Is fluctuating hydrodynamics stochastic?

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Introduction

In the following project I will observe the simple atomic system with monatomic viscous fluid based on Leonard Jones potential in equilibrium state. Firstly, we will derive correlation functions from HD theory, using linearized equations which follow from the conservation laws(the set of Navier-Stokes equations) (1). Next the atom's trajectory is computed by running MD simulation as trajectories display an exponentials sensitivity to even the most minute perturbation (2). Then on the basis of the resulting expression for correlation function we will examine the experimental data which can be interpreted in the HD fluctuation theory to obtain the information on the dynamic behavior of fluid system. In final step I will compute values of fluctuate stress tensor and heat flux. The method of ε-machine(3) will show how non-stochastic these values are. The main task of the project is experimentally explore our fluid system and to prove that fluctuations of main thermodynamic quantities in HD systems are chaotic instead of random.

The Navier-Stokes equations

In this section lets move to derivation of basic fluid dynamic equation.

The continuity equation which conservation of matter(1):

$$\frac{\partial\rho}{\partial t}+div(\rho v)=0;$$

The force equation – conservation of momentum:

$$\rho\frac{\partial v_i}{\partial t}+\rho v_k\frac{\partial v_i}{\partial x_k}=-\frac{\partial P}{\partial x_i}+\frac{\partial \boldsymbol{\sigma}'_{ik}}{\partial x_k};$$

The heat-exchange equation – conservation of energy:

$$\rho T\left(\frac{\partial s}{\partial t}+v\nabla s\right)=\frac{1}{2}\sigma'_{ik}\left(\frac{\partial v_i}{\partial x_k}+\frac{\partial v_k}{\partial x_i}\right)-div\boldsymbol{q};$$

$\boldsymbol{\sigma}'_{ik}$ - stress tensor, $\boldsymbol{q}$ – heat flux.

Expression for the stress tensor and the heat flux vector

$$\boldsymbol{\sigma}'_{ik}=\eta\left(\frac{\partial v_i}{\partial x_k}+\frac{\partial v_k}{\partial x_i}-\frac{2}{3}\delta_{ik}div\, v\right)+\xi\delta_{ik}div\, v+s_{ik};$$

$$q=-x\nabla T+g;$$

Where $\boldsymbol{\eta},\ \boldsymbol{\xi}$ – viscosity coefficient and $\boldsymbol{x}$ – thermal conductivity coefficient and s_{ik}, g – random stress tensor and heat flux. Finally the following formulas solve the problem of calculating the hydrodynamic fluctuations(1):

$$<s_{ik}(t_1,r_1)g_l(t_2,r_2)>=0;$$

$$<g_i(t_1,r_1)g_k(t_2,r_2)>=2xT^2\delta_{ik}\delta(r_1-r_2)\delta(t_1-t_2);$$

$$<s_{ik}(t_1,r_1)s_{im}>=$$

$$=2T[\eta(\delta_{il}\delta_{km}+\delta_{im}\delta_{kl})+(\xi-\frac{2\eta}{3})\delta_{il}\delta_{km}]\delta(r_1-r_2)\delta(t_1-t_2);$$

Pressure Tensor

MD simulation was carried out using a Leonard-Jones pair potential(4):

$$\phi(r_{ij})=4\epsilon[(\frac{\varpi}{r_{ij}})^{12}-(\frac{\varpi}{r_{ij}})^{6}],\ r_{ij}\le|r_c|$$

Where r_{ij} - the difference between the vectorial position of atom i located at r_i and j located at r_j. ϖ- molecular diameter and ϵ- the characteristic energy of the interaction. The **Irving Kirkwood equation for the pressure tensor is:**

$$\overline{\overline{\Pi}}=\sum_{i=1}^{N}\frac{1}{m_i}p_ip_i\delta(r-r_i)+\frac{1}{2}\sum_{i=1}^{N}\ \sum_{j\neq1}^{N}r_{ij}f_{ij}\int_0^1\delta(r-r_i+\lambda r_{ij})d\lambda,$$

Where the momenta $p_i=m_iv_i-u$, is the mass of the molecule, r_{ij} is the pair separation vector, and f_{ij} is the pair force. The spatial integral over the value in space gives the **control volume(CV)** form of PT:

$$\int_V\overline{\overline{\Pi}}dV=\sum_{i=1}^{N}\frac{1}{m_i}p_ip_i\gamma_i+\frac{1}{2}\sum_{i=1}^{N}\ \sum_{j\neq1}^{N}r_{ij}f_{ij}\int_0^1\gamma_\lambda d\lambda,$$

where γ_λ a functional with a value 1 when a part of the interaction between i and j is in CV and 0 otherwise.

Conclusion

The fundamental properties of fluid mechanics are contained in the conservation laws . To any conservation quantity we can associate a flux describing how that quantity is changed by the flow. The lows of the fluid mechanics are governed by the conservation equations for the three basis equations. There assumptions are quite important as I have began my first step of exploring properties of hydrodynamic fluctuations of the fluid. Also I came to certain conclusion that construction of a general theory of HD reduce to the formulation of the equations of motion for fluctuating quantities. My next step is to discover the atoms trajectories and illustrate them using software and numerical programming methods and analyze the results.

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