FLUCTUATION AND DISSIPATION IN DISCRETIZED FLUID DYNAMICS

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Coarse grained Langevin-type effective field equations may provide some guidance for the analysis of mesoscopic or microscopic molecular systems exhibiting fluctuations or for systems of hundreds to thousands of subatomic particles produced in high-energy nuclear collisions. Suggestions for consistent realization of random fluctuations in discretized fluid dynamics will be presented.

1 Introduction

It has been customary to treat systems with very large number of degrees of freedom as continua (e.g. electromagnetic field, fluid), and depending on their character the dynamics is described by field equations. The underlying microscopic nature is usually disregarded. However, in certain problems, ignoring completely the phenomena taking place at microscopic level can lead to inaccurate descriptions or even qualitatively different results.

The size of a system where fluctuations become important is the order of the mean distance between the constituent particles and the characteristic time of the dynamics of the system is comparable with the microscopic time scale. There are situations when the inclusion of fluctuations has a dramatic effect on the result. A good example is high energy nuclear physics. As long as the matter of the expanding fire-ball is interacting, fluid dynamical or transport calculations can be applied and they yield satisfactory explanations for a limited range of data. On the other hand, no matter how complicated equation of state is used, fluid dynamical calculations or the solutions of kinetic models as BUU, VUU or Landau-Vlasov models cannot reproduce some fundamental features of the data. An example for such a feature is the fragment mass distribution. Averaging is done during the dynamics and the resulting force fields are smooth. Therefore no realistic clusterization is possible, and the only mass distribution emerging from such calculations is the trivial one consistent with the mass of law action.

Unlike the above calculations quantum molecular dynamical descriptions and solution of Langevin type of dynamical equations do allow for clusterization. In both cases the averaging is done after the whole dynamics, meaning that the time-evolution of all the elements of the ensemble happens under the influence of fields that are different for each configuration. These fluctuating fields are responsible for the non-trivial fragment distributions yielded by these approaches.

Another phenomenon wherein fluctuations are crucial is sonoluminescence, ref.[1]. A micronsize bubble in water driven by ultrasound can periodically collapse and revive, each time emitting one short blue flash coming from the bubble's very center. The light emission is due to extremely high temperatures (up to 10^5 K) which means a concentration of energy density by a factor of 10^{12}. Sonoluminescence has already gained many applications in chemistry and medical physics, and some physicists speculate about the possibility of achieving nuclear fusion. The sphericity of the collapse imposes the most serious limitation on the temperature, density and size of the scorching central spot. The focusing mechanism can fail because of instabilities developing in both the liquid-gas interface and the surface of the converging shock-wave. The instabilities are partly of microscopic origin, i.e., as time goes on, the shrinking shock surface senses more an more the effect of molecular fluctuations.

Thus fluctuations due to the microscopic structure of the system under study may be of determining importance. Therefore, a proper inclusion of the fluctuations in the description of such systems becomes necessary.

As a first step we should get a deeper insight into what fluctuations are and try to develop some of the ideas that arise. Let us restrict ourselves to thermodynamical fluctuations, that is to systems for which $\tau \gg \hbar/kT$, where τ is the order of the characteristic time of the system, T is its temperature and $\hbar$ and k are the Planck and Boltzmann constants respectively. Such fluctuations are not due to the quantum mechanical uncertainty typical to small systems. By fluctuation one usually means an uncontrolled and therefore random variation of a quantity. The definition of randomness is not trivial, and we shall not get involved with it here. In classical systems it is connected to the lack of information regarding the system. Correlations appear in the intermediate state between the two extremes of complete randomness and determinism. The more we dig into the microstructure of the system in order to get more information about the events taking place at low level, the more information is needed to describe it and less and less chaotic the time-dependence of the studied quantities becomes. The main assumption of equilibrium statistical physics is molecular chaos and fluid dynamics means a further step into this direction of suppressing everything microscopical since local thermal equilibrium is required throughout in the bulk of the fluid. This stands at the basis of the one-particle Boltzmann transport equation which does not allow the study of any two particle correlations.

The main postulate of non-fluctuating statistical physics is that $N, V \to \infty$ while N/V remains finite, where N is the number of particles and V the volume of the system. In practical calculations these conditions are only approximately true but in the above mentioned two cases they break down. When the size of the system described as a fluid decreases and the characteristic size of its dynamics becomes comparable with the interparticle distance, the number of particles within a small volume in thermal equilibrium will be too low for disregarding fluctuations. The solution of the Navier Stokes equation is feasible only by numerical methods. The fluid is divided into small cells of size Δx and the field variables are Taylor expanded around each vertex. For a good accuracy Δx should be lot smaller than the characteristic length in the problem (e.g. wavelength). The Taylor expansion of the field variables in the Navier Stokes equation is not simply a mathematical trick but it leads back to the physical origin of the abstract partial differential equation. After discretization we will be left with a number of fluid cells that are pushing against each other and move accordingly. Therefore one has also a natural, physical lower limit on the size of the cells, namely, they should be big enough for still being considered a piece of fluid. This means continuum and thermal equilibrium that is, the number of particles should be large enough, $\Delta N \gg 1$, and the mean free path relatively small, $\lambda \ll \Delta x$. If the characteristic length of the studied phenomenon is not considerably bigger than the interparticle distance these conditions cannot be satisfied. What would take the place of the Navier Stokes equation in this case?

2 From Langevin equation to Navier-Stokes equation

The inclusion of fluctuations into dynamical equations is not a new idea. Langevin's equation for the damped motion of a Brownian particle can be found in ordinary textbooks [2]. Certain aspects of fluctuations in fluid dynamics have been discussed as well [3].

The motion of a fluid happens according to the interaction between the fluid elements. They exert on each other both a smoothly varying average force and also a fluctuating one due to the random-like momentum transfer.

2.1 Langevin equation for external heat-bath (Brownian motion)

Let us first take the simple example of the Brownian motion. We can conceive it as the thermal interaction of a small system with an external heat bath, Fig. 1. There is a random momentum exchange, F', between the system and the heat bath. "Randomness" does not exclude the presence of correlations. The dynamics of the Brownian particle is given by Langevin's equation

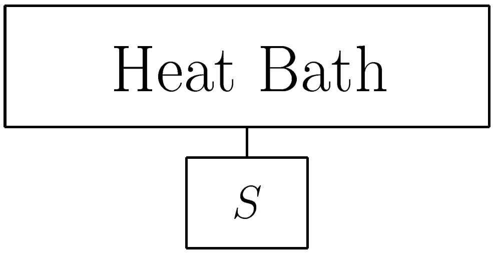

Figure 1: A small system, S, interacting with an external heat bath with random thermal interaction forces. This is the case for the Brownian motion.

$$m[v(t+\tau) - v(t)] = \mathcal{F}(t)\tau - \alpha v(t)\tau + \int_t^{t+\tau} F'(s)ds \ , \tag{1}$$

where m and v are the mass and velocity of the Brownian particle. While $\mathcal{F}$ is an external force, F', fluctuates satisfying the condition

$$\langle F'(s) \rangle = 0 \ .$$

The averaging is done over the whole ensemble of the gas. α is a dissipative coefficient which is related to the fluctuating force by the simple expression:

$$\alpha \equiv \frac{1}{2kT} \int_{-\infty}^{+\infty} \langle F'(0)F'(s) \rangle ds \tag{2}$$

Eq. (2) is the so-called *fluctuation dissipation theorem.* For (1) to apply one has to stipulate that τ is larger than the relaxation time in the gas that is, the collision time between the gas particles.

2.2 Langevin equation for internal heat-bath

Now, imagine many small systems in contact with each other via both conservative forces and random momentum transfer, Fig. 2. They are arranged such that they form a grid with inversion simmetry with respect to the gridpoints. When applying it to a fluid the systems stand for the fluid cells. Following ref. [4] the force acting on the μth cell due to its σth neighbours is

$$\mathbf{F}_\mu^{(\sigma)} = \frac{\mathbf{p}_{\mu-\sigma,\mu} - \mathbf{p}_{\mu,\mu+\sigma}}{\tau}$$

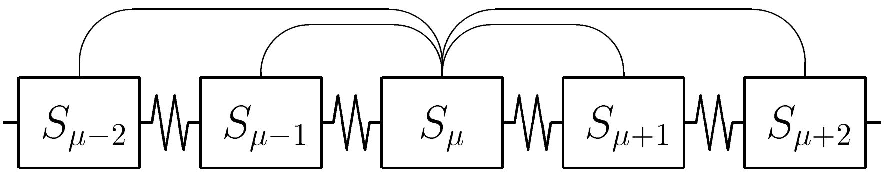

Figure 2: A series of small systems, $S_{\mu-1}$, S_μ, $S_{\mu+1}$, ..., interacting with each other with random thermal interaction forces (thin lines). The random forces are classified into forces interacting with nearest neighbour volumes of about 1 m.f.p. distance from the fluid element in discussion $F_\mu^{(1)}(t)$, with 2nd nearest neighbour volumes of about 2 m.f.p. distance from the fluid element in discussion, $F_\mu^{(2)}(t)$, ... , and so on. Furthermore, our small volume elements interact with their nearest neighbours via non-random, harmonic forces (heavy lines) also.

where $\mathbf{p}_{\mu,\nu}$ is the momentum received by element μ from ν. After reasonably long calculation, in the continuum limit we find that

$$\rho\frac{d\mathbf{v}}{dt} = -\nabla P + \eta\nabla^2\mathbf{v} + \left(\zeta + \frac{1}{3}\eta\right)\nabla(\nabla\cdot\mathbf{v}) + \mathbf{f}' \ ,$$

which is the Navier Stokes equation with a fluctuating force density included. The viscosity coefficients, η, ζ, can be found from fluctuation-dissipation theorem:

$$\eta = \frac{1}{120}\int_0^\infty ds \int d^3y y^2(4k_T + k_L), \quad \zeta = \frac{1}{72}\int_0^\infty ds \int d^3y y^2(k_L - 2k_T) \ , \tag{3}$$

where k_L and k_T are diagonal elements of the correlation matrix

$$\mathbf{K}^{(\sigma)}(s)\delta_{\mu\nu} = \langle \mathbf{p}_{\mu,\mu+\sigma}(t) \circ \mathbf{p}_{\nu,\nu+\sigma}(t-s)\rangle \ .$$

In the limit of large systems $\mathbf{f}'$ vanishes. The above result shows that theoretically, the inclusion of fluctuations for small systems is necessary and possible. What it doesn't show is how $\mathbf{f}'$ behaves and how it should be generated. There is nothing simpler than adding a randomly fluctuating force term to our fluid dynamical code. However, there are some fundamental problems that should be considered before one can take action.

3 Generation of fluctuating transports

A complete fluid dynamical calculation involves not only the Navier Stokes equation but also the continuity and energy equations and an appropriate equation of state. There is an exchange of all three conserved quantities, particle number, momentum and energy, between the fluid cells. These exchanges exhibit fluctuations when the cells are so small that the number of particles within their borders become too low. Adding to the Navier Stokes equation an arbitrarily fluctuating term that is completely unrelated to the molecular motion can only spoil the solution. Now, if we impose some trivial restriction on the fluctuations that would require the respectation of the conservation laws, the zero average, and fluctuation dissipation theorem (3), all this would still not mean an important step toward a more realistic description since it does not make use of the molecular motions. A more elaborate study of the fluctuating quantities would lead to a decreased stochastic character of the fluctuations and would give a more molecular dynamical character to the description. It is important to note that by no means we imply that the perfect description is the molecular dynamical one just because it involves more parameters that is, more detailed information about the system. Even if in principal this is true, it is well-known that in practice the great disadvantage of this method is that it cannot handle phase-transitions. Therefore what we are looking for is a *fluid-dynamical description with fluctuations* that are "clever" enough and yet their generation is feasible. However, the main idea, that more input results in more output, remains valid. In the next couple of sections this is illustrated by the case of a Brownian particle.

3.1 Simplest case. Dirac delta correlation function

For a one-dimensional Brownian motion one can generate a force which has a fixed magnitude and random diraction. It points either to the left or to the right. Obviously, such a fluctuation has a zero average. One can also fix the magnitude of the force from the fluctuation dissipation theorem (2) since the time-correlation will be $\langle F'(0)F'(s)\rangle = |F'|^2\delta(s)$ yielding $|F'| = 2kT\alpha$. In conclusion, we gained a fluctuating force which used in the Langevin equation would produce something like a Brownian motion and probably be useful for studying certain aspects of the phenomenon. But clearly, the obtained results will be far from what is observed experimentally.

3.2 Fluctuating force exhibiting time-correlation

A good support for the "more input, more output" intuitive truth is provided by a random force that is more "clever" than the previously seen flipping one. The force acting on the Brownian particle at a certain moment is determined by the state of the heat-bath which state is in causal relation with its foregoing states. Thus, when generating the force we should be aware of at least two properties of it: stochastic character and memory. Let us discretize the time such that $f(t) = f(n\Delta t) \equiv f_n, n = \overline{0,\infty}$. A simple ansatz for the force could be

$$f_n = \xi_n f_{n-1} + (1-\xi_n) r_n \ ,$$

where ξ_n and r_n are uncorrelated random variables with values $\xi_n = \{0,1\}$, $r_n = (-\infty, +\infty)$ and probabilities such that $P_\xi(0) \equiv 1 - \Delta t/\tau_{coll}, P_\xi(1) = \Delta t/\tau_{coll}, \langle r_n^m \rangle = const., \langle r_n^{2m+1} \rangle = 0, \forall n, m$. τ_{coll} is the collision time of the molecules in the gas. A detailed discussion and calculations can be found in ref.[5]. Summarizing the results:

$$\langle f(t) \rangle = 0 \ , \ \langle f^{2m}(t) \rangle = const. \ , \ \langle f^{2m+1}(t) \rangle = 0 \ ,$$

$$K(t,s) = \langle f(t) f(t+s) \rangle = \langle f^2(t) \rangle e^{-s/\tau_{coll}} \ , \ K(t,s) = K(s) = K(-s) \ .$$

We can conclude that indeed we got more "output" from this more complicated ansatz for the force. All the statistical momenta of the fluctuation have the expected behavior and it also shows time-correlation which exhibits the right properties. Using this force in a simulation will provide us with fairly realistic results. A similar kind of approach for a fluid is not readily feasible and it has some fundamental limitations. For details see ref.[5].

3.3 Generation of fluctuating transports for internal heat-bath

In this last and most important section we shall get a bit closer to the final goal of fluctuating fluid dynamics. We will suggesta simple minded way of generating a fairly "clever" fluctuation between one dimensional numerical fluid cells.

The change in the particle number and momentum of a cell at location k and at a certain timestep is made up from the individual contributions of the exchange transports between these cell and all the other. The transports reaching the cell at k originating from a cell l will suffer a certain amount of time delay because of the finite velocity of propagation of the constituent particles. This retardation is expected to account for the time correlation, therefore it cannot be disregarded when constructing the model. Time is discretized as well after being divided up to small intervals of length Δt. The changes ΔN_k and ΔP_k occuring in the cell at k and time $t_i \equiv i\Delta t$

$$\begin{aligned} \Delta N_k(t_i) &= \sum_l \Delta N_{l,k} \left(t_i - \frac{d_{l,k}}{\langle v_{th} \rangle} \right) - \Delta N_{k,l}(t_i) \ , \\ \Delta P_k(t_i) &= \sum_l \Delta P_{l,k} \left(t_i - \frac{d_{l,k}}{\langle v_{th} \rangle} \right) - \Delta P_{k,l}(t_i) \ , \end{aligned}$$

where $\Delta N_{l,k}$ is the particle transport originating from cell l and addressed to cell k, $\Delta N_{k,l}$ is the transport into the inverse direction and $\Delta P_{l,k}$ and $\Delta P_{k,l}$

are the corresponding momentum transfers. $d_{l,k}$ is the distance between the two cells, $\langle v_{th} \rangle$ is the thermal velocity and for the moment it is considered to be constant for the whole bulk of the gas. The summation is done over all cells apart from the one at k.

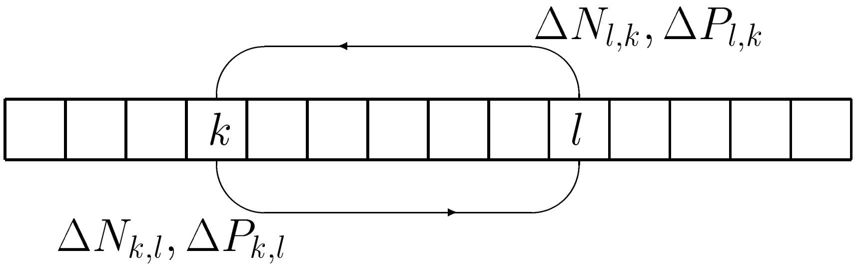

Figure 3: Exchange of particles and momentum between two cells in an one dimensional fluid

The random variables are $\Delta N_{l,k}$ and $\Delta P_{l,k}$ for all l and k so that $l \neq k$. They are generated from a Poisson distribution characterized by the mean values

$$\langle \Delta N_{l,k} \rangle = C_N(\lambda, \langle v_{th} \rangle) N_k N_l e^{-d_{lk}/\lambda} \ , \quad \langle \Delta P_{l,k} \rangle = C_P(\lambda, \langle v_{th} \rangle) \Delta N_{l,k} m \langle v_{th} \rangle \ ,$$

where λ is the mean free path in the gas taken as constant similarly to the thermal velocity. N_k, N_l are the total number of molecules in the corresponding cells and m is the mass of the constituent particles. The expressions for the two factors C_N and C_P represent the real modelling in the problem. Depending on how demanding the model of the physical problem is wanted and on the available computer power one can dig to arbitrary depths in the underlying kinetics.

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