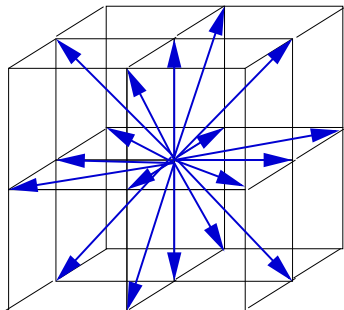


Theory of the Lattice Boltzmann Method

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B. D. and A. J. C. Ladd, arXiv:0803.2826v2,
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- \vec{c}_i small set of velocities
- $\vec{c}_i h$ connects two sites
- $n_i(\vec{r}, t)$: real number, mass density on site \vec{r} corresponding to velocity \vec{c}_i

- linearized Boltzmann equation (kinetic theory of gases)
- fully discretized
- sites \vec{r} , lattice spacing a
- time t , time step h

$$n_i(\vec{r} + \vec{c}_i h, t + h) = n_i^*(\vec{r}, t) = n_i(\vec{r}, t) + \Delta_i(\vec{r}, t)$$

Conservation laws, symmetries

$$n_i(\vec{r} + \vec{c}_i h, t + h) = n_i^*(\vec{r}, t) = n_i(\vec{r}, t) + \Delta_i \{n_i(\vec{r}, t)\}$$

$$\rho = \sum_i n_i$$

$$\vec{j} = \rho \vec{u} = \sum_i n_i \vec{c}_i$$

$$\sum_i \Delta_i = \sum_i \Delta_i \vec{c}_i = 0$$



mass conservation



momentum conservation



locality



rotational symmetry (lattice!)



Galilei invariance (finite number of velocities)

Low Mach number physics

- only $u \ll c_i$
- only $u \ll c_s$
- $Ma = u/c_s \ll 1$
- low Mach number \Rightarrow compressibility does not matter \Rightarrow equation of state does not matter \Rightarrow choose ideal gas!

m_p particle mass:

$$p = \frac{\rho}{m_p} k_B T$$

$$c_s^2 = \frac{\partial p}{\partial \rho} = \frac{1}{m_p} k_B T$$

$$p = \rho c_s^2$$

$$k_B T = m_p c_s^2$$

Where we want to get

in the continuum limit $a \rightarrow 0$, $h \rightarrow 0$:

$$\partial_t \rho + \partial_\alpha j_\alpha = 0$$

$$\partial_t j_\alpha + \partial_\beta (\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta) = \partial_\beta \sigma_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \eta_{\alpha\beta\gamma\delta} \partial_\gamma u_\delta$$

$$\eta_{\alpha\beta\gamma\delta} = \left(\zeta - \frac{2}{3} \eta \right) \delta_{\alpha\beta} \delta_{\gamma\delta} + \eta (\delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma})$$

- η shear viscosity
- ζ bulk viscosity

Difference equation \rightarrow differential equation

Example: consider

$$f(x+a) - f(x) = g(x)$$

small a :

$$a \frac{d}{dx} f(x) \approx g(x)$$

continuum limit $a \rightarrow 0$:

$$\frac{d}{dx} f(x) = \lim_{a \rightarrow 0} \frac{g(x)}{a}$$

watch out: if the rhs does not exist, then the continuum limit does not exist!

corrections to the leading behavior?

$$f(x+a) - f(x) = g(x)$$

set

$$D = a \frac{d}{dx}$$
$$g(x) = a(g_0(x) + ag_1(x) + a^2g_2(x) + \dots)$$

g_i independent of a

$$f(x_0+a) = f(x_0) + a \left. \frac{df}{dx} \right|_{x=x_0} + \frac{a^2}{2!} \left. \frac{d^2f}{dx^2} \right|_{x=x_0} + \dots$$
$$= \exp\left(a \frac{d}{dx}\right) f(x) \Big|_{x=x_0} = \exp(D) f(x) \Big|_{x=x_0}$$

$$\Rightarrow [\exp(D) - 1] f(x) = g(x)$$

$$f(x) = [\exp(D) - 1]^{-1} g(x)$$

$$Df(x) = D [\exp(D) - 1]^{-1} g(x)$$

now,

$$\frac{x}{\exp(x) - 1} = 1 - \frac{x}{2} + \frac{x^2}{12} - \frac{x^4}{720} + \frac{x^6}{30240} - + \dots = \sum_{k=0}^{\infty} \frac{B_k}{k!} x^k$$

Bernoulli numbers B_k

$$\begin{aligned} f(x+a) - f(x) &= g(x) \Leftrightarrow \\ Df(x) &= \left[1 - \frac{D}{2} + \frac{D^2}{12} + \dots \right] g(x) \\ \frac{d}{dx} f(x) &= \left[1 - \frac{D}{2} + \frac{D^2}{12} + \dots \right] \\ &\quad [g_0(x) + ag_1(x) + a^2g_2(x) + \dots] \end{aligned}$$

systematic expansion in powers of a !

LB continuum limit: how??

$a \rightarrow 0$, $h \rightarrow 0$ to be replaced by $\varepsilon \rightarrow 0$:

- wave-like scaling: $a/h = \text{const.}$

$$a = \varepsilon a_0$$

$$h = \varepsilon h_0$$

$$\vec{c}_i = \vec{c}_{i0}$$

$$n_i(\vec{r} + \varepsilon \vec{c}_{i0} h_0, t + \varepsilon h_0) - n_i(\vec{r}, t) = \Delta_i$$

- diffusive scaling: $a^2/h = \text{const.}$

$$a = \varepsilon a_0$$

$$h = \varepsilon^2 h_0$$

$$\vec{c}_i = \varepsilon^{-1} \vec{c}_{i0}$$

$$n_i(\vec{r} + \varepsilon \vec{c}_{i0} h_0, t + \varepsilon^2 h_0) - n_i(\vec{r}, t) = \Delta_i$$

Expanding the solution

lhs is $O(\varepsilon) \Rightarrow$ rhs must be $O(\varepsilon)$!

ansatz:

$$\begin{aligned}n_i &= n_i^{(0)} + \varepsilon n_i^{(1)} + O(\varepsilon^2) \\ \Delta_i \{n_i\} &= \Delta_i^{(0)} + \varepsilon \Delta_i^{(1)} + O(\varepsilon^2) \\ &= \Delta_i \{n_i^{(0)}\} + \varepsilon \sum_j \left. \frac{\partial \Delta_i}{\partial n_j} \right|_{n_i=n_i^{(0)}} n_j^{(1)} + O(\varepsilon^2) \\ &=: \varepsilon \sum_j L_{ij} n_j^{(1)} + O(\varepsilon^2)\end{aligned}$$

and

$$\Delta_i \{n_i^{(0)}\} = 0$$

conservation laws:

$$\sum_i \Delta_i^{(k)} = \sum_i \Delta_i^{(k)} \vec{c}_i = 0$$

$$0 = \Delta_i^{(0)} = \Delta_i \{n_i^{(0)}\}$$

- $\{n_i^{(0)}\}$ collisional invariant, $\{n_i^{(0)}\} = n_i^{eq}$
- no spurious conservation laws \Rightarrow
- $n_i^{(0)} = n_i^{(0)}(\rho, \vec{j})$

No expansion for conserved quantities!

$$n_i = n_i^{(0)} + \varepsilon n_i^{(1)} + O(\varepsilon^2)$$

$$\rho = \rho^{(0)} + \varepsilon \rho^{(1)} + O(\varepsilon^2)$$

$$\vec{j} = \vec{j}^{(0)} + \varepsilon \vec{j}^{(1)} + O(\varepsilon^2)$$

$$\begin{aligned} n_i^{(0)} &= n_i^{(0)}(\rho, \vec{j}) \\ &= n_i^{(0)}(\rho^{(0)} + \varepsilon \rho^{(1)} + O(\varepsilon^2), \vec{j}^{(0)} + \varepsilon \vec{j}^{(1)} + O(\varepsilon^2)) \end{aligned}$$

no expansion for $n_i^{(0)} \Rightarrow$

$$\rho^{(1)} = \rho^{(2)} = \dots = 0$$

$$\vec{j}^{(1)} = \vec{j}^{(2)} = \dots = 0$$

i. e.



$$\rho^{(0)} = \rho$$



$$\vec{j}^{(0)} = \vec{j}$$



$$\sum_i n_i^{eq} = \rho$$



$$\sum_i n_i^{eq} \vec{c}_i = \vec{j}$$

- mass density

$$\rho = \sum_i n_i$$

- momentum density

$$j_\alpha = \sum_i n_i c_{i\alpha}$$

- stress

$$\Pi_{\alpha\beta} = \sum_i n_i c_{i\alpha} c_{i\beta}$$

- 3rd moment

$$\Phi_{\alpha\beta\gamma} = \sum_i n_i c_{i\alpha} c_{i\beta} c_{i\gamma}$$

$$n_i(\vec{r} + \varepsilon \vec{c}_i h_0, t + \varepsilon h_0) - n_i(\vec{r}, t) = \Delta_i$$

set

$$D_i = \varepsilon h_0 \partial_t + \varepsilon h_0 c_{i\alpha} \partial_\alpha$$

$$D_i n_i = \left[1 - \frac{D_i}{2} + \frac{D_i^2}{12} + \dots \right] \Delta_i$$

• ε^1 :

$$(h_0 \partial_t + h_0 c_{i\alpha} \partial_\alpha) n_i^{(0)} = \Delta_i^{(1)}$$

• ε^2 :

$$(h_0 \partial_t + h_0 c_{i\alpha} \partial_\alpha) n_i^{(1)} = \Delta_i^{(2)} - \frac{1}{2} (h_0 \partial_t + h_0 c_{i\alpha} \partial_\alpha) \Delta_i^{(1)}$$

take zeroth and first velocity moment:

- ε^1 :

$$\begin{aligned}h_0 \partial_t \rho + h_0 \partial_\alpha j_\alpha &= 0 \\h_0 \partial_t j_\beta + h_0 \partial_\alpha \Pi_{\alpha\beta}^{(0)} &= 0\end{aligned}$$

or

$$\begin{aligned}\partial_t \rho + \partial_\alpha j_\alpha &= 0 \\ \partial_t j_\beta + \partial_\alpha \Pi_{\alpha\beta}^{(0)} &= 0\end{aligned}$$

- ε^2 :

$$\begin{aligned}0 &= 0 \\ h_0 \partial_\alpha \Pi_{\alpha\beta}^{(1)} &= -\frac{1}{2} h_0 \partial_\alpha \left(\Pi_{\alpha\beta}^{(1)*} - \Pi_{\alpha\beta}^{(1)} \right)\end{aligned}$$

or

$$\frac{1}{2} \partial_\alpha \left(\Pi_{\alpha\beta}^{(1)*} + \Pi_{\alpha\beta}^{(1)} \right) = 0$$

consequences:

- $\Pi^{(0)}$ depends only on ρ, \vec{j} (locally!!)
- $\Rightarrow \Pi^{(0)}$ must be the Euler stress!
- i. e.

$$\sum_i n_i^{eq} c_{i\alpha} c_{i\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

- stress relaxation at order ε^2 gives rise to “some sort of” dissipation, **but no relation** to the previous order
- i. e. relation to velocity gradients (viscous shear stresses) can not be established!
- we find: Euler equations at order ε^1 , but no useful results beyond!

can we at least adjust n_i^{eq} such that we get Euler in the leading order? **YES!**

The equilibrium populations

ansatz (Euler stress is a 2nd order polynomial in \vec{u}):

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho (1 + A \vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + C u^2)$$

w_i positive weights, identical within a shell. cubic symmetry:

$$\sum_i w_i = 1$$

$$\sum_i w_i c_{i\alpha} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} = \sigma_2 \delta_{\alpha\beta}$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = \kappa_4 \delta_{\alpha\beta\gamma\delta}$$

$$+\sigma_4 (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$$

mass:

$$\begin{aligned}\rho &= \sum_i n_i^{eq} \\ &= \rho \sum_i w_i (1 + A\vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + Cu^2)\end{aligned}$$

$$\begin{aligned}0 &= Bu_\alpha u_\beta \sum_i w_i c_{i\alpha} c_{i\beta} + Cu^2 \\ &= Bu_\alpha u_\beta \sigma_2 \delta_{\alpha\beta} + Cu^2 \\ &= (B\sigma_2 + C) u^2\end{aligned}$$

$$C + B\sigma_2 = 0$$

momentum:

$$\begin{aligned}\rho u_\alpha &= \sum_i n_i^{\text{eq}} c_{i\alpha} \\ &= \rho \sum_i w_i c_{i\alpha} (1 + A\vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + Cu^2) \\ &= \rho A u_\beta \sum_i w_i c_{i\alpha} c_{i\beta} \\ &= \rho A u_\beta \sigma_2 \delta_{\alpha\beta} \\ &= \rho A \sigma_2 u_\alpha \\ A \sigma_2 &= 1\end{aligned}$$

stress:

$$\begin{aligned}c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta &= \frac{1}{\rho} \sum_i n_i^{eq} c_{i\alpha} c_{i\beta} \\ &= \sum_i w_i c_{i\alpha} c_{i\beta} (1 + A \vec{u} \cdot \vec{c}_i + B (\vec{u} \cdot \vec{c}_i)^2 + C u^2) \\ &= (1 + C u^2) \sigma_2 \delta_{\alpha\beta} + B u_\gamma u_\delta \kappa_4 \delta_{\alpha\beta\gamma\delta} \\ &+ B u_\gamma u_\delta \sigma_4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma})\end{aligned}$$

hence $\kappa_4 = 0$ and

$$c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta = (\sigma_2 + C \sigma_2 u^2 + B \sigma_4 u^2) \delta_{\alpha\beta} + 2B \sigma_4 u_\alpha u_\beta$$

i. e. $\sigma_2 = c_s^2$, $C \sigma_2 + B \sigma_4 = 0$, $2B \sigma_4 = 1$

taken all together:

$$\kappa_4 = 0$$

$$\sigma_2 = c_s^2$$

$$2B\sigma_4 = 1$$

$$C\sigma_2 + B\sigma_4 = 0$$

$$C + B\sigma_2 = 0$$

$$A\sigma_2 = 1$$

six equations, six unknowns. multiply Eq. 5 with σ_2 and compare with Eq. 4. hence the solution is:

$$\kappa_4 = 0$$

$$\sigma_2 = c_s^2$$

$$\sigma_4 = c_s^4$$

$$A = 1/c_s^2$$

$$B = 1/(2c_s^4)$$

$$C = -1/(2c_s^2)$$

form of the equilibrium populations is

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho \left(1 + \frac{\vec{u} \cdot \vec{c}_i}{c_s^2} + \frac{(\vec{u} \cdot \vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right)$$

what are the weights? we need to satisfy the three conditions:

$$\begin{aligned} \sum_i w_i &= 1 \\ \kappa_4 &= 0 \\ \sigma_4 &= \sigma_2^2 \end{aligned}$$

therefore, at least three shells are needed! each shell is assigned its own σ_2 , σ_4 , κ_4 (assuming weight one).

- one zero velocity: $\vec{c}_i = 0$, weight w_0
- six nearest neighbors: $\vec{c}_i = (a/h)(\pm 1, 0, 0)$, $(a/h)(0, \pm 1, 0)$, $(a/h)(0, 0, \pm 1)$, weight w_I
- twelve next-nearest neighbors: $\vec{c}_i = (a/h)(\pm 1, \pm 1, 0)$, $(a/h)(\pm 1, 0, \pm 1)$, $(a/h)(0, \pm 1, \pm 1)$, weight w_{II}
- zeroth shell: velocity moments trivial

- first shell:

$$\sum_i c_{i1}^2 = 2(a/h)^2 = \sigma_2(l)$$

$$\sum_i c_{i1}^4 = 2(a/h)^4 = \kappa_4(l) + 3\sigma_4(l)$$

$$\sum_i c_{i1}^2 c_{i2}^2 = 0 = \sigma_4(l)$$

$$\sigma_2(l) = 2(a/h)^2$$

$$\sigma_4(l) = 0$$

$$\kappa_4(l) = 2(a/h)^4$$

- second shell:

$$\sum_i c_{i1}^2 = 8(a/h)^2 = \sigma_2(l)$$

$$\sum_i c_{i1}^4 = 8(a/h)^4 = \kappa_4(l) + 3\sigma_4(l)$$

$$\sum_i c_{i1}^2 c_{i2}^2 = 4(a/h)^4 = \sigma_4(l)$$

$$\sigma_2(l) = 8(a/h)^2$$

$$\sigma_4(l) = 4(a/h)^4$$

$$\kappa_4(l) = -4(a/h)^4$$

$$\begin{aligned}
0 &= \kappa_4 \\
&= w_I \kappa_4(I) + w_{II} \kappa_4(II) \\
&= 2w_I - 4w_{II} \\
w_I &= 2w_{II} \\
\sigma_2 &= w_I \sigma_2(I) + w_{II} \sigma_2(II) \\
&= w_{II} (2\sigma_2(I) + \sigma_2(II)) \\
&= w_{II} (a/h)^2 (2 \cdot 2 + 8) \\
&= 12w_{II} (a/h)^2 \\
\sigma_4 &= w_I \sigma_4(I) + w_{II} \sigma_4(II) \\
&= w_{II} (2\sigma_4(I) + \sigma_4(II)) \\
&= 4w_{II} (a/h)^4 \\
&= \sigma_2^2 \\
&= 144w_{II}^2 (a/h)^4
\end{aligned}$$

$$\begin{aligned}
 1 &= 36w_{II} \\
 w_{II} &= \frac{1}{36} \\
 w_I &= 2w_{II} = \frac{1}{18} \\
 1 &= w_0 + 6w_I + 12w_{II} \\
 &= w_0 + \frac{1}{3} + \frac{1}{3} \\
 w_0 &= \frac{1}{3} \\
 c_s^2 &= \sigma_2 \\
 &= 12w_{II}(a/h)^2 \\
 &= \frac{1}{3}(a/h)^2
 \end{aligned}$$

all coefficients of n_i^{eq} known!

$$n_i(\vec{r} + \varepsilon \vec{c}_{i0} h_0, t + \varepsilon^2 h_0) - n_i(\vec{r}, t) = \Delta_i$$

watch out: $\vec{c}_i = \varepsilon^{-1} \vec{c}_{i0}$! define moments wrt \vec{c}_{i0} , not \vec{c}_i ! e. g.
 $\vec{j} = \sum_i n_i \vec{c}_{i0}$ etc.!

set:

$$D_i = \varepsilon^2 h_0 \partial_t + \varepsilon h_0 c_{i0\alpha} \partial_\alpha$$

$$D_i n_i = \left[1 - \frac{D_i}{2} + \frac{D_i^2}{12} + \dots \right] \Delta_i$$

• ε^1 :

$$h_0 c_{i0\alpha} \partial_\alpha n_i^{(0)} = \Delta_i^{(1)}$$

• ε^2 :

$$h_0 \partial_t n_i^{(0)} + h_0 c_{i0\alpha} \partial_\alpha n_i^{(1)} = \Delta_i^{(2)} - \frac{1}{2} h_0 c_{i0\alpha} \partial_\alpha \Delta_i^{(1)}$$

$$h_0 c_{i0\alpha} \partial_\alpha n_i^{(0)} = \Delta_i^{(1)}$$

zeroth velocity moment:

$$\partial_\alpha j_\alpha = 0$$

first velocity moment:

$$\partial_\alpha \Pi_{\alpha\beta}^{(0)} = 0$$

$$h_0 \partial_t n_i^{(0)} + h_0 c_{i0\alpha} \partial_\alpha n_i^{(1)} = \Delta_i^{(2)} - \frac{1}{2} h_0 c_{i0\alpha} \partial_\alpha \Delta_i^{(1)}$$

zeroth velocity moment:

$$\partial_t \rho = 0$$

incompressible fluid!

1st velocity moment:

$$\begin{aligned} \partial_t j_\beta + \partial_\alpha \Pi_{\alpha\beta}^{(1)} &= -\frac{1}{2} \partial_\alpha \left(\Pi_{\alpha\beta}^{(1)*} - \Pi_{\alpha\beta}^{(1)} \right) \\ \partial_t j_\beta + \frac{1}{2} \partial_\alpha \left(\Pi_{\alpha\beta}^{(1)*} + \Pi_{\alpha\beta}^{(1)} \right) &= 0 \end{aligned}$$

Adding the equations

$$\begin{aligned}\partial_t \rho + \partial_\alpha j_\alpha &= 0 \\ \partial_t j_\beta + \partial_\alpha \Pi_{\alpha\beta}^{(0)} + \frac{1}{2} \partial_\alpha \left(\Pi_{\alpha\beta}^{(1)*} + \Pi_{\alpha\beta}^{(1)} \right) &= 0\end{aligned}$$

looks like Navier–Stokes; $\Pi^{(0)}$ Euler stress, $(1/2) (\Pi^{(1)*} + \Pi^{(1)})$ viscous stress; **BUT**

- dynamics with *constraints*:

$$\begin{aligned}\partial_\alpha j_\alpha &= 0 \\ \partial_\alpha \Pi_{\alpha\beta}^{(0)} &= 0 \\ \partial_t \rho &= 0\end{aligned}$$

- incompressible \rightarrow pressure as a Lagrange multiplier
- difficult to analyze! (Junk / Luo / Klar)

All these difficulties go away when one combines wave-like and diffusive scaling in a multiple time scale analysis!

So, what is this?

The idea of multiple time scale expansion

example: damped oscillator

$$\frac{d^2}{dt^2}x + \frac{1}{\tau} \frac{d}{dt}x + \frac{1}{T^2}x = 0$$

- T oscillation period
- τ frictional relaxation time
- consider $T \ll \tau$ (weak damping)
- try to treat

$$\varepsilon := \frac{T}{2\tau}$$

as a small parameter for **perturbation theory**

- unit system: set $T = 1$

$$\frac{d^2}{dt^2}x + 2\varepsilon \frac{d}{dt}x + x = 0$$

$$\frac{d^2}{dt^2}x + 2\varepsilon \frac{d}{dt}x + x = 0$$

- $x(t=0) = 1, \dot{x}(t=0) = -\varepsilon$
- exactly solvable

$$x(t) = \exp(-\varepsilon t) \cos\left(\sqrt{1 - \varepsilon^2}t\right)$$

ε dependence looks harmless, **but** ...

$$\frac{d^2}{dt^2}x + 2\varepsilon \frac{d}{dt}x + x = 0$$

$$x(t) = x_0(t) + \varepsilon x_1(t) + \varepsilon^2 x_2(t) + \dots$$

yields hierarchy:

$$\ddot{x}_k + x_k = -2\dot{x}_{k-1}$$

with (def.) $x_{-1} = 0$, plus corresponding hierarchy of initial conditions

- ε^0 :

$$x_0 = \cos t$$

- ε^1 :

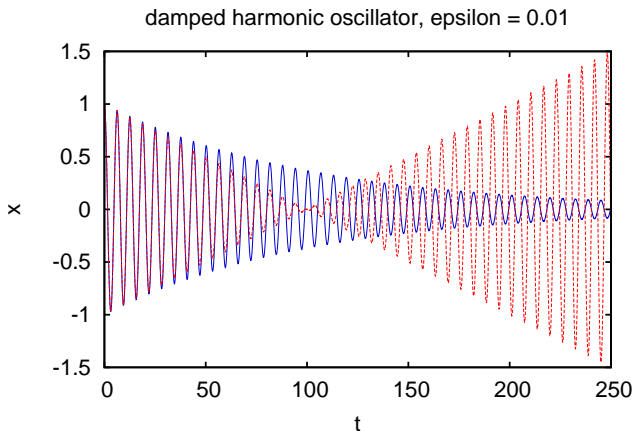
$$x_1 = -t \cos t$$

i. e., 1st order perturbation theory yields

$$x(t) = (1 - \varepsilon t) \cos t + O(\varepsilon^2)$$

identical with Taylor expansion of the exact solution!

For $t \gg 1/\varepsilon$ this becomes completely useless!!!



Deficiencies of naive perturbation theory:

- does not capture the presence of different time scales (here: fast oscillations vs. slow damping)
- typically, this occurs if one has *qualitatively different* behavior for $\varepsilon = 0$ and small $\varepsilon > 0$ (here: conservative vs. dissipative)
- “singular perturbation theory” needed

Multiple time scale analysis

Idea:

$$\begin{aligned}x(t) &= \exp(-\varepsilon t) \cos\left(\sqrt{1-\varepsilon^2}t\right) \\ &\approx \exp(-\varepsilon t) \cos t \\ &= \exp(-t_1) \cos t \\ &= x(t, t_1)\end{aligned}$$

with

$$t_1 = \varepsilon t$$

consider x as a function of *two independent* variables t, t_1

\Rightarrow should be able to grasp the time scale separation!

hence, study expansion

$$x(t, t_1) = x_0(t, t_1) + \varepsilon x_1(t, t_1) + \varepsilon^2 x_2(t, t_1) + \dots$$

with

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{\partial t_1}{\partial t} \frac{\partial}{\partial t_1} = \frac{\partial}{\partial t} + \varepsilon \frac{\partial}{\partial t_1}$$

again the damped oscillator:

$$\begin{aligned}\frac{d}{dt}x &= p \\ \frac{d}{dt}p &= -2\varepsilon p - x\end{aligned}$$

(expand both x and p)

ε^0 :

$$\begin{aligned}\frac{\partial}{\partial t}x_0 &= p_0 \\ \frac{\partial}{\partial t}p_0 &= -x_0 \\ x_0 &= A(t_1) \cos t + B(t_1) \sin t \\ p_0 &= -A(t_1) \sin t + B(t_1) \cos t\end{aligned}$$

$A(t_1)$, $B(t_1)$ not yet known

ε^1 :

$$\begin{aligned}\frac{\partial}{\partial t}x_1 &= p_1 - \frac{\partial}{\partial t_1}x_0 \\ \frac{\partial}{\partial t}p_1 &= -x_1 - \frac{\partial}{\partial t_1}p_0 - 2p_0\end{aligned}$$

ansatz

$$\begin{aligned}x_1 &= C(t, t_1) \cos t + D(t, t_1) \sin t \\ p_1 &= -C(t, t_1) \sin t + D(t, t_1) \cos t\end{aligned}$$

yields

$$\begin{aligned}\frac{\partial C}{\partial t} &= -\frac{\partial A}{\partial t_1} - 2A \sin^2 t + 2B \sin t \cos t \\ \frac{\partial D}{\partial t} &= -\frac{\partial B}{\partial t_1} - 2B \cos^2 t + 2A \sin t \cos t\end{aligned}$$

integrate wrt t , but the solution **should not explode!!!**

now,

$$\langle \sin^2 t \rangle = \langle \cos^2 t \rangle = \frac{1}{2}$$

hence

$$\frac{\partial A}{\partial t_1} + A = 0$$

$$\frac{\partial B}{\partial t_1} + B = 0$$

or

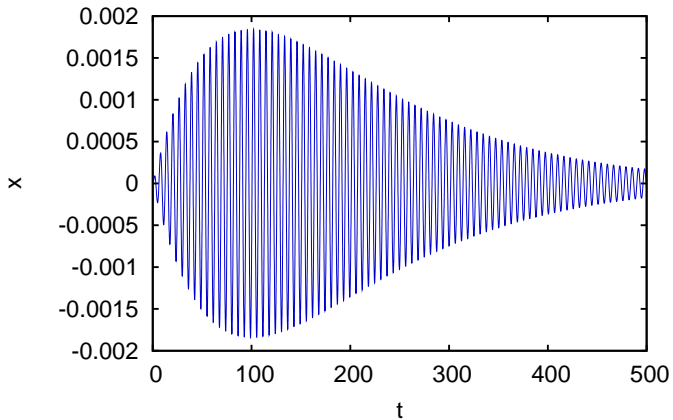
$$A = \hat{A} \exp(-t_1)$$

$$B = \hat{B} \exp(-t_1)$$

insert this into ε^0 solution, initial conditions:

$$x_0 = \exp(-\varepsilon t) \cos t$$

difference exact vs. perturbation theory, $\epsilon = 0.01$



Chapman–Enskog expansion

- original LBE:

$$n_i(\vec{r} + \vec{c}_i h, t + h) - n_i(\vec{r}, t) = \Delta_i$$

- desired: continuum limit $h \rightarrow 0$, \vec{c}_i fixed
- set $h = \varepsilon h_0$
- expansion parameter $\varepsilon \ll 1$, $\varepsilon \rightarrow 0$
- write $t_1 = t$, $\vec{r}_1 = \vec{r}$
- yields:

$$n_i(\vec{r}_1 + \vec{c}_i \varepsilon h_0, t_1 + \varepsilon h_0) - n_i(\vec{r}_1, t_1) = \Delta_i$$

- two time scales:
 - waves: time \sim length
 - diffusion: time \sim (length)²
- second time scale: $t_2 = \varepsilon t$

- study LBE:

$$n_i(\vec{r}_1 + \varepsilon \vec{c}_i h_0, t_1 + \varepsilon h_0, t_2 + \varepsilon^2 h_0) - n_i(\vec{r}_1, t_1, t_2) = \Delta_i$$

-

$$\frac{\partial}{\partial \vec{r}} = \frac{\partial}{\partial \vec{r}_1}$$

-

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_1} + \varepsilon \frac{\partial}{\partial t_2}$$

- set

$$D_i = \varepsilon h_0 c_{i\alpha} \partial_{1\alpha} + \varepsilon h_0 \partial_{t_1} + \varepsilon^2 h_0 \partial_{t_2}$$

$$D_i n_i = \left[1 - \frac{D_i}{2} + \frac{D_i^2}{12} + \dots \right] \Delta_i$$

- ε^1 :

$$(h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) n_i^{(0)} = \Delta_i^{(1)}$$

- ε^2 :

$$\begin{aligned} & h_0 \partial_{t2} n_i^{(0)} + (h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) n_i^{(1)} \\ = & \Delta_i^{(2)} - \frac{1}{2} (h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) \Delta_i^{(1)} \end{aligned}$$

or

$$h_0 \partial_{t2} n_i^{(0)} + \frac{1}{2} (h_0 c_{i\alpha} \partial_{1\alpha} + h_0 \partial_{t1}) (n_i^{(1)*} + n_i^{(1)}) = \Delta_i^{(2)}$$

Zerth velocity moment: Mass conservation

$$\partial_{t_1} \rho + \partial_{1\alpha} j_\alpha = 0$$

$$\partial_{t_2} \rho = 0$$

Hence,

👍 continuity equation OK!!!

First velocity moment: Momentum conservation

$$\partial_{t_1} j_\alpha + \partial_{1\beta} \Pi_{\alpha\beta}^{(0)} = 0$$

$$\partial_{t_2} j_\alpha + \frac{1}{2} \partial_{1\beta} \left(\Pi_{\alpha\beta}^{*(1)} + \Pi_{\alpha\beta}^{(1)} \right) = 0$$

comparison with Navier–Stokes:

Euler stress:

$$\Pi_{\alpha\beta}^{(0)} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

Newtonian viscous stress:

$$\frac{\varepsilon}{2} \left(\Pi_{\alpha\beta}^{*(1)} + \Pi_{\alpha\beta}^{(1)} \right) = -\sigma_{\alpha\beta}$$

Second velocity moment: A useful relation

$$\partial_{t_1} \Pi_{\alpha\beta}^{(0)} + \partial_{1\gamma} \Phi_{\alpha\beta\gamma}^{(0)} = h_0^{-1} \left(\Pi_{\alpha\beta}^{*(1)} - \Pi_{\alpha\beta}^{(1)} \right)$$

from explicit form of n_i^{eq} :

$$\Phi_{\alpha\beta\gamma}^{(0)} = \rho c_s^2 (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta})$$

use continuity and Euler for

$$\partial_{t_1} \Pi_{\alpha\beta}^{(0)} = \partial_{t_1} (\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta) = \dots$$

\Rightarrow (neglecting terms $O(u^3)$):

$$\Pi_{\alpha\beta}^{*(1)} - \Pi_{\alpha\beta}^{(1)} = h_0 \rho c_s^2 (\partial_\alpha u_\beta + \partial_\beta u_\alpha)$$

(details see next three slides)

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho \left(1 + \frac{\vec{u} \cdot \vec{c}_i}{c_s^2} + \frac{(\vec{u} \cdot \vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right)$$

hence

$$\begin{aligned}\Phi_{\alpha\beta\gamma} &= \frac{\rho}{c_s^2} u_\delta \sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} \\ &= \frac{\rho}{c_s^2} u_\delta c_s^4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \\ &= \rho c_s^2 (\delta_{\alpha\beta} u_\gamma + \delta_{\alpha\gamma} u_\beta + \delta_{\beta\gamma} u_\alpha)\end{aligned}$$

Equation of motion for the Euler stress

pure Euler hydrodynamics

$$\Pi_{\alpha\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

Euler equations:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_\gamma \partial_\gamma$$

$$\frac{D}{Dt} \rho = -\rho \partial_\gamma u_\gamma$$

$$\rho \frac{D}{Dt} u_\alpha = -c_s^2 \partial_\alpha \rho$$

$$\begin{aligned} \frac{D}{Dt} \Pi_{\alpha\beta} &= (c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta) \frac{D}{Dt} \rho + u_\alpha \rho \frac{D}{Dt} u_\beta + u_\beta \rho \frac{D}{Dt} u_\alpha \\ &= -\rho (c_s^2 \delta_{\alpha\beta} + u_\alpha u_\beta) \partial_\gamma u_\gamma - c_s^2 u_\alpha \partial_\beta \rho - c_s^2 u_\beta \partial_\alpha \rho \end{aligned}$$

neglect $O(u^3)$:

$$\frac{\partial}{\partial t} \Pi_{\alpha\beta} + u_\gamma c_s^2 \delta_{\alpha\beta} \partial_\gamma \rho = -c_s^2 \delta_{\alpha\beta} \rho \partial_\gamma u_\gamma - c_s^2 u_\alpha \partial_\beta \rho - c_s^2 u_\beta \partial_\alpha \rho$$

$$\begin{aligned}
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + c_s^2 \delta_{\alpha\beta} \partial_\gamma (\rho u_\gamma) + c_s^2 u_\alpha \partial_\beta \rho + c_s^2 u_\beta \partial_\alpha \rho = 0 \\
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + c_s^2 \delta_{\alpha\beta} \partial_\gamma (\rho u_\gamma) + c_s^2 \partial_\beta (\rho u_\alpha) + c_s^2 \partial_\alpha (\rho u_\beta) \\
= & c_s^2 \rho \partial_\beta u_\alpha + c_s^2 \rho \partial_\alpha u_\beta \\
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + \partial_\gamma \{ \rho c_s^2 (\delta_{\alpha\beta} u_\gamma + \delta_{\beta\gamma} u_\alpha + \delta_{\alpha\gamma} u_\beta) \} \\
= & c_s^2 \rho \partial_\beta u_\alpha + c_s^2 \rho \partial_\alpha u_\beta \\
& \frac{\partial}{\partial t} \Pi_{\alpha\beta} + \partial_\gamma \Phi_{\alpha\beta\gamma} = \rho c_s^2 (\partial_\alpha u_\beta + \partial_\beta u_\alpha)
\end{aligned}$$

$$\begin{aligned}\Delta_i &= \Delta_i^{(0)} + \varepsilon \Delta_i^{(1)} + O(\varepsilon^2) \\ &= \varepsilon \Delta_i^{(1)} + O(\varepsilon^2)\end{aligned}$$

$O(\varepsilon^2)$ does not contribute to hydrodynamics \Rightarrow ignore

$$\Delta_i^{(1)} = \sum_j \left. \frac{\partial \Delta_i}{\partial n_j} \right|_{\{n_k^0\}} n_j^{(1)} = \sum_j L_{ij} n_j^{(1)}$$

i. e.

$$\Delta_i = \sum_j L_{ij} (n_j - n_j^{eq})$$

The linear collision process

$$n_i^{neq} := n_i - n_i^{eq}$$

$$n_i^* = n_i + \sum_j L_{ij} n_j^{neq}$$

$$n_i^{neq*} = n_i^{neq} + \sum_j L_{ij} n_j^{neq}$$

$$\Gamma_{ij} := \delta_{ij} + L_{ij}$$

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$\Gamma = ???$

simplest choice: Lattice BGK:

$$\Gamma_{ij} = \left(1 - \frac{1}{\tau}\right) \delta_{ij}$$

study here the MRT (multi relaxation time) framework!

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$$\sum_i \Rightarrow$$

$$0 = \sum_j \left(\sum_i \Gamma_{ij} \right) n_j^{neq}$$

$$0 = \sum_i \Gamma_{ij}$$

$$e_{0i} := 1$$

$$e_{0j} \cdot 0 = \sum_i e_{0i} \Gamma_{ij}$$

i. e. \vec{e}_0 is left eigenvector, eigenvalue zero.

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$$\sum_i c_{ix} \Rightarrow$$

$$0 = \sum_j \left(\sum_i c_{ix} \Gamma_{ij} \right) n_j^{neq}$$

$$0 = \sum_i c_{ix} \Gamma_{ij}$$

$$e_{1i} := c_{ix}$$

$$e_{1j} \cdot 0 = \sum_i e_{1i} \Gamma_{ij}$$

i. e. \vec{e}_1 is left eigenvector, eigenvalue zero.

analogous: $e_{2i} = c_{iy}$, $e_{3i} = c_{iz}$

$$n_i^{neq*} = \sum_j \Gamma_{ij} n_j^{neq}$$

$\sum_i c_{i\gamma} c_{i\gamma}$ (bulk stress) \Rightarrow (bulk stress relaxation with γ_b):

$$\Pi_{\gamma\gamma}^{neq*} = \sum_j \left(\sum_i c_{i\gamma} c_{i\gamma} \Gamma_{ij} \right) n_j^{neq}$$

$$\Pi_{\gamma\gamma}^{neq*} = \gamma_b \Pi_{\gamma\gamma}^{neq} = \gamma_b \sum_j n_j^{neq} c_{j\gamma} c_{j\gamma} = \sum_j (\gamma_b c_{j\gamma} c_{j\gamma}) n_j^{neq}$$

$$\gamma_b c_{j\gamma} c_{j\gamma} = \sum_i c_{i\gamma} c_{i\gamma} \Gamma_{ij}$$

$$e_{4i} := c_{i\gamma} c_{i\gamma}$$

$$e_{4j} \gamma_b = \sum_i e_{4i} \Gamma_{ij}$$

i. e. \vec{e}_4 is left eigenvector, eigenvalue γ_b

... and so on! $\vec{e}_5, \dots, \vec{e}_9$: five shear stresses, eigenvalue γ_s (same value for symmetry reasons)

$\vec{e}_{10}, \dots, \vec{e}_{18}$ 9 “kinetic modes”, “ghost modes” (higher-order polynomials in the \vec{c}_i)

i. e. we do not know Γ directly, but its eigenvalues and eigenvectors!

generally (eigenvalues γ_i)

$$e_{kj}\gamma_k = \sum_i e_{ki}\Gamma_{ij}$$

$$|\gamma_i| \leq 1$$

for linear stability!

set

$$\begin{aligned}
 m_k &= \sum_j e_{kj} n_j \\
 m_k^{neq*} &= \sum_i e_{ki} n_i^{neq*} = \sum_i e_{ki} \sum_j \Gamma_{ij} n_j^{neq} \\
 &= \sum_j \left(\sum_i e_{ki} \Gamma_{ij} \right) n_j^{neq} = \sum_j e_{kj} \gamma_k n_j^{neq} = \gamma_k m_k^{neq}
 \end{aligned}$$

I. e. the relaxation process is simple in mode space!

- $\gamma_0 = \gamma_1 = \gamma_2 = \gamma_3 = 0$ (mass and momentum conservation)
- $\gamma_4 = \gamma_b$ (bulk stress)
- $\gamma_5 = \dots = \gamma_9 = \gamma_s$ (shear stress)
- $\gamma_{10} = \dots = \gamma_{18} = 0$ (simplest choice, not necessary)

scalar product:

$$\langle \vec{n}' | \vec{n} \rangle = \sum_i w_i n'_i n_i$$

Claim: It is possible to pick the eigenvectors in such a way that they satisfy

$$\langle \vec{e}_k | \vec{e}_l \rangle = \mathcal{N}_k \delta_{kl}$$

where the \mathcal{N}_k are just normalization constants.

Proof: Either you understand group theory pretty well, or you do an explicit Gram–Schmidt orthogonalization! Result is tabulated in the review!

$$\begin{aligned}
\delta_{kl} &= \frac{1}{\mathcal{N}_k} \sum_i w_i e_{ki} e_{li} \\
&= \sum_i \sqrt{\frac{w_i}{\mathcal{N}_k}} e_{ki} \sqrt{\frac{w_i}{\mathcal{N}_l}} e_{li} \\
\hat{e}_{ki} &:= \sqrt{\frac{w_i}{\mathcal{N}_k}} e_{ki} \\
\delta_{kl} &= \sum_i \hat{e}_{ki} \hat{e}_{li}
\end{aligned}$$

i. e. \hat{e}_{ki} is a standard orthogonal matrix with Euclidean scalar product!

$$\begin{aligned}
 m_k &= \sum_i e_{ki} n_i = \sum_i \sqrt{\frac{\mathcal{N}_k}{w_i}} \hat{e}_{ki} n_i \\
 \hat{m}_k &:= \frac{1}{\sqrt{\mathcal{N}_k}} m_k \\
 \hat{n}_i &:= \frac{1}{\sqrt{w_i}} n_i \\
 \hat{m}_k &= \sum_i \hat{e}_{ki} \hat{n}_i
 \end{aligned}$$

orthonormal transformation, trivial to invert!

$$\Pi_{\alpha\beta} = \bar{\Pi}_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta}\Pi_{\gamma\gamma}$$

$$\bar{\Pi}_{\alpha\beta}^{*neq} = \gamma_s \bar{\Pi}_{\alpha\beta}^{neq}$$

$$\bar{\Pi}_{\gamma\gamma}^{*neq} = \gamma_b \bar{\Pi}_{\gamma\gamma}^{neq}$$

$$\begin{aligned}\Pi_{\alpha\beta}^{*neq} - \Pi_{\alpha\beta}^{neq} &= \bar{\Pi}_{\alpha\beta}^{*neq} - \bar{\Pi}_{\alpha\beta}^{neq} + \frac{1}{3}\delta_{\alpha\beta} (\Pi_{\gamma\gamma}^{*neq} - \Pi_{\gamma\gamma}^{neq}) \\ &= (\gamma_s - 1) \bar{\Pi}_{\alpha\beta}^{neq} + \frac{1}{3}\delta_{\alpha\beta} (\gamma_b - 1) \bar{\Pi}_{\gamma\gamma}^{neq}\end{aligned}$$

on the other hand, we had derived

$$\begin{aligned}\Pi_{\alpha\beta}^{*neq} - \Pi_{\alpha\beta}^{neq} &= h\rho c_s^2 (\partial_\alpha u_\beta + \partial_\beta u_\alpha) \\ &= h\rho c_s^2 \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ &\quad + \frac{2}{3} h\rho c_s^2 \delta_{\alpha\beta} \partial_\gamma u_\gamma\end{aligned}$$

comparison:

$$\begin{aligned}(\gamma_s - 1) \bar{\Pi}_{\alpha\beta}^{neq} &= h\rho c_s^2 \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ (\gamma_b - 1) \Pi_{\gamma\gamma}^{neq} &= 2h\rho c_s^2 \partial_\gamma u_\gamma\end{aligned}$$

or

$$\begin{aligned}\bar{\Pi}_{\alpha\beta}^{neq} &= \frac{h\rho c_s^2}{\gamma_s - 1} \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ \Pi_{\gamma\gamma}^{neq} &= \frac{2h\rho c_s^2}{\gamma_b - 1} \partial_\gamma u_\gamma\end{aligned}$$

Chapman–Enskog told us: Newtonian viscous stress is

$$-\sigma_{\alpha\beta} = \frac{1}{2} \left(\Pi_{\alpha\beta}^{neq*} + \Pi_{\alpha\beta}^{neq} \right)$$

hence

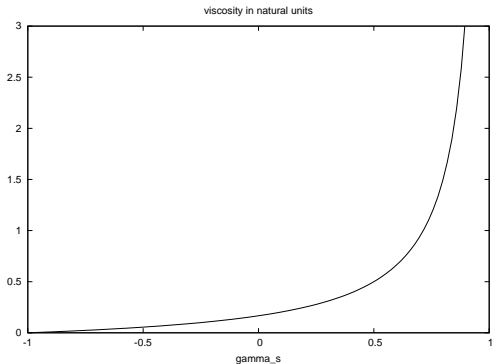
$$\begin{aligned} \frac{1}{2} \left(\bar{\Pi}_{\alpha\beta}^{neq*} + \bar{\Pi}_{\alpha\beta}^{neq} \right) &= \frac{1}{2} (\gamma_s + 1) \bar{\Pi}_{\alpha\beta}^{neq} \\ &= \frac{h\rho c_s^2}{2} \frac{\gamma_s + 1}{\gamma_s - 1} \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \\ &= -\eta \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma u_\gamma \right) \end{aligned}$$

and

$$\begin{aligned} \frac{1}{2} \frac{1}{3} \delta_{\alpha\beta} \left(\Pi_{\gamma\gamma}^{neq*} + \Pi_{\gamma\gamma}^{neq} \right) &= \frac{1}{2} \frac{1}{3} \delta_{\alpha\beta} (\gamma_b + 1) \Pi_{\gamma\gamma}^{neq} \\ &= \frac{h\rho c_s^2}{3} \frac{\gamma_b + 1}{\gamma_b - 1} \delta_{\alpha\beta} \partial_\gamma u_\gamma \\ &= -\zeta \delta_{\alpha\beta} \partial_\gamma u_\gamma \end{aligned}$$

read off viscosities:

$$\eta = \frac{h\rho c_s^2}{2} \frac{1 + \gamma_s}{1 - \gamma_s} \quad \zeta = \frac{h\rho c_s^2}{3} \frac{1 + \gamma_b}{1 - \gamma_b}$$



- $|\gamma_i| \leq 1 \Leftrightarrow$ positive viscosities!
- *any* viscosity values are accessible!