

Monte Carlo Methods and Numerical Solutions

Wolfgang Wagner

Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, D-10117 Berlin, Germany

Abstract. The purpose of this paper is to illustrate that direct simulation Monte Carlo methods can often be considered as rigorous mathematical tools for solving nonlinear kinetic equations numerically. First a convergence result for Bird's DSMC method is recalled. Then some sketch of the history of stochastic models related to rarefied gas dynamics is given. The model introduced by Leontovich in 1935 provides the basis for a rigorous derivation of the Boltzmann equation from a stochastic particle system. The last part of the paper is concerned with some recent directions of study in the field of Monte Carlo methods for nonlinear kinetic equations. Models with general particle interactions and the corresponding limiting equations are discussed in some detail. In particular, these models cover rarefied granular gases (inelastic Boltzmann equation) and ideal quantum gases (Uehling-Uhlenbeck-Boltzmann equation). Problems related to the order of convergence, to the approximation of the steady state solution, and to variance reduction are briefly mentioned.

DSMC AND THE BOLTZMANN EQUATION

Direct simulation Monte Carlo (DSMC) has been the most widely used numerical algorithm in kinetic theory. We refer to G.A. Bird's monograph [1, Sections 9.4, 11.1] concerning remarks on the historical development. The history of the subject is also well reflected in the proceedings of the bi-annual conferences on "Rarefied Gas Dynamics" ranging from [2] to the present volume.

The method is based on systems of particles

$$\left(x_1(t), v_1(t); \dots; x_n(t), v_n(t)\right), \quad t \geq 0, \quad n \geq 1, \quad (1)$$

imitating the behaviour of gas molecules in a probabilistic way. It includes several numerically motivated approximations. Independent motion (free flow) of the particles and their pairwise interactions (collisions) are separated using a splitting procedure with a time increment Δt . During the free flow step, particles move according to their velocities,

$$x_i(t + \Delta t) = x_i(t) + \int_t^{t+\Delta t} v_i(s) ds, \quad i = 1, \dots, n,$$

and do not collide. At this step boundary conditions are taken into account. During the collision step, particles do not change their positions. At this step some partition

$$D = \cup_{l=1}^{l_c} D_l$$

of the spatial domain into a finite number l_c of disjoint cells is introduced. In each cell a certain amount of binary collisions between particles is performed,

$$v_i, v_j \Rightarrow v_i^*, v_j^*.$$

The probabilistic rules of these transformations depend on the interaction potential between gas molecules.

The interest in studying the connection between stochastic simulation procedures in rarefied gas dynamics and the Boltzmann equation was stimulated by K. Nanbu's paper [3] (cf. the survey papers [4, 5]). Convergence for the Nanbu scheme and its modifications was studied in [6] (spatially homogeneous case) and [7] (spatially inhomogeneous case). Convergence for Bird's method was proved in [8]. It was established that the empirical measures related to the particle system (1),

$$\mu^{(n)}(t, dx, dv) = \frac{1}{n} \sum_{i=1}^n \delta_{x_i(t), v_i(t)}(dx, dv),$$

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converge (as $n \rightarrow \infty$) to a deterministic measure with some density \hat{f} , which is defined as follows.

Consider the time discretization $t_k = k \Delta t$, $k = 0, 1, \dots$, and auxiliary functions

$$f^{(1,k)}(t, x, v), \quad f^{(2,k)}(t, x, v), \quad t \in [t_k, t_{k+1}], \quad (x, v) \in D \times \mathcal{R}^3.$$

These functions are determined by two systems of equations coupled via their initial conditions. The first system, corresponding to the free flow simulation steps, has the form

$$\frac{\partial}{\partial t} f^{(1,k)}(t, x, v) + (v, \nabla_x) f^{(1,k)}(t, x, v) = 0, \quad (2)$$

with appropriate boundary conditions. Here ∇ denotes the vector of partial derivatives and (\cdot, \cdot) is the scalar product in the Euclidean space \mathcal{R}^3 . The initial conditions are

$$f^{(1,k)}(t_k, x, v) = f^{(2,k-1)}(t_k, x, v), \quad k = 1, 2, \dots, \quad f^{(1,0)}(0, x, v) = f_0(x, v),$$

where f_0 is some density function related to the initial state of the particle system (1). The second system of equations, corresponding to the collision simulation steps, has the form

$$\begin{aligned} \frac{\partial}{\partial t} f^{(2,k)}(t, x, v) = & \quad (3) \\ & \int_D \int_{\mathcal{R}^3} \int_{S^2} h(x, y) B(v, w, e) \left[f^{(2,k)}(t, x, v^*) f^{(2,k)}(t, y, w^*) - f^{(2,k)}(t, x, v) f^{(2,k)}(t, y, w) \right] de dw dy, \end{aligned}$$

where

$$h(x, y) = \frac{1}{|D_l|} \sum_{l=1}^{l_c} \chi_{D_l}(x) \chi_{D_l}(y), \quad (4)$$

$|\cdot|$ denotes the volume, χ_A is the indicator function of a set A and S^2 is the unit sphere in \mathcal{R}^3 . The collision kernel B is determined by the interaction potential between gas molecules. The initial conditions are

$$f^{(2,k)}(t_k, x, v) = f^{(1,k)}(t_{k+1}, x, v), \quad k = 0, 1, \dots$$

The limiting density \hat{f} is defined as

$$\hat{f}(t_k, x, v) = f^{(2,k-1)}(t_k, x, v), \quad k = 1, 2, \dots, \quad \hat{f}(0, x, v) = f_0(x, v).$$

HISTORY OF STOCHASTIC MODELS IN RGD

Statistical description

The basis for the statistical theory of gases was provided in the second half of the 19th century. James Clerk Maxwell (1831-1879) found the distribution function of the gas molecule velocities in thermal equilibrium,

$$f_{eq}(v) = \frac{1}{[2\pi T]^{3/2}} \exp\left(-\frac{\|v\|^2}{2T}\right), \quad v \in \mathcal{R}^3. \quad (5)$$

The positive number T corresponds to the temperature of the gas. Ludwig Boltzmann (1844-1906) studied the problem if a gas starting from any initial state reaches the Maxwellian distribution (5). In [9] he established the equation

$$\frac{\partial}{\partial t} f(t, x, v) + (v, \nabla_x) f(t, x, v) = \int_{\mathcal{R}^3} dw \int_{S^2} de B(v, w, e) \left[f(t, x, v^*) f(t, x, w^*) - f(t, x, v) f(t, x, w) \right] \quad (6)$$

governing the time evolution of the distribution function

$$f(t, x, v), \quad t \geq 0, \quad x \in D \subset \mathcal{R}^3, \quad v \in \mathcal{R}^3.$$

This function represents the relative amount of gas particles at time t having a position close to x and a velocity close to v . The collision transformation is

$$v^* = v + e(e, w - v), \quad w^* = w + e(e, v - w). \quad (7)$$

For the hard sphere model (billiard balls) the collision kernel takes the form

$$B(v, w, e) = c|(v - w, e)|, \quad \text{for some } c > 0.$$

Leontovich model

Consider a stochastic particle system

$$Z^{(n)}(t) = \left(X_1(t), V_1(t); \dots; X_n(t), V_n(t) \right), \quad t \geq 0, \quad (8)$$

determined by an infinitesimal generator of the form

$$\mathcal{A}^{(n)}(\Phi)(z) = \sum_{i=1}^n (v_i, \nabla_{x_i})(\Phi)(z) + \frac{1}{2n} \sum_{1 \leq i \neq j \leq n} \int_{\mathcal{S}^2} \left[\Phi(J(z, i, j, e)) - \Phi(z) \right] q^{(n)}(x_i, v_i, x_j, v_j, e) de,$$

where Φ is an appropriate test function,

$$z = (x_1, v_1; \dots; x_n, v_n), \quad x_i, v_i \in \mathcal{R}^3, \quad i = 1, \dots, n,$$

$q^{(n)}$ is an intensity function and

$$[J(z, i, j, e)]_k = \begin{cases} (x_k, v_k) & , \text{ if } k \neq i, j, \\ (x_i, v_i + e(e, v_j - v_i)) & , \text{ if } k = i, \\ (x_j, v_j + e(e, v_i - v_j)) & , \text{ if } k = j, \end{cases}$$

is the jump transformation. Here we assume $D = \mathcal{R}^3$ so that no boundary conditions are involved. We recall the pathwise behaviour of the system (8), which is a piecewise-deterministic process in the sense of [10, Section 2]. Starting at z the process moves according to the free flow, i.e.

$$Z^{(n)}(t) = \left(x_1 + t v_1, v_1; \dots; x_n + t v_n, v_n \right),$$

until a random jump time τ_1 is reached. The probability distribution of this time is determined by

$$\text{Prob}(\tau_1 > t) = \exp \left(- \int_0^t \lambda^{(n)}(Z^{(n)}(s)) ds \right), \quad t \geq 0,$$

where

$$\lambda^{(n)}(z) = \frac{1}{2n} \sum_{1 \leq i \neq j \leq n} \int_{\mathcal{S}^2} q^{(n)}(x_i, v_i, x_j, v_j, e) de.$$

At the random time τ_1 the process jumps into a state z_1 , which is obtained from the state $z' = (x'_1, v'_1; \dots; x'_n, v'_n)$ of the process just before the jump by a two-particle interaction. Namely, two indices i, j and a direction vector e are chosen according to the probability density

$$\frac{q^{(n)}(x'_i, v'_i, x'_j, v'_j, e)}{2n \lambda^{(n)}(z')} \quad (9)$$

and the velocities v'_i, v'_j are replaced using the collision transformation (7).

The study of the relationship between the process (8) and the Boltzmann equation (6) was started by M. A. Leontovich (1903-1981) in the paper [11] in 1935. Let $p^{(n)}(t, z)$ denote the n -particle distribution function of the process. Applying properties of the collision transformation (7) and some symmetry assumptions on $q^{(n)}$, the equation

$$\begin{aligned} \frac{\partial}{\partial t} p^{(n)}(t, z) + \sum_{i=1}^n (v_i, \nabla_{x_i}) p^{(n)}(t, z) = \\ \frac{1}{2n} \sum_{1 \leq i \neq j \leq n} \int_{S^2} \left[p^{(n)}(t, J(z, i, j, e)) - p^{(n)}(t, z) \right] q^{(n)}(x_i, v_i, x_j, v_j, e) de \end{aligned} \quad (10)$$

is obtained from Kolmogorov's forward equation. Using the method of generating functions, Leontovich first studied the cases of "monomolecular processes" (independent particles) and of "bimolecular processes" with discrete states (e.g., a finite number of velocities). Under some assumptions on the initial state, he showed that the expectations of the relative numbers of particles in the bimolecular scheme asymptotically (as $n \rightarrow \infty$) solve the corresponding deterministic equation. In the case of the full Boltzmann equation the stochastic process was described via (10) (even including a boundary condition of specular reflection). Concerning the asymptotic behaviour of the process, Leontovich noted that he was not able to prove a limit theorem in analogy with the discrete case, though he strongly believes that such theorem holds. However, he pointed out the following. Let $p_k^{(n)}$ denote the marginal distributions corresponding to the density $p^{(n)}$. If

$$\lim_{n \rightarrow \infty} p_2^{(n)}(t, x_1, v_1, x_2, v_2) = \lim_{n \rightarrow \infty} p_1^{(n)}(t, x_1, v_1) \lim_{n \rightarrow \infty} p_1^{(n)}(t, x_2, v_2) \quad (11)$$

and

$$\lim_{n \rightarrow \infty} q^{(n)}(x, v, y, w, e) = \delta(x-y) B(v, w, e), \quad (12)$$

where δ denotes Dirac's delta-function, then the function

$$f(t, x, v) = \lim_{n \rightarrow \infty} p_1^{(n)}(t, x, v)$$

solves the Boltzmann equation. For example, (12) is satisfied for

$$q^{(n)}(x, v, y, w, e) = h^{(n)}(x, y) B(v, w, e)$$

and

$$h^{(n)}(x, y) = \begin{cases} c_n^{-1}, & \text{if } \|x - y\| \leq \varepsilon^{(n)}, \\ 0, & \text{otherwise,} \end{cases}$$

where c_n is the volume of a ball with radius $\varepsilon^{(n)} \rightarrow 0$. In this case, according to (9), only those particles can collide which are closer to each other than the interaction distance $\varepsilon^{(n)}$.

Independently, the stochastic approach to the Boltzmann equation was developed by M. Kac (1914-1984) in the paper [12] in 1956 (see also the books [13] and [14]). The spatially homogeneous version of equation (10) is called "master equation" referring to [15]. The factorization property (11) is called "chaos property" (indicating asymptotic independence) and the statement of the basic theorem is "propagation of chaos". The spatially inhomogeneous case was treated by C. Cercignani in the paper [16] in 1983. He considered a system of "soft spheres", where "molecules collide at distances randomly given by a probability distribution", and proved propagation of chaos (modulo a uniqueness theorem). The limiting equation is the mollified Boltzmann equation (cf. [17, Section VIII.3])

$$\begin{aligned} \frac{\partial}{\partial t} f(t, x, v) + (v, \nabla_x) f(t, x, v) = \\ \int_D \int_{\mathcal{R}^3} \int_{S^2} h(x, y) B(v, w, e) \left[f(t, x, v^*) f(t, y, w^*) - f(t, x, v) f(t, y, w) \right] de dw dy, \end{aligned} \quad (13)$$

which reduces to the Boltzmann equation (6) if the "mollifier" h is a delta-function. Further references concerning the spatially inhomogeneous case are [18, 19, 20, 21, 22, 23, 24].

Stochastic numerics

Stochastic numerical procedures in rarefied gas dynamics go back to the papers [25] (homogeneous gas relaxation problem) and [26] (shock structure problem) by G.A. Bird in 1963 and 1965, respectively. An interesting development of the DSMC method was related to the “time counter” – the mechanism that determines the number of collisions during a time step. Several similar modifications were introduced under different names in [27] (null-collision technique), [28] (majorant frequency scheme), [29] (no time counter scheme). The basic idea of “fictitious jumps” is applicable in general situations (cf. [30, Section 4.2]). In [3] K. Nanbu derived a stochastic particle scheme starting directly from the Boltzmann equation. However, the original method suffered from certain deficiencies (quadratic effort in the number of particles, conservation of momentum and energy only on average). Later this approach was considerably improved (cf. [31, 6]) so that it did successfully work in applications like the reentry problem (cf. [32, 33]). Among the numerous Russian sources on stochastic algorithms for the Boltzmann equation we mention papers related to the Leontovich-Kac-process [34, 35, 36, 37], papers using branching processes [38, 39] and papers following Skorokhod’s approach via stochastic differential equations with respect to Poisson measures [40, 41].

Comments

Boltzmann’s equation (6) was derived from a model with deterministic interaction between particles. The origin of stochasticity (necessary for the interpretation of the solution) remained unclear. Statistical mechanics solves this problem via a random initial state of the system. Leontovich’s motivation for introducing his model was to provide a stochastic process such that the Boltzmann equation describes the limit (for the particle number going to infinity) of rigorously defined mathematical expectations. Moreover, this approach allows one to study fluctuations. He did not address the problem of the relationship between the stochastic process and the description of the system by quantum (or classical) mechanics. The main new point in this model are the stochastic interactions. Billiard balls can penetrate each other colliding only with a certain probability. This is a conceptual barrier, which Kac was not able to overcome. In 1959 he wrote [14, p.131]: “The primary disadvantage of the master equation approach ... lies in the difficulty (if not impossibility!) of extending it to the nonspatially uniform case.” In 1973 the message was the same [42, p.385]: “The master equation approach suffers from a major deficiency. It is limited to the spatially homogeneous case. It seems impossible to bring in streaming terms while at the same time treating collisions as random events.” Bird’s DSMC algorithm can be derived from the Leontovich model by introducing certain numerical approximations (splitting, cells). The problem of combining free flow with stochastic collisions is avoided (hidden) by the splitting procedure. Nevertheless, all particles in a cell collide according to some probabilistic rules and not according to their actual trajectories.

SOME RECENT DIRECTIONS OF STUDY

General interactions

Consider particles with types from a locally compact separable metric space \mathcal{Z} . Any event in the system consists in the interaction of at most R particles and produces as a result a finite number of particles. This includes, for example, the generation of new particles from a source, the extinction or transformation of single particles, the collision of two particles, as well as more complicated chemical reactions. Formally, we introduce the state space of the particle system as

$$E = \left\{ \sum_{i=1}^n \delta_{z_i} : n \geq 0, \quad z_i \in \mathcal{Z}, \quad i = 1, \dots, n \right\},$$

where δ_a denotes the delta-measure concentrated at a . The admissible subsequent states of $\nu \in E$ are denoted by

$$J_0(\nu, \xi) = \nu + \xi, \quad J_r(\nu, i_1, \dots, i_r, \xi) = \nu + \xi - \delta_{z_{i_1}} - \dots - \delta_{z_{i_r}}, \quad r = 1, \dots, R,$$

where i_1, \dots, i_r are pairwise distinct indices from $\{1, \dots, n\}$ and $\xi \in E$. The intensity of these events is determined by some compactly bounded kernels q_0, q_1, \dots, q_R depending on a corresponding number of arguments. The asymptotic

behaviour of such systems has been studied under appropriate assumptions in [43]. It turned out that they approximate the deterministic measure-valued solution of the equation

$$\frac{d}{dt} \langle \varphi, \mu(t) \rangle = \mathcal{G}(\varphi, \mu(t)), \quad t > 0. \quad (14)$$

The nonlinear operator is defined as

$$\mathcal{G}(\varphi, \mu) = \int_E \langle \varphi, \xi \rangle q_0(d\xi) + \sum_{r=1}^R \int_{\mathcal{Z}} \dots \int_{\mathcal{Z}} \int_E \left[\langle \varphi, \xi \rangle - \varphi(z_1) - \dots - \varphi(z_r) \right] q_r(z_1, \dots, z_r, d\xi) \mu(dz_1) \dots \mu(dz_r),$$

for continuous test functions φ with compact support and measures μ on \mathcal{Z} , where the notation $\langle \varphi, \nu \rangle = \int_{\mathcal{Z}} \varphi(z) \nu(dz)$ is used. As an example we consider the spatially homogeneous Boltzmann equation with dissipative collisions. Let $\mathcal{Z} = \mathcal{R}^d$, $d \geq 1$, and denote

$$v'(v, w, e, \theta) = \frac{v+w}{2} + \varepsilon(v, w, \theta) \frac{\|v-w\|e}{2}, \quad w'(v, w, e, \theta) = \frac{v+w}{2} - \varepsilon(v, w, \theta) \frac{\|v-w\|e}{2},$$

where $v, w \in \mathcal{R}^d$, $e \in \mathcal{S}^{d-1}$ (unit sphere), $\theta \in \Theta$ (measurable space) and ε is some measurable function. Note that

$$\|v'\|^2 + \|w'\|^2 = \|v\|^2 + \|w\|^2 - \frac{1 - \varepsilon(v, w, \theta)^2}{2} \|v-w\|^2,$$

i.e. energy is dissipated if $\varepsilon^2 < 1$, conserved if $\varepsilon^2 = 1$, and created if $\varepsilon^2 > 1$. Assuming

$$q_2(v, w, A) = \frac{1}{2} \int_{\Theta} \int_{\mathcal{S}^{d-1}} \chi_A(\delta_{v'(v, w, e, \theta)} + \delta_{w'(v, w, e, \theta)}) B(v, w, e) de \pi(d\theta),$$

where A is a measurable subset of E and π is some probability measure on Θ , equation (14) takes the form

$$\begin{aligned} \frac{d}{dt} \langle \varphi, \mu(t) \rangle = \\ \frac{1}{2} \int_{\mathcal{R}^d} \int_{\mathcal{R}^d} \int_{\Theta} \int_{\mathcal{S}^{d-1}} \left[\varphi(v'(v, w, e, \theta)) + \varphi(w'(v, w, e, \theta)) - \varphi(v) - \varphi(w) \right] B(v, w, e) de \pi(d\theta) \mu(t, dv) \mu(t, dw) \end{aligned}$$

and reduces to the weak form of the spatially homogeneous Boltzmann equation in the case $\varepsilon \equiv 1$.

An even more general class of stochastic models is obtained when the intensity of an individual interaction depends on the state of the whole system, e.g. via the particle density. Such systems approximate certain generalized Boltzmann equations. One example is the Uehling-Uhlenbeck-Boltzmann equation [44] related to ideal quantum gases. In the spatially homogeneous case this equation reads

$$\begin{aligned} \frac{\partial}{\partial t} f(t, v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de B(v, w, e) \left[[1 + \theta f(t, v)] [1 + \theta f(t, w)] f(t, v^*) f(t, w^*) - \right. \\ \left. [1 + \theta f(t, v^*)] [1 + \theta f(t, w^*)] f(t, v) f(t, w) \right]. \end{aligned} \quad (15)$$

It reduces to the Boltzmann equation in the case $\theta = 0$. Bose-Einstein statistics and Fermi-Dirac statistics are equilibrium distributions of equation (15) with $\theta = +1$ and $\theta = -1$, respectively. A DSMC method for this equation was studied in [45], where more details and further references can be found. A second example is the limiting equation for the Consistent Boltzmann Algorithm [46], a DSMC modification for dense gases. This equation takes the form

$$\begin{aligned} \frac{\partial}{\partial t} f(t, x, v) + (v, \nabla_x) f(t, x, v) = \\ \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de B(v, w, e) \left[Y(\varrho(t, x^*)) f(t, x^*, v^*) f(t, x^*, w^*) - Y(\varrho(t, x)) f(t, x, v) f(t, x, w) \right]. \end{aligned} \quad (16)$$

Here $\varrho(t, x) = \int_{\mathcal{R}^3} f(t, x, v) dv$ is the density and x^* denotes an appropriate displacement during collisions. The positive continuous function Y is going to infinity as the density reaches its close-packing value. Equation (16), which is closely related to the Enskog equation, has been studied in [47, 48], where more details and further references can be found (see [49, 50] concerning DSMC methods related to the Enskog equation). The derivation of equations (15) and (16) from corresponding particle systems was rather formal, and rigorous results would be of considerable interest.

Convergence order

The DSMC algorithm mentioned above depends on three main approximation parameters – the number of particles n , the splitting time step Δt and the cell size Δx . By taking the limit $n \rightarrow \infty$ one obtains the system of equations (2), (3), which depends on the remaining two parameters. In the limit $\Delta t \rightarrow 0$ this system transforms into equation (13) with h defined in (4). Finally, the Boltzmann equation (6) is obtained in the limit $\Delta x \rightarrow 0$. For numerical purposes the order of convergence with respect to the various parameters is important. The order with respect to n has been established in the context of general Markov processes in [20, 23]. Cell size dependence was studied in [51]. Second order with respect to time step was predicted in [52]. However, in [53, 54] the author noticed a mistake in the derivations of [52] and gave some specific example illustrating first order behaviour. On the other hand, rather thorough numerical experiments in [55] showed second order behaviour in many test cases (see also the derivation in [56]). This problem was further investigated in [57]. See also the contribution by M.A. Gallis and co-authors in these proceedings.

Steady state problems

In many applications studying the equilibrium behaviour of gas flows is of primary interest. To this end, time averaging over trajectories of the corresponding particle system is used,

$$\frac{1}{k} \sum_{j=1}^k \left[\frac{1}{n} \sum_{i=1}^n \varphi(x_i(t_j), v_i(t_j)) \right], \quad t_j = \bar{t} + j \Delta t,$$

where φ is some test function and \bar{t} is the starting time for averaging. To justify this procedure (for $k \rightarrow \infty$), one has to study the connection between the stationary density of the process and the stationary Boltzmann equation. From the results mentioned above one can obtain information about the limit $\lim_{t \rightarrow \infty} \lim_{n \rightarrow \infty} p_1^{(n)}(t, x, v)$ while here one is interested in the limit $\lim_{n \rightarrow \infty} \lim_{t \rightarrow \infty} p_1^{(n)}(t, x, v)$. The identity of both quantities is not at all obvious. Some result concerning the factorization of the equilibrium distribution was obtained in [58]. But in this field the state of the theory is rather unsatisfactory.

Variance reduction

A serious problem in many applications of DSMC (flows with high density gradients, or low Mach number flows) are large statistical fluctuations. For the purpose of variance reduction, a modification of DSMC called SWPM (stochastic weighted particle method) was proposed in [59]. In SWPM a system of weighted particles is used, which allows one to resolve low density regions with a moderate number of simulation particles (cf. [60]). A convergence proof for SWPM has recently been proposed in [61]. Further references related to weighted particles are [62, 63]. An “information preservation method” (cf. [64, 65]) has been developed for low Mach number flows occurring in micro-electro-mechanical systems (MEMS). Here the convergence issue is open.

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