

Towards a New Algorithm for Multiphase Lattice Boltzmann Simulations

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Some theology

The world of the quantum chemist
(according to Walter Thiel)

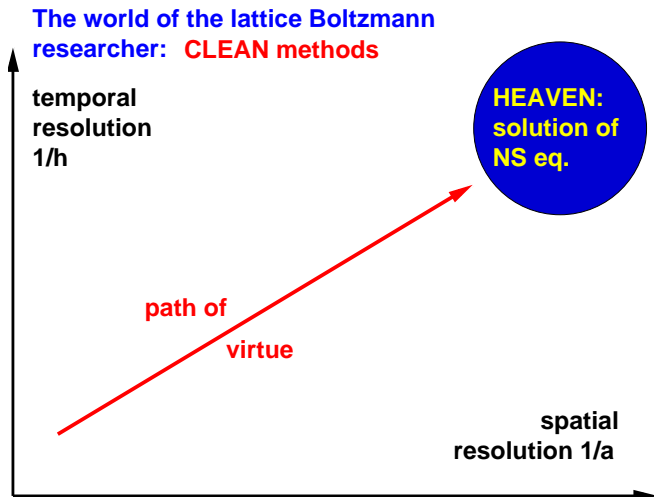
improved
electron–electron
correlations

path of
virtue

single–electron
orbitals

HEAVEN:
full solution
of $H\psi = E\psi$

Some theology



Some theology

The world of the lattice Boltzmann
researcher: **DIRTY** methods

temporal
resolution
 $1/h$

highway
to

HELL:
solution of
NS eq. + ??

spatial
resolution $1/a$

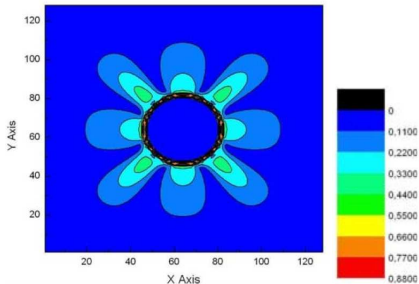


In short:

- ▶ **system:** single-component fluid, coexistence of gas and liquid phase
- ▶ **objectives:** develop thermodynamically and hydrodynamically fully consistent lattice Boltzmann algorithm for multiphase fluids
- ▶ **hope / expectation:** complete elimination of spurious currents

Droplet formation →

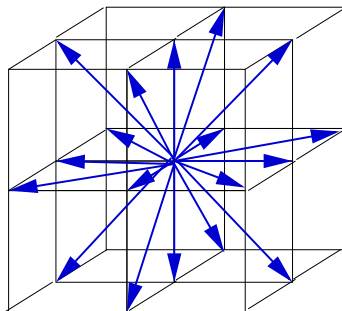
spurious currents: $\frac{|\vec{u}|}{c_s}$



Background and motivation:

Lattice Boltzmann for the ideal gas

Lattice Boltzmann



- ▶ \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:

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

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

$$p = \rho c_s^2$$

$$k_B T = m_p c_s^2$$

Desired asymptotic limit: Navier–Stokes

in the continuum limit $a \rightarrow 0$, $h \rightarrow 0$ (or: on large length and time scales)

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

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

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

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

- ▶ η shear viscosity
- ▶ ζ bulk viscosity

LB continuum limit: how??

in principle, only one parameter $\varepsilon \rightarrow 0$:

- ▶ 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: $a^2/h = \text{const.}$

$$a = \varepsilon a_0$$

$$h = \varepsilon^2 h_0$$

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

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

The idea of multiple time scale expansion

example:

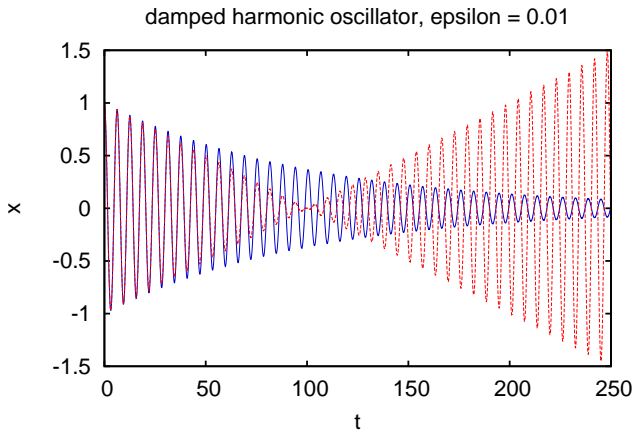
- ▶ weakly damped harmonic oscillator
- ▶ $\varepsilon \rightarrow 0$
- ▶ time scale separation: damping time \gg oscillation time

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

exact solution:

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

naive Taylor expansion wrt ε (1st order):



Multiple time scale analysis

Idea:

$$\begin{aligned}x(t) &= \exp(-\varepsilon t) \cos\left(\sqrt{1 - \varepsilon^2} t\right) \\&\approx \exp(-\varepsilon t) \cos t \\&= \exp(-t_2) \cos t_1 \\&= x(t_1, t_2)\end{aligned}$$

with

$$t_1 = t \quad t_2 = \varepsilon t$$

consider x as a function of two independent variables t_1, t_2

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

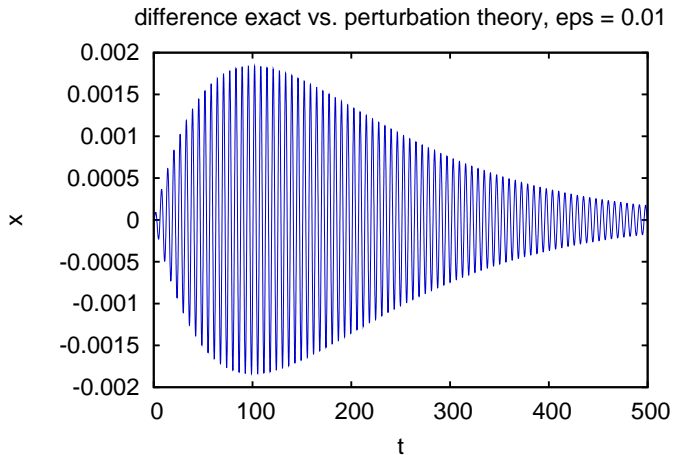
hence, study expansion

$$x(t_1, t_2) = x^{(0)}(t_1, t_2) + \varepsilon x^{(1)}(t_1, t_2) + \varepsilon^2 x^{(2)}(t_1, t_2) + \dots$$

with

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

result for leading order:



Chapman–Enskog expansion

- ▶ LBE:

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

- ▶

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

- ▶ exact re-write as a differential equation:

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

- ▶ $\vec{r}_1 = \varepsilon \vec{r}$
- ▶ $t_1 = \varepsilon t$ waves
- ▶ $t_2 = \varepsilon^2 t$ diffusion
- ▶ $n_i = n_i(\vec{r}_1, t_1, t_2)$

- ▶

$$\partial_\alpha = \varepsilon \partial_{1\alpha}$$

- ▶

$$\partial_t = \varepsilon \partial_{t1} + \varepsilon^2 \partial_{t2}$$

Expanding the solution

$$\begin{aligned}n_i &= n_i^{(0)} + \varepsilon n_i^{(1)} + O(\varepsilon^2) \\ \Delta_i \{n_i\} &= \Delta_i \{n_i^{(0)}\} + \varepsilon \sum_j L_{ij} n_j^{(1)} + O(\varepsilon^2) \\ &= \Delta_i \{n_i^{(0)}\} - \varepsilon(1 - \gamma)n_i^{(1)} + O(\varepsilon^2) \quad (\text{BGK})\end{aligned}$$

ε orders

- ▶ ε^0 : $n_i^{(0)}$ is collisional invariant, hence $n_i^{(0)} = n_i^{eq} = n_i^{eq}(\rho, \vec{j})$
- ▶ $n_i^{(0)}$ contains **NO GRADIENTS! THESE APPEAR AT HIGHER ORDER!**
- ▶ ε^1 : Continuity equation, dissipation-free NS
- ▶ isotropic NS requires

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

- ▶ 3 shells needed. D3Q19: $w_0 = 1/3$, $w_1 = 1/18$, $w_2 = 1/36$, $c_s^2 = a^2/(3h^2)$
- ▶ more freedom in the equation of state requires more shells
- ▶ ε^2 : Dissipative part of NS
- ▶

$$\eta = \frac{h}{2} \rho c_s^2 \frac{1 + \gamma}{1 - \gamma}$$

Gas-liquid systems, part 1:

Lattice Boltzmann setup and
the difference between ideal gas and nonideal gas

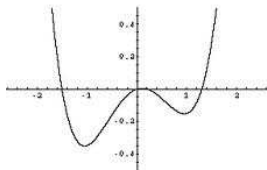
Desired limit: Model H

- ▶ Starting point: Landau–Ginzburg free energy functional
- ▶ In the absence of dissipation, this should be viewed as the conserved energy:

$$\mathcal{H} = \int_V dV \left[\frac{1}{2} \rho \vec{u}^2 + \rho e + \frac{\kappa}{2} (\nabla \rho)^2 \right]$$

$e(\rho)$ gives rise to a Maxwell loop in $p(\rho)$

e vs. ρ



Conservative dynamics:

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

$$\frac{\partial}{\partial t}(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p + f_\alpha$$

Choose force such that Hamiltonian is conserved:

$$\boxed{\frac{d}{dt} \mathcal{H} = 0} \rightarrow \int dV u_\alpha f_\alpha = -\frac{\kappa}{2} \int dV \frac{\partial}{\partial t} (\nabla \rho)^2$$

\Rightarrow

$$\boxed{f_\alpha^{int} = \kappa \rho \partial_\alpha \partial_\beta \partial_\beta \rho} \leftarrow \text{3rd order gradient!}$$

\Rightarrow Chapman-Enskog up to 3rd order is needed!
needed in LB:

$$\Delta_i = \Delta_i^{bulk} + \Delta_i^{int} + \Delta_i^{corr} = -(1 - \gamma)(n_i - n_i^{eq}) + \Delta_i^{int} + \Delta_i^{corr}$$

Equilibrium populations

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

Equation of state

Ideal gas:

$$p = \rho c_s^2 \rightarrow c_s^2 = \frac{p}{\rho} = \frac{\partial p}{\partial \rho}$$

Nonideal gas:

$$p(\rho) = \rho c_s^2(\rho) \rightarrow c_s^2(\rho) = \frac{p}{\rho} \neq \frac{\partial p}{\partial \rho}$$

Velocity moments

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

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

$$\begin{aligned} \sum_i n_i^{eq} c_{i\alpha} c_{i\beta} &= \pi_{\alpha\beta}^{(eq)} \\ &= p(\rho) \delta_{\alpha\beta} + \rho u_\alpha u_\beta \end{aligned}$$

Non-equil. moments: defined similarly up to 4th order.

Coefficients - IDEAL GAS

isotropic lattice tensors

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} = c_s^2 \delta_{\alpha\beta}$$

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} \\ = c_s^4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \text{perm.})$$

weights

D3Q19: Qian et al., EPL, 1992

$$(000) \quad w_0 = \frac{1}{3}$$

$$(100) \quad w_1 = \frac{1}{18}$$

$$(110) \quad w_2 = \frac{1}{36}$$

$$\blacktriangleright c_s^2 = 1/3$$

in lattice units

Coefficients - NONIDEAL GAS

isotropic lattice tensors

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} = c_s^2(\rho) \delta_{\alpha\beta}$$

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = c_s^4(\rho) (\delta_{\alpha\beta} \delta_{\gamma\delta} + \text{perm.})$$

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} c_{i\mu} c_{i\nu} = c_s^6(\rho) (\delta_{\alpha\beta} \delta_{\gamma\delta} \delta_{\mu\nu} + \text{perm.})$$

weights

D3Q19: Qian et al., EPL, 1992

$$(000) \quad w_0 = \frac{1}{3}$$

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Coefficients - NONIDEAL GAS

isotropic lattice tensors

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} = c_s^2(\rho) \delta_{\alpha\beta}$$

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = c_s^4(\rho) (\delta_{\alpha\beta} \delta_{\gamma\delta} + \text{perm.})$$

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

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} c_{i\mu} c_{i\nu} = c_s^6(\rho) (\delta_{\alpha\beta} \delta_{\gamma\delta} \delta_{\mu\nu} + \text{perm.})$$

weights

D3Q59: H. Chen et al., J. Sci. Comp., 2008

$$(000) \quad w_0 = 1 - \frac{2351}{720} c_s^2 + \frac{1081}{192} c_s^4 - \frac{363}{192} c_s^6$$

$$(100) \quad w_1 = 2c_s^2 \left(\frac{8}{45} - \frac{1}{3} c_s^2 + \frac{1}{6} c_s^4 \right)$$

$$(110) \quad w_2 = c_s^2 \left(\frac{8}{45} - \frac{1}{3} c_s^2 + \frac{1}{6} c_s^4 \right)$$

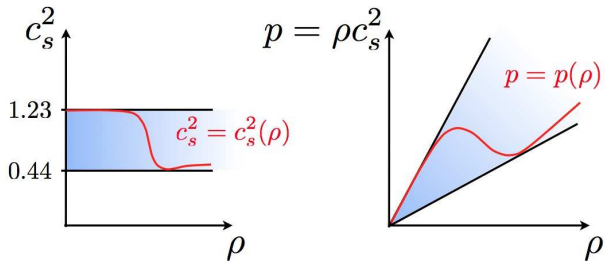
$$\blacktriangleright c_s^2 \in [0.44, 1.23] \quad (w_i > 0!)$$

in lattice units

further weights w_3, \dots, w_7 for

(111), (200), (220), (222), (400)

Allowed equation of state



Comparison to Swift-Yeomans

Swift-Yeomans

- ▶ determine pressure tensor:

$$P_{\alpha\beta}^{int}$$

- ▶ impose: $\sum_i n_i^{eq} c_{i\alpha} c_{i\beta} =$

$$\rho \delta_{\alpha\beta} + \rho u_{\alpha} u_{\beta} + P_{\alpha\beta}^{int}$$

Problem with S-Y model:

- ▶ $n_i^{eq} \rightarrow$ 0th order CE
- ▶ $P_{\alpha\beta}^{int} \rightarrow$ higher order CE because of gradients!

This work

- ▶ determine force density: f_{α}^{int}

- ▶ put it into the collision operator:

$$\Delta_i^{int} = w_i \frac{2h}{1+\gamma} \frac{f_{\alpha}^{int} c_{i\alpha}}{c_s^2}$$

Decouple bulk and interface terms:

- ▶ bulk \leftarrow local equilibrium populations
- ▶ interface \leftarrow force

Gas-liquid systems, part 2:
Chapman-Enskog analysis

Chapman–Enskog expansion

\vec{r}_1	$= \varepsilon \vec{r}$	scaling parameter ε
t_1	$= \varepsilon t$	sound waves
t_2	$= \varepsilon^2 t$	diffusion of momentum
t_3	$= \varepsilon^3 t$	coarsening

$$n_i(\vec{r}_1 + \vec{c}_i \varepsilon h, t_1 + \varepsilon h, t_2 + \varepsilon^2 h, t_3 + \varepsilon^3 h) - n_i(\vec{r}_1, t_1, t_2, t_3) = \Delta_i$$

From Boltzmann to Navier–Stokes

Lattice Boltzmann eq.:

$$\begin{aligned} n_i(\vec{r}_1 + \varepsilon \vec{c}_i h, t_1 + \varepsilon h, t_2 + \varepsilon^2 h, t_3 + \varepsilon^3 h) - n_i(\vec{r}_1, t_1, t_2, t_3) \\ = \Delta_i^{bulk} + \Delta_i^{int} + \Delta_i^{corr} \end{aligned}$$

Navier–Stokes eq.:

$$\partial_t j_\alpha + \partial_\beta (\rho(\rho) \delta_{\alpha\beta} + \rho u_\alpha u_\beta) - \partial_\beta \sigma_{\alpha\beta} = \kappa \rho \partial_\alpha \partial_\beta \partial_\beta \rho$$

Velocity moments

$$h f_\alpha = \frac{2}{1+\gamma} \sum_i \Delta_i^{int} c_{i\alpha}$$

Interface collision operator Δ_i^{int}

local collision operator - ideal gas:

$$\Delta_i(\vec{r}, t) = \Delta_i(\{n_i(\vec{r}, t)\} \quad)$$

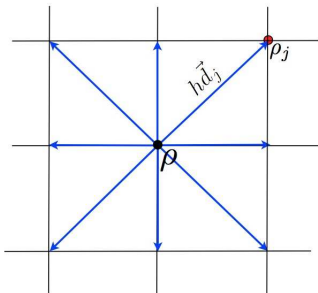
$$\rho = \rho(\vec{r}_1)$$

Interface collision operator Δ_i^{int}

Nonlocal collision operator - nonideal gas:

$$\Delta_i(\vec{r}, t) = \Delta_i(\{n_i(\vec{r}, t)\}, \{\rho_j\})$$

$$\rho = \rho(\vec{r}_1) \quad \rho_j \equiv \rho(\vec{r}_1 + \vec{d}_j \varepsilon h)$$



- ▶ new set of lattice vectors \vec{d}_j
- ▶ new set of weights τ_j
- ▶ interactions with neighboring sites

Adjust weights τ_i so that:

$$\sum_i \tau_i d_{i\alpha} = 0 \quad \sum_i \tau_i d_{i\alpha} d_{i\beta} d_{i\gamma} = 0$$

$$\sum_i \tau_i d_{i\alpha} d_{i\beta} = \tilde{\sigma}_2 \delta_{\alpha\beta} = 0$$

$$\sum_i \tau_i d_{i\alpha} d_{i\beta} d_{i\gamma} d_{i\delta} = \tilde{\sigma}_4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma})$$

\Rightarrow 3 shells of lattice vectors \vec{d}_j needed

Ansatz:

$$\Delta_i^{int} = \kappa \rho w_i c_{i\alpha} \sum_j \tau_j d_{j\alpha} \rho_j$$

$$\Delta_i^{int} = \kappa \rho w_i c_{i\alpha} \sum_j \tau_j d_{j\alpha} \rho_j$$

Does this Ansatz give us the right force?

$$\begin{aligned} \frac{1 + \gamma}{2} h f_\alpha^{int} &= \sum_i \Delta_i^{int} c_{i\alpha} \\ &= \kappa \rho c_s^2 \sum_j \tau_j d_{j\alpha} \rho_j \end{aligned}$$

$$\Delta_i^{int} = \kappa \rho w_i c_{i\alpha} \sum_j \tau_j d_{j\alpha} \rho_j$$

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$$\rho_j = \rho + \varepsilon h d_{j\alpha} \partial_{\alpha_1} \rho + \frac{\varepsilon^2 h^2}{2} d_{j\alpha} d_{j\beta} \partial_{\alpha_1} \partial_{\beta_1} \rho + \frac{\varepsilon^3 h^3}{6} d_{j\alpha} d_{j\beta} d_{j\gamma} \partial_{\alpha_1} \partial_{\beta_1} \partial_{\gamma_1} \rho$$

$$\tilde{\sigma}_2 = 0$$

$$\Delta_i^{int} = \kappa \rho w_i c_{i\alpha} \sum_j \tau_j d_{j\alpha} \rho_j$$

Does this Ansatz give us the right force?

$$\begin{aligned} \frac{1+\gamma}{2} h f_\alpha^{int} &= \sum_i \Delta_i^{int} c_{i\alpha} \\ &= \kappa \rho c_s^2 \sum_j \tau_j d_{j\alpha} \rho_j \\ &= \kappa \rho c_s^2 \tilde{\sigma}_4 h^3 \frac{1}{6} 3 \partial_\alpha \partial_\beta \partial_\beta \rho \end{aligned}$$

$$\Delta_i^{int} = \kappa \rho w_i c_{i\alpha} \sum_j \tau_j d_{j\alpha} \rho_j$$

Does this Ansatz give us the right force?

$$\begin{aligned} \frac{1+\gamma}{2} h f_\alpha^{int} &= \sum_i \Delta_i^{int} c_{i\alpha} \\ &= \kappa \rho c_s^2 \sum_j \tau_j d_{j\alpha} \rho_j \\ &= \kappa \rho c_s^2 \tilde{\sigma}_4 h^3 \frac{1}{6} 3 \partial_\alpha \partial_\beta \partial_\beta \rho \end{aligned}$$

► $f_\alpha^{int} = \kappa \rho \partial_\alpha \partial_\beta \partial_\beta \rho$

$$\Delta_i^{int} = \kappa \rho w_i c_{i\alpha} \sum_j \tau_j d_{j\alpha} \rho_j$$

Does this Ansatz give us the right force?

$$\begin{aligned} \frac{1+\gamma}{2} h f_\alpha^{int} &= \sum_i \Delta_i^{int} c_{i\alpha} \\ &= \kappa \rho c_s^2 \sum_j \tau_j d_{j\alpha} \rho_j \\ &= \kappa \rho c_s^2 \tilde{\sigma}_4 h^3 \frac{1}{6} 3 \partial_\alpha \partial_\beta \partial_\beta \rho \end{aligned}$$

- ▶ $f_\alpha^{int} = \kappa \rho \partial_\alpha \partial_\beta \partial_\beta \rho$
- ▶ $\Rightarrow \tilde{\sigma}_4 = \frac{1+\gamma}{h^2 c_s^2}$

Continuity equation

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

In order to get it correct up to 3rd order in the CE expansion, we need a
Re-defined momentum density

$$j_\alpha = \sum_i n_i c_{i\alpha} + \frac{\hbar}{2} f_\alpha - \varepsilon^2 \frac{\hbar}{12} \partial_{\beta_1} (\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)})$$

$$\frac{1}{\hbar} (\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)}) = p(\rho) (\partial_{\alpha_1} u_\beta + \partial_{\beta_1} u_\alpha) + \left(p(\rho) - \frac{\partial p(\rho)}{\partial \rho} \rho \right) (\partial_{\gamma_1} u_\gamma) \delta_{\alpha\beta}$$

Need an iterative algorithm to define $u_\alpha = j_\alpha / \rho$!

Navier-Stokes equation

$$\begin{aligned} & \partial_t j_\alpha + \partial_\beta \pi_{\alpha\beta}^{(0)} + \varepsilon \frac{1}{2} \frac{\gamma + 1}{\gamma - 1} \partial_\beta \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right) - \varepsilon \frac{h}{\gamma - 1} \partial_\beta \Sigma_{\alpha\beta}^{(1)} \\ & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[\frac{\gamma + 1}{\gamma - 1} \partial_{t_2} \pi_{\alpha\beta}^{(0)} + \frac{\gamma^2 + 4\gamma + 1}{3(\gamma - 1)^2} \partial_{t_1} \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right) \right] \\ & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[-h \frac{\gamma + 1}{(\gamma - 1)^2} \partial_{t_1} \Sigma_{\alpha\beta}^{(1)} - \frac{2}{\gamma - 1} \Sigma_{\alpha\beta}^{(2)} \right] - \varepsilon^3 \frac{1}{12} h^2 \partial_{t_1}^2 f_\alpha^{(1)} \\ & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[\frac{\gamma^2 + 4\gamma + 1}{3(\gamma - 1)^2} \partial_{\gamma_1} \left(\phi_{\alpha\beta\gamma}^{*(1)} - \phi_{\alpha\beta\gamma}^{(1)} \right) - h \frac{\gamma + 1}{(\gamma - 1)^2} \partial_{\gamma_1} \Xi_{\alpha\beta\gamma}^{(1)} \right] \\ & = \varepsilon f_\alpha^{(1)} + \varepsilon^2 f_\alpha^{(2)} + \varepsilon^3 f_\alpha^{(3)} \end{aligned}$$

Navier-Stokes equation

$$\begin{aligned} & \partial_t j_\alpha + \partial_\beta \pi_{\alpha\beta}^{(0)} + \varepsilon \frac{1}{2} \frac{\gamma + 1}{\gamma - 1} \partial_\beta \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right) - \varepsilon \frac{h}{\gamma - 1} \partial_\beta \Sigma_{\alpha\beta}^{(1)} \\ & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[\frac{\gamma + 1}{\gamma - 1} \partial_{t_2} \pi_{\alpha\beta}^{(0)} + \frac{\gamma^2 + 4\gamma + 1}{3(\gamma - 1)^2} \partial_{t_1} \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right) \right] \\ & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[-h \frac{\gamma + 1}{(\gamma - 1)^2} \partial_{t_1} \Sigma_{\alpha\beta}^{(1)} - \frac{2}{\gamma - 1} \Sigma_{\alpha\beta}^{(2)} \right] - \varepsilon^3 \frac{1}{12} h^2 \partial_{t_1}^2 f_\alpha^{(1)} \\ & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[\frac{\gamma^2 + 4\gamma + 1}{3(\gamma - 1)^2} \partial_{\gamma_1} \left(\phi_{\alpha\beta\gamma}^{*(1)} - \phi_{\alpha\beta\gamma}^{(1)} \right) - h \frac{\gamma + 1}{(\gamma - 1)^2} \partial_{\gamma_1} \Xi_{\alpha\beta\gamma}^{(1)} \right] \\ & = \varepsilon f_\alpha^{(1)} + \varepsilon^2 f_\alpha^{(2)} + \varepsilon^3 f_\alpha^{(3)} \end{aligned}$$

Navier-Stokes equation with force at 3rd order taking into account interfaces

Navier-Stokes equation

$$\begin{aligned}
 & \partial_t j_\alpha + \partial_\beta \pi_{\alpha\beta}^{(0)} + \varepsilon \frac{1}{2} \frac{\gamma + 1}{\gamma - 1} \partial_\beta \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right) - \varepsilon \frac{h}{\gamma - 1} \partial_\beta \Sigma_{\alpha\beta}^{(1)} \\
 & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[\frac{\gamma + 1}{\gamma - 1} \partial_{t_2} \pi_{\alpha\beta}^{(0)} + \frac{\gamma^2 + 4\gamma + 1}{3(\gamma - 1)^2} \partial_{t_1} \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right) \right] \\
 & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[-h \frac{\gamma + 1}{(\gamma - 1)^2} \partial_{t_1} \Sigma_{\alpha\beta}^{(1)} - \frac{2}{\gamma - 1} \Sigma_{\alpha\beta}^{(2)} \right] - \varepsilon^3 \frac{1}{12} h^2 \partial_{t_1}^2 f_\alpha^{(1)} \\
 & + \varepsilon^2 \frac{h}{2} \partial_\beta \left[\frac{\gamma^2 + 4\gamma + 1}{3(\gamma - 1)^2} \partial_{\gamma_1} \left(\phi_{\alpha\beta\gamma}^{*(1)} - \phi_{\alpha\beta\gamma}^{(1)} \right) - h \frac{\gamma + 1}{(\gamma - 1)^2} \partial_{\gamma_1} \Xi_{\alpha\beta\gamma}^{(1)} \right] \\
 & = \varepsilon f_\alpha^{(1)} + \varepsilon^2 f_\alpha^{(2)} + \varepsilon^3 f_\alpha^{(3)}
 \end{aligned}$$

Adjust correction collision operator \Rightarrow undesired terms = 0

$$h \Sigma_{\alpha\beta} = \sum_i \Delta_i^{corr} c_{i\alpha} c_{i\beta} \quad h \Xi_{\alpha\beta\gamma} = \sum_i \Delta_i^{corr} c_{i\alpha} c_{i\beta} c_{i\gamma}$$

Navier-Stokes equation




$$\partial_t j_\alpha + \partial_\beta \pi_{\alpha\beta}^{(0)} + \varepsilon \frac{1}{2} \frac{\gamma + 1}{\gamma - 1} \partial_\beta \left(\pi_{\alpha\beta}^{*(1)} - \pi_{\alpha\beta}^{(1)} \right)$$

$$= \varepsilon^3 f_\alpha^{(3)}$$





Navier-Stokes equation with force at 3rd order taking into account interfaces

Summary

▶ Good news

-  no spurious terms
-  6th rank isotropy
-  fully consistent method for gas-liquid coexistence can be constructed

▶ Bad news

-  many velocities needed (21 in 2D, 59 in 3D) + another set of velocities for interface collision operator (12 in 2D, 20 in 3D)
-  need for finite difference scheme to compute the correction collision operator
-  limited freedom for choosing the equation of state
-  need of iterative algorithm to calculate flow velocity

▶ Future

- ▶ test numerical implementation
- ▶ thermal fluctuations
- ▶ boundaries
- ▶ binary fluids