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STOCHASTIC QUASI GAS DYNAMICS EQUATIONS AS A BASE FOR PARTICLE METHODS

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Abstract. *Based on a system of stochastic differential equations, describing a gas at small Knudsen numbers, explicit equations of gas dynamics with additional small terms for the Fokker – Planck model of Boltzmann collision integral are obtained.*

1 INTRODUCTION

The accuracy of gas dynamic calculations can be increased by implementation of hierarchical algorithms based on micro – macro representations[1,2,3,4,5,6,7,8,9]. Usually one starts from the Boltzmann equation[2,3]

$$\frac{\partial F}{\partial t} + \mathbf{v}\frac{\partial F}{\partial \mathbf{x}} = \frac{1}{Kn}Q(F,F) \tag{1}$$

with a parameter Kn, depending on the space variable x. A whole computational domain, as a rule, has to be divided at subdomains possessing different properties. If Kn is of order 1 then it is the subdomain where Boltzmann equation has to be applied. In the regions, where Kn is small, one can use the Kolmogorov – Fokker – Planck equation (for moderate Kn)[1,2,3,10,12]

$$\frac{\partial F}{\partial t} + \mathbf{v}\frac{\partial F}{\partial \mathbf{x}} + \frac{1}{Kn}\frac{\partial(\mathbf{a}(F)F)}{\partial \mathbf{v}} = \frac{1}{Kn}\frac{1}{2}\frac{\partial^2(\sigma^2(F)F)}{\partial \mathbf{v}^2} \tag{2}$$

in which the coefficients (the vector $\mathbf{a}$ and the matrix σ^2) are defined by a collision model (we describe it bellow). It is nonlinear equation for seven – dimensional distribution function in phase space as well as the Boltzmann equation but with more simple structure of collision integral .

In the range of moderate numbers Kn it is possible to get a macroscopic description— stochastic quasi – gas dynamic equations[9,11]

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho V}{\partial x} &= \frac{1}{2}\frac{\partial^2}{\partial x^2}(Kn\frac{D^2}{\gamma^2}\rho) \\
\frac{\partial}{\partial t}(\rho V) + \frac{\partial}{\partial x}(V\rho V) &= -\frac{\partial}{\partial x}(\frac{D^2}{\gamma}\rho) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(Kn\frac{D^2}{\gamma^2}\rho V) \\
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x}(V\rho E) &= -\frac{\partial}{\partial x}(\frac{D^2}{\gamma}\rho V) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(Kn\frac{D^2}{\gamma^2}\rho E)..
\end{aligned} \tag{3}$$

Here they are written for 1D and in the case when the following connection with the coefficients of the above Kolmogorov – Fokker – Planck equation (2) is assumed[11]:

$$a(\cdot) \equiv \gamma(x,t), \quad \sigma(\cdot) \equiv D(x,t), \quad D^2/\gamma = RT, \quad \frac{D^2}{\gamma}\rho \equiv p.$$

For very small Kn these equations tends to Navier – Stokes equations.

In more general case the coefficients in the Kolmogorov – Fokker – Planck equation can be calculated under some simplifying assumption[10]: vector $\mathbf{a}$

$$\mathbf{a}(\mathbf{c}) = -\frac{\mathbf{c}}{c}\frac{\sqrt{\pi}}{4}[\sqrt{\pi}erf(c)(2c^2 + 2 - \frac{1}{2c^2}) + e^{-c^2}(2c + \frac{1}{c})],$$

the components of matrix σ^2

$$\sigma^2_{xx}(c) = \frac{\sqrt{\pi}}{4}[P(c) + c_x^2 S(c)],$$
$$\sigma^2_{xy}(c) = \frac{\sqrt{\pi}}{4} c_x c_y S(c),$$

$$P(c) = \sqrt{\pi} erf(c)(\frac{c^3}{3} + \frac{3}{2}c + \frac{3}{4c} - \frac{1}{8c^3}) + e^{-c^2}(\frac{c^2}{3} + \frac{4}{3} + \frac{1}{4c^2}),$$
$$S(c) = \sqrt{\pi} erf(c)(c + \frac{3}{2c} - \frac{3}{4c^3} + \frac{3}{8c^5}) + e^{-c^2}(1 + \frac{1}{c^2} - \frac{3}{4c^4}),$$

$c \equiv c'/\sqrt{T'}$, where $\mathbf{c}' = \mathbf{v}' - \mathbf{V}'$, $c' = |\mathbf{c}'|$ and T' are nondimensional thermal velocity, its absolute value and temperature,

$$erf(\beta) \equiv 2/\sqrt{\pi} \int_0^\beta e^{-\gamma^2} d\gamma.$$

That gives quite robust model.

The above micro – macro bridge is reached by the help of the theory of random processes[11] as it is presented in the next section.

2 STOCHASTIC MODELS

If a gas is treated as a collection of chaotically moving molecules rather than a continuous medium, then we obtain mathematical models based on the apparatus of the theory of stochastic differential equations[1,12].

2.1 Micro scale, $Kn \sim 1$

Ludwig Boltzmann derived his famous equation considering a gas as determined number of rigid spheres and introduced stochasticity by taking into account the hypothesis of molecular chaos – Stossanzahlanzatz[3]. Following A. V. Skorokhod[1] at the very beginning we regard the positions and velocities of the molecules as random time functions depending on random independent couple collisions. The equations of motions of the molecules fullfils a system of stochastic differential equations

$$dx_i(t) = v_i(t)dt,$$
$$dv_i(t) = \sum_{j=1}^{n} \int f(\theta, x_i(t), v_i(t), x_j, v_j) p_{ij}^{(n)}(d\theta \times dt), \tag{4}$$

where x_i and v_i determine the position and velocity of the particle in the phase space $R^3 \times R^3$ (for the sake of shortness let us note it by Z and the couple $(x_i(t), v_i(t))$ let us note by $z_i(t)$), the integral over the stochastic Poisson measure $p_{ij}^{(n)}$ at $\Theta \times [0, \infty)$ (Θ is the surface of unit sphere) is an impulse random force of interaction which change the

conditions of particles jump – likely (the impulses of the interacting particles change by jumps), namely the velocity of i – particle as a result of collision with j – particle is changed by the magnitude $f(\theta, x_i(t), v_i(t), x_j, v_j)$ which is called a jump function. The solution $(x_1(t), v_1(t), \ldots, x_n(t), v_n(t))$ is Markov process. Kolmogorov equation for distribution of the process (the direct equation) plays the role of Liouville equation. Let us introduce a "statistical" distribution function:

$$\mu_t^{(n)}(A) = \frac{1}{n}\sum_{i=1}^{n} \chi_A(x_i(t), v_i(t))$$

(χ_A – indicator of Borel set A of our phase space) and let us study a limit behaviour of that random measure at $n \to \infty$.

Let $\mathbf{E}p_{ij}^{(n)}(d\theta \times dt) = \frac{1}{n}m(d\theta)dt$, where m is a finite measure at Θ (its concrete expression will be established later). Then under some smoothness assumptions the following statements holds.

1) The measure $\mu_t^{(n)}(A)$ weakly converges to a non random measure $\lambda_t(A)$, for which an equation holds: for any quite smooth finite function $\phi(z)$

$$\frac{d}{dt}\int \phi(z)\lambda_t(dz) = \int (\frac{\partial}{\partial x}\phi(z), v)\lambda_t(dz)$$
$$+ \int\int\int [\phi(z + f(\theta, z, z')) - \phi(z)]m(d\theta)\lambda_t(dz')\lambda_t(dz), \tag{5}$$

which can be considered as generalized Boltzmann equation; if a density F of measure $\lambda_t(dz)$ exists then if satisfies the classical Boltzmann equation.

2) Let the initial values of functions $z_1^{(n)}(t), \ldots, z_k^{(n)}(t)$ (the solutions of the system (4) at given n) converge to $z_1^{(n)}(0), \ldots, z_k^{(n)}(0)$. Then a mutual distribution of the processes $(z_1^{(n)}(t), \ldots, z_k^{(n)}(t))$ at $n \to \infty$ converges to mutual distribution of k independent processes $(z_1(t), \ldots, z_k(t))$, each of which is a Markov process satisfying a system of stochastic differential equations

$$dx_i(t) = v_i(t)dt,$$
$$dv_i(t) = \int f(\theta, x_i(t), v_i(t), x', v')\hat{p}(d\theta \times dx' \times dv' \times dt), \tag{6}$$

where $\hat{p}$ is a Poisson measure at $\Theta \times Z \times [0, \infty)$. By the way, "Stossanzahlanzatz" follows from that statement.

If in the equation (5) we put formally:

$\theta = \xi$, $\xi \in \Xi$, $\Theta = \Xi$ is unit sphere,

$\xi = \{\cos\epsilon\sin\alpha, \sin\epsilon\sin\alpha, \cos\alpha\}$,

$m(d\theta) = d^2 \mid v' - v \mid\mid \cos\alpha \mid \sin\alpha d\alpha d\epsilon$, d is diameter of a molecule,

$0 < \alpha < \pi$,$0 < \epsilon < 2\pi$ are the angles of the local spherical coordinate system the axe z of which coincides with vector $v' - v$,

and to take jump function as $f(\cdot) = \xi(v - v', \xi)$, $(\cdot, \cdot)$ is inner product,

then the equation (5) turns in the generalized Boltzmann equation for gas of rigid spheres.

Let us assume now that the measure $\lambda_t(dx, dv)$ has a density $F(x, v, t)$ and nondimensionalize our problem:

$$t = t_* t', x = x_* x', v = v_* v', F = F_* F', n = n_* n', T = T_* T',$$

where

$$v_*^2 = 2RT_*, \quad t_* = x_*/v_*, \quad F_* = n_*/(2RT_*)^{3/2}.$$

As n_*, V_*, T_* let us take $n(x,t), V(x,t), T(x,t)$, a local macroscopic molecular number density, velocity and temperature. Then the local Maxwellian take the more convinient form

$$F_M = (1/\pi^{3/2}) \exp(-(v - V_1)^2),$$

and Kn is a function of x and t:

$$Kn(x,t) = 1/(d^2 n(x,t) x_*),$$

that coincides with usual determination of Knudsen number as the ratio of the mean free path (which can be taken to the accuracy of constant $\sqrt{2}\pi/4 \approx 1,11$ as $1/d^2 n(x,t)$, d is diameter of a molecule) to a character problem range x_*.

The only one free parameter is x_* which depends on a scale of each subdomains of a problem under consideration.

Below, the prime marks of the dimensionless variables will be discarded.

So we can consider one particle in a mean field and the basis for deriving a hierarchy of gas dynamics models is a stochastic process $\{x_1(t), v_1(t)\}$, describing the motion of a particle in the six-dimensional phase space. The stochastic process is governed by the system of stochastic differential equations[1,2]

$$\begin{aligned} dx_1(t) &= v_1(t)dt, \\ dv_1(t) &= \int\int\int f(\theta, x_1(t), v_1(t), x, v) p(d\theta \times dx \times dv \times dt), \end{aligned} \tag{7}$$

where the vector f is a function of the velocity jump due to a collision between molecules, p is a Poisson random measure with the expectation:

$$\mathbf{E}p(d\theta \times dx \times dv \times dt) = \frac{1}{Kn} m(d\theta) \lambda_t(dx, dv) dt,$$

$m(d\theta)$ is a given function determining a collision model, and $\lambda_t(dx, dv)$ is the measure generated by $\{x_1(t), v_1(t)\}$, (as a result, the problem belongs to the class of nonlinear Markov systems). The density of $\lambda_t(dx, dv)$ satisfies the classical Boltzmann equation (1). The nondimensionalization of the problem yields the parameter $Kn(x,t)$ (which can be considered as a local Knudsen number).

2.2 Meso scale, moderate Kn

The introduction of a centered measure

$$q(d\theta \times dx \times dv \times dt) = p(d\theta \times dx \times dv \times dt) - \frac{1}{Kn} m(d\theta)\lambda_t(dx, dv)dt,$$

yields the martingale statement:

$$\begin{aligned} x_1(t) &= x_1(0) + \int_0^t v_1(s)ds \\ v_1(t) &= v_1(0) + \int_0^t \int\int\int f(\theta, x_1(s), v_1(s), x, v)\frac{1}{Kn} m(d\theta)\lambda_s(dx, dv)ds \\ &+ \int_0^t \int\int\int f(\theta, x_1(s), v_1(s), x, v) q(d\theta \times dx \times dv \times ds), \end{aligned} \tag{8}$$

where the last term is the martingale and its characteristic is equal to (page 513 in [16]):

$$< I >_t = \int_0^t \int\int\int f^2(\theta, x_1(s), v_1(s), x, v)\frac{1}{Kn} m(d\theta)\lambda_s(dx, dv)ds. \tag{9}$$

Considering the martingale term in (8), let us introduce a random variable

$$\eta \equiv \int_t^{t+\Delta t} \int\int\int f(\theta, x_1(s), v_1(s), x, v) p(d\theta \times dx \times dv \times ds).$$

Its mathematical expectation

$$\mathbf{E}\eta = \int_t^{t+\Delta t} \int\int\int f(\theta, x_1(s), v_1(s), x, v)\frac{1}{Kn} m(d\theta)\lambda_s(dx, dv)ds,$$

and the square root of the covariance matrix

$$\mathbf{D}\eta = (\int_t^{t+\Delta t} \frac{1}{Kn}\sigma^2(s)ds)^{1/2},$$

where it is denoted that:

$$\sigma^2(s) \equiv \int\int\int f^2(\theta, x_1(s), v_1(s), x, v) m(d\theta)\lambda_s(dx, dv). \tag{10}$$

Let us consider the random variable

$$\zeta \equiv \mathbf{D}\eta^{-1} \cdot (\eta - \mathbf{E}\eta),$$

where $\mathbf{E}\eta = O(1/Kn),\ \mathbf{D}\eta = O(1/\sqrt{Kn})$. We assume that in accordance with the central limit theorem when the Knudsen number tends to zero it tends to the standard normally distributed vector $N(0, 1)$. Then, the martingale term in (8) can be represented as:

$$(\int_t^{t+\Delta t} \frac{1}{Kn}\sigma^2(s)ds)^{1/2} \cdot N(0, 1),$$

and if $\Delta t^{1/2}$ is small it can be approximated by the value

$$(\frac{1}{Kn}\sigma^2(t))^{1/2} \cdot \Delta w(t),$$

where $\Delta w(t)$ is the increment of a standard three – dimensional Wiener process.

Consider also the representation

$$\int\int\int f(\theta, x_1(s), (s), x, v)m(d\theta)\lambda_s(dx, dv) \equiv -a(\mid c \mid)c,$$

where $c = v_1 - V$ is the thermal velocity and $a(\cdot)$ is generally an operator. This representation naturally arises, for example, for a hard – sphere gas. Under a simplifying assumption about the form of $\lambda_s(dx, dv)$, this eightfold integral can be evaluated and the operator $a(\cdot)$ becomes a scalar function of the thermal velocity magnitude.

Therefore, our hypothesis consists of the assumption that this rather complex random process for small Knudsen numbers will be close to the increment in the diffusion process. Then the system (7) takes the following form:

$$\begin{aligned} dx_1(t) &= v_1(t)dt, \\ dv_1(t) &= \frac{1}{Kn}a(x_1(t), v_1(t), t)dt + \frac{1}{\sqrt{Kn}}\sigma(x_1(t), v_1(t), t)dw(t), \end{aligned} \tag{11}$$

where $\sigma = (\sigma^2)^{1/2}$ (the matrix σ is a square root of σ^2) and the stochastic differentials are understood in the sense of Ito.

A more accurate system of stochastic differential equations with respect to the asymptotics of the quantity $1/Kn$ can be obtained by using Berry – Essen inequalities for the approximation of random variable ζ.

The process $\{x_1(t), v_1(t)\}$ generates a measure whose density satisfies the Kolmogorov – Fokker – Planck equation (2), which can be shown on the basis of Ito's formula:

$$\frac{\partial F}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial F}{\partial x_i} - \frac{1}{Kn}\sum_{i=1}^{3}\frac{\partial(a_i(F)(v_i - V_i)F)}{\partial v_i} = \frac{1}{Kn}\frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2(\sigma_{ij}^2(F)F)}{\partial v_i \partial v_j}$$

Following A. V. Skorokhod[1] let us transform the second equation in (11):

$$\frac{a}{Kn}v_1 dt = \frac{a}{Kn}V dt + \int\int\int f(\theta, x_1(s), v_1(s), x, v)q(d\theta \times dx \times dv \times ds) - dv_1,$$

or, taking into account the first equation in (11),

$$dx_1(t) = V dt + a^{-1}Kn\int\int\int f(\theta, x_1(s), v_1(s), x, v)q(d\theta \times dx \times dv \times ds) - a^{-1}Kn dv_1,$$

which is a short form of an equation:

$$x_1(t+\Delta t) = x_1(t) + \int_t^{t+\Delta t} V dt + \int_t^{t+\Delta t} a^{-1} Kn \int\int\int f(\theta, x_1(s), v_1(s), x, v) q(d\theta \times dx \times dv \times ds) - \int_t^{t+\Delta t} a^{-1} Kn dv_1. \tag{12}$$

Let us make some simplifying remarks concerning the last term in equation (12) for the increment of space position of the particle under consideration:

$$\int_t^{t+\Delta t} a^{-1} Kn dv_1.$$

At small Knudsen numbers, dv_1 can be represented as a function of thermal velocity c:

$$dv_1(t) = -\frac{1}{Kn} a(c) c dt + \frac{1}{\sqrt{Kn}} \sigma(c) dw(t),$$

The function dv_1, standing under the integral sign, is a fast changing in time random value according to the sense of diffusion approximation. That integral term influence the increment of particle space position under action of chaotically moving surrounding medium. That is why it is possible to take for dv_1 under the integral sign its average value – zero.

Therefore, we obtain the system

$$\begin{aligned} dx_1(t) &= V dt + \sqrt{Kn} \left[a^{-1}(c) \left(\sigma(c) - \sigma(0) \right) \right] dw(t), \\ dv_1(t) &= -\frac{1}{Kn} a(c)(v(t) - V) dt + \frac{1}{\sqrt{Kn}} \sigma(c) dw(t), \end{aligned} \tag{13}$$

Denote: $\widetilde{\sigma} \equiv \sigma(c) - \sigma(0)$.

The process $\{x_1(t), v_1(t)\}$ generates a measure $\lambda_t(dx, dv)$ whose density $F(x, v, t)$ satisfies the Kolmogorov – Fokker – Planck equation (we conserve the same notations as for micro case inspite of that the measure is generated by diffusion and not Poisson process but still taking place in phase space):

$$\frac{\partial F}{\partial t} + \sum_{i=1}^{3} \frac{\partial V_i F}{\partial x_i} - \frac{1}{Kn} \sum_{i=1}^{3} \frac{\partial (a_i(F)(v_i - V_i) F)}{\partial v_i} = \frac{1}{Kn} \frac{1}{2} \sum_{i,j=1}^{3} \frac{\partial^2 (\widetilde{\sigma}_{ij}^2(F) F)}{\partial v_i \partial v_j} + \frac{1}{2} \sum_{i,j=1}^{3} \left[\frac{\partial^2 (a^{-1} \sqrt{Kn} \widetilde{\sigma})_{ij}^2 F}{\partial x_i \partial x_j} + 2 \frac{\partial^2 (a^{-1} \widetilde{\sigma})_{ij} \widetilde{\sigma}_{ji} F}{\partial x_i \partial v_j} \right], \tag{14}$$

where the additional second term in the righthand side is small regarding Kn in comparison to the first one.

The further simplification of the model (11), (13), (2), (14) can be attained by calculating the drift vector in phase space and the covariance matrix (10). This can be successfully done for a hard – sphere gas if under the integral in expression (11) the local Maxwellian is taken as the density measure of $\lambda_t(dx, dv)$.

We calculate the value σ^2_{xx} (the calculation of the drift vector **a** is similar and easier):

$$\sigma^2_{xx}(x_1(t), v_1(t), t) = \int\int\int f^2_x(\theta, x_1(t), v_1(t), x, v) m(d\theta)\lambda_t(dx, dv). \tag{15}$$

In order to obtain the expression for the x–component of the step function f_x of the local spherical coordinate system, variables should be substituted for the component of the unit vector ξ_x. In the global spherical coordinate system let the coordinates be determined by the polar angle ψ and the azimuth angle δ. Then, the conversion from the global system to the local one

$$\xi = A \cdot \xi_{loc}$$

is performed by means of the rotation matrix

$$A = \begin{array}{ccc} \cos\delta\cos\psi & -\sin\psi & \sin\delta\cos\psi \\ \cos\delta\sin\psi & \cos\psi & \sin\delta\sin\psi \\ \sin\delta & 0 & \cos\delta \end{array}$$

which is the product of the rotation matrix by the angle ψ about the axis z, and then by the angle δ about the axis y:

$$A = A_3(\psi) \cdot A_2(\delta).$$

Hence,

$$\xi_x = \cos\epsilon\sin\alpha\cos\delta\cos\psi - \sin\epsilon\sin\alpha\sin\psi + \cos\alpha\sin\delta\cos\psi,$$

$$f_x = \xi_x \mid v_1 - v \mid \cos\alpha.$$

Therefore, for the hard – sphere gas and the local Maxwellian distribution

$$\sigma^2_{xx} = (1/2)\int_{R^3}\int_0^{\pi}\int_0^{2\pi} \xi^2_x \mid v_1 - v \mid^3 \cos^2\alpha \mid \cos\alpha \mid F_M \sin\alpha d\epsilon d\alpha d^3v.$$

The multiplying factor $1/2$ arises because the integral must be taken over the half – sphere $(v - v_1, \xi) > 0$, which implies the counter motion of two molecules (resulting in a collision), and it is more convenient to take it over the entire sphere. This is a standard technique for the derivation of the Boltzmann equation.

The integration over the angles ϵ and α accompanied by the introduction of the designation $v - v_1 \equiv w$ and $v_1 - V_1 \equiv c$ (thermal velocity) yields:

$$\sigma^2_{xx} = \frac{\pi}{4}\frac{1}{\pi^{3/2}}\int_{R^3} \mid w \mid^3 (1/3 + \sin^2\delta\cos^2\psi) exp(-(c - w)^2) d^3w,$$

or

$$\sigma_{xx}^2 = \frac{1}{4\pi^{1/2}} \int_{R^3} ((1/3) \mid w \mid^3 + w_x^2 \mid w \mid) exp(-(c-w)^2) d^3w.$$

Incidentally, the same expression will be obtained if the representation of molecule collision is used in terms of the impact parameter and the scattering angle, and the tensor dimensionality considerations are employed, as was done by B.A. Trubnikov[13] for the Coulomb interaction in the paper, where the detailed discussion of the physical interpretation for the obtained equations is also given.

In order to calculate this integral, we change over to the coordinate system where the axis z coincides with the vector c of thermal velocity. Such a transition is performed by means of the same rotation matrix A, with the angles ψ and δ being substituted for the angles φ and θ, which determine the vector c in the global coordinate system:

$$w = A \cdot w_{loc}, \quad w_{loc} \equiv \{x, y, z\}^T.$$

Then,

$$w_x = \cos\theta \cos\varphi \; x - \sin\varphi \; y + \sin\theta \cos\varphi \; z.$$

In the new system, the vector $c = \{0, 0, |c|\}^T$, and the vector lengths and the element of the three – dimensional integration will not change. By computing

$$\int\int\int_{-\infty}^{\infty} x^2 \sqrt{x^2+y^2+z^2} \; e^{-x^2-y^2(|c|-z)^2} dxdydz$$

by means of the transition to the cylindrical coordinate system

$$= \frac{\pi}{4} \int_{-\infty}^{\infty} [3 \mid z \mid + \sqrt{\pi} e^{z^2} (3/2 - z^2)(1 - erf(\mid z \mid))] \; e^{-(|c|-z)^2} dz,$$

where

$$erf(\beta) \equiv 2/\sqrt{\pi} \int_0^{\beta} e^{-\gamma^2} d\gamma,$$

and changing the order of integration over z and γ

$$= \frac{\pi}{4} [\sqrt{\pi} erf(\mid c \mid)(2 \mid c \mid + \frac{2}{\mid c \mid} - \frac{1}{2 \mid c \mid^3}) + e^{-c^2}(2 + \frac{2}{c^2})],$$

and,

$$\int\int\int_{-\infty}^{\infty} z^2 \sqrt{x^2+y^2+z^2} \; e^{-x^2-y^2(|c|-z)^2} dxdydz$$

$$= [\sqrt{\pi} erf(\mid c \mid)(\mid c \mid^3 + 2 \mid c \mid - \frac{1}{4 \mid c \mid} + \frac{1}{4 \mid c \mid^3}) + e^{-c^2}(c^2 + 3/2 - \frac{1}{2c^2})],$$

we obtain the expression for σ_{xx}^2 presented in the beginning of this article. σ_{xy}^2 and other components of the diffusion matrix are calculated absolutely similarly.

2.3 Macro scale, small Kn

Under some simplifying assumptions, the operator $a(\cdot)$ becomes a scalar function of the thermal velocity magnitude and the eightfold integrals $a(\cdot)$ and $\sigma^2(\cdot)$ can be evaluated as it was shown just above. Moreover, further simplifications lead to $a(\cdot) = \gamma(x,t)$, $\sigma(\cdot) = D(x,t)$ and to the stochastic quasi – gas dynamic equations for this set of coefficients.

Specifically, we need to construct equations for the measures generated by the stochastic processes $\{x_1(t)\}$ and $\{v_1(t)\}$. The physical meaning of these measures is the evolution of the mass, momentum and energy distributions. By the help of Ito's formula, it can be shown that their densities $(\rho(x,t), \rho V(x,t), \rho E(x,t))$ satisfy the system:

$$\begin{aligned}
\frac{\partial}{\partial t}\rho + \sum_{j=1}^{3}\frac{\partial}{\partial x_j}(\rho V_j) &= \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2}{\partial x_i \partial x_j}(Kn\frac{D_{ij}^2}{\gamma^2}\rho), \\
\frac{\partial}{\partial t}(\rho V_i) + \sum_{j=1}^{3}\frac{\partial}{\partial x_j}(V_j \rho V_i) &= -\sum_{j=1}^{3}\frac{\partial}{\partial x_j}(\frac{D_{ij}^2}{\gamma}\rho) + \frac{1}{2}\sum_{k,j=1}^{3}\frac{\partial^2}{\partial x_k \partial x_j}(Kn\frac{D_{kj}^2}{\gamma^2}\rho V_i), \qquad (16) \\
& \qquad\qquad i = 1,2,3, \\
\frac{\partial \rho E}{\partial t} + \sum_{j=1}^{3}\frac{\partial}{\partial x_j}(V_j \rho E) &= -\sum_{j=1}^{3}\frac{\partial}{\partial x_j}(\frac{D_{ij}^2}{\gamma}\rho V_j) + \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2}{\partial x_i \partial x_j}(Kn\frac{D_{ij}^2}{\gamma^2}\rho E),
\end{aligned}$$

which holds for small Knudsen numbers. The righthand side reflects the "trace" left by the thermal motion of molecules.

Let us define a stochastic empirical measure $\mu_t(dx)$ by an expression: for any function $\psi \in C_b^{(2)}(\mathbf{R}^3)$ (a space of continuously differentiable finite functions)

$$\int \psi(x)\mu_t(dx) = \frac{1}{N}\sum_{l=1}^{N}\psi(x_l(t)), \qquad (17)$$

more precisely:

$$\forall \psi \in C_b^{(2)}(\mathbf{R}^3); \forall D \in \mathbf{R}^3 : \int_D \psi(x)\mu_t(dx) = \frac{1}{N}\sum_{l=1}^{N}\psi(x_l(t))\chi(x_l(t) \in D).$$

That expression, connecting the measure distribution to realizations of particle positions at time moment t, is a quadrature formula (the weights are known and the nodes are parameters) if to read if from left to right.

For obtaining an equation for measure $\mu_t(dx)$, let us take a stochastic differential from both of two sides of (17).

We'll use Ito's formula for complex function differentiation[12]:

$$d\psi(x) = \sum_{i=1}^{3}\frac{\partial \psi}{\partial x_i}dx_i + \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2 \psi}{\partial x_i \partial x_j}dx_i dx_j,$$

where stochastic differentials dx_i are taken from the system (13):

$$dx_i = V_i dt + \sqrt{Kn}\sum_{j=1}^{3}\left(\frac{D_{ij}-D_{ij}^{(0)}}{\gamma_i}\right)dw_j, \qquad (i=1,2,3),$$

$$\left(\frac{D_{ij}-D_{ij}^{(0)}}{\gamma_i}\right) \equiv \left(\widetilde{\frac{D}{\gamma}}\right)_{ij},$$

and because of definition of a standard three – dimensional Wiener process increment, the smallness of which is $\sqrt{dt}$:

$$dw_i dw_j = \delta_{ij}dt, \qquad dw_i dt = 0, \qquad dt^2 = 0, \tag{18}$$

δ_{ij} – Kronecker symbol, that leads to

$$\begin{aligned} dx_i dx_j &= Kn\sum_{m,n=1}^{3}\left(\frac{D_{im}-D_{im}^{(0)}}{\gamma_i}\right)\left(\frac{D_{jn}-D_{jn}^{(0)}}{\gamma_j}\right)\delta_{mn}dt \\ &= Kn\sum_{m=1}^{3}\left(\frac{D_{im}-D_{im}^{(0)}}{\gamma_i}\right)\left(\frac{D_{jm}-D_{jm}^{(0)}}{\gamma_j}\right)dt \\ = Kn\frac{1}{\gamma_i\gamma_j}&\left(D_{ij}^2 - \sum_{m=1}^{3}\left(D_{im}^{(0)}D_{jm} + D_{jm}^{(0)}D_{im}\right) + (D_{ij}^{(0)})^2\right)dt \\ &\equiv Kn\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}dt, \end{aligned}$$

which means that Ito's formula in our case turns out to be:

$$\begin{aligned} d\psi(x) = &\left(\sum_{i=1}^{3}V_i\frac{\partial\psi}{\partial x_i} + \frac{1}{2}Kn\sum_{i,j=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j}\right)dt \\ &+\sqrt{Kn}\sum_{i,j=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{ij}\frac{\partial\psi}{\partial x_i}dw_j. \end{aligned} \tag{19}$$

Then we get the stochastic differential from both of two sides (17):

$$\begin{aligned} d\int\psi(x)\mu_t(dx) = &\frac{1}{N}\sum_{l=1}^{N}\left\{\left[\sum_{i=1}^{3}V_i\frac{\partial\psi}{\partial x_i} + \frac{1}{2}Kn\sum_{i,j=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j}\right](x_l(t))\right\}dt \\ &+\frac{1}{N}\sum_{l=1}^{N}\left\{\sqrt{Kn}\left[\sum_{i,j=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{ij}\frac{\partial\psi}{\partial x_i}\right](x_l(t))dw_j\right\}, \end{aligned}$$

or, applying the formula (17) from right to left for the righthand side of the last expression,

$$d\int \psi(x)\mu_t(dx)$$
$$= \int \left\{ \left[\sum_{i=1}^{3} V_i(x,t)\frac{\partial \psi}{\partial x_i}(x) + \frac{1}{2}Kn(x,t)\sum_{i,j=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}(x,t)\frac{\partial^2\psi}{\partial x_i \partial x_j}(x)\right] dt \right\} \mu_t(dx)$$
$$+ \int \left\{ \sqrt{Kn(x,t)} \left[\sum_{i,j=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{ij}(x,t)\frac{\partial \psi}{\partial x_i}(x)\right] dw_j \right\} \mu_t(dx).$$

Assuming existence of a density $\rho(x,t)$ of stochastic empirical measure $\mu_t(dx)$, taking the usual steps while deriving from a generalizied equation an equation in partial derivatives, having integrated by parts one or two times in appropriate places, we get a stochastic continuity equation in the form:

$$d\rho = \left[-\sum_{i=1}^{3}\frac{\partial}{\partial x_i}(V_i\rho) + \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2}{\partial x_i \partial x_j}\left(Kn\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}\rho\right)\right] dt$$
$$- \sum_{i,j=1}^{3}\frac{\partial}{\partial x_i}\left(\sqrt{Kn}\left(\widetilde{\frac{D}{\gamma}}\right)_{ij}\rho\right) dw_j,$$

and having averaged over the time we get a deterministic continuity equation for averaged over the time deterministic mass density $\overline{\rho}(x,t)$:

$$\frac{\partial \overline{\rho}}{\partial t} + \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left(\overline{V_i\rho}\right) = \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2}{\partial x_i \partial x_j}\left(\overline{Kn\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}\rho}\right),$$

which is valid for small Knudsen numbers. The righthand side reflects the "trace" left by the thermal motion of molecules, or self – diffusion.

It is natural to regard the random values ρ, V_i and $\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}$ (which depends on thermal velocity c) independent, that gives the product of averaged values after the averaging procedure. If we assume that the time averaging leads to the values using by traditional gas dynamics, then we get a continuity equation taking into account the self – diffusion:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3}\frac{\partial}{\partial x_i}(V_i\rho) = \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2}{\partial x_i \partial x_j}\left(\overline{Kn\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}\rho}\right).$$

Let us get equations for an impulse and its density, connecting an impulse with a vector measure $\nu_t(dx)$ by:

$$\sum_{l:x_l\in D} v_l m_l = \int_D \nu_t(dx),$$

or, in generalized form:

$$\forall \psi \in C_b^{(2)}(\mathbf{R}^3): \quad \int \psi(x)\nu_{t,i}(dx) = \frac{1}{N}\sum_{l=1}^{N} v_i(x_l(t))\psi(x_l(t)) \qquad (i=1,2,3), \tag{20}$$

considering the process $v(t)$, the solution of (13), as a function of $x(t)$.

Let us take a stochastic differential from both of two sides of that equality.

We'll need a stochastic formula of product differentiation[12]

$$d(v_i\psi) = \psi dv_i + v_i d\psi + dv_i d\psi, \qquad (i=1,2,3).$$

The stochastic differentials dv_i are the equations of the system (13):

$$dv_i = -\frac{\gamma_i}{Kn}(v_i - V_i)dt + \frac{1}{\sqrt{Kn}}\sum_{j=1}^{3} D_{ij}dw_j, \qquad (i=1,2,3).$$

Applying Ito's formula (19) and the rules (18), calculate

$$\begin{aligned}
dv_i d\psi &= \left(-\frac{\gamma_i}{Kn}(v_i - V_i)dt + \frac{1}{\sqrt{Kn}}\sum_{j=1}^{3} D_{ij}dw_j\right) \\
&\left[\left(\sum_{i=1}^{3} V_i\frac{\partial\psi}{\partial x_i} + \frac{1}{2}Kn\sum_{i,j=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j}\right)dt + \sqrt{Kn}\sum_{i,j=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{ij}\frac{\partial\psi}{\partial x_i}dw_j\right] \\
&= \sum_{j=1}^{3} D_{ij}dw_j \sum_{m,n=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}dw_n \\
&= \sum_{j=1}^{3}\sum_{m,n=1}^{3} D_{ij}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}\delta_{jn}dt \\
&= \sum_{j=1}^{3}\sum_{m=1}^{3} D_{ij}\left(\widetilde{\frac{D}{\gamma}}\right)_{mj}\frac{\partial\psi}{\partial x_m}dt = \sum_{m=1}^{3}\left(\frac{D_{im}^2}{\gamma_m} - \sum_{j=1}^{3} D_{ij}\frac{D_{mj}^{(0)}}{\gamma_m}\right)\frac{\partial\psi}{\partial x_m}dt \\
&\equiv \sum_{m=1}^{3}\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\frac{\partial\psi}{\partial x_m}dt.
\end{aligned} \tag{21}$$

Rewrite as well

$$\begin{aligned}
\psi dv_i &= \left(-\frac{\gamma_i v_i}{Kn} + \frac{\gamma_i V_i}{Kn}\right)\psi dt + \frac{1}{\sqrt{Kn}}\sum_{n=1}^{3} D_{in}\psi dw_n, \\
v_i d\psi &= v_i\left(\sum_{m=1}^{3} V_m\frac{\partial\psi}{\partial x_m} + \frac{1}{2}Kn\sum_{m,n=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{mn}\frac{\partial^2\psi}{\partial x_m\partial x_n}\right)dt \\
&\quad + v_i\sqrt{Kn}\sum_{m,n=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}dw_n.
\end{aligned}$$

Then

$$d(v_i\psi) = \left(-\frac{\gamma_i v_i}{Kn} + \frac{\gamma_i V_i}{Kn}\right)\psi dt$$
$$+\left[v_i\left(\sum_{m=1}^{3} V_m\frac{\partial\psi}{\partial x_m} + \frac{1}{2}Kn\sum_{m,n=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{mn}\frac{\partial^2\psi}{\partial x_m\partial x_n}\right) + \sum_{m=1}^{3}\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\frac{\partial\psi}{\partial x_m}\right]dt$$
$$+\frac{1}{\sqrt{Kn}}\sum_{n=1}^{3} D_{in}\psi dw_n + v_i\sqrt{Kn}\sum_{m,n=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}dw_n.$$

Therefore, the stochastic differential from both of two sides of that equality (20) is:

$$d\int\psi(x)\nu_{t,i}(dx) = \frac{1}{N}\sum_{l=1}^{N}\left\{\left[-\frac{\gamma_i v_i}{Kn} + \frac{\gamma_i V_i}{Kn}\right](x_l(t))\right\}dt$$
$$+\frac{1}{N}\sum_{l=1}^{N}\left\{\left[v_i\sum_{m=1}^{3} V_m\frac{\partial\psi}{\partial x_m} + \sum_{m=1}^{3}\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\frac{\partial\psi}{\partial x_m}\right](x_l(t))\right\}dt$$
$$+\frac{1}{N}\sum_{l=1}^{N}\left\{\left[v_i\frac{1}{2}Kn\sum_{m,n=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{mn}\frac{\partial^2\psi}{\partial x_m\partial x_n}\right](x_l(t))\right\}dt$$
$$+\frac{1}{N}\sum_{l=1}^{N}\left\{\left[\frac{1}{\sqrt{Kn}}\sum_{n=1}^{3} D_{in}\psi dw_n + v_i\sqrt{Kn}\sum_{m,n=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}dw_n\right](x_l(t))\right\},$$

Remembering the definitions of the measures $\mu_t(dx)$ and $\nu_t(dx)$, we get the equation for the measure $\nu_{t,i}(dx)$:

$$d\int\psi(x)\nu_{t,i}(dx) = \left[-\int\frac{\gamma_i}{Kn}\psi\nu_{t,i}(dx) + \int\frac{\gamma_i}{Kn}\psi V_i(x,t)\mu_t(dx)\right]dt$$
$$+\left[\sum_{m=1}^{3}\int V_m\frac{\partial\psi}{\partial x_m}\nu_{t,i}(dx) + \sum_{m=1}^{3}\int\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\frac{\partial\psi}{\partial x_m}\mu_t(dx)\right]dt$$
$$+\frac{1}{2}\sum_{m,n=1}^{3}\int Kn\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{mn}\frac{\partial^2\psi}{\partial x_m\partial x_n}\nu_{t,i}(dx)dt$$
$$+\sum_{n=1}^{3}\int\frac{1}{\sqrt{Kn}}D_{in}\psi\mu_t(dx)dw_n + \sum_{m,n=1}^{3}\int\sqrt{Kn}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}\nu_{t,i}(dx)dw_n.$$

Denoting as $\rho V_i(x,t)$ a density of the measure $\nu_{t,i}(dx)$ and integrating by parts one or two times in appropriate places, we get a stochastic differential equation which is a stochastic analogue of Navier – Stokes equation:

$$d(\rho V_i) = -\sum_{m=1}^{3}\frac{\partial}{\partial x_m}\left(V_m\rho V_i\right)dt - \sum_{m=1}^{3}\frac{\partial}{\partial x_m}\left(\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\rho\right)dt$$

$$+\frac{1}{2}\sum_{m,n=1}^{3}\frac{\partial^2}{\partial x_m\partial x_n}\left(Kn\widetilde{\left(\frac{D^2}{\gamma^2}\right)}_{mn}\rho V_i\right)dt$$
$$+\sum_{n=1}^{3}\frac{1}{\sqrt{Kn}}D_{in}\rho dw_n+\sum_{m,n=1}^{3}\frac{\partial}{\partial x_m}\left(\sqrt{Kn}\widetilde{\left(\frac{D}{\gamma}\right)}_{mn}\rho V_i\right)dw_n,$$

if Knudsen numbers are small.

Taking mathematical expectation, at the same basis as at derivation of deterministic continuity equation with self – diffusion, we get deterministic quasi gas dynamics equations for the impulse density:

$$\frac{\partial}{\partial t}(\rho V_i)+\sum_{m=1}^{3}\frac{\partial}{\partial x_m}(V_m\rho V_i)=-\sum_{m=1}^{3}\frac{\partial}{\partial x_m}\left(\overline{\widetilde{\left(\frac{D^2}{\gamma}\right)}_{im}\rho}\right)$$
$$+\frac{1}{2}\sum_{m,n=1}^{3}\frac{\partial^2}{\partial x_m\partial x_n}\left(Kn\overline{\widetilde{\left(\frac{D^2}{\gamma^2}\right)}_{mn}\rho V_i}\right),\qquad(i=1,2,3).$$

Let us get equations for an energy.

Define a measure $\epsilon_t(dx)$:

$$\forall\psi\in C_b^{(2)}(\mathbf{R}^3):\quad\int\psi(x)\epsilon_t(dx)=\frac{1}{N}\sum_{l=1}^{N}\psi(x_l(t))\sum_{i=1}^{3}\frac{v_i^2}{2}(x_l(t)).\tag{22}$$

Take the stochastic formula of product differentiation

$$d(\frac{v_i^2}{2}\psi)=\psi d(\frac{v_i^2}{2})+\frac{v_i^2}{2}d\psi+d(\frac{v_i^2}{2})d\psi,$$

$$d(\frac{v_i^2}{2})=v_idv_i+\frac{1}{2}(dv_i)^2,$$

the system (13), Ito's formula (19), expressions (18):

$$\frac{1}{2}(dv_i)^2=\frac{1}{2Kn}\sum_{n=1}^{3}D_{in}dw_n\sum_{m=1}^{3}D_{im}dw_m=\frac{1}{2}\frac{D_{ii}^2}{Kn}dt,$$

the formula (21):

$$dv_id\psi=\sum_{m=1}^{3}\widetilde{\left(\frac{D^2}{\gamma}\right)}_{im}\frac{\partial\psi}{\partial x_m}dt,$$

$$d(\frac{v_i^2}{2}\psi) = \psi v_i dv_i + \frac{v_i^2}{2}d\psi + v_i dv_i d\psi + \psi\frac{1}{2}\frac{D_{ii}^2}{Kn}dt$$
$$= \psi\left[\left(-\frac{\gamma_i v_i^2}{Kn} + \frac{\gamma_i v_i V_i}{Kn} + \frac{1}{2}\frac{D_{ii}^2}{Kn}\right)dt + \frac{1}{\sqrt{Kn}}\sum_{m=1}^{3} D_{im}dw_m\right]$$
$$+\frac{v_i^2}{2}\left(\sum_{m=1}^{3} V_m\frac{\partial\psi}{\partial x_m} + \frac{1}{2}Kn\sum_{m,n=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{mn}\frac{\partial^2\psi}{\partial x_m\partial x_n}\right)dt$$
$$+\frac{v_i^2}{2}\sqrt{Kn}\sum_{m,n=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}dw_n$$
$$+v_i\sum_{m=1}^{3}\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\frac{\partial\psi}{\partial x_m}dt.$$

The stochastic differentiation of the formula (22) with account to the just obtained expressions leads to an equation for evolution of the expressions $\epsilon_t(dx)$ (we can put $\gamma_i = \gamma$):

$$d\int\psi(x)\epsilon_t(dx)$$
$$= \left[-2\int\psi\frac{\gamma}{Kn}\epsilon_t(dx) + \int\psi\frac{1}{2}\sum_{i=1}^{3}\frac{D_{ii}^2}{Kn}\mu_t(dx) + \int\psi\sum_{i=1}^{3}\frac{\gamma}{Kn}V_i(x,t)\nu_{t,i}(dx)\right]dt$$
$$+\int\left(\sum_{m=1}^{3} V_m\frac{\partial\psi}{\partial x_m} + \frac{1}{2}Kn\sum_{m,n=1}^{3}\left(\widetilde{\frac{D^2}{\gamma^2}}\right)_{mn}\frac{\partial^2\psi}{\partial x_m\partial x_n}\right)\epsilon_t(dx)dt$$
$$+\sum_{i,m=1}^{3}\left(\widetilde{\frac{D^2}{\gamma}}\right)_{im}\frac{\partial\psi}{\partial x_m}\nu_{t,i}(dx)dt$$
$$+\int\psi\frac{1}{\sqrt{Kn}}\sum_{i,m=1}^{3} D_{im}\mu_t(dx)dw_m + \int\sqrt{Kn}\sum_{m,n=1}^{3}\left(\widetilde{\frac{D}{\gamma}}\right)_{mn}\frac{\partial\psi}{\partial x_m}\epsilon_t(dx)dw_n.$$

Assuming existence of densities $\rho V_i(x,t)$ and $\rho E(x,t)$ of measures $\nu_{t,i}(dx)$ and $\epsilon_t(dx)$, we get for the term inside the first square brackets:

$$[-\int\psi\frac{2\gamma}{Kn}\left(\rho E - \sum_{i=1}^{3}(\frac{\rho V_i^2}{2} + \frac{D_{ii}^2}{4\gamma})\right)dx].$$

For ideal gas, because of the fluctuation – dissipation theorem[3], we can write: $D^2/2\gamma = RT$ (in dimensional form for clearness). That, together with the definition of temperature and total energy,

$$\rho E = \frac{\rho V^2}{2} + \frac{3}{2}RT$$

brings zero to this expression after averaging.

Then a stochastic differential equation for energy density looks like

$$d\rho E = \left[-\sum_{j=1}^{3} \frac{\partial}{\partial x_j}(V_j \rho E) - \sum_{i,j=1}^{3} \frac{\partial}{\partial x_j} \left(\left(\widetilde{\frac{D^2}{\gamma}} \right)_{ij} \rho V_i \right) \right] dt$$
$$+ \frac{1}{2} \left[\sum_{i,j=1}^{3} \frac{\partial^2}{\partial x_i \partial x_j} \left(Kn \left(\widetilde{\frac{D^2}{\gamma^2}} \right)_{ij} \rho E \right) \right] dt$$
$$+ \frac{1}{\sqrt{Kn}} \sum_{i,m=1}^{3} D_{im} \rho dw_m + \sqrt{Kn} \sum_{m,n=1}^{3} \frac{\partial}{\partial x_m} \left(\left(\widetilde{\frac{D}{\gamma}} \right)_{mn} \rho E \right) dw_n,$$

and its deterministic part

$$\frac{\partial \rho E}{\partial t} + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}(V_j \rho E) = - \sum_{i,j=1}^{3} \frac{\partial}{\partial x_j} \left(\overline{\left(\widetilde{\frac{D^2}{\gamma}} \right)_{ij}} \rho V_i \right)$$
$$+ \frac{1}{2} \sum_{i,j=1}^{3} \frac{\partial^2}{\partial x_i \partial x_j} \left(Kn \overline{\left(\widetilde{\frac{D^2}{\gamma^2}} \right)_{ij}} \rho E \right),$$

if Knudsen numbers are small.

The numerical examples[14] give nearly the same results as benchmark Navier – Stokes calculations in the proper range of parameters.

3 PARTICLE METHODS

The models presented can be used to construct optimal hierarchical shock-capturing algorithms for gas dynamic simulation based on both stochastic and deterministic particle methods[15].

The well known Monte – Carlo method for solving Boltzmann equation is equal to numerical realization of system (7) which can be called a stochastic (Poisson) particle method[2].

The system (13), (14) can be solved both by stochastic (Wiener) particle method or by deterministic particle method for the Kolmogorov – Fokker – Planck equation[2].

Solving the system (16) by deterministic particle method[15], to our opinion, is more efficient than the usual difference or FE methods especially for discontinuous 3D cases.

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