Portrait: Adaptive Resolution Molecular Dynamics Simulation

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Pioneers

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References

Motivation—Features of Soft Matter

Intrinsic multi-scale & Hierarchical features

Computational capability for solution state

Solute molecule

Solvent molecules
Motivation—Multi-Scale Model

Atomistic MD

Coarse-grained MD

Toluene

Densely packed cluster with modest phase separation
Linking Different Levels of Resolution

Quantum mechanism + Molecular mechanism

Atomistic MD + Coarse-grained MD

Forbid to switch between different levels of resolution

Dual-scale model of BPA-PC on a nickel surface
Problems of Combining AMD with CGMD

If molecules can freely exchange between atomistic region & coarse-grained region, ...

- Number of degrees of freedom (DOF) changes.
- Free energy \( A \) associated with DOFs is unequal in the two regions.
- Non-equilibrium & inducing driving force:

\[
A_A \neq A_B, \quad \mu_A \neq \mu_B, \quad P_A \neq P_B, \quad T_A \neq T_B
\]
Idea of Adaptive Resolution Scheme

Geometry induced first-order phase transition

- Keep the equilibrium
  \[ \mu_A = \mu_B, \quad P_A = P_B, \quad T_A = T_B \]

- Difference of free energy ≡ latent heat

- No net flux

The free energy \( A \) associated with DOFs explicitly considered in a simulation as a function of \( x \).
Introducing the Transition Regime

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*Intermolecular force acting between the molecules α and β*

\[
\mathbf{F}_{\alpha\beta} = w(x_\alpha)w(x_\beta)\mathbf{F}_{\alpha\beta}^{\text{atom}} + \left[1 - w(x_\alpha)w(x_\beta)\right]\mathbf{F}_{\alpha\beta}^{\text{CG}}
\]

- \(\alpha, \beta\): index of the molecules
- \(w(x)\): weighting function
- \(\mathbf{F}_{\alpha\beta}^{\text{atom}}\): sum of all pair atom interactions between explicit atoms of the molecule \(\alpha\) and \(\beta\)
- \(\mathbf{F}_{\alpha\beta}^{\text{CG}}\): effective pair force between the two molecules

\[
\mathbf{F}_{\alpha\beta}^{\text{atom}} = \sum_{i\alpha, j\beta} \mathbf{F}_{i\alpha j\beta}^{\text{atom}} = -\nabla U_{i\alpha j\beta}^{\text{atom}} \quad ; \quad \mathbf{F}_{\alpha\beta}^{\text{CG}} = -\nabla U_{\alpha\beta}^{\text{CG}}
\]
Introducing the Transition Regime

Intermolecular force acting between the molecules $\alpha$ and $\beta$

$$F_{\alpha\beta} = w(x_\alpha)w(x_\beta)F^{\text{atom}}_{\alpha\beta} + \left[1 - w(x_\alpha)w(x_\beta)\right]F^{\text{CG}}_{\alpha\beta}$$

Weighting function

$$w(x) = \begin{cases} 
1 & , -d > x \geq -L \\
0 & , +L > x \geq +d \\
\cos^2\left[\frac{\pi}{2d}(x + d)\right], & +d > x \geq -d 
\end{cases}$$
Validation of AdResS

RDF & order parameter

Number density profile

Diffusion profile over different time origins

Equation of state

Mean square displacement

- Radius of gyration of the solute (polymer)
- Diffusivity of the solute (polymer)
Progress

2005

Slab model
Tetrahedral molecule

2006

Spherical model
Tetrahedral molecule
Pressure & density correction

2007

Polymer in media of
tetrahedral molecules

w/o correction
w/ correction
**Progress**

**2007**
1. Liquid water
2. Applying electrostatic interaction via reaction field method

**2012**
Within AMD & hybrid regions
1. C$_{60}$ in toluene
2. Implementation of the AdResS into GROMACS

**2014**
1. Protein in Martini water
2. Bundled-water model

Mathematical expression:

$$F^{\text{atom}}_C(r_{i\alpha j\beta}) = \frac{e_{i\alpha} e_{j\beta}}{4\pi \varepsilon_0} \left[ \frac{1}{r_{i\alpha j\beta}^3} - \frac{1}{R_c^3} \left( 1 + 2\varepsilon_\text{RF} \right) \right] r_{i\alpha j\beta}.$$
Conclusion

- AdResS allows the free exchange of particles among full-atom region and coarse-grained region, and reduce the computational effort massively.

- AdResS provides a chance to investigate many interesting problems in soft materials which are inherently multiscale.