Scaling in DPD

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DPD

$$\frac{d\boldsymbol{r_i}}{dt} = \boldsymbol{v_i} \qquad \frac{d\boldsymbol{v_i}}{dt} = \boldsymbol{f_i} \tag{1}$$

$$\boldsymbol{f_i} = \sum_{j \neq i} (\boldsymbol{F^C_{ij}} + \boldsymbol{F^D_{ij}} + \boldsymbol{F^R_{ij}}) \tag{2}$$

$$\boldsymbol{F^C_{ij}} = a_{ij} \omega^C(r_{ij}) \boldsymbol{\hat{r}_{ij}} \tag{3}$$

$$\boldsymbol{F^D_{ij}} = -\gamma \omega^D(r_{ij})(\boldsymbol{\hat{r}_{ij}} \cdot \boldsymbol{v_{ij}}) \boldsymbol{\hat{r}_{ij}} \tag{4}$$

$$\boldsymbol{F^R_{ij}} = \sigma \omega^R(r_{ij}) \theta_{ij} \boldsymbol{\hat{r}_{ij}} \tag{5}$$

Usually,

$$\omega^C(r) = 1 - \frac{r}{r_c} \tag{6}$$

$$\omega^D(r) = [\omega^R(r)]^2 = (1 - \frac{r}{r_c})^2 \tag{7}$$

DPD

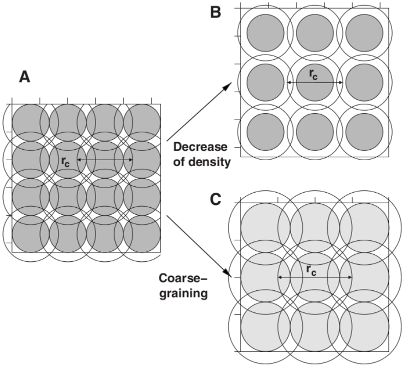
How to choose a, γ, and σ?

- scaling: different coarse grain level?
- match experimental parameters?

References

- Groot & Warren, J. Chem. Phys, 1997.
- Pivkin, J. Chem. Phys, 2006.
- Qiao & He, J. Chem. Phys, 2008.
- Fuchslin, J. Chem. Phys, 2009.

- coarse graining level
  $\nu \equiv \frac{N_{phys}}{N}$
- scaling ratio $\phi \equiv \frac{\nu'}{\nu} = \frac{N}{N'}$
- mass of a DPD particle
  $m' = \phi m$
- $r'_c = \phi^{\frac{1}{d}} r_c$
  d is dimension



B: the mutual overlap of the soft particles is smaller.

Potential energy $U_0 = \sum_i^N \sum_{j>i} \frac{a}{2r_c}(r_{ij} - r_c)^2$
For an isotropically compressed system, $L \to (1-\delta)L$, $\delta \ll 1$
Assume $\Delta r_{ij}(\delta) = \delta r_{ij} + O(\delta^2)$

$$U_\delta = \sum_i^N \sum_{j>i} \frac{a}{2r_c}(r_{ij} - \Delta r_{ij}(\delta) - r_c)^2$$

$$\Delta U = U_\delta - U_0 = \sum_i^N \sum_{j>i} a(1 - \frac{r_{ij}}{r_c})\delta r_{ij}$$

ΔU is invariant under scaling

$$\sum_i^N \sum_{j>i} a(1 - \frac{r_{ij}}{r_c})\delta r_{ij} = \sum_i^{N'} \sum_{j>i} a'(1 - \frac{r'_{ij}}{r'_c})\delta r'_{ij}$$

$$a' = \phi^{1-\frac{1}{d}} a$$

- $T' = T$
- nondimensional $\tilde{a} = a\frac{r_c}{\epsilon}$ is invariant
  $\rightarrow$ energy unit $\epsilon' = \phi\epsilon$
- $\epsilon = m\frac{{r_c}^2}{\tau^2}$
  $\rightarrow$ time unit $\tau' = \phi^{\frac{1}{d}}\tau$
- nondimensional $\tilde{\gamma} = \gamma\frac{r_c^2}{\epsilon\tau}$ is invariant
  $\rightarrow \gamma' = \phi^{1-\frac{1}{d}}\gamma$
- $\sigma^2 = 2k_B T\gamma$
  $\rightarrow \sigma' = \phi^{1-\frac{1}{2d}}\sigma$

$$N' = \phi^{-1} N, \quad a' = \phi^{1-1/d} a,$$

$$m' = \phi m, \quad \gamma' = \phi^{1-1/d} \gamma,$$

$$r_c' = \phi^{1/d} r_c, \quad \sigma' = \phi^{1-1/(2d)} \sigma,$$

$$\tau' = \phi^{1/d} \tau, \quad \epsilon' = \phi \epsilon.$$

$$[\Delta \boldsymbol{v_i}]' = \sum_{j \neq i} \frac{[\boldsymbol{F_{ij}}]'}{m'} \Delta t'$$

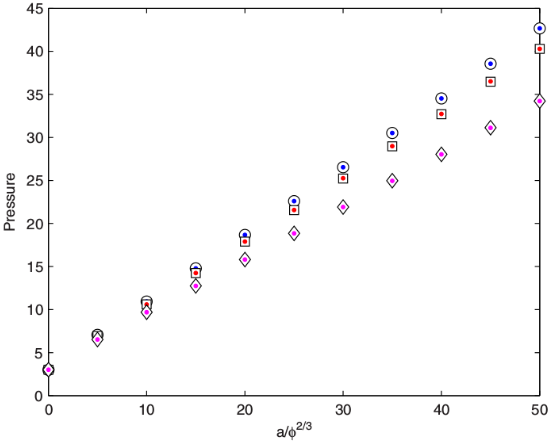
$$= \frac{\phi^{1-1/d} \phi^{1/d}}{\phi} \sum_{j \neq i} \frac{\boldsymbol{F_{ij}}}{m} \Delta t = \Delta \boldsymbol{v_i}$$

$$\Delta \tilde{\boldsymbol{v}}_{\boldsymbol{i}} = \Delta \boldsymbol{v_i} \frac{\tau}{r_c}$$

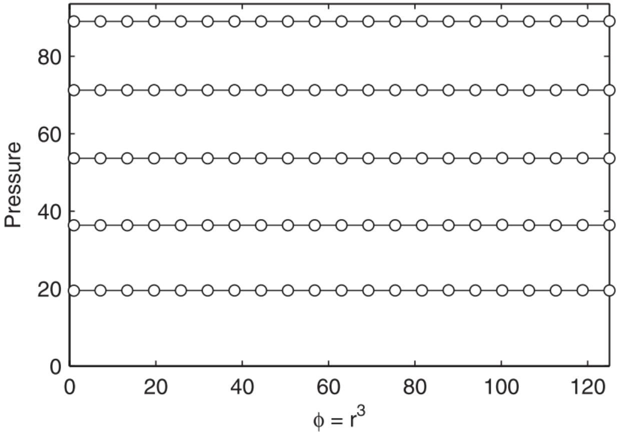
$$\rightarrow \Delta \tilde{\boldsymbol{v}}_{\boldsymbol{i}} = \Delta \tilde{\boldsymbol{v}}_i'$$

$$\rightarrow \tilde{\boldsymbol{r}}(\tilde{t}) = \tilde{\boldsymbol{r}}'(\tilde{t}')$$

at $\phi = 1,\ r_c = 1, m = 1, \rho = 3, \gamma = 4.5, \sigma = 3$
a in $[0,\ \frac{50}{\phi^{2/3}}]$
$\phi = 1$ (circles), 8 (squares), 125 (diamonds)
BC: reflective walls



periodic BC
a in $[0, \frac{100}{\phi^{2/3}}]$, ϕ in [1, 125]



Compressibility and a

$$\kappa^{-1} = \left(\frac{1}{n k_B T \kappa_T}\right)_{phys} = \frac{1}{\nu k_B T}\left(\frac{\partial p}{\partial \rho}\right)_T$$

n: number density of physical molecules, for water, $3.337 \times 10^{28}\,\mathrm{m}^{-3}$

$$p = \rho k_B T + \frac{2\pi}{3}\rho^2 \int_0^1 r f(r) g(r) r^2 dr$$

$$\rightarrow p = \rho k_B T + \alpha a \rho^2 \qquad \alpha = 0.101 \pm 0.001$$

$$\rightarrow a = k_B T \frac{\kappa^{-1}\nu - 1}{2\alpha\rho} \qquad \rho \geq 3 r_c^{-3}$$

Conclusions

Map parameters from one DPD system to another

$$N' = \phi^{-1} N, \quad a' = \phi^{1-1/d} a,$$

$$m' = \phi m, \quad \gamma' = \phi^{1-1/d} \gamma,$$

$$r_c' = \phi^{1/d} r_c, \quad \sigma' = \phi^{1-1/(2d)} \sigma,$$

$$\tau' = \phi^{1/d} \tau, \quad \epsilon' = \phi \epsilon.$$

Determine a by compressibility

$$a = k_B T \frac{\kappa^{-1} \nu - 1}{2 \alpha \rho}$$