Particle-Based Multiscale Coupling of Fluids

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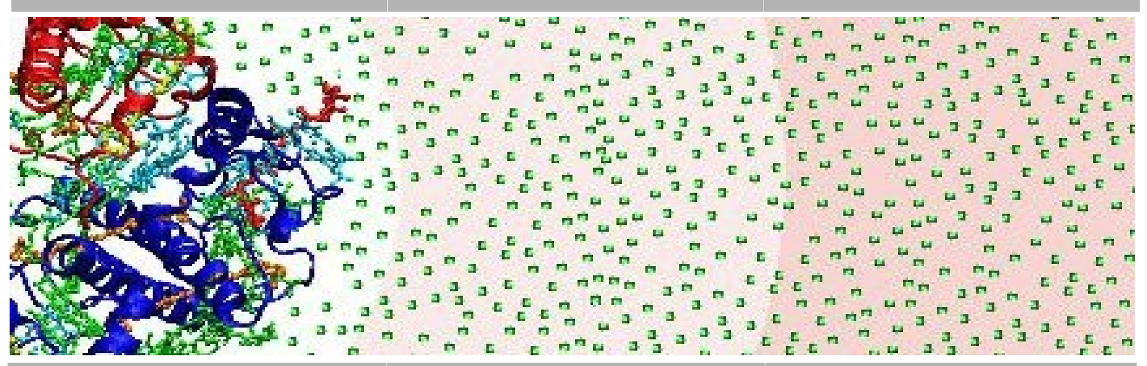
Aim: coupling between the atomistic fluid (Lennard-Jones model, LJ) and the mesoscopic hydrodynamis method (Multi-Particle CollisionDynamics, MPC)

How:	by using a buffer-zone, where particles gradually change their identity while tracing the interface
Why:	adjusting the level of resolution in the system "on the fly", i.e. enabling a more detailed view of the area of interest, while keeping the larger surroundings on a coarser level

Detailed Description	Buffer Zone	Coarse-grain Description



Molecular Dynamics		Multi-Particle Collision Dynamics

Methods to be coupled

Molecular Dynamics

pair interaction between neutral particles

(Lennard-Jones potential)

$$U_{ij}^{LD} = 4\varepsilon\left(\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right)$$

$$\vec{f}_{ij}^{LD} = -\nabla U_{LD}$$

integrating the Equations of Motion:

$$\vec{r}_i(t+\delta t) = \vec{r}_i(t) + \vec{v}_i(t)\delta t + \frac{\vec{f}_i(t)}{2m}\delta t^2$$

$$\vec{v}_i(t+\delta t) = \vec{v}_i(t) + \vec{f}_i(t)\delta t$$

Multiparticle Collision Dynamics (MPC)

Free Streaming Step:

$$\vec{r}(t+\Delta t) = \vec{r}(t) + \vec{v}(t)\Delta t$$

particles perform a ballistic motion without interacting with each other

Cell Filling Step:

-grid is superimposed over simulation box

-particles are assigned to collision cells

-collision grid is shifted randomly after each time step

Multiparticle Collision Step:

$$\vec{v}_{i,c}(t+\Delta t) = \vec{v}_{i,c}(t) + R\{\vec{v}_{i,c}(t) - \vec{v}_{cm,c}(t); n, \alpha\}$$

particle velocities are rotated relative to the centre of mass velocity of a given angle around a random rotation axis

Matching the Systems

Physical Properties

$$\rho^{MD} = \rho^{MPC}, \left(\frac{3}{2}k_B T\right)_{MD} = \left(\frac{3}{2}k_B T\right)_{MPC}$$

Transport Properties

$$D_{MD} = \int_0^\infty \langle v_{\alpha i}(t) v_{\alpha i}(0)\rangle dt \qquad D_{MPC} = D_{MPC}(a, \Delta t)$$

$$\eta_{MD} = \frac{1}{k_B T V}\int_0^\infty \langle \sigma_{\alpha\beta}(t)\sigma_{\alpha\beta}(0)\rangle dt \qquad \eta_{MPC} = \eta_{MPC}(a, \Delta t, \alpha)$$

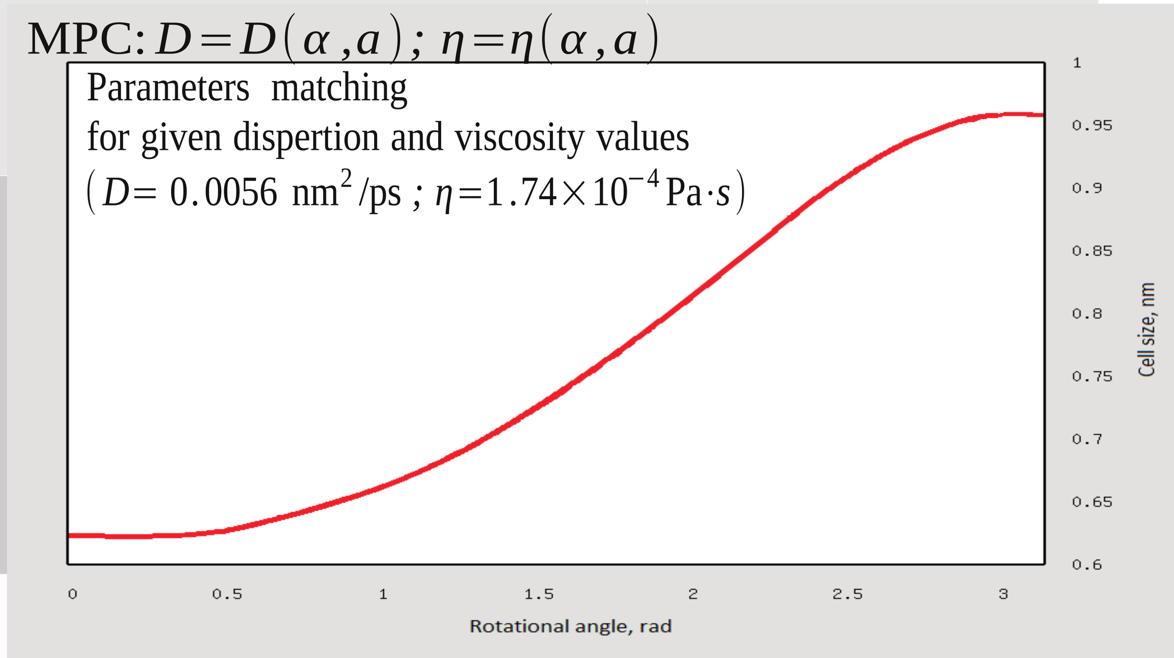
$$\sigma_{\alpha\beta}(t) = \sum_i^N \frac{p_{\alpha i}(t) p_{\beta i}(t)}{m_i} + \sum_{i<j}^N r_{\alpha i}(t) F_{\beta i}(t)$$

a : cell site

Δt : time step

α : rotation angle

MPC: $D = D(\alpha, a)$; $\eta = \eta(\alpha, a)$



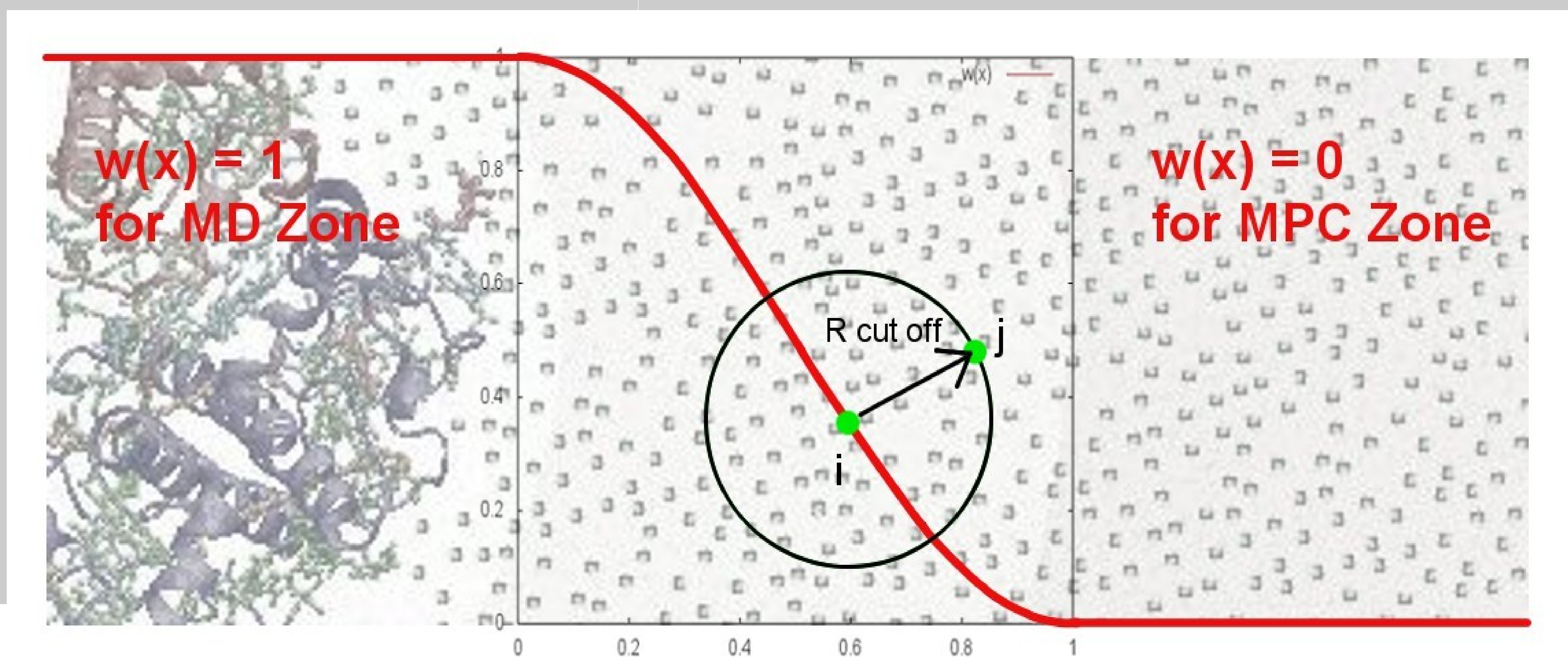
The Coupling

Switching function w(x)

MD: $\vec{f}_{ij} = w(x_i) w(x_i) \vec{f}_{ij}^{LD}$

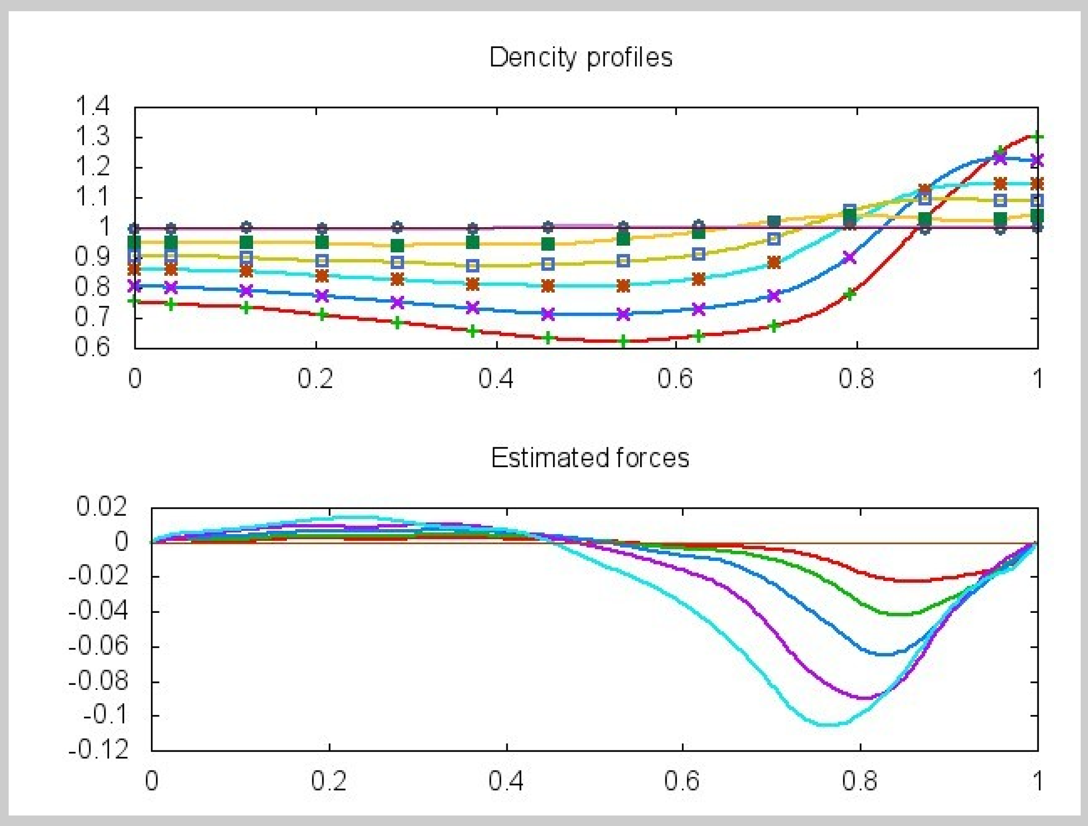
$$f_i = \sum_{j\neq i} \vec{f}_{ij} = w(x_i) \sum_{j\neq i} w(x_i) \vec{f}_{ij}^{LD}$$

MPC: collision probability $P = 1 - w(x_{c.m.})$



External Force in the Buffer Zone

Restraining force proportional to the local density difference



Do we still have hydrodynamics in the system?

Long time tail of velocity correlation function

A simulation was performed with a set of systems composed of particles with intermediate identity (left) or identity according to a random walk in w(x) (right). The velocity auto-correlation function for each system was calculated.

The long time tail of the velocity correlation functions show the typical $t^{-3/2}$ asymptotic behavior, showing that hydrodynamics is preserved across the buffer zone.