Liquid crystals

- Liquid Crystals (LCs)
  - phase in the state between solid and liquid.
- Unique optical characteristics
  - Many technological-applications.

1

Liquid Crystal Display

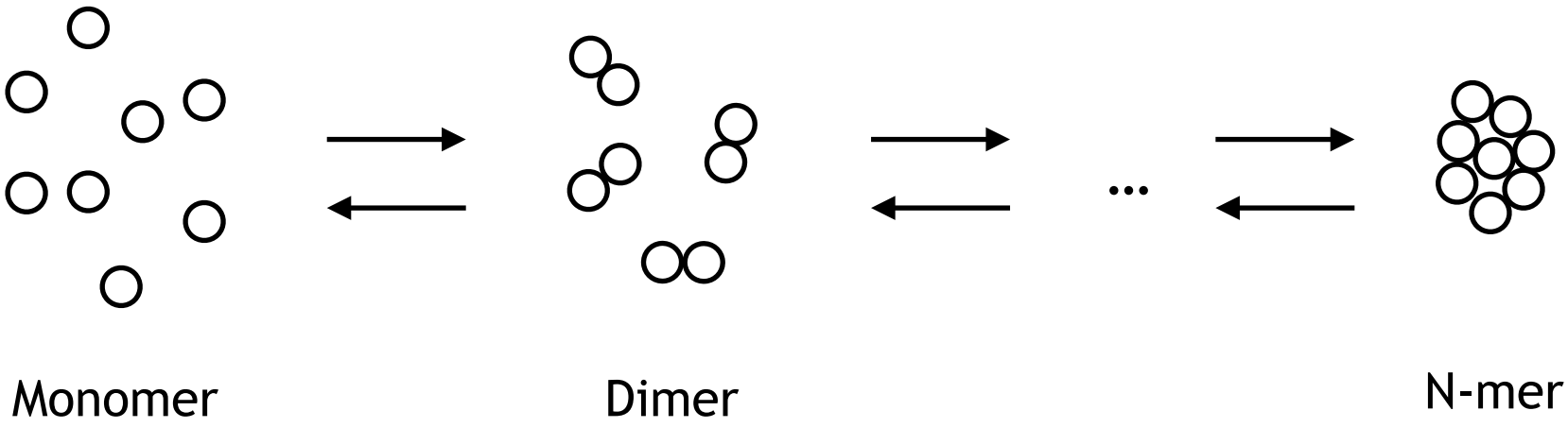
2

Optical effect
by LC structure

Nucleation

- an early-stage process of phase transitions

molecular condensation



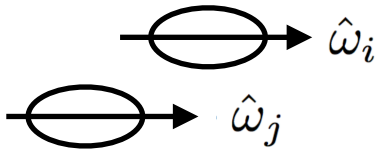
Molecular model

- Hess-Su model

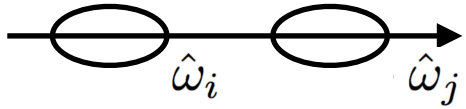
$$u(r_{ij}, \hat{\omega}_i, \hat{\omega}_j) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} (1 + \Psi) \right],$$

$$\Psi = 5\epsilon_1 P_2 \left(\hat{\omega}_i \cdot \hat{\omega}_j \right) + 5\epsilon_2 \left[P_2 \left(\hat{\omega}_i \cdot \hat{r}_{ij} \right) + P_2 \left(\hat{\omega}_j \cdot \hat{r}_{ij} \right) \right]. \qquad P_2(x) = \frac{1}{2} \left(3x^2 - 1 \right).$$

Prefer parallel



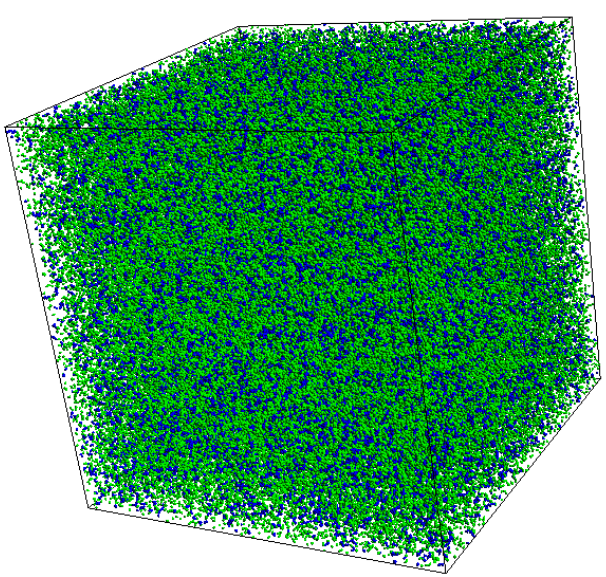
Prefer parallel and colinear

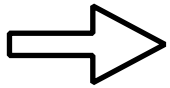


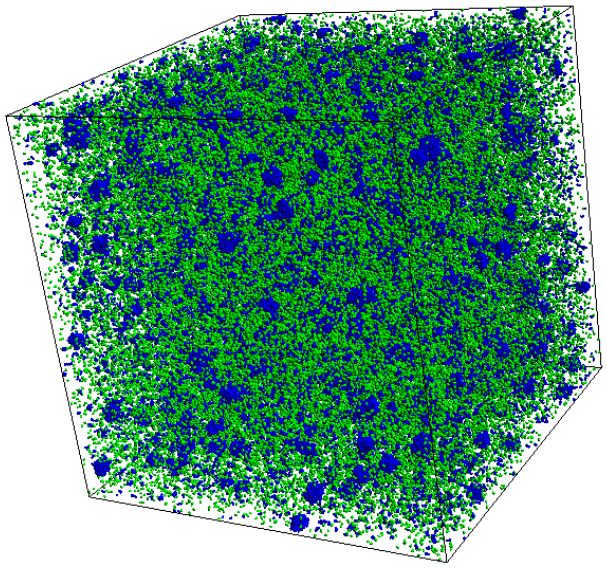
- Number of molecules
  - LCs 2.56E+5 (ρ_m = 0.012), Carrier gas 4.27E+5 (ρ_c = 0.02)

Simulation conditions

- NVT MD simulation with Hess-Su model
- Yasuoka-Matsumoto method [K. Yasuoka et al., *J. Chem. Phys.*, 109, 19 (1998).]
- Monomer, Cluster, Carrier gas (not shown)





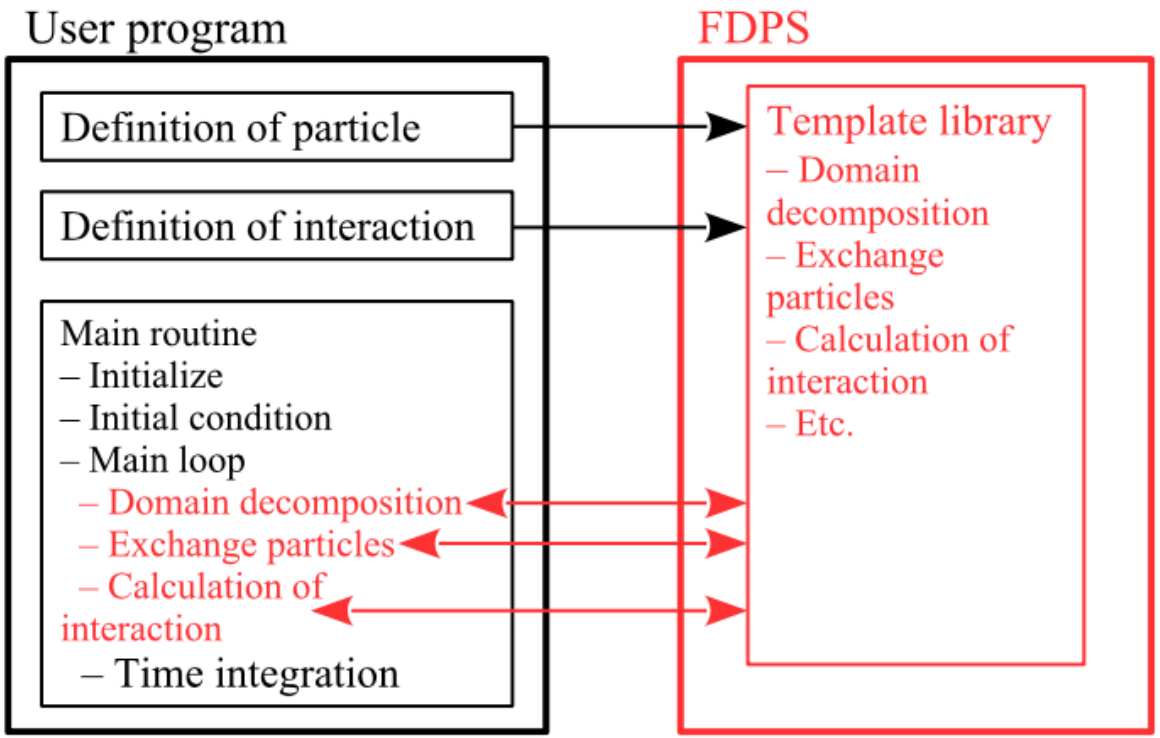


T^* = 1.25

T^* = 0.67

Implementation

Framework for developing particle simulator (FDPS)



Basic concept of FDPS. Colored text corresponds to FDPS APIs.

M. Iwasawa et al., *Publications of the Astronomical Society of Japan*, **68**, 4 (2016).

https://github.com/FDPS/FDPS