carried out by Lecot [43,44], with additional references in the Proceedings of the 17th Rarefied Gas Dynamics Symposium.

A different modification of the DSMC method has been developed by Goldstein, Sturtevant and Broadwell [26]. They consider a gas in which the velocities are discrete and can be described on a multi-dimensional integer lattice. Then the computations of collisions can all be performed in integer arithmetic, which provides savings by a factor of 7 or so.

These numerical methods, especially Bird's DSMC method have been used for a wide variety of flow computations with considerable success; see for example the many articles in International Symposium on Rarefied Gas Dynamics from 1990 and earlier years. Computational comparisons of Bird's and Nanbu's methods have been performed in [16], which show smaller errors

for Bird's method, apparently due to the random variations of energy and momentum for the latter method.

One of the main advantages of the particle methods in general and of the DSMC method in particular is that additional physical effects can be added easily. These could include internal degrees of freedom in the molecules, chemical reactions and ionization. Inclusion of these effects, as well as a critical comparison of DSMC with molecular dynamics, is described in [13].

There has been a lot of discussion of whether the various particle methods are derived from the Boltzmann equation or from the underlying Master equation. This issue is important from the physical point of view, since it affects how new physical effects are included and how the results are interpreted. From the numerical analysis point of view however, the formal resemblance of the numerical method to the Boltzmann or Master equation is less important than the complexity of the method and its accuracy as a simulation scheme. As stated in the introduction, we are always thinking of the Boltzmann equation as the system to be simulated. Note on the other hand that, as new physical effects are included, the DSMC and other particle methods can be formulated even if there is no Boltzmann equation, as pointed out by Bird [14].

Completely deterministic particle methods have also been developed. In the method of Mas-Gallic [46], the distribution function is represented as

$$F_N(\cdot\ ,\xi,t) = \sum_{n=1}^{N} a_n(t)\delta(\xi - \xi_n(t))\delta(x - x_n(t)) \tag{4.5}$$

with weights $a_n(t)$. In each time step, the positions $x_n(t)$ are changed according to the velocities $\xi_n(t)$. Collisions are simulated by changing the weights $a_n(t)$. Since particle locations are discrete while the collision process is local, a spatial smoothing is introduced, so that particles at distance Δx have a probability of colliding that decreases as Δx increases. A convergence proof for this method for the linear Boltzmann equation has been carried out in [46].

A somewhat different deterministic particle method has been developed by Russo [55] in several contexts, including pure diffusion and the Vlasov-Fokker-Planck equation. In this method the collisions are represented by changing the velocities $\xi_n(t)$. Convergence results and numerical trials for this method are presented in [55].

5 Convergence Results for Particle Methods

Convergence of particle methods for transport equations is only possible in the sense of weak convergence. If the distribution $F(x,\xi,t)$ is represented as the sum

$$F_N(x,\xi,t) = \sum_{n=1}^{N} \delta(\xi - \xi_n(t))\delta(x - x_n(t)) \tag{5.1}$$

then $F_N \rightharpoonup F$ in the weak sense if

$$\int \phi F_N d\xi d. \;\rightarrow \int \phi F_N d\xi d. \tag{5.2}$$

as $N \rightarrow \infty$, for any continuous function $\phi(x,\xi)$. Note that since F_N is a sum of delta functions, it cannot converge to F pointwise.

Particle methods for fluid dynamics have received considerable attention from numerical analysts. For example the deterministic blob and point vortex methods for inviscid, incompressible flow have been shown to converge in a variety of contexts, see for example [1,8,28] and references therein. For the random vortex method simulating viscous, incompressible flow, convergence has been proved in a more restrictive set of regimes [27,32,45]. The difficulty of the random methods is caused by the interactions of the particles.

Convergence theory of direct simulation methods for the nonlinear Boltzmann equation is only partly developed. Here we describe two recent results:

The first such convergence result was by Babovsky and Illner [6] for Nanbu's method. Their result is based on a new formulation of the weak form of the Boltzmann equation. Consider the spatially homogeneous Boltzmann with discretized time, which can be written as an equation for F_{j+1}, the distribution after $j+1$ time steps, in terms of F_j. The weak formulation of the equation is represented by integration of this equation against a function $\phi(\xi)$. They found that it can be reformulated as

$$\int \phi(\xi)F_{j+1}(\xi)d\xi = \int\int K_{\xi,\eta}[\phi]F_j(\xi)F_j(\eta)d\xi d\eta. \tag{5.3}$$

In this equation $K_{\xi,\eta}[\phi]$ is a linear operator on the function ϕ evaluated at the velocity pair (ξ,η) defined by

$$K_{\xi,\eta}[\phi] = \left(1 - \Delta t \int k(|\xi-\eta|,\theta)d\omega\right)\phi(\xi) + \Delta t \int k(|\xi-\eta|,\theta)\phi(\xi')d\omega \tag{5.4}$$

The significance of this representation is that the nonlinear integral on the right hand side of (5.3), which represents the effect of collisions on the change in F over one time step, is in a form of an integral against the density function $F(\xi)F(\eta)$. This integral can be evaluated by the Monte Carlo method. In particular this requires choice of velocity pairs (ξ, η) for the integral in (5.3) and choice of points ω for the integral in (5.4). If F is represented by a collection of velocities $\{\xi_n : 1 \leq n \leq N\}$, then the pair (ξ, η) can be chosen from the collection of pairs $\{(\xi_m, \eta_n) : 1 \leq m \leq N, 1 \leq n \leq N\}$. This shows that in a direct simulation method the choice of two particles for a collision amounts to a procedure for representation of the pair distribution $F(\xi)F(\eta)$ for Monte Carlo evaluation of the outer integral of (5.3); while the choice of scattering parameters ω is for evaluation of the integral in (5.4). Following this interpretation, a direct simulation method can be thought of as a series of Monte Carlo evaluations of integrals.

Using this interpretation, Babovsky and Illner [6] were able to prove weak convergence of Nanbu's method to a solution of the Boltzmann equation. The main step is use of the central limit theorem to obtain convergence of the Monte Carlo representations of the integrals. As usual in such numerical analysis theorems, convergence is proved under the assumption that a Boltzmann solution exists. This result seems to be restricted to Nanbu's method because it does not deal with the correlations between particles that could develop in Bird's method.

For Bird's Direct Simulation Monte Carlo method with the time-counter technique, a partial convergence theorem has been proved by Wagner [62]. He first discretizes time and space so that Boltzmann equation with full space and time dependence is replaced by a sequence of spatially homogeneous Boltzmann equations on spatial cells, followed by convection of particles between cells. Each of these processes occurs successively on cells of size Δx^3 over a time period of size Δt. This exactly corresponds to the discretization of space and time in the DSMC and other particle methods. Wagner then uses a Markov jump process which represents the solution of the spatially homogeneous Boltzmann equation over each space cell and time step. This Markov process can be described as the solution of a stochastic differential equation with respect to a Poisson measure. Ito's formula then gives the Boltzmann equation as a Martingale representation of the solution.

This jump process and its representation provide the propagation of chaos that is needed for convergence to the Boltzmann equation; they were developed earlier by a series of authors [3,62] and references therein. Although Wagner does not consider the continuum limit $\Delta t \to 0, \Delta x \to 0$, we

expect that standard numerical analysis methods would apply to this limit, as in [6], to show that the discrete solution converges to a solution of the full Boltzmann equation, provided that one exists.

6 Quasi-Random Sequences

As described in the previous section 5, the solution of most transport problems can be reduced to a problem of integration over a domain, usually with a fairly large dimension. Moreover since the integration usually simulates a decision of whether or not a collision should occur, the integrand is often a discontinuous function. The subject of this section is *quasi-random* sequences, which are an alternative to pseudo-random sequences for Monte-Carlo integration and transport calculations.

Integration using a regular grid of points in a domain of high dimension encounters several practical difficulties: First, although in principle a high order method can give results with errors of size $N^{-\alpha}$ for any α, in practice there are precision problems which make the convergence rate quite slow. It is just not possible to put very many points in any one direction if the domain has high dimension s. A second difficulty is that a regular grid cannot be refined incrementally. In dimension s a refinement in all directions requires that the number of points N be increased by a factor of 2^s, which does not allow the computation to be very adaptive.

Monte Carlo integration using pseudo random sequences avoids these difficulties. Points are added incrementally and the resulting error decreases at a rate $\sigma N^{-1/2}$. This rate is usually faster than that achieved for a grid in high dimension, apparently because the points are distributed uniformly throughout the domain rather than being rigidly prescribed. On the other hand the error rate of $N^{-1/2}$ is rather slow and is due to clustering of the points.

An improved procedure for choosing the points for a Monte Carlo integration is to use quasi-random points. These have the advantage that they can be added incrementally and that they are not rigidly prescribed, yet they do not cluster as badly as the pseudo-random sequences so that errors of size N^{-1} can be achieved, at least in principle. For a straightforward Monte Carlo integration method it is impossible to do better than N^{-1}, since that is the contribution from just a single point. Basic references on the theory of quasi-random sequences are [34,40,50,51,52]; more applied dis-

cussions are presented in [47,54]. A general reference on the Monte Carlo method is [37,34].

The simplest example of a quasi-random sequence is the van der Corput sequence

$$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}, \frac{1}{8}, \frac{5}{8}, \frac{3}{8}, \frac{7}{8}, \cdots . \tag{6.1}$$

The Halton sequence [33] is a generalization of this to an arbitrary prime p and is given by

$$0, \frac{1}{p}, \frac{2}{p}, \ldots, \frac{1}{p^2}, \frac{1}{p}+\frac{1}{p^2}, \frac{2}{p}+\frac{1}{p^2}, \ldots, \frac{2}{p^2}, \frac{1}{p}+\frac{2}{p^2}, \frac{2}{p}+\frac{2}{p^2}, \cdots . \tag{6.2}$$

More complicated sequences, such as the Faure [24] and Sobol[56,57] sequences, are described in [47]. A quasi-random sequence in $\mathcal{R}^s$ is formed by taking each component to be from a Halton sequence with a different prime p.

The theoretical accuracy of quasi-random sequences is based on the *discrepancy*. Consider integration over the unit cube I^s in $\mathcal{R}^s$. Denote E to be the set of all subcubes in I^s and E^* to be the set of all subcubes with one corner at 0. For any "nice" set $J \subseteq I^s$ and any sequence of N points $\{x_n\}$ in I^s, the error in representing the volume of J is

$$R_N(J) = \frac{1}{N}(\sum_{n=1}^{N} \chi_J(x_n) - m(J)) \tag{6.3}$$

in which χ_J is the characteristic function of the set J and $m(J)$ is the volume of J. The L_∞ and L_2 discrepancies for the sequence $\{x_n\}$ are

$$\begin{aligned} D_N &= \sup_{J \epsilon E} |R_N(J)| \\ T_N &= \{\int_{(x,y)\epsilon I^2, x_i<y_i} (R_N(J(x,y)))^2 dxdy\}^{1/2} \end{aligned} \tag{6.4}$$

in which $J(x,y)$ is the cube with one corner at x and another at y. The *-discrepancies are

$$\begin{aligned} D_N^* &= \sup_{J \epsilon E^*} |R_N(J)| \\ T_N^* &= \{\int_{I^s} (R_N(J(x)))^2 dx\}^{1/2} \end{aligned} \tag{6.5}$$

in which $J(x)$ is the cube with one corner at 0 and another at x. It is easy to show that

$$D_N^* \leq D_N \leq 2^s D_N^*$$
$$T_N^* \leq D_N^*; \tag{6.6}$$

additional discrepancy inequalities, including a discrepancy taken over convex sets, are found in [50].

For a given set of integration points $\{x_n\}$, the Monte Carlo approximation to the integral is

$$I(f) = \frac{1}{N} \sum_{n=1}^{N} f(x_n) \tag{6.7}$$

and the resulting integration error is

$$E(f) = \left| \int_{I^s} f(x)dx - \frac{1}{N} \sum_{n=1}^{N} f(x_n) \right|. \tag{6.8}$$

The basic error bound for quasi-random integration is given by the Koksma-Hlawka inequality

$$E(f) \leq V(f) D_N^*. \tag{6.9}$$

In this inequality $V(f)$ is the variation of f, which in one dimension is defined by

$$V(f) = \int_0^1 |df| \tag{6.10}$$

and in dimension s is defined by

$$V(f) = \sum_{k=1}^{s} \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq s} \int_{I^k} \left| \frac{\partial^k f}{\partial_{y_1} \ldots \partial_{y_k}} \right| dy, \tag{6.11}$$

in which f is evaluated at $y_j = 1$ for $j \neq i_k$. Note that the discrepancy is infinite for functions that are not sufficiently smooth, such as the characteristic function of any non-rectangular set in dimension greater than one.

A direct relation between the integration error $E(f)$ and the L^2 discrepancy has been derived by Wozniakowski [63]. He showed that T_N^* is equal to the average integration error, i.e.

$$T_N^* = Av(E(f)). \tag{6.12}$$

The average is taken over function space with a measure given by the "Brownian sheet" measure, which is a generalization of Brownian motion with s-dimensional "time." In particular the measure is concentrated on functions that are roughly half-differentiable, so that they have infinite variation. This shows that the Koksma-Hlawka inequality is a vast overestimate, at least for this class of functions. These functions $f(t_1, ..., t_s)$ are also required to vanish if any $t_k = 0$, i.e. on half of the faces of the unit cube, which may be an unrealistic restriction.

The derivation of (6.12) in [63] was simply a calculation of each side of the equation. Here we present a new derivation that follows naturally the properties of the Brownian sheet measure. First rewrite the integration error $E(f)$ using integration by parts, following the proof of the Koksma-Hlawka inequality [50]. First note that

$$dR_N(J(x)) = \{\frac{1}{N}\sum_{n=1}^{N}\delta(x - x_n) - 1\}dx. \tag{6.13}$$

Now assume that $f(x) = 0$ if $x^{(i)} = 1$ for any component $x^{(1)}, ..., x^{(s)}$ of x. Note that $R_N(x) = 0$ if $x^{(i)} = 0$ for any i, which implies that the boundary terms all disappear in the following integration by parts:

$$\begin{aligned} E(f) &= \left|\int_{I^s} f(x)dx - \tfrac{1}{N}\textstyle\sum_{n=1}^{N} f(x_n)\right| \\ &= \left|\int_{I^s}\{1 - \tfrac{1}{N}\textstyle\sum_{n=1}^{N}\delta(x - x_n)\}f(x)dx\right| \\ &= \left|\int_{I^s} R_N(J(x))df(x)\right|. \end{aligned} \tag{6.14}$$

A basic property of the Brownian sheet measure used in (6.12) is that

$$Av(df(x)df(x')) = \delta(x - x')dxdx'. \tag{6.15}$$

Thus the average square error is

$$\begin{aligned} Av(E(f)^2) &= Av((\int_{I^s} R_N(J(x))df(x))^2) \\ &= Av((\int_{I^s} R_N(J(x))df(x)(\int_{I^s} R_N(J(x'))df(x')) \\ &= \int_{I^s\times I^s} R_N(J(x))R_N(J(x'))Av(df(x)df(x') \\ &= \int_{I^s} R_N(J(x))^2dx \\ &= (T_N^*)^2. \end{aligned} \tag{6.16}$$

The discrepancy for the Halton sequence in $\Re^s$ with primes p_k has the bound

$$D_N^* \leq C_s \frac{(\log N)^s}{N} + O\left(\frac{(\log N)^{s-1}}{N}\right) \tag{6.17}$$

in which the constant C_s depends on the primes p_k. There are similar bounds on the discrepancies for the Faure and Sobol sequences. This bound and the Koksma-Hlawka inequality(6.9) indicate that the quasi-random Monte Carlo integration has error decreasing like N^{-1} for smooth functions. On the other hand these bounds are not very useful for large s, as pointed out by Morokoff [47]. In fact the bound (6.17) is worse than the trivial bound $D_N^* \leq 1$ for $N \leq e^s$.

Extensive computational tests were performed by Morokoff [47] to determine the dependence of quasi-random Monte Carlo integration error on dimension of the domain, smoothness of the integrand and choice of the quasi-random sequence. For integration of smooth functions the error is almost always much better than that of pseudo-random Monte Carlo integration. Nevertheless as the dimension increases, the rate of error decrease in a fixed range of N goes from N^{-1} to the pseudo-random rate $N^{-1/2}$. This loss of decay is more dramatic for functions that are not smooth, such as a characteristic function of a non-rectangular set. But even for such functions the errors are still much better than the pseudo-random error.

General conclusion on the comparison on different quasi-random sequences are that in low dimension ($s \leq$ *approximately* 6) Halton is superior, while in high dimension Sobol is better. Many previous comparative studies of quasi-random sequences were found to be flawed in that the primary errors came from transients, such as a sequence started at a special point at which the integrand was unusually large.

Quasi-random sequences have been used in a number of transport computations. In the simplest problem, Morokoff [47] used quasi-random sequences for a diffusion problem in $\Re^s$. At each time step and for each particle, a quasi-random vector is used to decide what the next step should be. In one dimension ($s = 1$) errors of size N^{-1} were achieved by reordering the particle labels according to their position, so that the quasi-random numbers were used in this order. If such relabeling is not used, then the ordering of the quasi-random numbers is effectively randomized, since the particles arrange themselves in a random order, which can lead to non-convergence for the simulation. In higher dimension this reordering is only partly possible, so that larger errors are encountered.

7 Methods with the Correct Diffusion Limit

One of the most difficult problems of transport theory is that there may be wide variation of mean free paths within a single problem. In regions where the mean free paths are large there are few collisions, so that large numerical time steps may be taken; whereas in regions where the mean free path is small, the time and space steps must be small. Thus the highly collisional regions determine the numerical time step, which may make computations impractically slow. On the other hand much of the extra effort in the collisional regions seems wasted, since in those regions the gas will be nearly in fluid dynamic equilibrium, so that a fluid dynamic description should be valid.

A partial remedy to this problem is to use a numerical method that converts to a numerical method for the correct fluid equations in regions where the mean free time is small. This allows large, fluid dynamic time steps in the collisional region and large collisional time steps in the large mean free time region. Such a method has been developed for neutron transport, as described below. We also describe an application of the same ideas to the Broadwell model of the nonlinear Boltzmann equation for rarefied gas dynamics.

The one-dimensional, one-speed transport equation in an isotropic material is

$$\varepsilon\partial_t\Psi^\varepsilon + \mu\partial_x\Psi^\varepsilon + \varepsilon^{-1}\sigma_T\Psi^\varepsilon = (\varepsilon^{-1}\sigma_T - \varepsilon\sigma_A)\Phi^\varepsilon + \varepsilon Q \tag{7.1}$$

in which the scalar flux is

$$\Phi^\varepsilon(t,x) = \frac{1}{2}\int_{-1}^{1}\Psi^\varepsilon(t,x,\mu')d\mu'. \tag{7.2}$$

As $\varepsilon \to 0$, the solution of (7.1) has the expansion

$$\Psi^\varepsilon = \Theta - \varepsilon\frac{\mu}{\sigma_T}\partial_x\Theta \ + 0(\varepsilon^2), \tag{7.3}$$

in which Θ solves the diffusion equation

$$\partial_t\Theta - \partial_x\left(\frac{1}{3\sigma_T}\partial_x\Theta\right) + \sigma_A\Theta = \frac{1}{2}Q. \tag{7.4}$$

For neutron transport, this is the analogue of the the fluid dynamic limit for rarefied gas dynamics.

Now consider a discretization of the transport equation (7.1) with discrete space and time scales Δx and Δt, and a discretization of the scattering integral (7.2) with a discretization size $\Delta\mu$. If Δx, Δt, $\Delta\mu$ are much smaller than ε, then the discrete solution is nearly a solution of the transport equation (7.1). On the other hand in regions of small mean free time, we want to let the discretization scale be much larger than the collision scale ε. So we consider the limit in which the numerical parameters Δx, Δt, $\Delta\mu$ are held fixed, while $\varepsilon \to 0$. We say that the discretized equation has the correct diffusion limit, if in this limit the solution of the discrete equations for (7.1) goes to the solution for a discretization of the diffusion equation (7.4).

Larsen, Morel and Miller [42] have investigated this diffusion limit for a variety of difference schemes for (7.1) and have found that many of them have the correct diffusion limit only in special regimes. They have constructed some alternative methods that always have the correct diffusion limit. Jin and Levermore [36] have applied a similar procedure to an interface problem to get a constraint on the quadrature set for the discretization of the scattering integral (7.2). So far generalization of these ideas to multidimensional problems has not been successful [15]. Another class of methods that use information from the diffusion limit to improve a numerical transport methods is that of the "diffusion synthetic acceleration methods" [41].

As a first step in applying these ideas to nonlinear rarefied gas dynamics, consider the equations of the Broadwell model:

$$\begin{aligned} f_t \;+f_x \;&= \frac{1}{\varepsilon}(h^2 - fg) \\ g_t \;-g_x \;&= \frac{1}{\varepsilon}(h^2 - fg) \\ h_t \;\;\;\;\;\;\;\;&= -\frac{1}{\varepsilon}(h^2 - fg). \end{aligned} \tag{7.5}$$

The fluid dynamic variables for this system are $\rho = f+2h+g$ and $m = f-g$. Denote also $z = f + g$. Then (7.5) can be rewritten as

$$\begin{aligned} \rho_t + m_x &= 0 \\ m_t + z_x &= 0 \\ z_t + m_x &= \tfrac{1}{2\varepsilon}(\rho^2 + m^2 - 2\rho z). \end{aligned} \tag{7.6}$$

The Euler equation corresponding to (7.5) is just the first two equations of (7.6) in which z is replaced by $z_0(\rho, m) = (\rho^2 + m^2)/2\rho$, which makes the

right side of the third equation vanish [17],i.e.

$$\begin{aligned} \rho_t + m_x &= 0 \\ m_t + \frac{1}{2}(\rho + m^2/\rho)_x &= 0. \end{aligned} \tag{7.7}$$

The corresponding Navier-Stokes equations are found by replacing z by

$$z_1(\rho, m) = z_0(\rho, m) + \varepsilon(z_{0\rho}\partial_x m + z_{0m}\partial_x z_0 - \partial_x m)/2\rho \tag{7.8}$$

which makes the third equation of (7.6) vanish to $O(\varepsilon)$.

Now consider difference schemes for the Broadwell equations (7.5) and look at the fluid dynamic limit $\varepsilon \to 0$, as the numerical parameters are held fixed. The most natural difference schemes do not necessarily have the correct fluid dynamic limit. A simple scheme with the correct Euler and Navier-Stokes limits is the following centered difference scheme: Define the centered difference operators

$$\begin{aligned} D_t f(k,n) &= \frac{1}{2\Delta t}(f(k,n+1) - f(k,n-1)) \\ D_x f(k,n) &= \frac{1}{2\Delta x}(f(k+1,n) - f(k-1,n)). \end{aligned} \tag{7.9}$$

The centered difference method for (7.5) is

$$\begin{aligned} D_t f \quad + D_x f \quad &= \frac{1}{\varepsilon}(h^2 - fg) \\ D_t g \quad - D_x g \quad &= \frac{1}{\varepsilon}(h^2 - fg) \\ D_t h \qquad\quad &= -\frac{1}{\varepsilon}(h^2 - fg) \end{aligned} \tag{7.10}$$

for each (k, n).

The difference scheme can be rewritten in the form (7.6) as

$$\begin{aligned} D_t\rho + D_x m &= 0 \\ D_t m + D_x z &= 0 \\ D_t z + D_x m &= \tfrac{1}{2\varepsilon}(\rho^2 + m^2 - 2\rho z). \end{aligned} \tag{7.11}$$

As $\varepsilon \to 0$ with Δt and Δx held fixed the solution of (7.11) satisfies

$$z = z_0(\rho, m) + \varepsilon(z_{0\rho}D_x m + z_{0m}D_x z_0 - D_x m)/2\rho. \tag{7.12}$$

It follows that the first two equation of (7.11) go to difference equations for the model Euler or Navier Stokes equations, at least away from transition regions.

This formal analysis leaves many questions unanswered, such as the following:

(1) What happens to the difference scheme in transition regions, such as shock and boundary layers, where the mean free path is small but the gas is not in equilibrium? Perhaps the method of Jin and Levermore [36] can be generalized to this problem.

(2) Can the difference scheme (7.11) be modified to preserve positivity and still have the correct diffusion limit?

(3) Are there particle methods for the Broadwell equations or the full Boltzmann equation which have the correct diffusion limit?

We believe that a method such as this which uses fluid dynamic information to improve the collisional step for rarefied gas dynamic computations could be of great utility.

References

[1] C.R. Anderson and C. Greengard. On vortex methods. *SIAM J. Num. Anal.*, 22:413–440, 1985.

[2] K. Aoki. Numerical analysis of rarefied gas flows by finite-difference method. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 297–322. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.

[3] A.A. Arsenyev. On the approximation of the solution of the Boltzmann equation by solutions of the ito stochastic differential equations. *USSR Computational Mathematics and Mathematical Physics*, 27:51–59, 1987.

[4] Hans Babovsky. On a simulation scheme for the Boltzmann equation. *Mathematical Methods in the Applied Sciences*, 8:223–233, 1986.

[5] Hans Babovsky, F. Gropengeisser, H. Neunzert, and J. Struckmeier. Low-discrepancy methods for the Boltzmann equation. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics*,

pages 85–99. 16th International Symposium on Rarefied Gas Dynamics, 1988.

[6] Hans Babovsky and Reinhard Illner. A convergence proof for Nanbu's simulation method for the full Boltzmann equation. *SIAM Journal on Numerical Analysis*, 26:45–65, 1989.

[7] C. Bardos, F. Golse, and C.D. Levermore. On the asymptotic limits of kinetic theory leading to incompressible fluid dynamics. *preprint.*

[8] J.T. Beale and A. Majda. Vortex methods I: convergence in three dimensions. *Math. Comp.*, 39:1–27, 1982.

[9] O.M. Belotserkovskii, A.I. Erofeev, and V.E. Yanitskii. A non-stationary method of direct statistical modeling of rarefied flows. *USSR Computational Mathematics and Mathematical Physics*, 1980:82–112, 20(5).

[10] G.A. Bird. Direct simulation and the Boltzmann equation. *Physics of Fluids*, 13:2672–2681, 1970.

[11] G.A. Bird. *Molecular Gas Dynamics.* Oxford U. Press, London, 1976.

[12] G.A. Bird. MonteCarlo simulation of gas flows. *Ann. Rev. Fl. Mech.*, 10:11–31, 1978.

[13] G.A. Bird. Direct simulation of gas flows at the molecular level. *Communications in Applied Numerical Methods*, 4:165–172, 1988.

[14] G.A. Bird. Perception of numerical methods in rarefied gasdynamics. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 211–222. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.

[15] Christoph Borgers, Edward W. Larsen, and Marvin L. Adams. The asymptotic diffusion limit of a linear discontinuous discretization of a two-dimensional linear transport equation. *Journal of Computational Physics*, 1990, to appear.

[16] I.D. Boyd and J.P.W. Stark. Statistical fluctuations in Monte-Carlo calculations. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 245–257. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.

[17] Russel E. Caflisch. Fluid dynamics and the Boltzmann equation. In E.W. Montroll and J.L. Lebowitz, editors, *Studies in Statistical Mechanics, 10, Nonequilibrium Phenomena I: The Boltzmann equation*, pages 193–223. North Holland, 1983.

[18] Carlo Cercignani. A variational principle for boundary value problems in kinetic theory. *Physics of Fluids*, 9:1167–1173, 1966.

[19] F.G. Cheremisin. Numerical methods for the direct solution of the kinetic Boltzmann equation. *USSR Computational Mathematics and Mathematical Physics*, 25(6):156–166, 1985.

[20] A.J. Chorin. Numerical solution of Boltzmann's equation. *Communications on Pure and Applied Mathematics*, 25:171–186, 1972.

[21] A. De Masi, R. Esposito, and J.L. Lebowitz. Incompressible Navier-Stokes and Euler limits of the Boltzmann equation. *Communications on Pure and Applied Mathematics*, 42:1189–1214, 1989.

[22] S.M. Deshpande and R. Narasimha. The Boltzmann collision integrals for a combination of Maxwellians. *Journal of Fluid Mechanics*, 36:545–554, 1969.

[23] R. DiPerna and P.L. Lions. On the cauchy problem for Boltzmann equations: Global existence and weak stability. *Annals of Mathematics*, 130:321–366, 1989.

[24] Henri Faure. Discrépance de suites associées à un système de numération (en dimension s). *Acta Arithmetica*, 41:337–351, 1982.

[25] D.H. Fujii, R.O. Barrachina, and C.R. Garibotti. Iteration scheme for the solution of the nonlinear spatially homogeneous Boltzmann equation. In V. Boffi and C. Cercignani, editors, *Proceedings of the 15th International Symposium on Rarefied Gas Dynamics*, pages 514–520. Teubner, 1986.

[26] D. Goldstein, B. Sturtevant, and J.E. Broadwell. Investigations of the motion of discrete-velocity gases. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 100–117. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.

[27] J. Goodman. Convergence of the random vortex method. *Communications on Pure and Applied Mathematics*, 40:189–220, 1987.

[28] J. Goodman, T.Y. Hou, and J. Lowengrub. Convergence of the point vortex method for the 2-d Euler equations. *Communications on Pure and Applied Mathematics*, 43:415–430, 1990.

[29] Harold Grad. Singular and nonuniform limits of the Boltzmann equation. In *SIAM-AMS Proceedings I Transport Theory*, pages 296–308. 1969.

[30] C. Greengard and L. Reyna. Drift of second moments in Nanbu's simulation scheme for the Boltzmann equation. *preprint.*

[31] F. Gropengiesser, H. Neunzert, and J. Struckmeier. Computational methods for the Boltzmann equation. In R. Spigler, editor, *The State of the Art in Appl. and Industrial Math.*, 1989.

[32] O.H. Hald. Convergence of vortex methods for Euler's equations, iii. *SIAM J. Num. Anal.*, 24:538–582, 1987.

[33] J. H. Halton. On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals. *Numer. Math*, 2:84–90, 1960.

[34] J. M. Hammersley. *Monte Carlo Methods.* Methuen, London, 1964.

[35] M.S. Ivanov, S. V. Rogasinsky, and V. Ya. Rudyak. Direct statistical simulation method and master kinetic equation. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 171–181. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.

[36] Shi Jin and C. David Levermore. The discrete-ordinate method in diffusive regimes. *preprint*, 1991.

[37] Malvin H. Kalos and Paula A. Whitlock. *Monte Carlo Methods, Volume I.* John Wiley and Son, New York, 1986.

[38] K. Koura. Null-collision technique in the direct-simulation Monte Carlo method. *Physics of Fluids*, 29:3509–3511, 1986.

[39] M. Krook and T.T. Wu. Exact solutions of the Boltzmann equation. *Physics of Fluids*, 20:1589–1595, 1977.

[40] L. Kuipers and H. Niederreiter. *Uniform Distribution of Sequences.* John Wiley and Son, New York, 1976.

[41] Edward W. Larsen. Diffusion-synthetic acceleration methods for discrete-ordinates problems. *Transport Theory and Statistical Physics*, 13:107–126, 1984.

[42] Edward W. Larsen, J.E. Morel, and Warren F. Miller, Jr. Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes. *Journal of Computational Physics*, 69:283–324, 1987.

[43] Christian Lecot. A direct simulation Monte Carlo scheme and uniformly distributed sequences for solving the Boltzmann equation. *Computing*, 41, 1989.

[44] Christian Lecot. Low discrepancy sequences for solving the Boltzmann equation. *Journal of Computational and Applied Mathematics*, 25:237–249, 1989.

[45] D.G. Long. Convergence of the random vortex method in two dimensions. *preprint*, 1988.

[46] S. Mas-Gallic. A deterministic particle method for the linearized Boltzmann equation. *Transport Theory and Statistical Physics*, 16:855–887, 1987.

[47] William J. Morokoff. *Quasi-Monte Carlo Methods for Numerical Integration and Simulation.* PhD thesis, New York University, 1991.

[48] K. Nanbu. Theoretical basis of the direct simulation Monte Carlo method. In V. Boffi and C. Cercignani, editors, *Proceedings of the 15th International Symposium on Rarefied Gas Dynamics*, pages 369–383, 1986.

[49] R. Narasimha and P. Das. The infinitely strong shock. In V. Boffi and C. Cercignani, editors, *Proceedings of the 15th International Symposium on Rarefied Gas Dynamics*, pages 293–307. Teubner, 1986.

[50] H. Niederreiter. Quasi-Monte Carlo methods and pseudo-random numbers. *Bull. Amer. Math. Soc.*, 84:957 – 1041, 1978.

[51] H. Niederreiter. Point sets and sequences with small discrepancy. *Monatsh. Math.*, 104:273–337, 1987.

[52] H. Niederreiter. Quasi-Monte Carlo methods for multidimensional numerical integration. In H. Brass and G.Hammerlin, editors, *Numerical Integration III, International Series of Numerical Math. 85.* Birkhauser Verlag, 1988.

[53] A. Nordsieck and B.L. Hicks. Monte Carlo evaluation of the Boltzmann collision integral. In Brundin, editor, *Rarefied Gas Dynamics*, pages 695–710. Academic Press, 1967.

[54] William H. Press and Saul A. Teukolsky. Quasi- (that is, sub-) random numbers. *Computers in Physics*, pages 76–79, 1989.

[55] G. Russo. A particle method for collisional kinetic equations. I. basic theory and one dimensional results. *Journal of Computational Physics*, to appear.

[56] I. M. Sobol'. The distribution of points in a cube and the approximate evaluation of integrals. *U.S.S.R. Computational Math. and Math. Phys.*, 7:86–112, 1967.

[57] I. M. Sobol'. Uniformly distributed sequences with additional uniformity property. *U.S.S.R. Computational Math. and Math. Phys.*, 16:1332–1337, 1976.

[58] G.A. Sod. A numerical solution of Boltzmann's equation. *Communications on Pure and Applied Mathematics*, 1977:391–419, 30.

[59] Y. Sone, T. Ohwada, and K. Aoki. Evaporation and condensation on a plane condensed phase: Numerical analysis of the linearized Boltzmann equation for hard-sphere molecules. *Physics of Fluids A*, 1:1398–1405, 1989.

[60] K. Sugano and A. Sakurai. Finite element solution of the linearized Boltzmann equation through its variational principle. In V. Boffi and C. Cercignani, editors, *Proceedings of the 15th International Symposium on Rarefied Gas Dynamics*, pages 492–501. Teubner, 1986.

[61] Z. Tan, Y.K. Chen, P.L. Varghese, and J.R. Howell. New numerical strategy to evaluate the collision integral of the Boltzmann equation. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 359–373. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.

[62] Wolfgang Wagner. A convergence proof for Bird's Direct Simulation Monte Carlo method for the Boltzmann equation. *Communications on Mathematical Physics*, 1991, to appear.

[63] H. Wozniakowski. Average case complexity of multivariate integration. *Bulletin of the AMS*, 24:185–194, 1991.

[64] S.M. Yen. Application of Monte Carlo methods to near-equilibrium problems. In E.P. Muntz, D.P.Weaver, and D.H. Campbell, editors, *Rarefied Gas Dynamics:Theoretical and Computational Techniques, Progress in Aeronautics and Astronautics, v. 118*, pages 323–336. Proceedings of the 16th International Symposium on Rarefied Gas Dynamics, 1988.