Numerical Methods in Fluid Dynamics

Edited by
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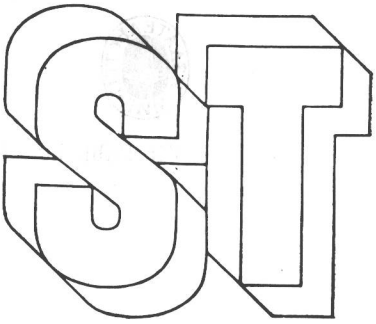

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CONTENTS

PREFACE

Experience in applied mathematics has shown that many classes of scientific problems, particularly in fluid dynamics, cannot be solved unless new methods of computational mathematics are developed. The development of efficient methods for solving fluid dynamic equations is important for many branches of modern science.

This collection of papers gives the reader an insight into the state-of-art of the numerical methods in fluid dynamics.

In the paper by Belotserkovsky, Erofeyev, and Yanitsky a numerical method is presented for the direct statistical computer simulation of transport processes in rarefied gases and turbulent fluids. The statistical model proposed in the paper is in a sense a statistical variant of the particle-in-cell method and is based on a synthesis of concepts of splitting (in a statistical interpretation) and on Kac's idea of the existence of models asymptotically equivalent to the Boltzmann equation.

The paper by Kovenya and Yanenko presents a method of splitting with respect to physical processes and spatial directions for the numerical solution of multidimensional gas-dynamics problems. A class of efficient difference schemes is proposed for numerically solving multidimensional gas-dynamics equations and the Navier-Stokes equations for a compressible heat-conducting gas.

The paper by Berezin presents numerical models for studying the formation and evolution of shock waves in a rarefied plasma with a magnetic field. Transport coefficients are defined using the effective frequency of collisions due to both Coulomb and collective interactions. The study is made using two models: a gas dynamic one (with subcritical amplitudes) and a combined one (with supercritical amplitudes). Efficient numerical algorithms are developed and a detailed analysis of the evolution and structure of shock waves is presented.

In the contribution by Sofronov, Rasskazova, and Nesterenko procedures are described for calculating two-dimensional nonstationary problems in gas dynamics on nonregular nets.

The contribution by Bakhrakh *et al.* describes a finite-difference method for calculating two-dimensional heterogeneous flows in Eulerian coordinates. Contact discontinuities are determined using the mass concentrations of substances and a special algorithm for

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computing the mass fluxes across cells containing several substances. Results are presented of calculations for two-dimensional gas flows with large deformations.

In the contribution by Yelesin, Troshchiyev, and Yudintsev, an iterative method is developed for the numerical solution of nonstationary spectral problems of thermal-radiation transport and based on applying correction-type operators to cause simple iterations over temperature to converge quickly, the operators having no spectral dependence. The method is justified analytically and verified by numerical experiments.

The paper by Marchuk, Chubarov, and Shokin reviews work on the numerical simulation of tsunamis that have really occurred in the ocean. Results are given of calculations for tsunami generation, propagation and run-up using the equations of shallow-water theory.

The paper by Sidorov reviews some results on the representation of solutions of hyperbolic gas-dynamics equations as characteristic series. The paper surveys justifications of their convergence and their effective application to the solution of three-dimensional problems in gas dynamics.

In the paper by Kuropatenko a method is proposed for investigating the dissipative properties of difference schemes in gas dynamics using the notions of M and S-conservatism, and the strong and the weak dissipative properties. The writer analyses the dissipative properties of some known difference schemes.

In their paper Ivanov, Fedotova, and Shokin use the differential approximation method to investigate the property of complete conservatism of a many-parameter family of difference schemes for gas-dynamics equations in Eulerian coordinates.

The paper by Bondarenko, Zmushko, and Stenin uses the operator-difference (energy) method to investigate stability from initial data of "Cross"-type difference schemes for solving gas-dynamics equations in Lagrangian coordinates. The investigation took artificial viscosity in the one and the two-dimensional cases into account. In one dimension, nearly exact nonlocal stability conditions are obtained that effectively take into account the presence of local nonhomogeneities in the scheme. In two dimensions, local stability conditions are obtained for arbitrary quadrangular grids, taking into account the shape of the quadrangular cells at a given point on the grid, as well as the velocity of sound and the viscosity distribution.

In their paper Ismailova and Kondrashov suggest that left-hand side and right-hand side sweep coefficients of the corresponding spectral systems of equations should be used for investigating the spectral properties of difference schemes. This approach makes it possible to allow for the variability of the coefficients of the scheme

and for the presence in difference equations of various inhomogeneities (at both the interior and limiting points of a space grid) and to obtain practical stability criteria for a finite computational grid.

In the contribution by Yanenko, Kuznetsov, and Smagulov the behaviour of a strong solution of equations with small parameters approximating the Navier-Stokes equations for an incompressible fluid is considered and the stability and convergence of fractional-step type difference schemes for the Navier-Stokes equations are investigated.

The paper by Lar'kin, Novikov, and Yanenko considers problems in the theory of variable-type nonlinear equations. This class of equations has lately been the subject of growing interest in connection with the simulation of complex phenomena in continuum mechanics.

This collection of papers will be useful for applied mathematicians, in particular those working on numerical methods for continuum mechanics.

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1 Direct Statistical Simulation of Problems in Aerohydrodynamics

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1.1 DIRECT STATISTICAL SIMULATION METHOD

1.1.1 Introduction

1. We present here a numerical method for the direct statistical computer simulation of the transport processes in rarefied gases and turbulent fluids. The method is developed with a view to applying the approaches to problems in fluid mechanics. There are actually no appropriate mathematical models for most of the practically important problems in this field and ours is an attempt at designing new statistical models. These models should satisfy two requirements: (1) they must adequately describe the phenomenon under consideration and (2) they must lend themselves to study using existing computing techniques. Two classes of problems are investigated here: stationary multidimensional rarefied gas dynamics (RGD) problems (including methodical calculations associated with the development of the method and a wide range of flow problems) and nonstationary turbulent problems. The latter have only begun to be simulated comparatively recently.

We shall give at the outset a general definition of the direct numerical simulation method to be presented below. Using a set of a few particles used to represent a medium and Monte Carlo methods as the numerical techniques, a simulation model of a phenomenon is constructed (without solving the kinetic equation) which adequately reflects the features of the flow. We repeat, a kinetic equation (of one sort or another) is used to construct the simulation model. The numerical computer simulation itself, however, is carried out using statistical techniques without resorting to the kinetic equation. Thus one of the central problems in this approach is the necessity of proving the adequacy of the simulation process and of the corresponding kinetic equation.

2. The numerical algorithms are constructed using a splitting method, the basic principles of which are formulated below. Recently workers at the Computing Centre of the USSR Academy of Sciences and those at the Moscow Institute of Physical Engineering have developed a group of numerical approaches (e.g. the "large particle" and "flux" methods) which split the physical process using time step Δt and allow the process to reach the steady state to solve stationary

problems [1]. These algorithms, implementation of which borders on conducting a numerical experiment, can be effectively applied to solve both Euler and Navier-Stokes equations. The basic ideas of this approach seem promising for the solution of RGD and turbulence problems. In this paper we present the basic principles of our statistical particle-in-cell method for computing spatially inhomogeneous and nonstationary flows as described by kinetic equations.

The first (basic) category of problems are investigations of multidimensional rarefied gas flows. We have in this case the universal kinetic Boltzmann equation (see, for example, [2]). It is a nonlinear, integro-differential equation closed under the distribution function $f(t, \boldsymbol{x}, \boldsymbol{c})$, which in the simplest case of a monatomic gas defines the density of the particles in the phase space of a molecule. The difficulty of solving the Boltzmann equation is that there are a large number of independent variables (seven in the general case: t, $\boldsymbol{x}$, $\boldsymbol{c}$), that the collision integral J is complicated (with a multiplicity of no less than five) and that the integrand is essentially nonlinear.

When investigating problems in turbulence, additional difficulties arise due to the nonstationarity of the process and the absence of a universal kinetic equation.

An efficient numerical solution of the Boltzmann kinetic equation by classical methods is hardly possible with current computer capacities. Statistical methods [3] began to be widely used. However, most of the conventional Monte Carlo methods of solving the "unsimplified" Boltzmann equation have a serious drawback limiting their application to one-dimensional flows or the simplest plane problems. Their main disadvantage is that they require too large a working storage, a capacity considerably exceeding the working storage of modern computers.

The most general analytical method of solving the Boltzmann equation, the Chapman-Enskog theory, can only be applied at small Knudsen numbers Kn*. At the same time many important applications are in the transient region of flow where Kn $\sim$ 1**. Calculations of transient flows are also mainly done using numerical methods but here again great difficulties are encountered and overcome in general by a variety of methods.

We propose the following classification of RGD numerical methods [4, 5] into three main groups:

(a) regular methods, where difference approximations of the kinetic equations are solved, the integrals of the distribution function

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* The Knudsen number $\mathrm{Kn} = \lambda/L$ is the ratio of the mean free path of molecules of a fluid to a characteristic length.

** At altitudes $H \approx$ 90-120 km the local value of the molecular mean free path is of the same order of magnitude as the characteristic length of a flying vehicle; the flow regime at these heights is called transient (Kn $\sim$ 1).

being replaced by common (Simpson, Gauss, etc.) quadrature formulas;

(b) semiregular methods, which differ from regular ones in that they use Monte Carlo quadrature formulas to evaluate the integrals of the distribution function;

(c) statistical simulation methods, which use the Monte Carlo method directly to simulate rarefied flows without resorting at any stage to solutions of the kinetic equations.

A detailed analysis of all the three groups of methods is contained in the review by Belotserkovsky and Yanitsky [4, 5]. The regular numerical methods as applied to model equations like the Krook equation have been developed somewhat. The semiregular methods of numerically solving the Boltzmann equation directly are used mainly for one-dimensional problems and other methods will be compared with them. The statistical method (direct rarefied flow simulation) has turned out to be the most fruitful. This has been demonstrated by the many numerical experiments of Bird [6, 7] including calculations of a number of practically important problems. One of the computational advantages of this approach is its comparatively low storage requirement.

The statistical model proposed in this paper avoids, to our mind, a number of the fundamental shortcomings of Bird's heuristic model. Computationally our method is as efficient as Bird's but approximates the Boltzmann equation better and has a deeper probabilistic justification. The model is in a sense a statistical modification of Harlow's "particle-in-cell" method [8]. Basically it synthesizes the ideas of splitting (in a statistical treatment) and Kac's ideas about the existence of models asymptotically equivalent to the Boltzmann equation.

3. We will summarize the essence of these approaches. The general principle of splitting according to physical processes is as follows [1]:

The fluid to be simulated can be replaced by a system of N particles (fluid particles in the case of a continuous medium and molecules in the discrete case) which are distributed at the initial moment of time over Euler grid cells in a coordinate space according to the initial data. The evolution of the system during a period of time Δt may be split into two stages: changes in the internal states of the subsystems in the cells assuming that each subsystem is "frozen" or fixed (the "Euler" stage for a continuum and the collision relaxation stage for a discrete medium), and a subsequent displacement of all the particles to distances proportional to the time step Δt and velocities without changing their internal state (the "Lagrange" stage for a continuum and free molecule motion for a discrete medium).

The stationary distribution of all parameters of the medium is evaluated after the process has reached the steady state in time.

A feature of the statistical particle-in-cell method considered here

is that the state of every particle is characterized by coordinate and velocity vectors $\boldsymbol{r}$ and $\boldsymbol{c}$ respectively. In addition, a Monte Carlo method is used for the numerical implementation of the first stage (particle collision in cells) as well as that of the second stage of splitting (collisionless displacement). It is evident that the greatest difficulty lies in the implementation of the first stage.

The basic ideas of the method are illustrated using problems of rarefied gas dynamics.

1.1.2 The Basic Principles of the Method

1. It is assumed that the rarefied flow around a body can be found using a distribution function and that the gas is monatomic. Then any macroparameter of the gas flow $\Psi(t, \boldsymbol{x})$ that is related to the molecular constant $\psi(\boldsymbol{c})$ is a functional of the form

$$\Psi(t, \boldsymbol{x}) = \frac{1}{n(t, \boldsymbol{x})} \int \psi(\boldsymbol{c}) f(t, \boldsymbol{x}, \boldsymbol{c})\, d\boldsymbol{c}, \tag{1.1.1}$$

where $f(t, \boldsymbol{x}, \boldsymbol{c})$ is the molecule distribution function in the 6-dimensional space $(\boldsymbol{x}, \boldsymbol{c})$ of particle coordinates and velocities.

If Ω denotes the control volume, and Γ is the boundary of Ω, which includes the surface of a body in stream, then the problem reduces to finding the solution $f(t, \boldsymbol{x}, \boldsymbol{c})$ of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{c}\frac{\partial f}{\partial \boldsymbol{x}} = \int (f' f_1' - f f_1)\, g\, d\sigma\, d\boldsymbol{c}_1 \equiv J[f \cdot f_1], \tag{1.1.2}$$

satisfying the initial conditions

$$f(t = 0, \boldsymbol{x}, \boldsymbol{c}) = f_0(\boldsymbol{x}, \boldsymbol{c}), \quad \boldsymbol{x} \in \Omega, \quad -\infty < c_{x,\,y,\,z} < +\infty \tag{1.1.3}$$

and the boundary conditions

$$f(t, \boldsymbol{x}_\Gamma, \boldsymbol{c}) = \int K(\boldsymbol{c}, \boldsymbol{c}_1) f(t, \boldsymbol{x}_\Gamma, \boldsymbol{c}_1)\, d\boldsymbol{c}_1, \tag{1.1.4}$$

$$\boldsymbol{c} \cdot \boldsymbol{n}(\boldsymbol{x}_\Gamma) > 0, \quad \boldsymbol{c}_1 \cdot \boldsymbol{n}(\boldsymbol{x}_\Gamma) < 0,$$

where $\boldsymbol{n}(\boldsymbol{x}_\Gamma)$ is the normal to the surface Γ at the point $\boldsymbol{x}_\Gamma \in \Gamma$ directed into the volume Ω, the form of the kernel K is given by the gas-surface interaction law [2], and $g = |\boldsymbol{c} - \boldsymbol{c}_1|$, σ is the collision cross-section of the molecules.

To obtain an approximate solution of problems thus set we construct a statistical model of an ideal monatomic gas containing N particles with coordinates $\boldsymbol{r}_i$ and velocities $\boldsymbol{c}_i$ $(i = 1, \ldots, N)$ such that the evolution equation for this model approximates equation (1.1.2) subject to only one additional assumption, viz. the molecular-chaos hypothesis, i.e.

$$f_2(t, \boldsymbol{x}, \boldsymbol{c}_1, \boldsymbol{c}_2) = f_1(t, \boldsymbol{x}, \boldsymbol{c}_1) f_1(t, \boldsymbol{x}, \boldsymbol{c}_2), \tag{1.1.5}$$

where

$$f_s(t, x, c_1, \ldots, c_s) \equiv \frac{N}{(N-s)!} F_s(t, r_1, \ldots, r_s, c_1, \ldots, c_s)$$

for $r_1 = r_2 = \ldots = r_s = x$, with F_s being an s-particle distribution function in $6N$-dimensional phase space.

If we denote the state of the model at time t by $\{\boldsymbol{R}(t), \boldsymbol{C}(t)\} = \{r_1(t), c_1(t), \ldots, r_N(t), c_N(t)\}$, then the solution of the problem reduces to a numerical implementation of a finite number of paths $\{\boldsymbol{R}(t), \boldsymbol{C}(t)\}$ with the initial data corresponding to (1.1.3), the simulation of the interaction of particles with a boundary Γ being performed in accordance with a given kernel K [4]. Given a set of paths, we can evaluate any macroparameter (1.1.1) using consistent estimates from the Monte Carlo method for the integrals [9].

By synthesizing the basic ideas of the particle-in-cell method [1, 10, 11] and those of Kac's statistical model [12], the model we want $\{\boldsymbol{R}(t), \boldsymbol{C}(t)\}$ can be constructed for the spatially inhomogeneous case where $\partial f/\partial x \neq 0$ [13, 14, 15].

The distinctive feature of this model is that during the first stage (collision relaxation) a subsystem in a cell is regarded as Kac's N-particle model [12] and hence the simulation of the collisions reduces to the Monte Carlo implementation of the evolution of Kac's model or its approximation. It is important to note that the basic equation of Kac's model is linear and this considerably facilitates a numerical solution. In addition, Kac's model calculates the times between collisions in proper correspondence with the statistics of collisions in an ideal monatomic gas.

2. We shall now consider the numerical algorithm. A fixed coordinate grid $\{\lambda_\beta\}$ is fixed in space, and continuous time t is replaced by discrete time t_α. At the initial moment the control volume is filled with N particles ($N \sim 10^3$-10^4), each particle being described by a position vector r_i and velocity c_i. It is these quantities that are calculated by the Monte Carlo method according to the initial distribution function $f_0(\boldsymbol{r}, \boldsymbol{c})$. Thus, at every instant the state of simulation model is characterized by a $6N$-dimensional vector $\{\boldsymbol{R}, \boldsymbol{C}\}$.

Calculation of how the model has evolved at time step Δt is split into two main stages.

Stage I. Every cell of the space is scanned in turn and the particle collisions in each are statistically simulated by changing the velocities while leaving the coordinates unchanged.

Stage II. The displacements of all the particles in the model $\{r_1, c_1, \ldots, r_N, c_N\}$ are simulated. They are displaced by distances proportional to the time step Δt and their velocities c_i. It is here that particle boundary interactions are simulated.

Alternating the two main stages makes it possible in principle to

follow the simulation path in $6N$-dimensional phase space over any time interval. If the problem is to determine the macroscopic parameters of a steady flow, then we carry out periodic calculations of the average momenta and thermal kinetic energies of the particles in each cell, and after averaging over the number of measurements we find the field of momentum and internal energy distribution over the cells. The nonstationary problem is more involved. To obtain macroparameters at time t here, it is necessary to follow a quite larger number of paths (from zero to t) and only then do we average over the ensemble of the paths.

The direct simulation method for rarefied flows is thus equivalent to a numerical solution of the Boltzmann equation according to the following two-stage splitting scheme:

Stage I:

$$\frac{\partial f_\beta^*}{\partial t} = J(f_\beta^*), \quad \text{where } f_\beta^*(t = t_\alpha) = f_\beta^\alpha.$$

Stage II:

$$\frac{\partial f_\beta}{\partial t} + cL(f_\beta) = 0, \quad \text{where } f_\beta^{\alpha+1} = f_\beta^*(t = t_{\alpha+1}),$$

where $L(f_\beta)$ is the difference approximation of the space derivative $c\frac{\partial}{\partial x}$, and f^* is the "intermediate" value of the distribution function for Stage I.

This simulation scheme essentially uses the ideas of splitting a computational process into physically meaningful stages, and this allows us to reduce the problem at every time instant to the successive solution of the Boltzmann equation for the spatially homogeneous case (Stage I) and a free-molecule flow (Stage II). The splitting principle for differential operators was justified by Yanenko [16] and Marchuk [17]. As applied to kinetic equations, it was also treated by Godunov and Sultangazin [18]. The application of this principle virtually solves the problem of high dimensionality of a phase space for the kinetic equation. The multidimensionality of a phase space affects only Stage II (of free-molecule shift), but it is known that for this stage it is easy to generalize algorithms to two and three space variables.

3. It is, to our mind, important that an accurate approximation of the Boltzmann convection-free equation be carried out (Stage I), and this appears to be central to the approach. Here, as already noted, the Boltzmann equation is replaced by the Kac statistical model [12].

The Kac model describes the collision relaxation of an isolated system of a finite number of N identical atom-particles in the spatially homogeneous case. The state of the model is considered only in the velocity space and hence is characterized by the $3N$-dimensional vector $\{c_1, \ldots, c_N\} = C(t)$. The process $C(t)$ is strictly Marko-

vian. The basic equation of the model is written out for the evolution of the density $\varphi(t, c)$ of the probability distribution of all velocities $\{c\}$ simultaneously. It is of the form [13]

$$\frac{\partial \varphi(t, C)}{\partial t} = \frac{1}{V} \sum_{1 \leqslant l < m \leqslant N} g_{lm} \int [\varphi(t, C'_{lm}) - \varphi(t, C)] \, d\sigma_{lm}, \qquad (1.1.6)$$

where $C'_{lm} = \{c_1, \ldots, c_{l-1}, c'_l, c_{l+1}, \ldots, c_{m-1}, c'_m, c_{m+1}, \ldots, c_N\}$, $g_{lm} \equiv | c_l - c_m |$, and c'_l and c'_m denote the velocities of the lth and mth particles after colliding, $d\sigma_{lm}$ is the differential cross-section of the elastic scattering of the particle pair (c_l, c_m) and the normalization parameter V is determined by the choice of the units of measurements and can be interpreted as the cell volume.

If we introduce the distribution function

$$f_s(t, c_1, \ldots, c_s) = \frac{N!}{(N-s)! \, V^s} \int \varphi(t, C) \prod_{i=s+1}^{N} dc_i, \qquad (1.1.7)$$

then by integrating (1.1.6) it is not difficult to obtain

$$\frac{\partial f_1(t, c_1)}{\partial t} = \int [f_2(t, c'_1, c'_2) - f_2(t, c_1, c_2)] \, g_{12} \, d\sigma_{12} \, dc_2,$$

which coincides with the Boltzmann equation for zero convective derivative when equation (1.1.5) holds.

The algorithm for implementing Stage I when the evolution of the spatially inhomogeneous model is being calculated corresponds to the Monte Carlo numerical method for solving the basic Kac equation (1.1.6), which is (unlike the Boltzmann equation) linear. When deriving the basic equation of the Kac model the same prerequisites are used as when deriving the Boltzmann equation, except for the molecular chaos hypothesis.

Using the Kac equation at Stage I makes it possible to avoid a straightforward calculation of the collision integral J in the Boltzmann equation (1.1.2) (this being the main obstacle when directly solving the Boltzmann equation), and the construction of strictly Markovian processes makes this approach very efficient.

The relation between the Boltzmann equation and Kac model has been the subject of several probabilistic analyses ([13-15], etc.), the most complete of the relevant theorems being proved by Grünbaum [15] in 1971. The essence of these studies is that, as $N \to \infty$, the Kac model is equivalent to the spatially homogeneous Boltzmann equation, but for a finite number of particles N it is in principle possible that the assumption about the statistical independence of the particle (the molecular chaos hypothesis) could be violated, and this is the only difference between the Kac model and the Boltzmann equation. In numerical calculations this discrepancy is evaluated every time for the various numbers of particles in the cell N_0.

It has been shown that in rarefied flow calculations by the proposed method the dependence on N is very weak [13, 14].

Thus our theoretical scheme assumes two successive approximations of the Boltzmann equation. The first approximation corresponds to the split of the differential operator according to the physical processes, the second corresponds to the replacement of the spatially homogeneous Boltzmann equation in each cell by the Kac model. Computationally, this way of simulating particle collisions in cells is a statistical implementation of the Kac model. Of course, there is only one exact way of doing this, but many approximate schemes can be constructed.

4. The principal feature of the numerical algorithms developed in [10-15] is that the queueing time T for the next collision is defined following the statistics of the collision (Markovian and strictly Markovian processes*).

The algorithm for simulating collisions by a strictly Markovian process may be described, for example, in the following way [13, 15].

(i) A pair of collision partners (c_i, c_j) is chosen at random from the total number N of particles in a cell and assigned a probability proportional to $g\sigma$. The queueing time T for the collision between the chosen pair is sought,

$$P(T > \theta) = \exp(-\lambda\theta), \quad \lambda = \frac{1}{V} \sum_{1 \leqslant i < j \leqslant N} g_{ij}\sigma_{ij}.$$

(ii) The time interval is summed into an accumulator

$$\sum_{i=1}^{n} T_i = s_n.$$

If it is found that $s_n \leqslant \Delta t$, then the collision is accepted and the velocities of (c_i, c_j) are converted to their values (c_i', c_j') after collision, and the simulation process returns to (i)). If, however, it turns out that $s_n > \Delta t$, then the collision of the pair is rejected, and the entire process of simulating collisions in the cell is terminated.

It can be shown [13] that the basic kinetic equation for the evolution of the $3N$-dimensional vector $C(t) = \{c_1, \ldots, c_N\}$ that is determined by this algorithm when simulating a collision process is the Kac equation. This is derived directly from the algorithm

* Recall that by definition (see, for example, [19]) a process is Markovian if the queueing time T for the next collision is defined by the state of the entire subsystem of N particles in a cell at a given time before the collision, and hence it is the same regardless of what pair m is being considered; the exponential law for the distribution of time T makes this process strictly Markovian. Bird's scheme [6, 7] generates a typical semi-Markovian process in which the queueing time depends on the future state of the system (on the index number of the pair m which is to collide, and hence on the state of the system after the collision).