

MESO - MACRO MODELS FOR A HARD SPHERE GAS

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Abstract. *Macroscopic system of gas dynamic equations, differing from Navier – Stokes and quasi gas dynamic ones, is derived from a stochastic microscopic model of a hard sphere gas in a phase space. The model is diffusive in velocity space and valid for moderate Knudsen numbers. The main peculiarity of our derivation is more accurate velocity averaging due to analytical solving stochastic differential equations with respect to Wiener measure which describe our original meso model. It is shown at an example of a shock wave front structure that our approach leads to larger than Navier – Stokes front widening that corresponds to reality. The numerical solution is performed by a (well suited to high performance computer applications) special "discontinuous" particle method.*

1 INTRODUCTION

A description of gas dynamic phenomena at the base of hierarchies of micro – macro models has become a long time ago a classical part of theoretical physics as well as a foundation for high performance industrial calculations [1]. In the last years more attention was drawn to "meso" models in the phase space. That models are often called Kolmogorov – Fokker – Planck equations. They are used by theoreticians [2] and applied mathematicians [3, 4]. The last ones mostly implement the models of so-called maxwellian molecules, not hard sphere ones, that lead to considerably different results [5].

We consider a model valid, on our opinion, at moderate Knudsen numbers (Kn), transient between a molecular description and an imagination of a gas as continuous medium. Kn is a parameter of nondimensionalization depending on a space subdomain. Its physical meaning is a ratio of an average mean free pass to a character dimension of the subdomain. Our model [6, 7, 8, 9] is a system of stochastic differential equations (SDE) with respect to Wiener measure $dw(t)$ describing a movement of a particle ($x(t)$ is its position and $v(t)$ is its velocity) in the phase space at moderately small Kn :

$$\begin{aligned} dx(t) &= v(t)dt, \\ dv(t) &= -\frac{1}{Kn}a(c)(v(t) - V)dt + \frac{1}{\sqrt{Kn}}\sigma(c)dw(t), \end{aligned} \quad (1)$$

where c is an absolute value of the dimensionless heat velocity $\mathbf{c} \equiv v(t) - V$, $V(x, t)$ is a macroscopic velocity, the coefficients in the second equation (vector $\mathbf{a}(c) = a(c)\mathbf{c}$ and matrix $\sigma(c)$) will be determined later.

The realisations of that random process (the set of trajectories) generate a measure with a density $F(x, v, t)$ which satisfies an equation of Kolmogorov – Fokker – Planck's type:

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

We study that, computationally more efficient than Boltzmann equation, diffusive in velocity space gas model which is a link in a chain of multiscale algorithms based on micro – macro models depending on different subdomains (distinguished by their Knudsen numbers) of a whole problem under consideration. That model, from one side, is connected to microscopic model and, from the other side, leads to more accurate macroscopic equations [6, 7, 8, 9].

That equation is well known as an heuristic model Boltzmann equation with Fokker – Planck collision integral [10, 11, 12]. But before now its coefficients a , σ^2 and the limits of its applicability were not specified. In [8] it was shown that Boltzmann equation can be approximated by Kolmogorov – Fokker – Planck one (2) at moderate Knudsen numbers. Its coefficients are integrals in phase space representing moments of a jump random process describing molecules collisions formulized by means of stochastic integration with respect to Poisson measures [13]:

$$\mathbf{a}(x_1(t), v_1(t), t) = \int \int \int \mathbf{f}(\theta, x_1(s), v_1(s), \tilde{x}, \tilde{v}) m(d\theta) F d\tilde{x} d\tilde{v}, \quad \mathbf{a} \equiv a(c)\mathbf{c}$$

$$\sigma^2(x_1(t), v_1(t), t) = \int \int \int f^2(\theta, x_1(s), v_1(s), \tilde{x}, \tilde{v}) m(d\theta) F d\tilde{x} d\tilde{v}.$$

Here \mathbf{f} is a jump function (a molecule velocity increment as a result of a collision with another one), θ is a goal parameter, m is an intensity of random collision process, F is a distribution

function, v, v_1 are velocity vectors, x, x_1 are position vectors. For a gas of hard spheres and with assumption of jump function locality in x the integrals take the following form:

$$\mathbf{a}(x_1(t), v_1(t), t) = \frac{\pi}{2} \int_{\mathbf{R}^3} (v_1 - v) |v_1 - v| \delta(x - x_1) F dx dv,$$

$$\sigma_{ij}^2(x_1(t), v_1(t), t) = \frac{1}{4\sqrt{\pi}} \int_{\mathbf{R}^3} \left(\frac{1}{3} |v_1 - v|^3 + (v_i - v_{1i})(v_j - v_{1j}) |v_1 - v| \right) \delta(x - x_1) F dx dv,$$

$\delta(x)$ is Dirac delta - function.

At small Kn for hard spheres gas (at an assumption of distribution function F local maxwellity and isotropy by thermal velocity c inside eight – foled integrals calculations of "drift" vector \mathbf{a} and "diffusion" matrix σ^2 in velocity space), these coefficients in equations (1), (2) are obtained as follows:

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

$$\begin{aligned} \sigma_{ij}^2(c) &= T^{3/2} \frac{\sqrt{\pi}}{4} [\delta_{ij} P(c) + c_i c_j S(c)], \\ P(c) &= \sqrt{\pi} \operatorname{erf}(c) \left(\frac{c^3}{3} + \frac{3}{2}c + \frac{3}{4c} - \frac{1}{8c^3} \right) + e^{-c^2} \left(\frac{c^2}{3} + \frac{4}{3} + \frac{1}{4c^2} \right), \\ S(c) &= \sqrt{\pi} \operatorname{erf}(c) \left(c + \frac{3}{2c} - \frac{3}{4c^3} + \frac{3}{8c^5} \right) + e^{-c^2} \left(1 + \frac{1}{c^2} - \frac{3}{4c^4} \right), \end{aligned} \quad (3)$$

T is dimensionless temperature, δ_{ij} is Kronecker symbol.

A square root σ of matrix σ^2 is found by the standard way with the implementation of orthonormal basis of eigenvectors:

$$\begin{aligned} \sigma_{ij}(c) &= T^{3/4} \pi^{1/4} / 2 [\delta_{ij} \sqrt{\lambda_2} + c_i c_j / c^2 (\sqrt{\lambda_1} - \sqrt{\lambda_2})], \\ \lambda_1 &= c^2 S(c) + P(c), \lambda_2 = \lambda_3 = P(c). \end{aligned}$$

The computations [14] have shown that these coefficients are quite adequate for gas description at moderate Knudsen numbers. So we are continuing to develop that model.

In the present paper we'll try to get more accurate, than in [8] and than Navier – Stokes system, of macroscopic gas dynamics equations in case of hard sphere gas. The higher in [8] accuracy is based on analytical solving system (1), more precisely, its version, simplified to a handwriting level.

Note also that our approach with the help of SDE technique differs from other approaches for obtaining gas dynamics equations connected to application of deterministic equations for distribution function in phase space [15, 16, 17, 18] as well as other hierarchical models [19]. The models like ours with the coefficients \mathbf{a} and σ depending on velocity are in use by the physics theoreticians for the study of phenomena in turbulent flows (f. e. [20]).

2 SDE SYSTEM

We'll rearrange the system (1) in a way that makes it possible to get macroscopic equations keeping at the same time maximum of microscopic information. The system (1) is a system

of equations for unknown functions $x(t)$ and $v(t)$. Express $v(t)$ through $x(t)$ from the second equation and substitute it in the first one having got an equation only for $x(t)$.

That equation will give us macroscopic equations. To do it we need to make some simplifications. Analytical solving SDE is more difficult than solving ordinary differential equations. Only some successful examples are known. Let lead our equation to one of it.

The coefficients (3) at large c behave themselves as $\mathbf{a}(\mathbf{c}) \sim a_1 \mathbf{c}$, $a_1 \equiv \pi/2$ and $\sigma \sim \sigma_1 c^{3/2}$ (we denote $\sigma_1 \equiv (2\sqrt{\pi}/(3\sqrt{3}))T^{1/4}$). To derive them to a form enabling to get an exact solution let us put $\sigma = k\sigma_1 c$, introducing a parameter k which can be taken, for example, so that one of the terms in our macro – model coincides with the thermodynamical equation of state. We'll do it later. Underline that the introduction of the parameter k was done to get an analytical solution, we do not need the thermodynamical equation of state – all the coefficients in our equations are obtained from the model of hard spheres. Moreover, let us restrict ourselves to the matrix σ in a diagonal form not taking into consideration the elements out of the diagonal because of their smallness in the assumption of the isotropy in velocity space of the distribution function and further averaging. Then the system (1) takes the form:

$$\begin{aligned} dx_i &= v_i dt, \\ dv_i &= -\frac{1}{Kn} a_{1i} c (v_i - V_i) dt + \frac{1}{\sqrt{Kn}} k \sigma_{1ij} c dw_j, \\ x_i|_{t=0} &= x_{i0}, \quad v_i|_{t=0} = v_{i0}, \quad i = 1, 2, 3, \end{aligned}$$

Here $c = \sqrt{c_1^2 + c_2^2 + c_3^2}$ is an absolute value of dimensionless thermal velocity. Because of its presence the second equation can still not be solved exactly, so let us continue our simplifications.

Let $c_i > 0$, then:

$$\begin{aligned} dc_i &= -\frac{1}{Kn} a_0 c_i^2 dt + \frac{\sigma_0}{\sqrt{Kn}} c_i dw(t), \\ c_i|_{t=0} &= c_{i0}, \quad i = 1, 2, 3, \end{aligned}$$

we've replaced c by $3\sqrt{c_i}$, consequently: $a_0 = \sqrt{3}a_{1i}$, $\sigma_0 = \sqrt{3}k\sigma_{1ij}$. For reducing transformations assume that $dc_i = dv_i$, instead of $dc_i = dv_i - \partial V/\partial t dt$ because of slowness of V changing in comparison to c . To take into account $\partial V/\partial t$ technically is not difficult but we'll not do it here.

The exact solution of this equation (see Appendix 1) has the form:

$$\begin{aligned} c_i &= \frac{\exp\left(\frac{\sigma_0}{\sqrt{Kn}} w_t - \frac{\sigma_0^2}{2Kn} t\right)}{c_{0i}^{-1} + \frac{a_0}{Kn} \int_0^t \exp\left(\frac{\sigma_0}{\sqrt{Kn}} w_s - \frac{\sigma_0^2}{2Kn} s\right) ds}, \\ v_i &= V_i + \frac{\exp\left(\frac{\sigma_0}{\sqrt{Kn}} w_t - \frac{\sigma_0^2}{2Kn} t\right) (v_{0i} - V_{0i})}{1 + \frac{a_0(v_{0i} - V_{0i})}{Kn} \int_0^t \exp\left(\frac{\sigma_0}{\sqrt{Kn}} w_s - \frac{\sigma_0^2}{2Kn} s\right) ds}, \quad i = 1, 2, 3. \end{aligned}$$

where $w_t = w(t)$, $w_s = w(s)$.

Transform obtained v_i expanding the exponent in Taylor – Ito series near $t = 0$:

$$e^{-\frac{\alpha^2}{2}t + \alpha w_t} = 1 + \alpha w_t + \frac{1}{2!} \alpha^2 (w_t^2 - t) + \frac{1}{3!} \alpha^3 (w_t^3 - 3tw_t) + \dots$$

Taking it into account we get

$$v_i = V_i + \frac{\left(1 + \frac{\sigma_0}{\sqrt{Kn}} w_t + \frac{1}{2!} \frac{\sigma_0^2}{Kn} (w_t^2 - t) + \frac{1}{3!} \frac{\sigma_0^3}{Kn\sqrt{Kn}} (w_t^3 - 3tw_t) + \dots\right) (v_{0i} - V_{0i})}{1 + \frac{a_0(v_{0i} - V_{0i})}{Kn} \int_0^t \left(1 + \frac{\sigma_0}{\sqrt{Kn}} w_s + \frac{1}{2} \frac{\sigma_0^2}{Kn} (w_s^2 - s) + \dots\right) ds},$$

$$v_i = V_i + \frac{\left(Kn + \sigma_0\sqrt{Kn}w_t + \frac{1}{2}\sigma_0^2(w_t^2 - t) + \frac{\sigma_0^3}{6} \frac{1}{\sqrt{Kn}} (w_t^3 - 3tw_t) + \dots\right) (v_{0i} - V_{0i})}{Kn + a_0(v_{0i} - V_{0i}) \left(t + \int_0^t \frac{\sigma_0}{\sqrt{Kn}} w_s ds + \dots\right)}.$$

Rejecting the terms of order Kn :

$$v_i = V_i + \frac{\left(\sigma_0\sqrt{Kn}w_t + \frac{1}{2}\sigma_0^2(w_t^2 - t) + \frac{\sigma_0^3}{6} \frac{1}{\sqrt{Kn}} (w_t^3 - 3tw_t) + \dots\right)}{a_0 \left(t + \frac{\sigma_0}{\sqrt{Kn}} \eta \frac{t^{\frac{3}{2}}}{\sqrt{3}} + \dots\right)},$$

$\eta \sim \mathcal{N}(0, 1)$ is a standard normally distributed random value.

At $t \rightarrow 0$ we get finally:

$$v_i = V_i + \frac{\sigma_0\sqrt{Kn}}{a_0} \frac{w_t}{t} + \frac{\sigma_0^2}{2a_0} \left(\frac{w_t^2}{t} - 1\right),$$

$$dx_i = v_i dt.$$

In the same manner, for the case $c_i < 0$:

$$v_i = V_i + \frac{\sigma_0\sqrt{Kn}}{a_0} \frac{w_t}{t} - \frac{\sigma_0^2}{2a_0} \left(\frac{w_t^2}{t} - 1\right),$$

$$dx_i = v_i dt.$$

So:

$$v_i = V_i + \frac{\sigma_0\sqrt{Kn}}{a_0} \frac{w_t}{t} + \text{sign}(c) \frac{\sigma_0^2}{2a_0} \left(\frac{w_t^2}{t} - 1\right),$$

$$dx_i = v_i dt.$$

$$x_i = \int v_i dt = x_0 + V_i t + \frac{\sigma_0\sqrt{Kn}}{a_0} \int_0^t \frac{w_s}{s} ds + \text{sign}(c) \frac{\sigma_0^2}{2a_0} \int_0^t \left(\frac{w_s^2}{s} - 1\right) ds.$$

The calculation of integral $\int_0^t w_s/s ds$ is shown in Appendix 2:

$$\int_0^t w_s/s ds = \sqrt{t}(\varepsilon + \tilde{\varepsilon}),$$

where $\varepsilon, \tilde{\varepsilon} \sim \mathcal{N}(0, 1)$ are independent random values normally distributed with zero mean and unit dispersion.

$$x_i = x_{0i} + V_i t + \frac{\sigma_0\sqrt{Kn}}{a_0} (\varepsilon + \tilde{\varepsilon}) \sqrt{t} + \text{sign}(c) \frac{\sigma_0^2}{2a_0} \int_0^t \left(\frac{w_s^2}{s} - 1\right) ds.$$

Our goal is an obtaining macroscopic equations for non – random macro – parameters, that's why we'll not take into account in the last expression the fast changing sign, blinking term with the mean equal to zero. Then:

$$dx_i = V_i dt + \frac{\sigma_0 \sqrt{Kn}}{a_0} dw_t + \frac{\sigma_0 \sqrt{Kn}}{a_0} d\tilde{w}_t,$$

$$dw_t dw_t = dt, \quad d\tilde{w}_t d\tilde{w}_t = dt, \quad dw_t d\tilde{w}_t = 0.$$

So we're coming to the system:

$$\begin{aligned} dx(t) &= V dt + \sqrt{Kn} \tilde{\sigma} (dw + d\tilde{w}), \\ dv(t) &= -\frac{1}{Kn} a(v(t) - V) dt + \frac{1}{\sqrt{Kn}} \sigma dw, \end{aligned} \quad (4)$$

where:

$$\tilde{\sigma}_{ij} \equiv \sigma_{0ij} / a_{0i} = 0,43 \, kT^{1/4}, \quad (5)$$

and V is vector with the coordinates $V_i, i = 1, 2, 3$.

In the second equation instead of $a(c)$ and $\sigma(c)$ from (3) we take their computed values, averaged in velocity space with respect to the local maxwellian:

$$a \approx 2,979 \, T^{1/2}, \quad \sigma \approx 1,73 \, T^{3/4}. \quad (6)$$

The choice of coefficients depending only on x and t is frequently used, for instance, in the context of model collision integral in Fokker – Planck form [12]. Note, that from (6) with our simplifications we get Einstein's fluctuation – dissipation relation (in dimensional form for explicitity): $\sigma^2/a = 2RT$.

The presence of the increment of stochastic term in the first equation in the form of two independent processes, which has appeared at the calculation of $\int_0^t w_s / s ds$, is not trivial, at our glance. That is a significant step forward comparing to our previous results.

Let us derive the equations of stochastic gas dynamics for that set of coefficients. It means that we need to construct the equations for measures in 3D space which are generated by the random processes $x(t)$ and $v(t)$ belonging to the phase space. A physical meaning of that measures is the evolution of mass, momentum and energy distributions.

3 CONTINUITY EQUATION WITH SELF DIFFUSION

An amount of gas in a domain D is, from one side, a whole mass of molecules and, from the other side, an integral with respect to a measure: $\sum_{l: x_l \in D} m_l = \int_D \mu_t(dx)$, or, if all the particles possess the equal masses $1/N$: $\frac{1}{N} \sum_{l=1}^N \chi(x_l(t) \in D) = \int_D \mu_t(dx)$, where χ is a characteristic function. N can be considered as a number of realizations of the random process $x(t)$ which is a solution of the system (4).

We 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)

$$\int \psi(x) \mu_t(dx) = \frac{1}{N} \sum_{l=1}^N \psi(x_l(t)), \quad (7)$$

more precisely: $\forall \psi \in C_b^{(2)}(\mathbf{R}^3)$ and $\forall D \in \mathbf{R}^3$

$$\int_D \psi(x) \mu_t(dx) = \frac{1}{N} \sum_{l=1}^N \psi(x_l(t)) \chi(x_l(t) \in D).$$

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

For obtaining an equation for measure $\mu_t(dx)$, let us take a stochastic differentials from both of two sides of (7). We'll use Ito's formula for complex function differentiation

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

where stochastic differentials dx_i are taken from the system (4):

$$dx_i = V_i dt + \sqrt{Kn} \sum_{j=1}^3 \tilde{\sigma}_{ij} (dw_j + d\tilde{w}_j),$$

and because of definition of a standard three – dimensional Wiener process increment, the smallness of which is \sqrt{dt} [21]:

$$dw_i dw_j = \delta_{ij} dt, \quad dw_i dt = 0, \quad dt^2 = 0, \quad (8)$$

that leads to

$$dx_i dx_j = 2Kn \sum_{m,n=1}^3 (\tilde{\sigma}_{im} \tilde{\sigma}_{jn}) \delta_{mn} dt = 2Kn \sum_{m=1}^3 (\tilde{\sigma}_{im} \tilde{\sigma}_{jm}) dt \equiv 2Kn \tilde{\sigma}_{ij}^2 dt,$$

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

$$\begin{aligned} d\psi(x) = & \left(\sum_{i=1}^3 V_i \frac{\partial \psi}{\partial x_i} + Kn \sum_{i,j=1}^3 \tilde{\sigma}_{ij}^2 \frac{\partial^2 \psi}{\partial x_i \partial x_j} \right) dt \\ & + \sqrt{Kn} \sum_{i,j=1}^3 \tilde{\sigma}_{ij} \frac{\partial \psi}{\partial x_i} (dw_j + d\tilde{w}_j). \end{aligned} \quad (9)$$

Then we get the stochastic differentials from both of two sides of (7):

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

or, applying the formula (7) from right to left for the right hand side of the last expression:

$$\begin{aligned} d \int \psi(x) \mu_t(dx) = & \int \left[\left(\sum_{i=1}^3 V_i(x, t) \frac{\partial \psi}{\partial x_i}(x) \right. \right. \\ & \left. \left. + Kn(x, t) \sum_{i,j=1}^3 \tilde{\sigma}_{ij}^2(x, t) \frac{\partial^2 \psi}{\partial x_i \partial x_j}(x) \right) dt \right] \mu_t(dx) \\ & + \int \left\{ \sqrt{Kn(x, t)} \left[\sum_{i,j=1}^3 \tilde{\sigma}_{ij}(x, t) \frac{\partial \psi}{\partial x_i}(x) \right] (dw_j + d\tilde{w}_j) \right\} \mu_t(dx). \end{aligned}$$

Assuming existence of a density $\rho(x, t)$ of stochastic empirical measure $\mu_t(dx)$ (taking the usual steps while deriving from a generalized 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:

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

and having averaged over the time (taking mathematical expectation and having in mind that the mathematical expectations of the terms with $dw_j, d\tilde{w}_j$ are equal to zero ([16], theorem 3.2.1)) we get a deterministic continuity equation for time averaged deterministic mass density $\bar{\rho}(x, t)$:

$$\frac{\partial \bar{\rho}}{\partial t} + \sum_{i=1}^3 \frac{\partial}{\partial x_i} (\bar{V}_i \rho) = \sum_{i,j=1}^3 \frac{\partial^2}{\partial x_i \partial x_j} (Kn \overline{\tilde{\sigma}_{ij}^2} \rho),$$

which is valid for small Knudsen numbers. The right hand side reflects the trace left by the thermal motion of molecules, or self – diffusion. It does not destroy conservation because it describes diffusion and has a divergent form. So the doubts on the absence of the conservation law in our macro – model, marked in [22], seems to be not correct.

It is natural to regard the random values ρ, V_i and $\tilde{\sigma}_{ij}^2$ (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 (we omit the lines denoting time averaging above the macroparameters):

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

If to perform our derivations for a gas of maxwellian molecules, the self – diffusion corrector in the right hand side will vanish.

4 MOMENTUM EVOLUTION

Let us get equations for momentum and its density. We connect an amount of movement of a gas in D 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 a generalized form:

$$\forall \psi \in C_b^{(2)}(\mathbf{R}^3) : \int \psi(x) \nu_{t,i}(dx) = \frac{1}{N} \sum_{l=1}^N v_i(x_l(t)) \psi(x_l(t)) \quad (i = 1, 2, 3), \quad (10)$$

considering the process $v(t)$ (the solution of (6)) as a function of $x(t)$.

Let us take stochastic differentials from both of two sides of that equality. We'll need a stochastic formula for product differentiation [21]:

$$d(v_i \psi) = \psi dv_i + v_i d\psi + dv_i d\psi.$$

The stochastic differentials dv_i are the equations of the system (4):

$$dv_i = -\frac{a_i}{Kn} (v_i - V_i) dt + \frac{1}{\sqrt{Kn}} \sum_{j=1}^3 \sigma_{ij} dw_j$$

Applying Ito's formula (9) and the rules (8), calculate:

$$\begin{aligned}
 dv_i d\psi &= \left(-\frac{a_i}{Kn} (v_i - V_i) dt + \frac{1}{\sqrt{Kn}} \sum_{j=1}^3 \sigma_{ij} dw_j \right) \\
 &\times \left[\left(\sum_{i=1}^3 V_i \frac{\partial \psi}{\partial x_i} + Kn \sum_{i,j=1}^3 \tilde{\sigma}_{ij}^2 \frac{\partial^2 \psi}{\partial x_i \partial x_j} \right) dt + \sqrt{Kn} \sum_{i,j=1}^3 \tilde{\sigma}_{ij} \frac{\partial \psi}{\partial x_i} (dw_j + d\tilde{w}_j) \right] \\
 &= \sum_{j=1}^3 \sigma_{ij} dw_j \sum_{m,n=1}^3 \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} dw_n = \sum_{j=1}^3 \sum_{m,n=1}^3 \sigma_{ij} \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} \delta_{jn} dt \\
 &= \sum_{j=1}^3 \sum_{m=1}^3 \sigma_{ij} \tilde{\sigma}_{mj} \frac{\partial \psi}{\partial x_m} dt \equiv \sum_{m=1}^3 \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m} dt. \tag{11}
 \end{aligned}$$

Rewrite as well:

$$\begin{aligned}
 \psi dv_i &= \left(-\frac{a_i v_i}{Kn} + \frac{a_i V_i}{Kn} \right) \psi dt + \frac{1}{\sqrt{Kn}} \sum_{n=1}^3 \sigma_{in} \psi dw_n, \\
 v_i d\psi &= v_i \left(\sum_{m=1}^3 V_m \frac{\partial \psi}{\partial x_m} + Kn \sum_{m,n=1}^3 \tilde{\sigma}_{mn}^2 \frac{\partial^2 \psi}{\partial x_m \partial x_n} \right) dt \\
 &\quad + v_i \sqrt{Kn} \sum_{m,n=1}^3 \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} (dw_n + d\tilde{w}_n).
 \end{aligned}$$

Then:

$$\begin{aligned}
 d(v_i \psi) &= \left(-\frac{a_i v_i}{Kn} + \frac{a_i V_i}{Kn} \right) \psi dt + [v_i \left(\sum_{m=1}^3 V_m \frac{\partial \psi}{\partial x_m} + Kn \sum_{m,n=1}^3 \tilde{\sigma}_{mn}^2 \frac{\partial^2 \psi}{\partial x_m \partial x_n} \right) \\
 &\quad + \sum_{m=1}^3 \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m}] dt + \frac{1}{\sqrt{Kn}} \sum_{n=1}^3 \sigma_{in} \psi dw_n + v_i \sqrt{Kn} \sum_{m,n=1}^3 \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} (dw_n + d\tilde{w}_n).
 \end{aligned}$$

Therefore, the stochastic differentials from both of two sides of that equality (10) is:

$$\begin{aligned}
 d \int \psi(x) \nu_{t,i}(dx) &= \frac{1}{N} \sum_{l=1}^N \left\{ \left[-\frac{a_i v_i}{Kn} + \frac{a_i V_i}{Kn} \right] (x_l(t)) \right\} dt \\
 &+ \frac{1}{N} \sum_{l=1}^N \left\{ \left[v_i \sum_{m=1}^3 V_m \frac{\partial \psi}{\partial x_m} + \sum_{m=1}^3 \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m} \right] (x_l(t)) \right\} dt \\
 &+ \frac{1}{N} \sum_{l=1}^N \left\{ \left[v_i Kn \sum_{m,n=1}^3 \tilde{\sigma}_{mn}^2 \frac{\partial^2 \psi}{\partial x_m \partial x_n} \right] (x_l(t)) \right\} dt \\
 &+ \frac{1}{N} \sum_{l=1}^N \left[\left(\frac{1}{\sqrt{Kn}} \sum_{n=1}^3 \sigma_{in} \psi dw_n + v_i \sqrt{Kn} \sum_{m,n=1}^3 \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} (dw_n + d\tilde{w}_n) \right) (x_l(t)) \right],
 \end{aligned}$$

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

$$d \int \psi(x) \nu_{t,i}(dx) = \left[- \int \frac{a_i}{Kn} \psi \nu_{t,i}(dx) + \int \frac{a_i}{Kn} \psi V_i(x, t) \mu_t(dx) \right] dt$$

$$\begin{aligned}
 & + \left[\sum_{m=1}^3 \int V_m \frac{\partial \psi}{\partial x_m} \nu_{t,i}(dx) + \sum_{m=1}^3 \int \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m} \mu_t(dx) \right] dt \\
 & + \sum_{m,n=1}^3 \int Kn \tilde{\sigma}_{mn}^2 \frac{\partial^2 \psi}{\partial x_m \partial x_n} \nu_{t,i}(dx) dt \\
 & + \sum_{n=1}^3 \int \frac{1}{\sqrt{Kn}} \sigma_{in} \psi \mu_t(dx) dw_n + \sum_{m,n=1}^3 \int \sqrt{Kn} \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} \nu_{t,i}(dx) (dw_n + d\tilde{w}_n).
 \end{aligned}$$

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:

$$\begin{aligned}
 d(\rho V_i) = & - \sum_{m=1}^3 \frac{\partial}{\partial x_m} (V_m \rho V_i) dt - \sum_{m=1}^3 \frac{\partial}{\partial x_m} (\sigma_{im} \tilde{\sigma}_{im} \rho) dt \\
 & + \sum_{m,n=1}^3 \frac{\partial^2}{\partial x_m \partial x_n} (Kn \tilde{\sigma}_{mn}^2 \rho V_i) dt \\
 & + \sum_{n=1}^3 \frac{1}{\sqrt{Kn}} \sigma_{in} \rho dw_n + \sum_{m,n=1}^3 \frac{\partial}{\partial x_m} (\sqrt{Kn} \tilde{\sigma}_{mn} \rho V_i) (dw_n + d\tilde{w}_n),
 \end{aligned}$$

if Knudsen numbers are small.

Taking a mathematical expectation, using the same arguments as at derivation of deterministic continuity equation with self – diffusion, we get deterministic quasi gas dynamics equations for the momentum density (omitting the lines above gas dynamics values):

$$\begin{aligned}
 \frac{\partial}{\partial t} (\rho V_i) + \sum_{m=1}^3 \frac{\partial}{\partial x_m} (V_m \rho V_i) = & - \sum_{m=1}^3 \frac{\partial}{\partial x_m} (\overline{\sigma_{im} \tilde{\sigma}_{im} \rho}) \\
 & + \sum_{m,n=1}^3 \frac{\partial^2}{\partial x_m \partial x_n} (Kn \overline{\tilde{\sigma}_{mn}^2} \rho V_i), \quad (i = 1, 2, 3).
 \end{aligned}$$

5 ENERGY DISTRIBUTION

Let us get equations for energy density. Define a measure $\epsilon_t(dx)$:

$$\forall \psi \in C_b^{(2)}(\mathbf{R}^3) : \quad \int \psi(x) \epsilon_t(dx) = \frac{1}{N} \sum_{l=1}^N \psi(x_l(t)) \sum_{i=1}^3 \frac{v_i^2}{2} (x_l(t)). \quad (12)$$

Take the stochastic formula for product differentiation

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

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

the system (4), Ito's formula (9), expressions (8):

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

the formula (11):

$$\begin{aligned}
 dv_i d\psi &= \sum_{m=1}^3 \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m} dt, \\
 d\left(\frac{v_i^2}{2} \psi\right) &= \psi v_i dv_i + \frac{v_i^2}{2} d\psi + v_i dv_i d\psi + \psi \frac{1}{2} \frac{\sigma_{ii}^2}{Kn} dt \\
 &= \psi \left[\left(-\frac{a_i v_i^2}{Kn} + \frac{a_i v_i V_i}{Kn} + \frac{1}{2} \frac{\sigma_{ii}^2}{Kn} \right) dt + \frac{1}{\sqrt{Kn}} \sum_{m=1}^3 \sigma_{im} dw_m \right] \\
 &\quad + \frac{v_i^2}{2} \left(\sum_{m=1}^3 V_m \frac{\partial \psi}{\partial x_m} + Kn \sum_{m,n=1}^3 \tilde{\sigma}_{mn}^2 \frac{\partial^2 \psi}{\partial x_m \partial x_n} \right) dt \\
 &\quad + \frac{v_i^2}{2} \sqrt{Kn} \sum_{m,n=1}^3 \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} (dw_n + d\tilde{w}_n) + v_i \sum_{m=1}^3 \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m} dt.
 \end{aligned}$$

The stochastic differentiation of the formula (12) with account to the just obtained expressions leads to an equation for evolution of the measure $\epsilon_t(dx)$ (regarding to assumed isotropy in velocity space we can put $a_i = a$):

$$\begin{aligned}
 d \int \psi(x) \epsilon_t(dx) &= \left[-2 \int \psi \frac{a}{Kn} \epsilon_t(dx) + \int \psi \frac{1}{2} \sum_{i=1}^3 \frac{\sigma_{ii}^2}{Kn} \mu_t(dx) + \int \psi \sum_{i=1}^3 \frac{a}{Kn} V_i(x, t) \nu_{t,i}(dx) \right] dt \\
 &\quad + \int \left(\sum_{m=1}^3 V_m \frac{\partial \psi}{\partial x_m} + Kn \sum_{m,n=1}^3 \tilde{\sigma}_{mn}^2 \frac{\partial^2 \psi}{\partial x_m \partial x_n} \right) \epsilon_t(dx) dt + \sum_{i,m=1}^3 \sigma_{im} \tilde{\sigma}_{im} \frac{\partial \psi}{\partial x_m} \nu_{t,i}(dx) dt \\
 &\quad + \int \psi \frac{1}{\sqrt{Kn}} \sum_{i,m=1}^3 \sigma_{im} \mu_t(dx) dw_m + \int \sqrt{Kn} \sum_{m,n=1}^3 \tilde{\sigma}_{mn} \frac{\partial \psi}{\partial x_m} \epsilon_t(dx) (dw_n + d\tilde{w}_n).
 \end{aligned}$$

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:

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

For ideal gas, because of the fluctuation – dissipation theorem [12, 23], we can write: $\sigma^2/2a = RT$ (in dimensional form for clearness). That, together with the definition of temperature and total energy density

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

brings zero to this expression after averaging.

Then a stochastic differential equation for energy density looks like

$$\begin{aligned}
 d(\rho E) &= \left[- \sum_{j=1}^3 \frac{\partial}{\partial x_j} (V_j \rho E) - \sum_{i,j=1}^3 \frac{\partial}{\partial x_j} (\sigma_{ij} \tilde{\sigma}_{ij} \rho V_i) \right] dt + \left[\sum_{i,j=1}^3 \frac{\partial^2}{\partial x_i \partial x_j} (Kn \tilde{\sigma}_{ij}^2 \rho E) \right] dt \\
 &\quad + \frac{1}{\sqrt{Kn}} \sum_{i,m=1}^3 \sigma_{im} \rho dw_m + \sqrt{Kn} \sum_{m,n=1}^3 \frac{\partial}{\partial x_m} (\tilde{\sigma}_{mn} \rho E) (dw_n + d\tilde{w}_n),
 \end{aligned}$$

and its deterministic part

$$\frac{\partial(\rho E)}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j} (V_j \rho E) = - \sum_{i,j=1}^3 \frac{\partial}{\partial x_j} (\overline{\sigma_{ij} \tilde{\sigma}_{ij}} \rho V_i) + \sum_{i,j=1}^3 \frac{\partial^2}{\partial x_i \partial x_j} (Kn \overline{\tilde{\sigma}_{ij}^2} \rho E),$$

6 STOCHASTIC GAS DYNAMICS SYSTEM

Let us write the obtained system in Cartesian coordinates:

$$\begin{aligned}\frac{\partial}{\partial t}\rho + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(\rho V_j) &= \sum_{i,j=1}^3 \frac{\partial^2}{\partial x_i \partial x_j} (Kn \overline{\tilde{\sigma}_{ij}^2} \rho), \\ \frac{\partial}{\partial t}(\rho V_i) + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(V_j \rho V_i) &= - \sum_{j=1}^3 \frac{\partial}{\partial x_j} (\overline{\sigma_{ij} \tilde{\sigma}_{ij}} \rho) + \sum_{k,j=1}^3 \frac{\partial^2}{\partial x_k \partial x_j} (Kn \overline{\tilde{\sigma}_{kj}^2} \rho V_i), \\ \frac{\partial}{\partial t}(\rho E) + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(V_j \rho E) &= - \sum_{i,j=1}^3 \frac{\partial}{\partial x_j} (\overline{\sigma_{ij} \tilde{\sigma}_{ij}} \rho V_j) + \sum_{i,j=1}^3 \frac{\partial^2}{\partial x_i \partial x_j} (Kn \overline{\tilde{\sigma}_{ij}^2} \rho E).\end{aligned}$$

Denote and compute taking into account (5), (6): $A \equiv \overline{\tilde{\sigma}_{ij}^2} = 0.085 T^{1/2}$, $B \equiv \overline{\sigma_{ij} \tilde{\sigma}_{ij}} = 0.5 T$. The latter means our choice of the parameter $k = 0.675$ for denoting a combination (we'll find it in the second equation of the system below) $B\rho$ as p calling it "pressure". Then the equality $p = B\rho$ or $p = \rho RT$ (in dimensional form) can be called an equation of state. So:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(\rho V_j) &= \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2} (Kn A \rho) \\ \frac{\partial(\rho V_i)}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(V_j(\rho V_i)) &= - \frac{\partial}{\partial x_i} (B\rho) + \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2} (Kn A(\rho V_i)), \\ \frac{\partial(\rho E)}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(V_j(\rho E)) &= - \sum_{j=1}^3 \frac{\partial}{\partial x_j} (B(\rho V_j)) + \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2} (Kn A(\rho E)).\end{aligned}$$

Introducing the notions $p \equiv B\rho$, $\nu \equiv KnA$ and calling p by pressure and ν by coefficient of kinematic viscosity, we'll have the macroscopic system in traditional form:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(\rho V_j) &= \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2} (\nu \rho) \\ \frac{\partial(\rho V_i)}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(V_j(\rho V_i)) &= - \frac{\partial p}{\partial x_i} + \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2} (\nu(\rho V_i)), \quad i = 1, 2, 3 \\ \frac{\partial(\rho E)}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial x_j}(V_j(\rho E)) &= - \sum_{j=1}^3 \frac{\partial(p V_j)}{\partial x_j} + \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2} (\nu(\rho E)).\end{aligned}$$

7 A NUMERICAL EXAMPLE USING DISCONTINUOUS PARTICLE METHOD

We take a well known problem of shock wave structure as a test. Strictly speaking, it is not a test for macroscopic models because of quite high value of Knudsen number.

The original model (1) is of interest not only because of the possibility to construct new stochastic and deterministic macro – models but also is a base for direct modeling by the help of stochastic particle method [8], attractable for high performance simulation. In the present paper we use a deterministic particle method, alternative to stochastic one, free from parasitic fluctuations.

The applied explicit particle method [24] has a minimal dissipation that makes it possible to get a solution with high accuracy for correct comparison of different models. Here we'll describe our method shortly, paying attention at algorithmic peculiarities.

Divide a 1D computational domain in equal intervals. The heights of particles of three types (representing mass, momentum and energy densities) are taken equal to values of initial $\rho(x, 0)$, $\rho v(x, 0)$, $\rho E(x, 0)$ in points $x_i(0)$. The heights of particles with number i at j time step are denoted by ρ_i^j , ρv_i^j , ρE_i^j ; p_i^j and T_i^j are the values of pressure and temperature in a particle with number i at j time step.

1. Predictor. A system for positions of mass, momentum and energy particles is solved

$$\frac{dx_i}{dt} = v_i; \quad x_i(0) = x_{i0}.$$

by explicit Euler scheme (its accuracy is quite enough because the main source of error is transport nonlinearity):

$$x_i^{j+1} = x_i^j + \tau * v_i^j; \quad v_i^j = \rho v_i^j / \rho_i^j$$

2. Corrector (the main step to struggle with nonlinearity and the main peculiarity of our "discontinuous" method). As a result of particles movements "overlaps" and "gaps" occurs. It destroys the approximation of a function by discrete set of particles. To avoid it let us use the particles reconstruction from [24].

3. The pressure calculation. The difference of pressures leads to the particles volumes change (see more in [24]).

4. The account of viscosity. To do it we take a standard difference approximation for the second derivative at nonuniform grid:

$$\frac{\partial^2(\nu u)}{\partial x^2} \approx (\nu u)_{\bar{x}\bar{x}} \equiv \frac{\nu}{\bar{h}_i} \left(\frac{u_{i+1} - u_i}{h_{i+1}} - \frac{u_i - u_{i-1}}{h_i} \right),$$

where $\bar{h}_i = 0.5(h_i + h_{i+1})$.

We do not use limiters as in [24] because of sufficient natural viscosity. Our system turned out to be less demanding to the values of time steps than Navier – Stokes one.

We consider a one – atom gas ($\gamma = 5/3$, $Pr = 2/3$) at inlet flow Mach number $M = 1.55$. At Fig.1 the profiles of the normed density for the stochastic gas dynamics (SDE) and Navier – Stokes systems are given.

$$\rho' = \frac{\rho - \rho_1}{\rho_2 - \rho_1}.$$

where ρ_1 and ρ_2 are the values at infinity.

Note that our system gives a result close to the experiment [25].

8 CONCLUSIONS

Regardless to our quite severe simplifications we obtained a gas dynamics system which has clear microscopic origin and gives more adequate than usual results at the well known test. Moreover, we've got the hierarchy of micro – macro stochastic and deterministic models each of which has its own place in a row of unified solvers.

9 APPENDIX 1. EQUATION $dx_t = \beta x_t^\gamma dt + \alpha x_t dw_t$

Consider a stochastic differential equation:

$$dx_t = \beta x_t^\gamma dt + \alpha x_t dw_t, \quad \text{where } \alpha, \beta, \gamma - \text{const.} \quad (13)$$

Introduce an integrating multiplier ([21], chapter 5)

$$F_t = \exp \left(-\alpha w_t + \frac{\alpha^2}{2} t \right).$$

Multiply by it both sides of the equation:

$$F_t dx_t = \beta x_t^\gamma F_t dt + \alpha x_t F_t dw_t, \quad F_t dx_t - \alpha x_t F_t dw_t = \beta x_t^\gamma F_t dt,$$

and show that

$$F_t dx_t - \alpha x_t F_t dw_t = d(F_t x_t).$$

By the formula of product stochastic differentiation

$$d(F_t x_t) = F_t dx_t + x_t dF_t + dx_t dF_t.$$

Apply Ito formula for a function $g(t, x) = \exp \left(-\alpha x + \frac{\alpha^2}{2} t \right)$

$$dF_t = \frac{\partial g}{\partial t} dt + \frac{\partial g}{\partial x} dw_t + \frac{1}{2} \frac{\partial^2 g}{\partial x^2} (dw_t)^2,$$

$$dt dt = 0, \quad dt dw_t = 0, \quad dw_t dt = 0, \quad (dw_t)^2 = dt,$$

$$\frac{\partial g}{\partial t} = F_t \frac{\alpha^2}{2}, \quad \frac{\partial g}{\partial x} = (-\alpha) F_t, \quad \frac{\partial^2 g}{\partial x^2} = \alpha^2 F_t.$$

Then:

$$dF_t = \frac{\alpha^2}{2} F_t dt + (-\alpha) F_t dw_t + \frac{\alpha^2}{2} F_t dt = \alpha^2 F_t dt + (-\alpha) F_t dw_t.$$

Replace dx_t using equation (13):

$$dx_t dF_t = -\alpha^2 F_t x_t dt,$$

$$d(F_t x_t) = F_t dx_t + \alpha^2 F_t x_t dt - \alpha F_t x_t dw_t - \alpha^2 F_t x_t dt = F_t dx_t - \alpha F_t x_t dw_t.$$

So, equation (13) is equivalent to equation:

$$d(F_t x_t) = \beta x_t^\gamma F_t dt. \tag{14}$$

Denote $F_t(\xi) x_t(\xi) = y_t(\xi)$ considering ξ as a parameter, then $x_t = F_t^{-1} y_t$, and equation (14) can be written as a deterministic differential equation with respect to a function $t \rightarrow y_t(\xi)$ for each ξ [21]:

$$\begin{aligned} \frac{dy_t(\xi)}{dt} &= F_t(\xi) h(t, F_t^{-1}(\xi) y_t(\xi)) \\ y|_{t=0} &= x_0(\xi), \end{aligned} \tag{15}$$

where $h(t, x_t) = \beta x_t^\gamma$. Solve equation (15) for $y_t(\xi)$.

$$x_t = F_t^{-1} y_t = \exp \left(\alpha w_t - \frac{\alpha^2}{2} t \right) y_t,$$

$$dy_t/dt = \exp \left(-\alpha w_t + \frac{\alpha^2}{2} t \right) \beta y_t^\gamma / \left(\exp \left(-\alpha w_t + \frac{\alpha^2}{2} t \right) \right)^\gamma,$$

$$\frac{dy_t}{y_t^\gamma} = \beta \left(\exp \left(-\alpha w_t + \frac{\alpha^2}{2} t \right) \right)^{1-\gamma} dt,$$

$$\frac{y_t^{-\gamma+1}}{-\gamma+1} = \beta \int_0^t \exp \left(\left(-\alpha w_s + \frac{\alpha^2}{2} s \right) (1-\gamma) \right) ds,$$

$$y_t = \left(y_0^{1-\gamma} + (1-\gamma) \beta \int_0^t \exp \left(\left(-\alpha w_s + \frac{\alpha^2}{2} s \right) (1-\gamma) \right) ds \right)^{\frac{1}{1-\gamma}}.$$

Finally, for x_t we get:

$$x_t = \exp \left(\alpha w_t - \frac{\alpha^2}{2} t \right) \left(y_0^{1-\gamma} + (1-\gamma) \beta \int_0^t \exp \left(\left(-\alpha w_s + \frac{\alpha^2}{2} s \right) (1-\gamma) \right) ds \right)^{\frac{1}{1-\gamma}}.$$

We are interested in values $\gamma = 2$ and $\alpha = \frac{\sigma_0}{\sqrt{Kn}}$, $\beta = -\frac{a_0}{Kn}$:

$$x_t = \exp \left(\alpha w_t - \frac{\alpha^2}{2} t \right) \left(x_0^{-1} - \beta \int_0^t \exp \left(\alpha w_s - \frac{\alpha^2}{2} s \right) ds \right)^{-1}.$$

10 APPENDIX 2. CALCULATION OF INTEGRAL $\int_0^t w_s/s ds$.

Show that

$$\int_0^t f(s) w_s ds = \sigma(t) \eta,$$

where $f(t)$ is an arbitrary function, $\sigma^2(t) = \int_0^t \left(\int_s^t f(\tau) d\tau \right)^2 ds$ is a dispersion [26],

$$\sigma^2(t) = \left\langle \int_0^t f(\tau) w_\tau d\tau, \int_0^t f(\tau) w_\tau d\tau \right\rangle,$$

a random value η is not independent of Wiener wandering w_t , where $w_t = \varepsilon \sqrt{t}$, η can be represented as $\eta = \rho \varepsilon + \sqrt{1-\rho^2} \tilde{\varepsilon}$ where ε and $\tilde{\varepsilon}$ are independent random values, ρ is correlation coefficient:

$$\rho = \langle \varepsilon, \eta \rangle = \left(1 / \left(\sigma(t) \sqrt{t} \right) \right) \int_0^t \left(\int_s^t f(\tau) d\tau \right) ds$$

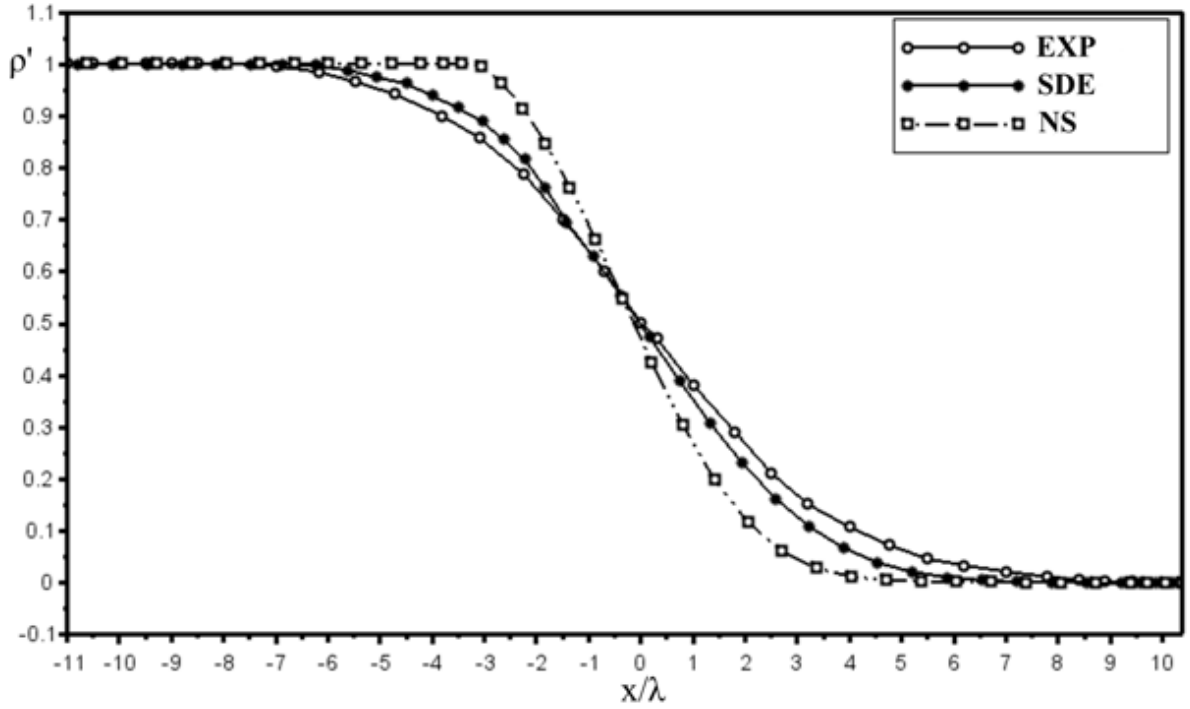


Figure 1: The profiles of the normed density in a shock wave for the stochastic gas dynamics (SDE) and Navier – Stokes (NS) systems, compared to EXPeriment.

Determine the integral by an integral sum S_n .

Let $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n$ are independent random values, having normal distribution with zero mean and unit dispersion: $\varepsilon_i \sim \mathcal{N}(0, 1)$. Divide a segment $[0; t]$ in n segments of length $\Delta t = t/n$. The values of Wiener process at the end k -th segment is equal to a sum of k independent random Gaussian increments at each segment $k = 1, 2, \dots, n$. Denote $f_i \equiv f((i-1)\Delta t)$, then

$$S_n = (f_1\varepsilon_1 + f_2(\varepsilon_1 + \varepsilon_2) + \dots + f_{n-1}(\varepsilon_1 + \varepsilon_2 + \dots + \varepsilon_{n-1}))\sqrt{\Delta t}\Delta t,$$

and its dispersion:

$$\begin{aligned} \sigma_n^2 &= \langle S_n, S_n \rangle = \langle ((f_1\varepsilon_1 + f_2(\varepsilon_1 + \varepsilon_2) + \dots + f_{n-1}(\varepsilon_1 + \varepsilon_2 + \dots + \varepsilon_{n-1}))\sqrt{\Delta t}\Delta t), \\ &\quad ((f_1\varepsilon_1 + f_2(\varepsilon_1 + \varepsilon_2) + \dots + f_{n-1}(\varepsilon_1 + \varepsilon_2 + \dots + \varepsilon_{n-1}))\sqrt{\Delta t}\Delta t) \rangle \\ &= \langle \Delta t^{\frac{3}{2}}((f_1 + f_2 + \dots + f_{n-1})\varepsilon_1 + (f_2 + f_3 + \dots + f_{n-1})\varepsilon_2 + \dots + f_{n-1}\varepsilon_{n-1}), \\ &\quad \Delta t^{\frac{3}{2}}((f_1 + f_2 + \dots + f_{n-1})\varepsilon_1 + (f_2 + f_3 + \dots + f_{n-1})\varepsilon_2 + \dots + f_{n-1}\varepsilon_{n-1}) \rangle \\ &= \Delta t((f_1 + f_2 + \dots + f_{n-1})^2\Delta t^2 + (f_2 + f_3 + \dots + f_{n-1})^2\Delta t^2 + \dots + f_{n-1}^2\Delta t^2). \end{aligned}$$

At $\Delta t \rightarrow 0$

$$\lim_{\Delta t \rightarrow 0} (f_k + f_{k+1} + \dots + f_{n-1})^2\Delta t^2 = \left(\int_{t_k}^t f(\tau) d\tau \right)^2,$$

$$\begin{aligned} \sigma^2(t) &= \lim_{\Delta t \rightarrow 0} \Delta t \left(\left(\int_{t_0}^t f(\tau) d\tau \right)^2 + \left(\int_{t_1}^t f(\tau) d\tau \right)^2 + \dots + \left(\int_{t_k}^t f(\tau) d\tau \right)^2 \right) \\ &= \int_0^t \left(\int_s^t f(\tau) d\tau \right)^2 ds, \end{aligned}$$

Let's calculate $\sigma^2(t)$ and $\rho(t)$ for $f(t) = 1/t$.

$$\begin{aligned}\sigma^2 &= \int_0^t \left(\int_s^t f(\tau) d\tau \right)^2 ds = \int_0^t \left(\int_s^t 1/\tau d\tau \right)^2 ds = \int_0^t \left((\ln |\tau|)|_s^t \right)^2 ds \\ &= \int_0^t (\ln t - \ln s)^2 ds = t \int_0^t \ln^2(s/t) d(s/t) \\ &= t(s/t \ln^2(s/t) - 2s/t \ln(s/t) + 2s/t)|_0^t = 2t,\end{aligned}$$

An integral $I = \int_0^t (\int_s^t 1/\tau d\tau) ds$:

$$\begin{aligned}I &= \int_0^t (\ln |\tau|)|_s^t ds = \int_0^t (\ln t - \ln s) ds = -t \int_0^t \ln(s/t) d(s/t) \\ &= -t(s/t \ln(s/t) - s/t)|_0^t = t,\end{aligned}$$

then $\rho = 1/\sqrt{2}$, $\eta = (\varepsilon + \tilde{\varepsilon})/\sqrt{2}$.

Finally, we have $\int_0^t w_s/s ds = \sqrt{t}(\varepsilon + \tilde{\varepsilon})$.

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