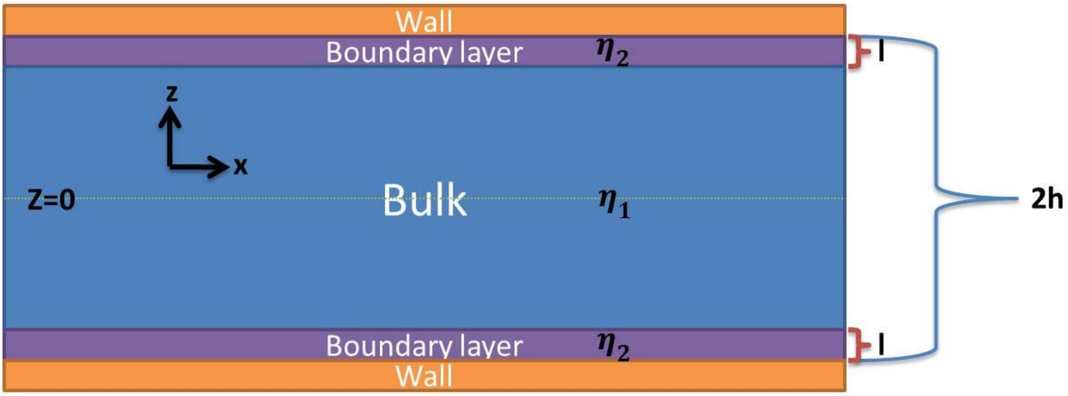
Green-Kubo formula for boundary momentum density fluctuation

System is shown in the figure below. Here, we consider the anti-symmetric fluctuating modes for incompressible fluid.



The fluctuating transverse momentum density is defined as $J(z,t)=\rho_0 v(z,t)$.

Its components $j_n(z,t)$ can be obtained by solving the incompressible NS equation

$$\frac{\partial}{\partial t} j_n(z,t)=\frac{\eta}{\rho_0}\frac{\partial^2}{\partial z^2} j_n(z,t)$$

The equation may be solved through separation of variables $j_n(z,t)=Z_n(z)T_n(t)$:

$$\frac{1}{Z_n(z)}\frac{d^2 Z_n(z)}{dz^2}+k_n^2=0$$

$$\frac{\rho_0}{\eta T_n(t)}\frac{dT_n(t)}{dt}+k_n^2=0$$

Because only the anti-symmetric modes are considered here, we get $Z_n(z)=A_n\sin(k_n z)$ in bulk $[0,h-l]$, where the coefficient A_n can be determined from the initial condition of equipartition. For each mode k_n, the corresponding Z component in the boundary layers may be assumed to have a linear form that fulfills no-slip boundary condition $Z_n(z=\pm h)=0$, and a slip velocity $v_{Sn}=V_{Sn}/\rho_0$ defined at the boundary-bulk interfaces. That is, in the upper boundary layer $[h-l,h]$,

$Z_n(z)=\frac{V_{Sn}}{l}(h-z)$. V_{Sn} can also be determined from the initial condition of equipartition. (Because of the anti-symmetric nature of the modes, only one side of the system needs to be considered.) At the boundary-bulk interfaces, the tangential stresses and transverse momentum densities must be equal for each mode:

$$V_{Sn}=A_n\sin\left(k_n\left(h-l\right)\right) \qquad (1)$$

$$-\eta_2\frac{V_{Sn}}{l}=\eta_1 A_n k_n\cos\left(k_n\left(h-l\right)\right) \qquad (2)$$

Divided (1) by (2), we get the eigenvalue equation

$$\tan\left(k_n\left(h-l\right)\right)=-\frac{\eta_1 k_n l}{\eta_2} \qquad (3)$$

This equation can be solved numerically.

Apply the equipartition.

$$2S\int_0^h Z_n\left(z\right)^2 dz=\rho_0 k_B T$$

$$2S\left[\int_0^{h-l}A_n^2\sin^2\left(k_n z\right)dz+\int_{h-l}^{h}\left(\frac{V_{Sn}}{l}\left(h-z\right)\right)^2 dz\right]=\rho_0 k_B T \qquad (4)$$

The first and second terms in the left hand side (LHS) represents the bulk and boundary contributions, respectively, and “2” is because of the anti-symmetry. Substituting (1) into (4), we get

$$A_n^2=\frac{\rho_0 k_B T}{2S\left[\int_0^{h-l}\sin^2\left(k_n z\right)dz+\int_{h-l}^{h}\left(\frac{\sin\left(k_n\left(h-l\right)\right)}{l}\left(h-z\right)\right)^2 dz\right]}$$

$$=\frac{\rho_0 k_B T}{S\left[h-l-\frac{\sin\left(2k_n\left(h-l\right)\right)}{2k_n}+\frac{2l\sin^2\left(k_n\left(h-l\right)\right)}{3}\right]} \qquad (5)$$

and

$$V_{Sn}^2=\frac{\sin^2\left(k_n\left(h-l\right)\right)\rho_0 k_B T}{S\left[h-l-\frac{\sin\left(2k_n\left(h-l\right)\right)}{2k_n}+\frac{2l\sin^2\left(k_n\left(h-l\right)\right)}{3}\right]} \qquad (6)$$

From Equation (3), we can get

$$\sin\left(2k_n\left(h-l\right)\right)=\frac{2\tan\left(k_n\left(h-l\right)\right)}{1+\tan^2\left(k_n\left(h-l\right)\right)}=-\frac{2\eta_1\eta_2 l k_n}{\eta_2^2+\eta_1^2 l^2 k_n^2} \qquad (7)$$

and

$$\sin^2\left(k_n\left(h-l\right)\right)=\frac{1}{2}\left(1-\frac{1-\tan^2\left(k_n\left(h-l\right)\right)}{1+\tan^2\left(k_n\left(h-l\right)\right)}\right)=\frac{\eta_1^2 l^2 k_n^2}{\eta_2^2+\eta_1^2 l^2 k_n^2} \qquad (8)$$

According to the FD theorem for viscosity, we calculate the following quantity:

$$2S\int_0^{+\infty}dt\int_0^h dz\left\langle\eta\left(\frac{\partial J\left(z,t=0\right)}{\partial z}\right)\left(\frac{\partial J\left(z,t\right)}{\partial z}\right)\right\rangle \qquad (9)$$

It is reasonable to assume no correlation between different modes of which J is composed. That is $\left\langle\eta\left(\frac{\partial j_m\left(z,t=0\right)}{\partial z}\right)\left(\frac{\partial j_n\left(z,t\right)}{\partial z}\right)\right\rangle=0$ when $m\neq n$. It then follows that (9) can be expressed as

$$2S\int_0^{+\infty}dt\int_0^h dz\left(\eta\sum_{n=0}^{N}\left\langle\left(\frac{\partial j_n\left(z,t=0\right)}{\partial z}\right)\left(\frac{\partial j_n\left(z,t\right)}{\partial z}\right)\right\rangle\right)=2S\sum_{n=0}^{N}\int_0^h dz\left(\eta\left(\frac{\partial Z_n\left(z\right)}{\partial z}\right)^2\right)\int_0^{+\infty}dtT_n\left(t\right)$$

(9a)

Now we calculate $2S\int_0^h\eta\left(\frac{\partial Z_n\left(z\right)}{\partial z}\right)^2 dz\int_0^{+\infty}T_n\left(t\right)dt$ For each mode.

The spatial component can be evaluated as

$$2S\int_0^h\eta\left(\frac{\partial Z_n\left(z\right)}{\partial z}\right)^2 dz=2S\left[\int_0^{h-l}\eta_1 A_n^2 k_N^2\cos^2\left(k_n z\right)dz+\int_{h-l}^{h}\eta_2\left(\frac{V_{Sn}}{l}\right)^2 dz\right]$$

$$=S\eta_1 A_n^2 k_N^2\left(h-l+\frac{\sin\left(2k_n\left(h-l\right)\right)}{2k_n}\right)+\frac{2S\eta_2 V_{Sn}^2}{l}$$

Let's look at the boundary contribution first. Using Equation (6), (7), and (8), and assuming that $h\gg l$ and $\frac{\eta_2}{l}=\beta$ is constant, we obtain

$$\frac{2S\eta_2 V_{Sn}^2}{l}=S\beta\left(2V_{Sn}^2\right)=\frac{2\beta\eta_1^2 k_n^2\rho_0 k_B T}{h\left(\beta^2+\eta_1^2 k_n^2\right)\left(1-\frac{l}{h}+\frac{\eta_1\beta}{h\left(\beta^2+\eta_1^2 k_n^2\right)}+\frac{l}{h}\frac{2\eta_1^2 k_n^2}{3\left(\beta^2+\eta_1^2 k_n^2\right)}\right)} \qquad (10)$$

$$\rightarrow\frac{\eta_1 k_n^2\rho_0 k_B T}{1+\frac{\eta_1\beta}{h\left(\beta^2+\eta_1^2 k_n^2\right)}}\times\frac{2\eta_1\beta}{h\left(\beta^2+\eta_1^2 k_n^2\right)}=D_n^{boundary}$$

For the bulk, we have

$$S\eta_1 A_n^2 k_N^2 \left(h - l + \frac{\sin\left(2k_n\left(h-l\right)\right)}{2k_n} \right)$$

$$= \frac{\eta_1 k_n^2 \rho_0 k_B T}{1 - \frac{l}{h} + \frac{\eta_1 \beta}{h\left(\beta^2 + \eta_1^2 k_n^2\right)} + \frac{l}{h}\frac{2\eta_1^2 k_n^2}{3\left(\beta^2 + \eta_1^2 k_n^2\right)}} \times \left(1 - \frac{l}{h} - \frac{\eta_1 \beta}{h\left(\beta^2 + \eta_1^2 k_n^2\right)} \right) \qquad (11)$$

$$\to \frac{\eta_1 k_n^2 \rho_0 k_B T}{1 + \frac{\eta_1 \beta}{h\left(\beta^2 + \eta_1^2 k_n^2\right)}} \times \left(1 - \frac{\eta_1 \beta}{h\left(\beta^2 + \eta_1^2 k_n^2\right)} \right) = D_n^{bulk}$$

It is therefore straightforward to show that with the boundary slip, the Green-Kubo formula still holds (we evaluate (9) when $T_n\left(t\right) = e^{-\eta_1 k_n^2 t/\rho_0}$ to be equal to $N\rho_0^2 k_B T$ where N denotes the number of modes). It is stressed that boundary dissipation as indicated by Equation (10) that does not vanish when $h \gg l$ has to be considered together with the bulk contribution. That is, the Green-Kubo formula for one mode has to be written, in current case, as

$$2S\left[\int_0^h \eta_1 \left(\frac{\partial Z_n\left(z\right)}{\partial z} \right)^2 dz + \beta\left(\rho_0 v_{Sn}\right)^2 \right] \int_0^{+\infty} T_n\left(t\right) dt = \rho_0^2 k_B T \qquad (12)$$

It is also noted that with no boundary slip ($v_{Sn} = 0$), the above calculation leads to exactly the Green-Kubo formula of viscosity for one mode

$$2S\int_0^h \eta_1 \left(\frac{\partial Z_n\left(z\right)}{\partial z} \right)^2 dz \int_0^{+\infty} T_n\left(t\right) dt = \rho_0^2 k_B T \qquad (12a)$$

Further calculation shows that Equation (12a) leads to identity of the two sides $\eta_1 == \eta_1$, which can be demonstrated below:

$$\eta_1 = \frac{\rho_0^2 k_B T}{2S\int_0^h \left(\frac{\partial Z_n\left(z\right)}{\partial z} \right)^2 dz \int_0^{+\infty} T_n\left(t\right) dt}$$

$$= \frac{\rho_0^2 k_B T}{2S A_n^2 k_n^2 \int_0^h \cos^2\left(k_n z\right) dz \int_0^{+\infty} e^{-\eta_1 k_n^2 t/\rho_0} dt}$$

$$= \frac{\rho_0^2 k_B T}{2S \frac{\rho_0 k_B T}{Sh} k_n^2 \cdot \frac{h}{2} \cdot \frac{\rho_0}{\eta_1 k_n^2}} == \eta_1$$

We define a dimensionless boundary dissipation number:

$$C_n = \frac{1}{2}\frac{D_n^{boundary}}{D_n^{bulk} + D_n^{boundary}} = \frac{\eta_1 \beta}{h\left(\beta^2 + \eta_1^2 k_n^2\right) + \eta_1 \beta}$$

The Green-Kubo formula for boundary momentum density fluctuation for one mode can be written as

$$S\beta\left(\rho_0 v_{Sn}\right)^2 \int_0^{+\infty} T_n\left(t\right)dt = C_n \rho_0^2 k_B T$$

Or in general

$$\int_0^{+\infty} \left\langle j_n\left(z=h,t=0\right) j_n\left(z=h,t\right)\right\rangle dt = \frac{C_n \rho_0^2 k_B T}{S\beta} \qquad (13)$$

We calculate the total bulk and boundary dissipation. From (12), it follows

$$\begin{aligned}
&2S\sum_{n=0}^{N}\left[\int_0^h \eta_1\left(\frac{\partial Z_n\left(z\right)}{\partial z}\right)^2 dz\int_0^{+\infty} T_n\left(t\right)dt + \beta\left(\rho_0 v_{Sn}\right)^2 \int_0^{+\infty} T_n\left(t\right)dt\right] \\
&= 2S\int_0^{+\infty} dt\int_0^h dz\left\langle \eta_1\left(\frac{\partial J\left(z,t=0\right)}{\partial z}\right)\left(\frac{\partial J\left(z,t\right)}{\partial z}\right)\right\rangle + 2S\beta\int_0^{+\infty} dt\left\langle J\left(z=h,t=0\right)J\left(z=h,t\right)\right\rangle \\
&= \sum_{n=0}^{N}\left(1-2C_n\right)\rho_0^2 k_B T + \sum_{n=0}^{N} 2C_n \rho_0^2 k_B T
\end{aligned} \qquad (14)$$

Here we use

$$\left\langle J\left(z=h,t=0\right)J\left(z=h,t\right)\right\rangle = \sum_{n=0}^{N} j_n\left(z=h,t=0\right) j_n\left(z=h,t\right) = \sum_{n=0}^{N}\left(\rho_0 v_{Sn}\right)^2 T_n\left(t\right)$$

In Equation (13), the first terms in line 2 and line 3 represent the bulk contribution, and it gives

$$\boxed{\int_0^{+\infty} dt\int_0^h dz\left\langle\left(\frac{\partial J\left(z,t=0\right)}{\partial z}\right)\left(\frac{\partial J\left(z,t\right)}{\partial z}\right)\right\rangle = \sum_{n=0}^{N}\frac{\left(1-2C_n\right)\rho_0^2 k_B T}{2S\eta_1}} \qquad (15)$$

And the second terms in line 2 and line 3 represent the boundary contribution, giving

$$\boxed{\int_0^{+\infty}\left\langle J\left(z=h,t=0\right)J\left(z=h,t\right)\right\rangle dt = \sum_{n=0}^{N}\frac{C_n \rho_0^2 k_B T}{S\beta}} \qquad (16)$$

Note that N is determined by an upper cutoff in k_n which is $\sim \frac{\beta}{\eta_1}$.

From equipartition in z-space

If we suppose the initial state of the system is in equilibrium, $C(z,z^{'},t=0)$ is simply given by

$$C(z,z^{'},t=0)=\left\langle J\left(z,t=0\right)J\left(z',t=0\right)\right\rangle=\rho_0 k_B T\delta(z-z^{'})$$

Then we chose normalized $Z_n\left(z\right)$, which is denoted by $z_n\left(z\right)$ with $\int_0^h z_n^2(z)dz=h$ to serve as a set of basis. Note, determination of $z_n\left(z\right)$ uses the same process as in (4).

Then $\left\langle J\left(z,t=0\right)J\left(z',t=0\right)\right\rangle=\sum_{n=0}^{N} a_n\left(z'\right)z_n\left(z\right)$ Here we have applied the fact that $\left\langle z_m\left(z\right)z_n\left(z\right)\right\rangle=0$ when $m\neq n$.

And $$\alpha_n(z^{'})=\frac{\int_0^h dz C(z,z^{'},t=0)z_n(z)}{h}=\frac{\int_0^h dz k_B T\rho_0\delta(z-z^{'})z_n(z)}{h}=k_B T\rho_0 z_n(z^{'})$$

We get the finial expression:

$$C(z,z^{'},t)=\rho_0 k_B T\sum_{n=0}^{N} z_n(z)z_n(z^{'})T_n\left(t\right)$$

So the coefficients determined here is the same as previous ones