Visualising and controlling the flows in biomolecular systems at and between multiple scales: from atoms to hydrodynamics at different locations in time and space

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The project

Title: 'Using next generation computers and algorithms for modelling the dynamics of large biomolecular systems'

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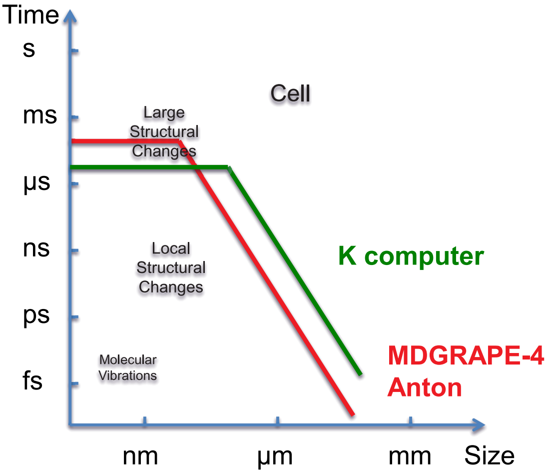
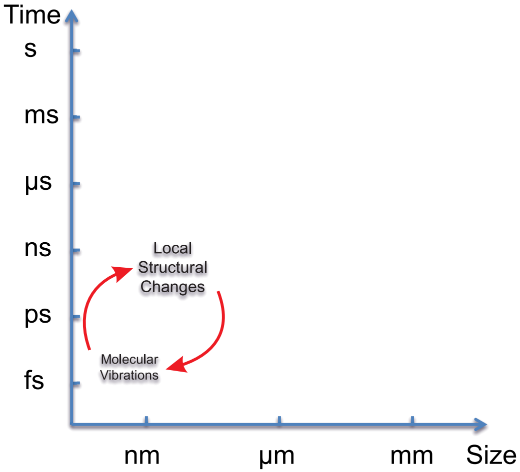
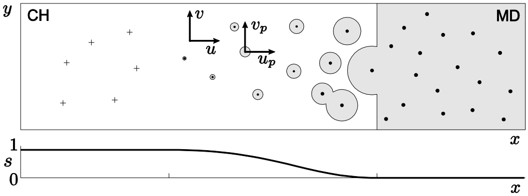
Biomolecular scales



Scales coupling: cyclic



Our framework



- The end domains HD and MD are described by purely hydrodynamic and purely Newtonian equations of motion respectively.
- In the hybrid domain the fluid consists of two “phases”:
  - HD phase is a continuum water with volume fraction $s = \frac{V_1}{V}$,
  - MD phase is a phase that incorporates atoms, its volume fraction is $(1 - s)$.
- The parameter $s = s(x)$ is the function of space coordinates, such that $s = 1$ in the HD domain, $s = 0$ in the MD domain.

Mass conservation

For HD phase:

$$\frac{\partial}{\partial t}(s\rho) + \frac{\partial}{\partial x_i}(u_i s\rho) = J,$$

For MD phase:

$$\frac{\partial}{\partial t}\left((1-s)\sum_{p=1,N(t)} \rho_p\right) + \frac{\partial}{\partial x_i}\left((1-s)\sum_{p=1,N(t)} \rho_p u_{ip}\right) = -J,$$

where $\rho_p = m_p/V$ is the density of MD particles and J is the birth/death rate due to the coupling between the phases.

Restricted dynamics

$$\tilde{\rho} = s\rho + (1-s)\sum_{p=1,N(t)} \rho_p$$

The deviations of $\tilde{\rho}$ are driven towards the correct value $\sum_{p=1,N(t)} \rho_p$:

$$\frac{D}{Dt_0}\left(\tilde{\rho} - \sum_{p=1,N(t)} \rho_p\right) = L^{(\rho)} \cdot \left(\tilde{\rho} - \sum_{p=1,N(t)} \rho_p\right),$$

where $\frac{D}{Dt_0}\cdot = \frac{\partial}{\partial t}\cdot + \nabla(\mathbf{u}\cdot)$.

Restricted dynamics

$\tilde{\rho}$ is diffused towards $\sum_{p=1,N(t)} \rho_p$:

$$L^{(\rho)}.\left(\tilde{\rho} - \sum_{p=1,N(t)} \rho_p\right) = \frac{\partial}{\partial x_i}\left(s(1-s)\alpha\frac{\partial}{\partial x_i}\left(\tilde{\rho} - \sum_{p=1,N(t)} \rho_p\right)\right).$$

Modified MD equations

For known sources J, MD equations are modified to preserve macroscopic conservation laws:

$$\frac{dx_{ip}}{dt} = u_{ip} + s(u_i - u_{ip}) + s(1-s)\alpha \frac{\partial}{\partial x_i}\left(\tilde{\rho} - \sum_{p=1,N(t)} \rho_p\right)\frac{1}{\rho_p N(t)},$$

$$\begin{aligned}\frac{du_{jp}}{dt} &= (1-s)F_{jp}/\rho_p \\ &+ \frac{\partial}{\partial x_i}\left(s(1-s)\alpha \sum_{p=1,N(t)} u_{jp}/N(t)\frac{\partial}{\partial x_i}\left(\tilde{\rho} - \sum_{p=1,N(t)} \rho_p\right)\right)\frac{1}{\rho_p N(t)} \\ &- \frac{\partial}{\partial x_i}\left(s(1-s)\beta\frac{\partial}{\partial x_i}\left(\tilde{u}_j\tilde{\rho} - \sum_{p=1,N(t)} u_{jp}\rho_p\right)\right)\frac{1}{\rho_p N(t)},\end{aligned}$$

Results