Fluctuating Navier-Stokes equations

We already discussed the fluctuating hydrodynamic equation for diffusive systems

$$\partial_t \rho = \nabla \cdot \left[\chi \nabla \rho + (2\chi\rho)^{1/2} \mathcal{W}(t) \right]$$

which fits our generic Langevin equation

$$\begin{cases} \partial_t x = -N(x) \cdot \dfrac{\partial H}{\partial x} + (2k_B T)^{1/2} B \cdot \mathcal{W}(t) \\ \quad \text{(Ito)} \qquad\qquad + (k_B T) \dfrac{\partial}{\partial x} \cdot N^*(x) \end{cases}$$

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and the fluctuation - dissipation balance condition

self adjoint

$$\boxed{BB^* = \frac{1}{2}(N + N^*) = M(x) = M^*(x)}$$

where $M(x)$ is the dissipative part of the mobility operator $N(x)$. The remaining part is conservative dynamics

skew adjoint

$$\boxed{L = \frac{1}{2}(N^* - N) = -L^*}$$

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$$\frac{dH(x)}{dt} = \frac{\partial H}{\partial x} \cdot \frac{\partial x}{\partial t} = \frac{\partial H}{\partial x} \cdot M \cdot \frac{\partial H}{\partial x} \leq 0$$

Now we want to generalize this to more realistic fluids, where fluid flow is important.

As coarse-grained variables we must choose slow variables, and physical intuition suggests the conserved fields

$$X \equiv \begin{bmatrix} \rho(r,t) \\ \vec{j}(r,t) \\ e(r,t) \end{bmatrix} \begin{array}{l} \text{mass} \\ \text{momentum} \\ \text{energy} \end{array} \Bigg\} \text{ density}$$

Defining these coarse variables precisely is rather non-trivial (see Thomas's talk), but intuitively:

$$\begin{bmatrix} \rho(\vec{r}) \\ \vec{j} = \rho\vec{v} \\ e = \frac{1}{2}\rho v^2 + \varepsilon \end{bmatrix} \approx \sum_{i=1}^{N} \begin{bmatrix} m_i \\ m_i \vec{v}_i \\ m_i \frac{v_i^2}{2} \end{bmatrix} \delta_a(\vec{r}-\vec{r}_i)$$

internal energy

particles

Here $\delta_a(r)$ is a molified delta function of compact support of size a = coarse-graining scale

We will consider here a simplified <u>isothermal</u> model

$$T = \text{const}$$

which means we will assume that temperature is a <u>fast</u> variable maintained by contact with an external thermal (heat bath) and thus the internal energy

$$\mathcal{E}(\rho, T) \simeq \mathcal{E}(\rho)$$

and $$X \equiv \begin{bmatrix} \rho \\ j = \rho v \end{bmatrix}$$ $\leftarrow$ fluid velocity

We postulate that the coarse-grained Hamiltonian or free-energy functional is

$$H[\rho, j] = \int \left[\underbrace{\frac{j^2}{2\rho}}_{\equiv\, \rho\frac{v^2}{2}} + \epsilon(\rho) \right] dr$$

(center-of-mass kinetic energy)

and that the equilibrium Gibbs distribution is

$$P(x) = Z^{-1} \exp\left\{ - \frac{H[\rho, j]}{k_B T} \right\}$$

The coarse-grained dynamics is

$$\partial_t x = - N(x) \cdot \frac{\partial H}{\partial x} + \text{fluctuations}$$

where

$$\frac{\partial H}{\partial x} = \begin{bmatrix} \frac{\partial H}{\partial \rho} \\ \frac{\partial H}{\partial j} \end{bmatrix} = \begin{bmatrix} -\frac{j^2}{2\rho^2} + \varepsilon'(\rho) \\ \frac{j}{\rho} = \vec{v} \end{bmatrix}$$

Now we need the mobility operator

$$N(x) = \left[\begin{array}{c|c} N_{\rho\rho} & N_{\rho v} \\ \hline N_{v\rho} & N_{vv} \end{array}\right]$$

In fluids, mass is transported by <u>advection</u> (or convection), meaning, by directed (instead of diffusive) transport. Mass conservation is thus microscopically exact and we postulate/state (see Landau-Lifshitz) that

MASS CONSERVATION

$$\boxed{\partial_t \rho = -\nabla \cdot (j) = -\nabla \cdot (\rho v)}$$

CONTINUITY EQUATION

which can in fact be thought of as the correct definition for v.

So we have

(1) $N_{\rho\rho} = 0$ and $\boxed{N_{\rho v} = -\frac{\partial}{\partial r} \cdot \rho}$

so that $N_{\rho v} \cdot \frac{\partial H}{\partial j} = -\nabla \cdot \left(\rho \frac{j}{\rho} \right) = -\nabla \cdot (j)$

for the continuity equation

(2) The reverse coupling $N_{v\rho}$ must be the skew adjoint of $N_{\rho v}$ since there is no dissipation associated with density, i.e., since $N_{\rho\rho} = 0$

$$N_{v\rho} = -N_{\rho v}^{*} = -\rho \frac{\partial}{\partial r}$$

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This gives a term in the momentum equation

$$\partial_t j = -\rho \frac{\partial}{\partial r}\left(\frac{\partial H}{\partial \rho}\right) + \ldots =$$

$$= \rho \frac{\partial}{\partial r}\left(\frac{v^2}{2}\right) - \rho \frac{\partial}{\partial r}\left[\varepsilon'(\rho)\right]$$

To write the second term more explicitly, we write

$$\rho \frac{\partial}{\partial r}\left[\varepsilon'(\rho)\right] = \rho \frac{\nabla P}{\rho} = \nabla P$$

where $\boxed{P(\rho) = \rho \varepsilon'(\rho) - \varepsilon(\rho)}$ is the pressure

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For the momentum-momentum coupling N_{vv} we just state the result:

$$L_{vv} = \frac{\partial}{\partial r} j + j \frac{\partial}{\partial r} = -\left(\frac{\partial}{\partial r} j + j \frac{\partial}{\partial r} \right)^T$$

advective or non-dissipative part of the dynamics (skew-adjoint)

Component-wise

$$\left(L_{vv}\right)_{\alpha\beta} = -\frac{\partial}{\partial r_\beta} j_\alpha - j_\beta \frac{\partial}{\partial r_\alpha}$$

$$\left[(L v v)\cdot \frac{\partial H}{\partial j} + \overbrace{\rho \frac{\partial}{\partial r}\left(\frac{v^2}{2}\right)}^{\text{from } \rho}\right]_\alpha =$$

$$\rho \frac{\partial}{\partial r_\alpha}\left(\frac{v_\beta v_\beta}{2}\right) - \frac{\partial}{\partial r_\beta} j_\alpha v_\beta - j_\beta \frac{\partial v_\beta}{\partial r_\alpha}$$

$$= \rho (\nabla v)\cdot v - \nabla\cdot(v j) - (\nabla v)\cdot j$$

$$= (\nabla v)\cdot j - \nabla\cdot(v j) - (\nabla v)\cdot j = -\nabla\cdot(v j)$$

which is a divergence of an <u>advective</u> <u>flux</u> $\boxed{v\cdot j}$ as expected.

Putting the pieces together, we get for the non-dissipative (reversible, conservative, Hamiltonian) dynamics the <u>Euler</u> equations

$$\begin{cases} \partial_t \rho = -\nabla\cdot(\rho v) \\ \partial_t(\rho v) = -\nabla\cdot(\rho v v) - \nabla P(\rho) + \begin{matrix}\text{dissipation}\\ \text{fluctuation}\end{matrix} \end{cases}$$

$\Downarrow$

$$\begin{cases} \rho(\partial_t v + v\cdot\nabla v) = -\nabla P \\ \partial_t \rho + v\cdot\nabla\rho = -\rho(\nabla\cdot v) \end{cases}$$

Momentum, unlike mass, is transferred between particles via <u>interactions</u> (collisions, forces), i.e, non-advectively. This would lead to additional <u>stress</u> terms in the momentum equation:

$$\partial_t \vec{j} = -\nabla\cdot\left(\overleftrightarrow{\sigma}\right) + \text{advective}$$

$$= \vec{\nabla}\cdot\left[\overleftrightarrow{\eta}\;\overleftarrow{\nabla}\left(\frac{\partial H}{\partial \vec{j}}\right)\right] = \nabla\cdot\left(\overleftrightarrow{\eta}\;\overleftarrow{\nabla}\vec{v}\right)$$

rank four <u>viscosity tensor</u> ≥ 0

For isotropic fluids (simple Newtonian liquids and gases), it can be shown by symmetry arguments that

$$\overleftrightarrow{\eta}\left(\overleftarrow{\nabla}\overleftrightarrow{v}\right) = \underset{\text{\underline{shear} viscosity}}{\eta}\left(\overleftarrow{\nabla}\overrightarrow{v} + \overleftarrow{\nabla}^T\overrightarrow{v}\right) + \underset{\text{\underline{bulk} viscosity}}{K}\left(\overrightarrow{\nabla}\cdot\overleftarrow{v}\right)\overleftrightarrow{I}$$

$$M = \frac{1}{2}(N+N^*) = -\frac{\partial}{\partial r}\cdot\overleftrightarrow{\eta}\,\frac{\partial}{\partial r} = BB^*$$

$$\Rightarrow \boxed{B = \frac{\partial}{\partial r}\cdot\overleftrightarrow{\eta}^{1/2}}$$

This means that the fluctuating or stochastic stress tensor $\tilde{\sigma}$ is

$$(2k_BT)^{1/2}\,B\cdot W(t) = \nabla\cdot\left(\tilde{\sigma}\right)$$

$$\tilde{\sigma} = \left(2k_BT\,\overleftrightarrow{\eta}\right)^{1/2} W(r,t)$$

white noise

giving the equations of fluctuating hydrodynamics

$$\rho\left(\partial_t v + v\cdot\nabla v\right) = -\nabla P + \nabla\cdot\left[\overleftrightarrow{\eta}\,\nabla v + \left(2k_BT\,\overleftrightarrow{\eta}\right)^{1/2} W(r,t)\right]$$

$\equiv$

or $\rho(D_t v)$ ← material derivative

$$D_t\rho = -\rho(\nabla\cdot v) = 0 \text{ if incompressible}$$

These equations revert to the usual compressible isothermal Navier-Stokes equations when fluctuations are neglected.

The stochastic terms ensure that the Gibbs distribution (canonical ensemble) is preserved

$$P_{eq} = Z^{-1} \exp\left[-\frac{1}{k_B T}\int\left(\frac{\rho v^2}{2} + \mathcal{E}(\rho)\right)dr\right]$$

Consider fluctuations at equilibrium

$$(\rho, v) = (\rho_0 + \delta\rho, \delta v)$$

and linearize to leading order in the fluctuations

$$\mathcal{H} = \int \left[\rho \frac{v^2}{2} + \mathcal{E}(\rho) \right] dr \approx \int \left[\rho_0 \frac{(\delta v)^2}{2} + \frac{\mathcal{E}''(\rho_0)}{2} (\delta \rho)^2 \right] dr$$

$$\Rightarrow P_{eq} \sim \exp \int dr \left[\frac{(\delta v)^2}{2\,(k_B T / \rho_0)} + \frac{(\delta \rho)^2}{2\,(k_B T / \mathcal{E}''(\rho_0))} \right]$$

This means (see earlier lecture) that at equilibrium both the density and the velocity are <u>spatially-white</u> and uncorrelated

$$\boxed{\begin{aligned} \langle v(r)\, v(r') \rangle &= \frac{k_B T}{\rho_0} I_d \cdot \delta(r-r') \\ \langle \rho(r)\, \rho(r') \rangle &= k_B T / \mathcal{E}''(\rho_0)\, \delta(r-r') \end{aligned}}$$

In terms of physical parameters

$$\varepsilon''(\rho_0) = \frac{1}{\rho} \frac{dP(\rho)}{d\rho} = \frac{c^2}{\rho}$$

where c is the isothermal speed of sound. The density fluctuations are

$$\langle (\delta \rho_{\Delta V})^2 \rangle = \frac{(k_B T)\rho_0}{(\Delta V)c^2} \rightarrow 0 \text{ if } c \rightarrow \infty$$

(incompressible fluid)

For an ideal gas $c^2 = \frac{k_B T}{m} \Rightarrow$

$$\langle (\delta \rho_{\Delta V})^2 \rangle = \frac{\rho_0 m}{\Delta V} = \langle \delta N_{\Delta V}^2 \rangle \frac{m^2}{\Delta V^2} = \frac{m^2 N_{\Delta V}}{\Delta V^2}$$

$$\Rightarrow \langle (\delta N_{\Delta V})^2 \rangle = N_{\Delta V} \leftarrow \text{number of molecules in volume } \Delta V$$

Poisson process

Note that these are the same sort of fluctuations that arise for diffusive dynamics but here there is no diffusion of mass (only momentum).

The fluctuating hydrodynamics formalism and equations obtained here can be extended to many other cases (non-isothermal, fluid mixtures, etc.).