Open Molecular Dynamics

Rafael Delgado-Buscalioni

Universidad Autónoma de Madrid

Dresden, September 2010
Domain decomposition: connecting models, connecting open systems

Open boundary conditions:
OUTSIDE WORLD
steady state,
thermodynamic reservoir
Multiscale approaches for complex liquids

**Domain decomposition**
- type A
  - Molecular detail, interfaces, surfaces, macromolecule - fluid interaction

**Eulerian-Lagrangian**
- Solute-solvent hydrodynamic coupling

**Patch dynamics**
- HMM
- Velocity-Stress coupling
  - type B
  - Non-Newtonian fluids
    - Unknown constitutive relation
    - polymer melts...

**Coarse-grained dynamics**

**shear flows**
- sound, heat
- large molecules
- multispecies
- electrostatics

Point particle approximation:
- Stokes drag (point particle), Faxen terms (finite size effects)
- Basset memory effects...
- Force Coupling
- particles of finite size
- Direct simulation
- Immersed boundaries

**How to reduce the degrees of freedom and keep the underlying dynamics**

**MD nodes used to evaluate the local stress for the Continuum solver.**
- Continuum solver provides the local velocity gradient imposed at each MD node.

**diffusion viscosity anisotropy**
- (nematics...)

FIG. 3: Sketch of the simulation setup.
Open systems
Beyond periodic boundary conditions

Objetives
- Avoid finite size effects (wrapped hydrodynamic fields)
Open systems
Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
Open systems
Beyond periodic boundary conditions

Objectives
- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
Open systems
Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
Open systems
Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
Open systems
Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.
Open systems
Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.
Open systems
Beyond periodic boundary conditions

Objectives
- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.

Open model
- Molecular Dynamics
Open systems

Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.

Open model

- Molecular Dynamics
- Continuum fluid dynamics, Fluctuating hydrodynamics
Open systems
Beyond periodic boundary conditions

Objectives
- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.

Open model
- Molecular Dynamics
- Continuum fluid dynamics, Fluctuating hydrodynamics
- Particle hydrodynamics (Eulerian-Lagrangian hybrids)
Open systems
Beyond periodic boundary conditions

Objectives

- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.

Open model

- Molecular Dynamics
- Continuum fluid dynamics, Fluctuating hydrodynamics
- Particle hydrodynamics (Eulerian-Lagrangian hybrids)
Open systems
Beyond periodic boundary conditions

Objectives
- Avoid finite size effects (wrapped hydrodynamic fields)
- Reduce computational cost (smaller systems).
- Generalize ensemble (e.g. grand-canonical)
- Inlet/Outlet boundary conditions: pipe, tube flows
- Heat control through system’s boundaries.
- Hybrid based on domain decomposition.

Open model
- Molecular Dynamics
- Continuum fluid dynamics, Fluctuating hydrodynamics
- Particle hydrodynamics (Eulerian-Lagrangian hybrids)

Purpose: reduce unphysical artifacts at boundaries.
Outline of the talk

- Open Fluctuating Hydrodynamics OPEN FH
Outline of the talk

- Open Fluctuating Hydrodynamics: OPEN FH
- Open Molecular Dynamics: OPEN MD
Outline of the talk

- Open Fluctuating Hydrodynamics (OPEN FH)
- Open Molecular Dynamics: (OPEN MD)
  - Imposing state variables
Outline of the talk

- Open Fluctuating Hydrodynamics
- Open Molecular Dynamics:
  - Imposing state variables
  - Imposing fluxes
Outline of the talk

- Open Fluctuating Hydrodynamics \textit{open FH}
- Open Molecular Dynamics: \textit{open MD}
  - Imposing state variables
  - Imposing fluxes
  - The particle buffer
Outline of the talk

- **Open Fluctuating Hydrodynamics** OPEN FH
- **Open Molecular Dynamics:** OPEN MD
  - Imposing state variables
  - Imposing fluxes
  - The particle buffer
  - Using Adaptive Resolution: the *mesoscopic layer.*
Outline of the talk

- Open Fluctuating Hydrodynamics \textit{OPEN FH}
- Open Molecular Dynamics: \textit{OPEN MD}
  - Imposing state variables
  - Imposing fluxes
  - The particle buffer
  - Using Adaptive Resolution: the \textit{mesoscopic layer}.
- Connection with a continuum solver: the hybrid particle-continuum scheme
Open Fluctuating hydrodynamics

Power spectra of density fluctuations: liquid argon @ equilibrium
NRBC = Non-Reflecting boundary conditions

![Graph showing density power spectra with different boundary conditions and box sizes.](image-url)
Open Fluctuating hydrodynamics
Evacuation of sound waves using non-reflecting boundaries

Open Fluctuating hydrodynamics

Non-reflecting boundary conditions in terms of sound modes.

- Amplitude of sound waves

\[
A_{IN} = \frac{1}{2} \left( \frac{\delta p}{\rho_e c} - \delta u \right) \quad \text{moving } \leftarrow
\]

\[
A_{OUT} = \frac{1}{2} \left( \frac{\delta p}{\rho_e c} + \delta u \right) \quad \text{moving } \rightarrow
\]

with \( \delta p = p - p_e, \delta u = u - u_e \), pressure and velocity fluctuations.
Open Fluctuating hydrodynamics
Non-reflecting boundary conditions for sound modes

- **Linear Navier-Stokes Eqs.**, normal-to-boundary direction,

\[
\frac{\partial A_i}{\partial t} = (u \pm c) \frac{\partial A_i}{\partial x} \pm \frac{1}{\rho_e} \frac{\partial P_{xx}}{\partial x}
\]

with \( i = \text{IN} \rightarrow + \) and \( i = \text{OUT} \rightarrow - \)

- Amplitude variations:

\[
\frac{L_i}{\rho_e c} = (u \mp c) \frac{\partial A_i}{\partial x}
\]
Open Fluctuating hydrodynamics

\[
\frac{\partial A_i}{\partial t} + \frac{L_i}{\rho_e c} = \pm \frac{1}{\rho_e} \frac{\partial P_{xx}}{\partial x}
\]

Amplitude variations,

\[
L_{OUT} = (u - c) \frac{\partial A_{OUT}}{\partial x} \quad \text{Measured within domain}
\]

\[
L_{IN} = K(\rho c A_{IN}) \quad \text{Modelled}
\]

\[
K = \frac{\nu_L}{(0.4\Delta x)^2} \quad \text{Satisfies FD balance}
\]
Open Fluctuating hydrodynamics

\[ \frac{\partial A_i}{\partial t} + \frac{L_i}{\rho_e c} = \pm \frac{1}{\rho_e} \frac{\partial P_{xx}}{\partial x} \]

Amplitude variations,

\[ L_{OUT} = (u - c) \frac{\partial A_{OUT}}{\partial x} \quad \text{Measured within domain} \]

\[ L_{IN} = K(\rho c A_{IN}) \quad \text{Modelled} \]

\[ K = \frac{\nu_L}{(0.4\Delta x)^2} \quad \text{Satisfies FD balance} \]

**NRBC Eqs. for boundary cells,**

- density: \[ \frac{\partial \rho}{\partial x} = 0 \]
- velocity: \[ \frac{\partial u}{\partial t} + \frac{1}{2\rho_e c}(L_{OUT} - L_{IN}) = 0 \]
NRBC Reflection coefficient.
Open MD via external forces

\[ m \ddot{r}_i = f_i(\{r\}) + f_i^{\text{ext}} \]
State-Coupling

(see: Thomsom and O’Connel and Mark Robbins' group)

Scope

- **CFD Research**: effects of molecular domain onto the mean flow.
- **Priority**: The external flow imposed into the molecular region.
- **Mass flux**: Imposed to MD using continuum expression: \( A \rho V_n \).
- **NO molecular fluctuations**
- **Impose** external velocity \( \mathbf{V} \) at the buffer \( \bar{\mathbf{v}} \equiv \frac{1}{N_B} \sum_{i \in B} \mathbf{v}_i \)
**State-Coupling**

**Method**
- Constrained dynamics: \( m\ddot{r}_i = (f_i - \bar{f}) - \xi (v_i - V) \)
- External force: \( f_{i}^{\text{ext}} = -\bar{f} - \xi (v_i - V) \)
- Mean buffer velocity:

\[
\frac{d\bar{v}}{dt} = -\gamma (\bar{v} - V)
\]

\( \bar{v} \) converges to \( V \) exponentially (at rate \( \gamma = \xi / M_B \)); and instantaneously if \( \gamma = 1/\Delta t \)
Thermodynamics of State-Coupling

Input power

\[ \dot{E} = \sum_{i \in B} f_{i}^{\text{ext}} \cdot \mathbf{v}_i \]

External force

\[ f_{i}^{\text{ext}} = -\bar{f} - \xi (\mathbf{v}_i - \mathbf{V}) \]

where

\[ \bar{f} = \frac{1}{N} \sum_{i \in B} f_i = M \frac{d\bar{v}}{dt} \]
Assume $\bar{v} \simeq V$

$$\dot{E} = -N\bar{f} \cdot \bar{v} - \xi \sum_{i \in B} (v_i - \bar{v})^2$$

Use equipartition $3kT = \langle (v_i - \bar{v})^2 \rangle$ and $\langle \bar{f} \bar{v} \rangle = M \langle \frac{d\bar{v}}{dt} \bar{v} \rangle = 0$ to get:
Assume $\bar{v} \simeq V$

$$\dot{E} = -N\bar{f} \cdot \bar{v} - \xi \sum_{i \in B} (v_i - \bar{v})^2$$

Use equipartition $3kT = \langle (v_i - \bar{v})^2 \rangle$ and $\langle f\bar{v} \rangle = M\langle \frac{d\bar{v}}{dt} \bar{v} \rangle = 0$ to get:

$$\frac{d\langle E \rangle}{dt} = -3\frac{\xi}{m} NkT$$

Exponential freezing (very fast, $\xi/m >> \xi/M = \gamma$).

**Hard thermostatting is required** (simple velocity rescaling!)
Flux-Coupling

(See: Flekkoy, RD-B and Coveney, Phys. Rev. E, 72, 026703 (2005))

Scope

- **Molecular research**: effects of flow on molecular domain.
- **Priority**: avoid external artifacts into molecular domain
- **Mass flux**: Measured from MD; naturally arises from pressure gradient across the interface
- **Molecular fluctuations** (mass, momentum, energy)
- **Imposes**: Flux across interface of area A and (inwards) surface vector \( n \)
- **Momentum flux** (force/area) \( P_n = P \cdot n \)
- **Heat flux** (energy/time) \( \dot{Q}_e = q \cdot n \)
 Flux-Coupling

(PRE, 72, 026703 (2005) Method

- External force to buffer particles: $f_{i}^{\text{ext}} = \bar{f}_{\text{ext}} + \tilde{f}_{\text{ext}}$
- Momentum transfer by the average external force
  \[ \bar{f}_{\text{ext}} = P_{n} A / N_{B} \]
- Heat transfer by the fluctuating external force
  \[ \tilde{f}_{\text{ext}} = \sum_{i \in B} v_{i}^{2} \dot{Q}_{e} \]
- Momentum and energy due to particle insertion/deletions can be taken into account (exact balance).
Thermodynamics of Flux-Coupling

Energy input over $\Delta t$

$$\Delta E = \sum_{i \in B} f_{i}^{\text{ext}} \cdot v_{i} \Delta t + \sum_{k} e_{k}$$

$$f_{i}^{\text{ext}} = \frac{\mathbf{P} \cdot n}{N} + \frac{v_{i}}{\sum_{i \in B} v_{i}^{2}} \dot{Q}_e$$

$$\Delta E = \mathbf{P} \cdot \bar{v} \Delta t + \dot{Q}_e \Delta t + \sum_{k} e_{k}$$
**Thermodynamics of Flux-Coupling**

Energy input over $\Delta t$

$$\Delta E = \sum_{i \in B} f_{i}^{\text{ext}} \cdot v_i \Delta t + \sum_{k} e_k$$

$$f_{i}^{\text{ext}} = A \mathbf{P}_n/N + \frac{v_i}{\sum_{i \in B} v_i^2} \dot{Q}_e$$

$$\Delta E = A \mathbf{P}_n \cdot \bar{v} \Delta t + \dot{Q}_e \Delta t + \sum_{k} e_k$$

Entropy change (quasi-stationary, $\dot{Q}_e$ not so large)

$$T \Delta S' = \sum_{k} e_k - \mu \Delta N \text{ Particle insertions}$$

$$T \Delta S = \dot{Q}_e \Delta t + T \Delta S' \text{ Total}$$
**Thermodynamics of Flux-Coupling**

Energy input over $\Delta t$

\[
\Delta E = \sum_{i \in B} \mathbf{f}_{i}^{\text{ext}} \cdot \mathbf{v}_i \Delta t + \sum_k e_k
\]

\[
\mathbf{f}_{i}^{\text{ext}} = \mathbf{A} \mathbf{P}_n / N + \frac{\mathbf{v}_i}{\sum_{i \in B} v_i^2} \dot{\mathbf{Q}}_e
\]

\[
\Delta E = \mathbf{A} \mathbf{P}_n \cdot \bar{\mathbf{v}} \Delta t + \dot{\mathbf{Q}}_e \Delta t + \sum_k e_k
\]

Entropy change (quasi-stationary, $\dot{\mathbf{Q}}_e$ not so large)

\[
T \Delta S' = \sum_k e_k - \mu \Delta N \text{ Particle insertions}
\]

\[
T \Delta S = \dot{\mathbf{Q}}_e \Delta t + T \Delta S' \text{ Total}
\]

\[
\Delta E = \mathbf{A} \mathbf{P}_n \cdot \bar{\mathbf{v}} \Delta t + T \Delta S + \mu \Delta N
\]
Energy input

\[ \Delta E = AP_n \cdot \bar{v} \Delta t + T \Delta S + \mu \Delta N \]

Pressure and stress (tangential external force)

\[ P_n = p_n + P_t \]
\[ AP_n \cdot \bar{v} \Delta t = p(A\bar{v} \cdot n \Delta t) + AP_t \bar{v} \cdot t \Delta t \]

Hence,

\[ \Delta E = -p \Delta V + T \Delta S + \mu \Delta N + \text{Heat dissipated by shear} \]

Flux coupling is consistent with equilibrium thermodynamics for open systems.
**Flux-coupling:** OPEN MD in generalized ensembles

- The amount of **heat** and **work** done into the MD system is exactly controlled
Flux-coupling: OPEN MD in generalized ensembles

- The amount of heat and work done into the MD system is exactly controlled.
- The system communicates with the exterior at its boundaries, like a real system.
Flux-coupling: open MD in generalized ensembles

- The amount of heat and work done into the MD system is exactly controlled.
- The system communicates with the exterior at its boundaries, like a real system.
Flux-coupling: **OPEN MD in generalized ensembles**

- The amount of **heat** and **work** done into the MD system is exactly controlled.
- The system communicates with the exterior at its boundaries, like a real system.

**Grand canonical** $\mu_B VT$  

**Dynamics of confined systems**
Flux-coupling: Open MD in generalized ensembles

- The amount of heat and work done into the MD system is exactly controlled.
- The system communicates with the exterior at its boundaries, like a real system.

Grand canonical $\mu_B VT$

Isobaric ensemble $P_n = p_n$

Dynamics of confined systems

Outlet B.C., Hybrids
Flux-coupling: Open MD in generalized ensembles

- The amount of heat and work done into the MD system is exactly controlled.
- The system communicates with the exterior at its boundaries, like a real system.

**Grand canonical** $\mu_B VT$

**Isobaric ensemble** $P_n = p_n$

**Constant enthalpy** $\dot{Q}_e = 0$

$(\Delta N = 0)$

$\Delta H = \Delta E + p\Delta V = 0$

Dynamics of confined systems

Outlet B.C., Hybrids

Joule-Thompson, MD-calorimeter
Flux-coupling: **OPEN MD in generalized ensembles**

- The amount of **heat** and **work** done into the MD system is exactly controlled.
- The system communicates with the exterior at its boundaries, like a real system.

**Grand canonical** $\mu B VT$

**Isobaric ensemble** $P_n = p_n$

**Constant enthalpy** $\dot{Q}_e = 0$

$(\Delta N = 0)$

$\Delta H = \Delta E + p\Delta V = 0$

**Constant heat flux**: $\dot{Q}_e$

**Dynamics of confined systems**

**Outlet B.C., Hybrids**

**Joule-Thompson, MD-calorimeter**

**Melting, ice formation, heat exchange at complex surfaces**
Density fluctuations (MD-FH hybrid)

Standard deviation of argon density, $T = 300 K$

RDB and G. Fabritiis et al. PRE, 76 (2007)
Density fluctuations (Full MD)

Standard deviation of argon density, $T = 300K$

Subvolume of a large PBC box
Open MD
Density profile at the buffer

The external force on a molecule \( i \) in the buffer:

\[
\mathbf{f}_{i}^{\text{ext}} = \frac{g(x_i)}{\sum_{i \in B} g(x_i)} \mathbf{F}^{\text{ext}} \quad \text{(with } \mathbf{F}^{\text{ext}} = A \mathbf{P} \cdot \mathbf{n})
\]
The external force on a molecule $i$ in the buffer:

$$f_{i}^{\text{ext}} = \frac{g(x_i)}{\sum_{i \in B} g(x_i)} F_{\text{ext}} \quad (\text{with } F_{\text{ext}} = A \mathbf{P} \cdot \mathbf{n})$$

The buffer density profile is controlled by the force distribution $g(x)$. 
**Open MD**

**Density profile at the buffer**

- **The external force** on a molecule $i$ in the buffer:

  $$ f_{i}^{ext} = \frac{g(x_i)}{\sum_{i \in B} g(x_i)} F^{ext} \quad \text{(with } F^{ext} = AP \cdot n) $$

- The buffer density profile is controlled by the force distribution $g(x)$.

- Any $g(x) \neq \text{cte}$ introduces **spurious heat** into the system and requires thermostats.
Open MD

Density profile at the buffer

\[ f_{i}^{\text{ext}} = \frac{g(x_i)}{\sum_{i \in B} g(x_i)} F^{ext} \quad (\text{with} \quad F^{ext} = A \mathbf{P} \cdot \mathbf{n}) \]
Open MD

Mass control at the buffer

The average buffer mass is controlled to a fixed value $\langle M_B \rangle$

$$\frac{\Delta M_B}{\Delta t} = \frac{1}{\tau_B} (\langle M_B \rangle - M_B)$$

with $\tau_B \simeq [10 – 100] fs$ (faster than any hydrodynamic time).

- **Deletion**: $\Delta M_B < 0$ (also particles crossing the buffer-end)
- **Insertion**: $\Delta M_B > 0$
  - Small solvent molecules: **USHER algorithm** for
  - Large molecules (star polymers): **Adaptive Resolution**
Open MD

Mass control at the buffer

Particle insertion by the **USHER** algorithm


- Insert a new molecule at target potential energy $E_T$ (usually $E_T = e(\rho, T)$ mean energy per particle)
Open MD

Mass control at the buffer

Particle insertion by the USHER algorithm


- Insert a new molecule at target potential energy $E_T$ (usually $E_T = e(\rho, T)$ mean energy per particle)
- Easy to implement Based on a modified Newton-Raphson method in the potential energy landscape.
Open MD
Mass control at the buffer
Particle insertion by the **USHER algorithm**


- Insert a new molecule at target potential energy $E_T$ (usually $E_T = \epsilon(\rho, T)$ mean energy per particle)
- **Easy to implement** Based on a modified Newton-Raphson method in the potential energy landscape.
- **Thermodynamic control**: local ENERGY, TEMPERATURE and PRESSURE are kept at the proper equation of state.
Open MD

Mass control at the buffer

Particle insertion by the USHER algorithm


- Insert a new molecule at target potential energy $E_T$ (usually $E_T = e(\rho, T)$ mean energy per particle)
- Easy to implement: Based on a modified Newton-Raphson method in the potential energy landscape.
- Thermodynamic control: local ENERGY, TEMPERATURE and PRESSURE are kept at the proper equation of state.
- Negligible insertion cost $< 1\%$ total CPU (LJ), $\sim 3\%$ (water).
Open MD

Mass control at the buffer

Particle insertion by the USHER algorithm


- Insert a new molecule at target potential energy $E_T$ (usually $E_T = e(\rho, T)$ mean energy per particle)
- Easy to implement Based on a modified Newton-Raphson method in the potential energy landscape.
- Thermodynamic control: local ENERGY, TEMPERATURE and PRESSURE are kept at the proper equation of state.
- Negligible insertion cost < 1% total CPU (LJ), ~ 3% (water).
- Very fast: water into water at low energy ($E_T = e$) requires 100 iterations ($10^5$ faster than random insertion)
Adaptive Resolution Scheme


center of mass

\[ R_\alpha = \frac{\sum m_{i\alpha} r_{i\alpha}}{M_\alpha} \]

\[ V_\alpha = \frac{\sum m_{i\alpha} v_{i\alpha}}{M_\alpha} \]
Adaptive Resolution Scheme

\[ R_{\alpha} = \frac{\sum_{i\alpha} m_{i\alpha} r_{i\alpha}}{M_{\alpha}} \]
\[ V_{\alpha} = \frac{\sum_{i\alpha} m_{i\alpha} v_{i\alpha}}{M_{\alpha}} \]

\[ \mathbf{F} = w(x_{\alpha})w(x_{\beta}) \sum_{i\alpha j\beta} \mathbf{F}_{i\alpha j\beta}^{\text{atom}} + [1 - w(x_{\alpha})w(x_{\beta})] \mathbf{F}_{\alpha\beta}^{\text{c.m.}} \]

\[ \mathbf{F}_{i\alpha j\beta}^{\text{atom}} = -\frac{\partial U_{\text{atom}}}{\partial \mathbf{r}_{i\alpha j\beta}} \quad \text{Atomistic} \]
\[ \mathbf{F}_{\alpha\beta}^{\text{c.m.}} = -\frac{\partial U_{\text{c.m.}}}{\partial \mathbf{R}_{\alpha\beta}} \quad \text{Coarse – Grained} \]
HybridMD-AdResS triple scale

(a) Coarse-grained buffer

(b) Adaptive buffer
Open MD with AdResS

The adaptive buffer
does not require accurate fits for the CG and HYB models

Viscosities (oxygen-LJ units)
- CG $\eta=20$
- EX $\eta=45$ Flexible TIP3P water model

Radial distribution functions (center of masses)
HybridMD-AdResS triple scale

HybridMD-AdResS triple scale

Melts of star polymers via *Open MD-AdResS*
Melts of star polymers via \textsc{Open MD-AdResS}

(to be submitted)

\[ \phi = 0.2 \]

\[ \text{Force} + 1 \]

\[ \text{attractive} \]

\[ \text{repulsive} \]

\[ \text{Star 12-6} \]

\[ \text{RDF} \]

\[ \text{MD} \]

\[ \text{DPD using} <F_{\mu \nu} \cdot e_{\mu \nu}>^R \]

\[ \text{DPD using} <F_{\mu} \cdot e_{\mu \nu}>^R \]
Hybrid particle-continuum schemes: 
alternatives

- **State scheme:** Non-conservative, no fluctuations (requires averaging), incompressible.
- **Flux scheme:** Conservative, fluctuations, compressible.
Hybrid particle-continuum schemes: set-up

State-coupling

Flux-coupling
Continuity in flux schemes

The continuum solver, schematically

\[ \Delta \Phi_i = \Delta t_{NS} \{ \Phi_j \} + \delta_{fC} \Delta \phi^{MD} \]

Relaxation of particle transfers towards C

\[ \Delta M^{MD} = \frac{\Delta t_c}{\tau_M} \left( \Delta M_{H}^{MD} - \Delta M_{H}^{NS} \right) \]

where \[ \Delta M_{H}^{NS} = -A\rho_H \mathbf{V}_H \cdot \mathbf{n} \Delta t \]

\[ \Delta \mathbf{V}^{MD} = \frac{\Delta t_c}{\tau_v} \left( \langle \mathbf{v}_C^{MD} \rangle_{[\delta t, \tau]} - \langle \mathbf{V}_C \rangle_{[\Delta t, \tau]} \right) \]
Hybrid particle-continuum schemes: Time coupling
Hybrid MD-Fluctuating Hydrodynamics

Matching stress fluctuations via Green-Kubo relations

- **Molecular dynamics**: decorrelation time $\tau_c \sim 100$fs (simple liquids)

  \[
  \langle J_{MD}^2 \rangle = \frac{\eta k_B T}{V \tau_c} \quad \text{with,} \quad \tau_c \equiv \frac{\int_0^\infty \langle J(t)J(0) \rangle dt}{\langle J(0)^2 \rangle}
  \]

- **Fluctuating hydrodynamics**: decorrelation time $\Delta t_{FH}/2$,

  \[
  \langle J_{FH}^2 \rangle = \frac{2\eta k_B T}{V \Delta t_{FH}}
  \]

Balance stress fluctuations, $\langle J_{MD}^2 \rangle = \langle J_{FH}^2 \rangle$:

$\Delta t_{FH} = 2\tau_c = \delta t_s$  Sampling time = twice MD decorrelation time

In general, $\Delta t_c = n_{FH} \Delta t_{FH} = N_s \delta t_s$
Hybrid MD-Fluctuating Hydrodynamics

Some test cases: sound

**liquid argon**

**water**

![Graphs](image)
Hybrid MD-Fluctuating Hydrodynamics

Some test cases: sound
Hybrid MD-Fluctuating Hydrodynamics
Collision of sound waves against DMPC lipid layer

Simulations of open systems is required for many applied problems: Confined systems, flow in nanotubes, sound-soft matter interaction, melting...

- **Open FH**
- **Open MD**
- **Hybrid MD**
- Use in combination with **AdResS** to work with large molecules