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Pressure Control in Dissipative Particle Dynamics and its Application in Simulating Micro- and Nano-bubbles

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Outline

- **Introduction**
- **Barostat in DPD & MDPD**
  - **Berendsen barostat in DPD**
  - **Partial Berendsen barostat in DPD & MDPD**
- **Bubble dynamics in DPD & MDPD**
  - **Application in multi-component system**
  - **Bubble Collapse & Oscillation**
- **Summary**

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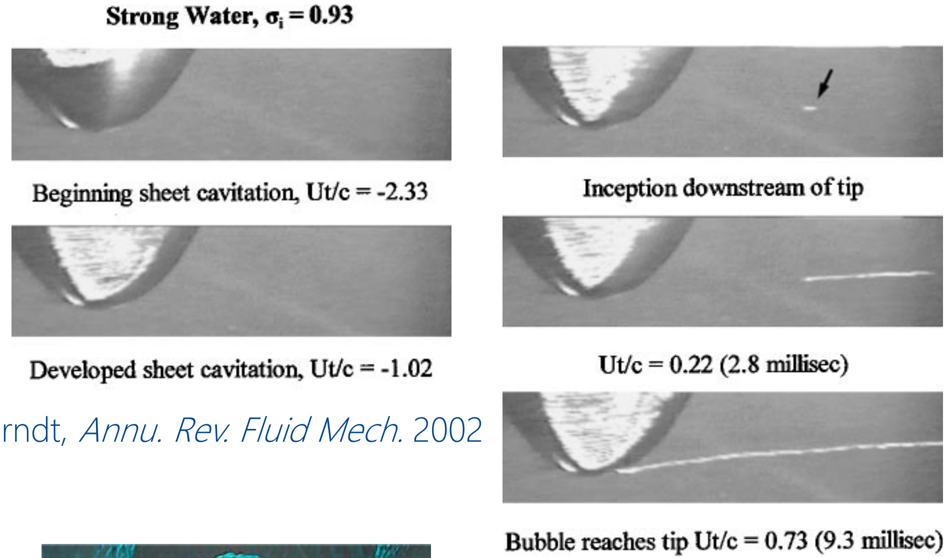
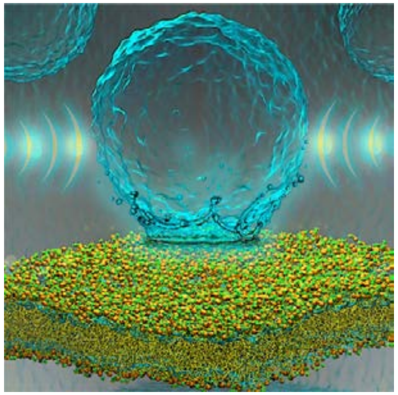
Introduction – Bubbles

- Cavitation Inception – Hydrodynamics of Propeller:
  - Liquid to Vapor Phase Transition;
  - Gaseous Nucleation.



Arndt, *Annu. Rev. Fluid Mech.* 2002

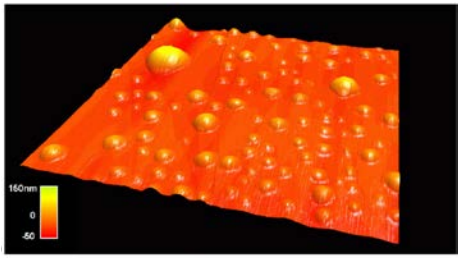
- Sonoporation – Drug Delivery:
  - Ultrasound Contrast Agent;
  - Drug Delivery & Noninvasive Therapy.

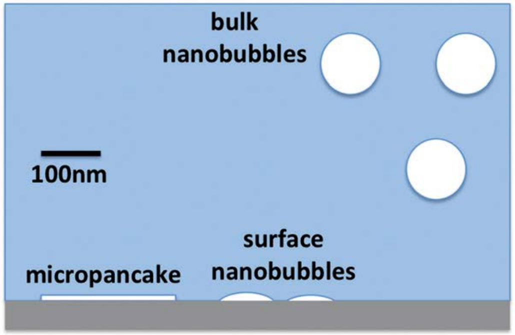


Fu *et al.*, *J. Phys. Chem. Lett.* 2015

Introduction – Bubbles

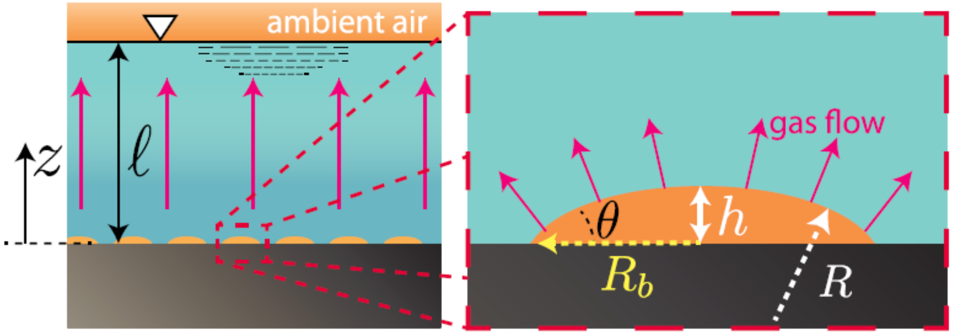
- Nanobubbles (surface or bulk):
  - Stability of their long life (days & weeks);
  - Current MD simulation is limited to several **tens of nanometers**, resulting in lifetimes of order **100 ns**.





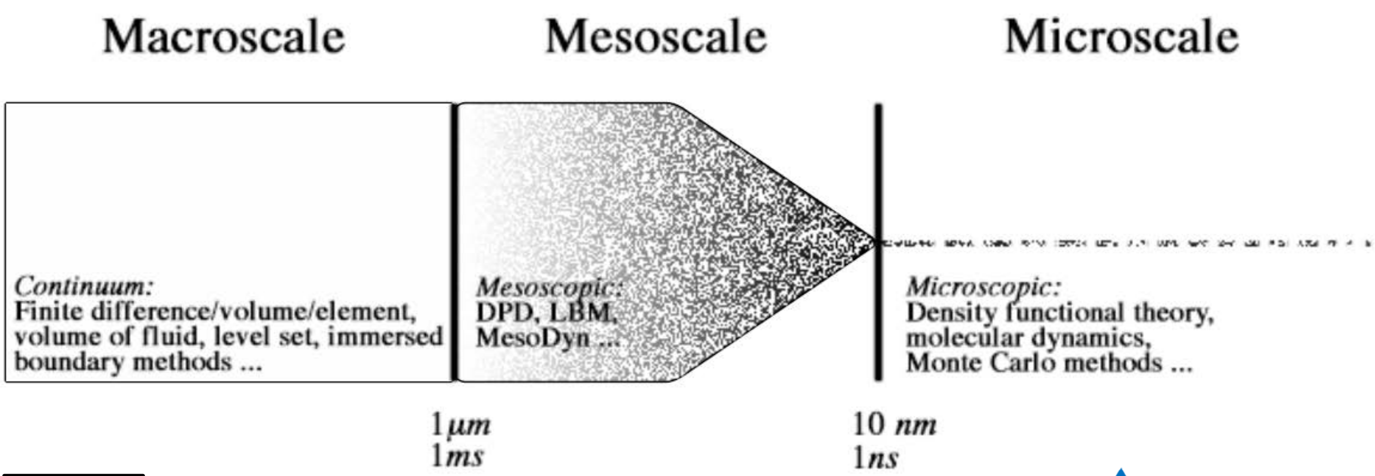
Seddon *et al.*, *ChemPhysChem*, 2012

Lohse & Zhang, *Rev. Mod. Phys.*, 2015



Weijs and Lohse, *Phys. Rev. Lett.*, 2013

Introduction – Dissipative Particle Dynamics



DPD

Colloidal suspensions *[Koelman and Hoogerbrugge, 1993, Boek et al., 1997]*

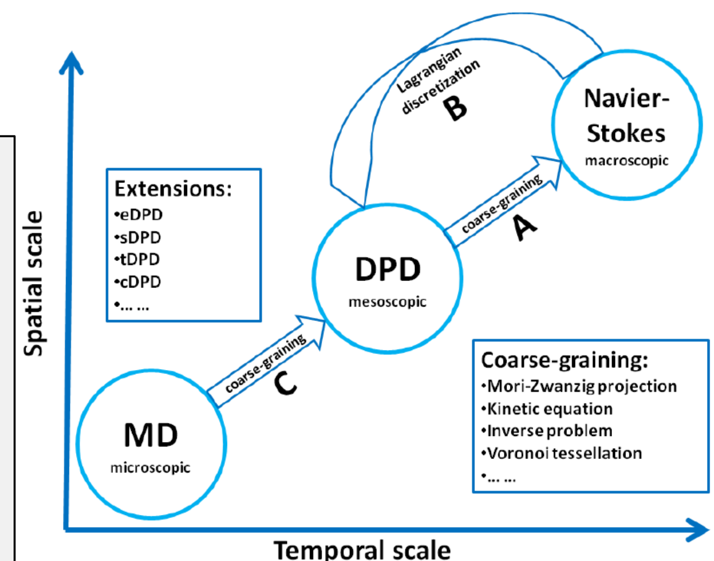
Ploymer solution *[Kong et al., 1997, Spenley, 2000, Jiang et al., 2007]*

Two-phase flow *[Pan et al., 2016, Warren, 2003]*

Surfactant *[Groot, 2000, Groot, 2003, Rekvig et al., 2003]*

Membranes *[Yang and Ma, 2010, Dutt et al., 2011, Li et al., 2012]*

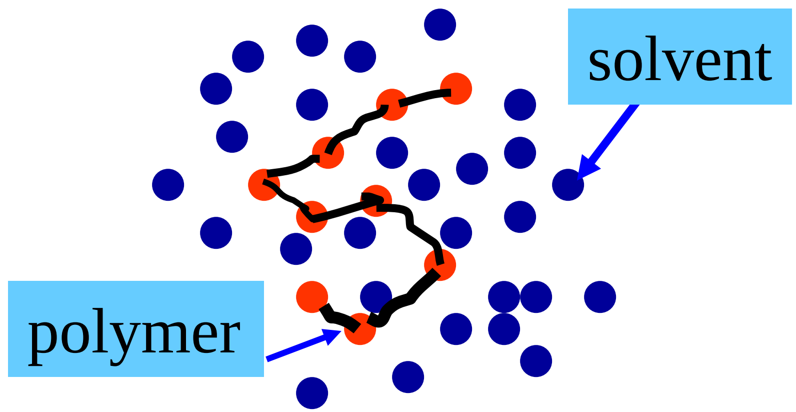
Drug delivery *[Tomasini and Tomassone, 2012, Patterson et al., 2011, Masoud and Alexeev, 2011, Delcea et al., 2011]*

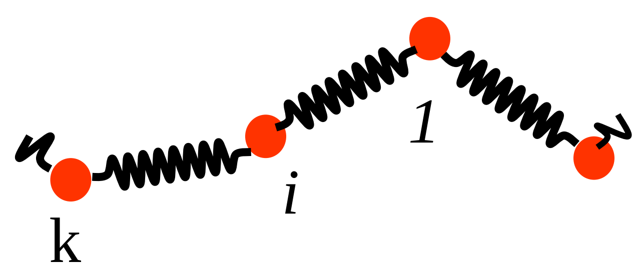


Standard DPD Method

- Basic Theory
  - $\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i$; $\frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i + \mathbf{F}_e$.
  - $\mathbf{f}_i = \sum_{j \neq i} \left(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \right)$.
  - $\mathbf{F}_{ij}^C = \begin{cases} a_{ij}(1 - r_{ij})\hat{\mathbf{r}}_{ij}, & r_{ij} < 1 \\ 0, & r_{ij} \geq 1 \end{cases}$;
  - $\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij})\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}\mathbf{r}_{ij}$;
  - $\mathbf{F}_{ij}^R = \sigma w^R(r_{ij})\theta_{ij}\hat{\mathbf{r}}_{ij}$.

- Fluctuation-Dissipation Theorem:
  - $\gamma = \frac{\sigma^2}{2k_BT}$;
  - $w^D(r) = [w^R(r)]^2 = \begin{cases} (1 - r/r_C)^s, & r_{ij} < r_C \\ 0, & r_{ij} \geq r_C \end{cases}$.



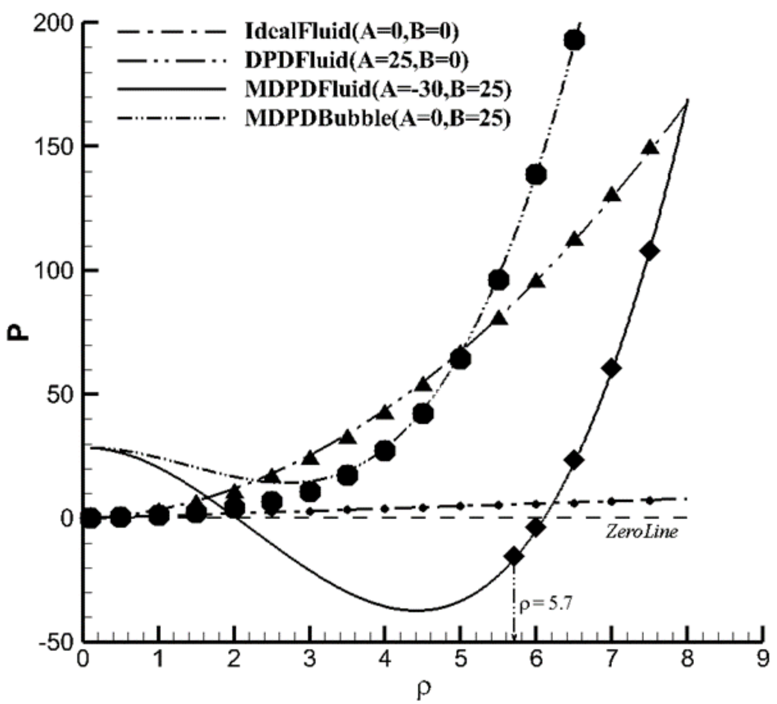


Many-body DPD

- Basic Theory
  - $\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i; \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i + \mathbf{F}_e.$
  - $\mathbf{f}_i = \sum_{j\neq i}\left(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R\right).$
  - $\mathbf{F}_{ij}^C =$

    $[A_{ij}w^C(r_{ij}) + B_{ij}(\bar{\rho}_i + \bar{\rho}_j)w^d(r_{ij})]$
  - $\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij})\mathbf{v}_{ij}\cdot\mathbf{r}_{ij}\mathbf{r}_{ij}$;
  - $\mathbf{F}_{ij}^R = \sigma w^R(r_{ij})\theta_{ij}\hat{\mathbf{r}}_{ij}$.

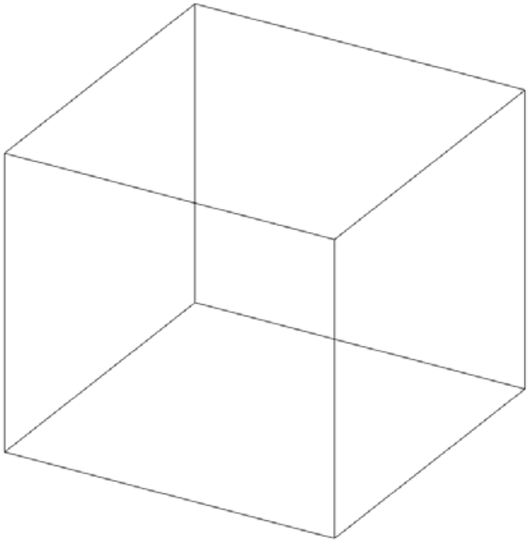
- Equations of State (EoS) :
- ***DPD:*** $P = \rho k_B T + \alpha A\rho^2$
- ***MDPD***: $P = \rho k_B T + \alpha A\rho^2 + 2\alpha B r_d^4(\rho^3 - c\rho^2 + d)$



Introduction – Pressure control

- The boundary condition(BC) in Particle methods
  - Periodic BC
  - No-slip wall BC
  - Pressure BC?
  - …

Cube system



MD → DPD

Pressure control（barostat）

DPD

- Andersen barostat [*Trofimov et al., 2005*]
- Berendsen barostat [*Atashafrooz and Mehdipour, 2016,Seaton et al., 2013*]
- SSA: Shardlow-splitting algorithm [*Lísal et al., 2011*]
- Langevin piston approach [*Jakobsen, 2005*]

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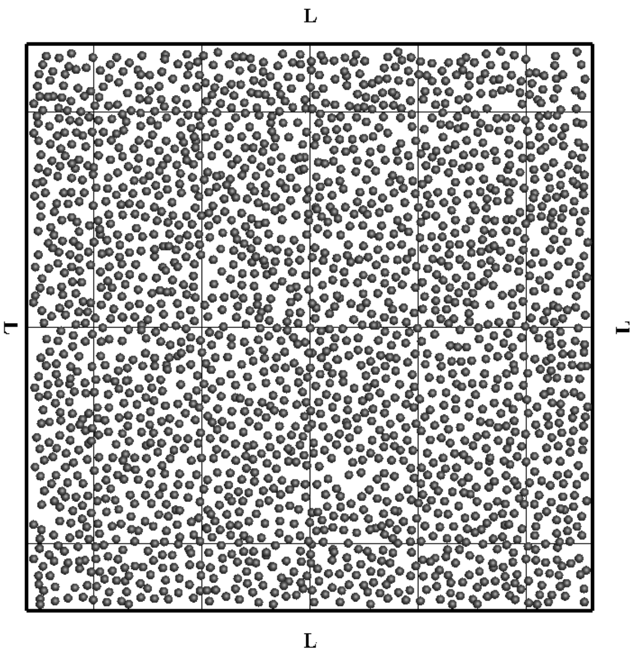
Berendsen Barostat theory

- The Berendsen barostat's scale factor,

$$\mu = \left[1 - \frac{\Delta t}{\tau_p}\left(P - P_0\right)\right]^{1/3}$$

- Consider a cubic system which contains N molecules and its volume is $V = L^3$.

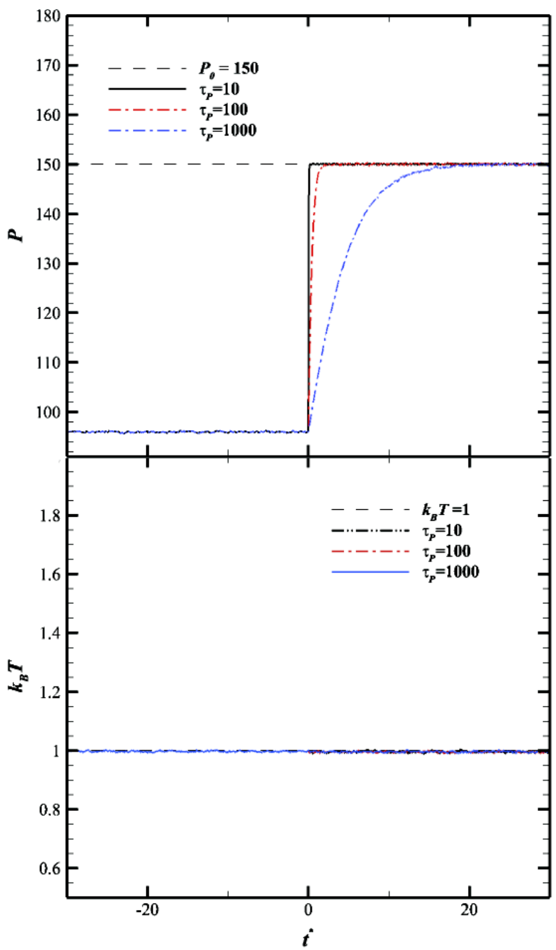


$$\left.\begin{aligned} r_i &\to \mu r_i \left(i = 1, 2, 3, \ldots, N\right) \\ L &\to \mu L\left(L = L_x = L_y = L_z\right) \end{aligned}\right\}$$

$$\Leftrightarrow \begin{cases} \left(r_x, r_y, r_z\right)_i \to \left(\mu r_x, \mu r_y, \mu r_z\right)_i \\ \left(L_x, L_y, L_z\right) \to \left(\mu L_x, \mu L_y, \mu L_z\right) \end{cases}$$

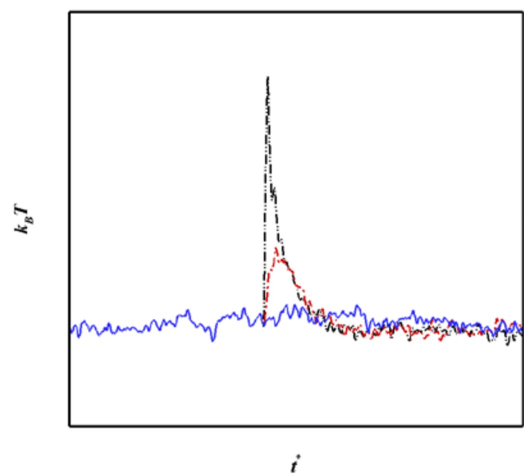
Here, t is the time step, τ_p is the "rise time" of the barostat, and P_0 is the desired pressure.

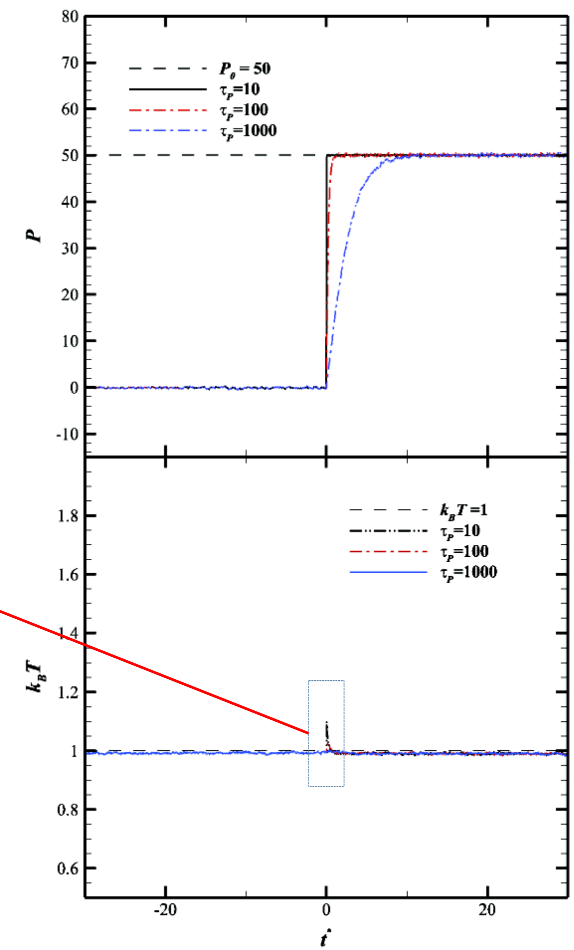
Berendsen barostat applys in single component system



DPD

t=0* : Start the implement of pressure control.

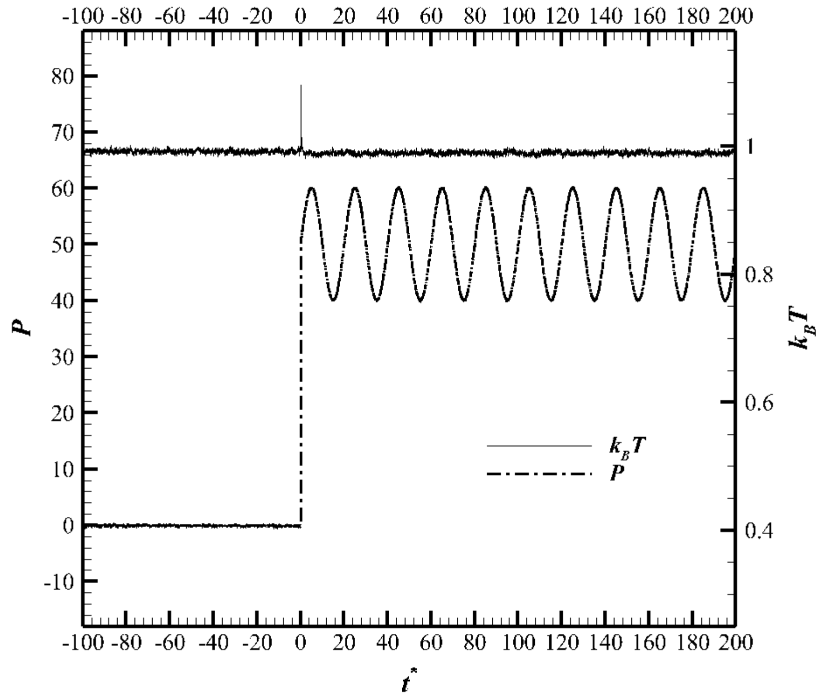




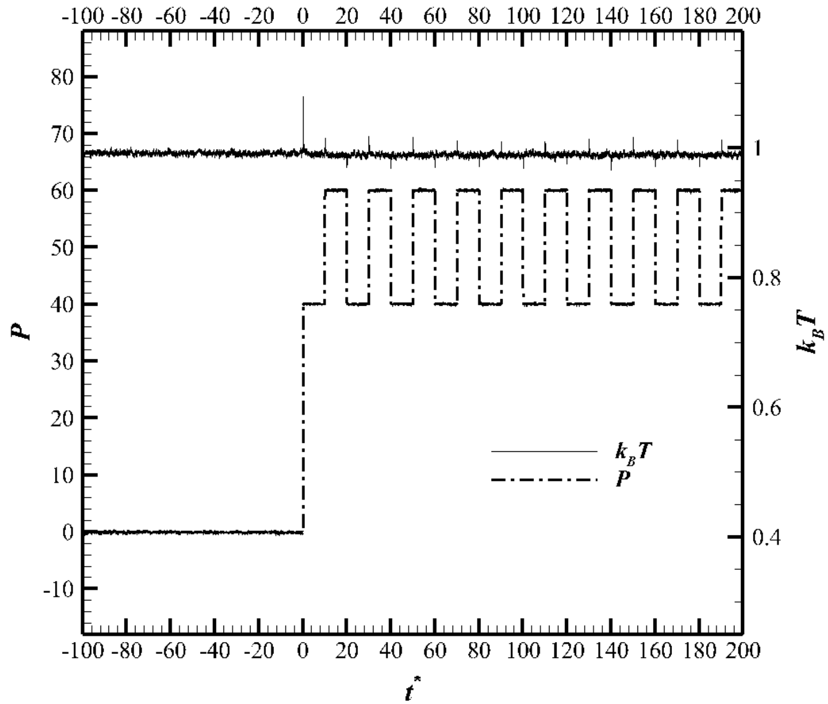
MDPD

Berendsen barostat - Nonequilibrium dynamics

$$P_0^* = P_0 + P_a sin(2\pi f \cdot t^*)$$



$$P_0^* = P_0 - P_a(-1)^{[2f \cdot t^*]}$$



Here, f is the frequency, P_a *is the* amplitude. And P_0 is the constant part of desired pressure $P_0{}^*$

Berendsen barostat limitation

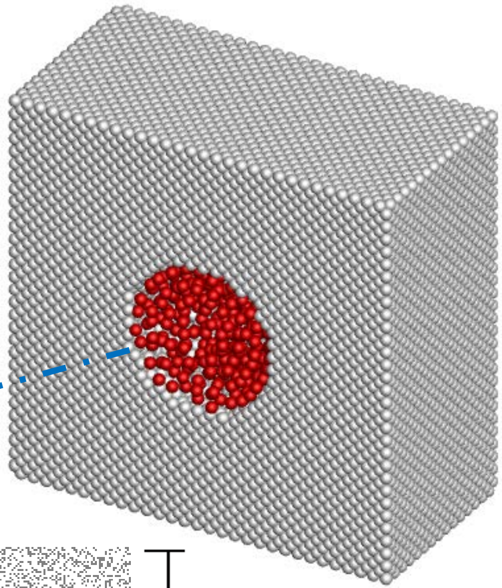
- Particle displacement rescaling

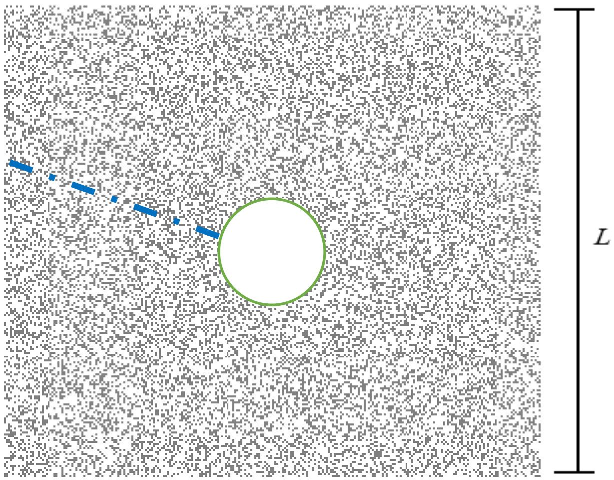
$$r_i \to \mu r_i \left(i = 1, 2, 3, \ldots, N \right)$$

- Region size rescaling

$$L \to \mu L \left(L = L_x = L_y = L_z \right)$$

Bring an artificial effect on the multi-component system interface.



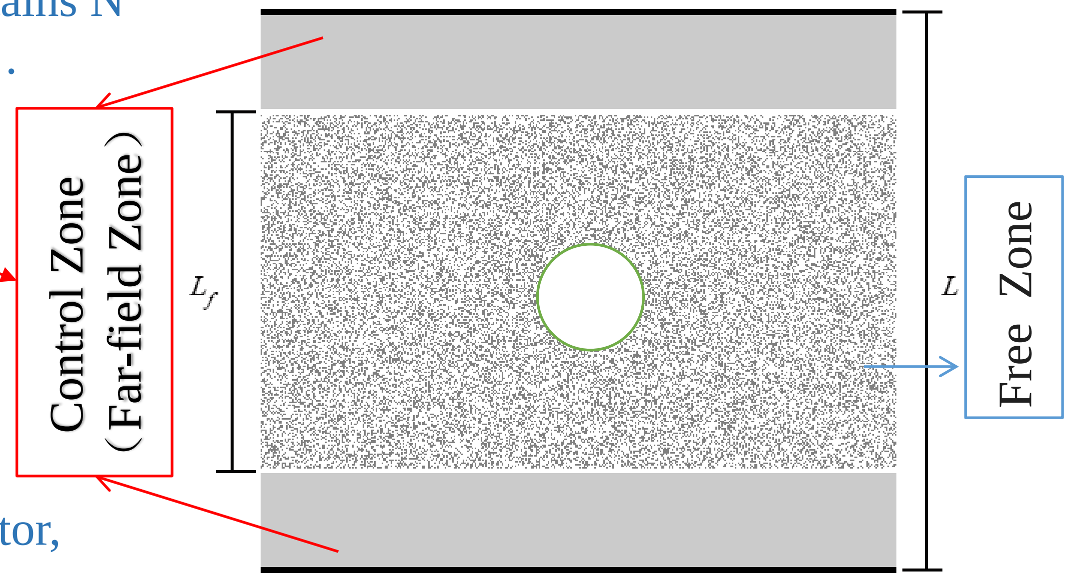


Partial Berendsen Barostat

- Consider a cubic system which contains N molecules and its volume is $V = L^3$.

$$
\left.\begin{array}{l}
\boxed{r_i \to \mu r_i \left(i = 1, 2, 3, \dots, N\right)} \\
L \to \mu L \left(L = L_x = L_y = L_z\right)
\end{array}\right\}
$$

$$
\Leftrightarrow \begin{cases}
\left(r_x, r_y, r_z\right)_i \to \left(\mu r_x, \mu r_y, \mu r_z\right)_i \\
\left(L_x, L_y, L_z\right) \to \left(\mu L_x, \mu L_y, \mu L_z\right)
\end{cases}
$$



- The Berendsen barostat's scale factor,

$$
\mu = \left[1 - \frac{\Delta t}{\tau_p}\left(P - P_0\right)\right]^{1/3}
$$

Here, t is the time step, τ_p is the "rise time" of the barostat, and P_0 is the desired pressure.

Define a new variable: $\delta = \dfrac{L_f}{L}$

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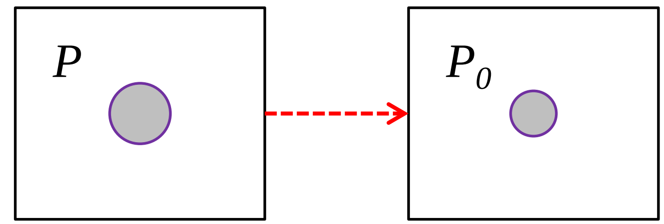
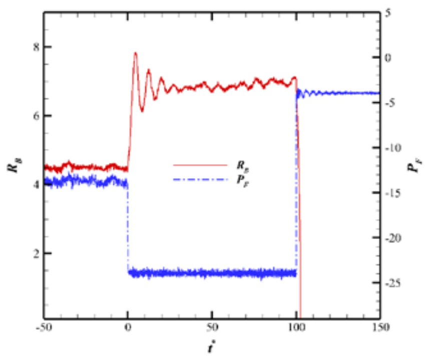
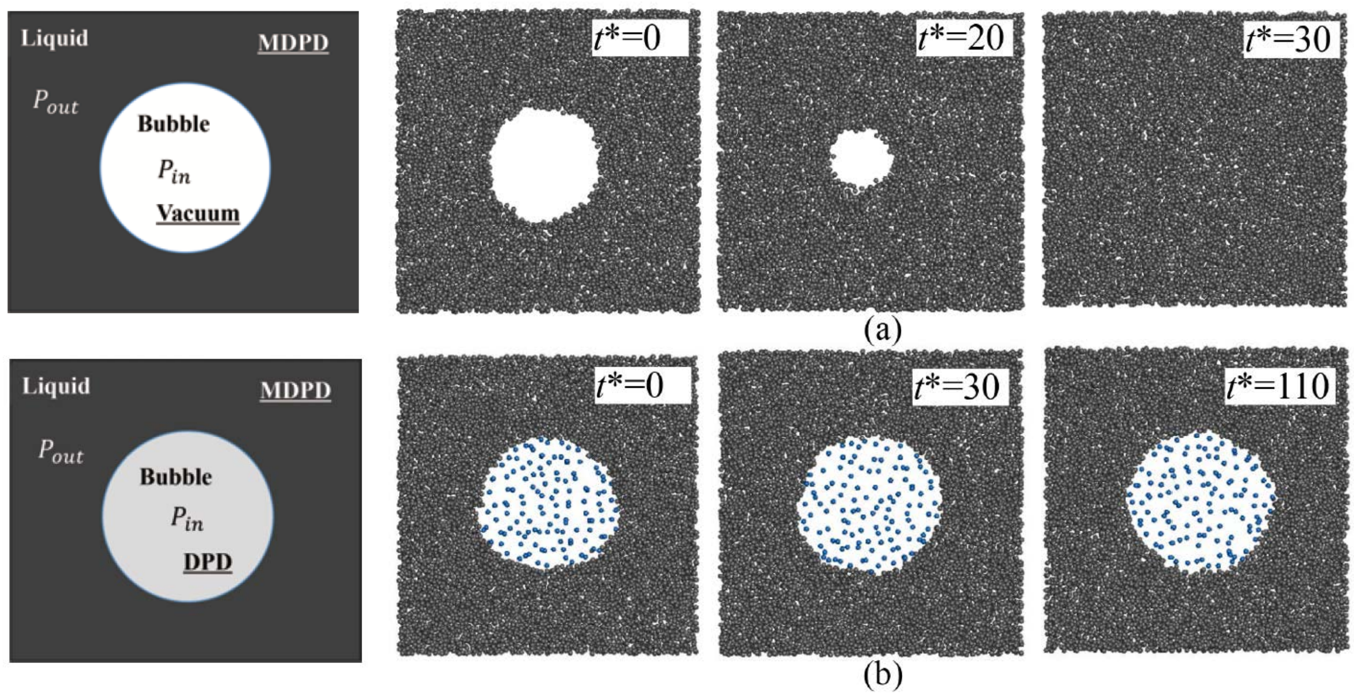
Vacuum and Gaseous bubble

- Control the surrounding fluid pressure become the constatnt value P_0.





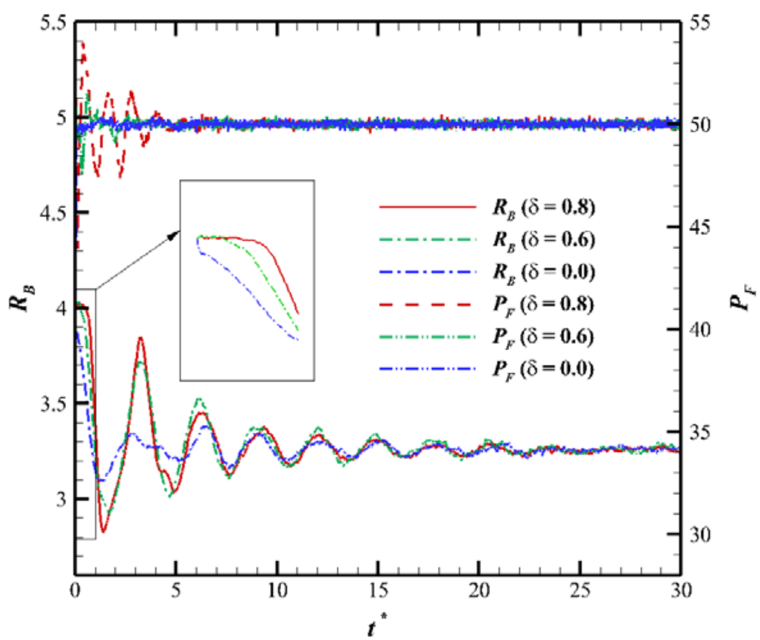
Collapse quickly

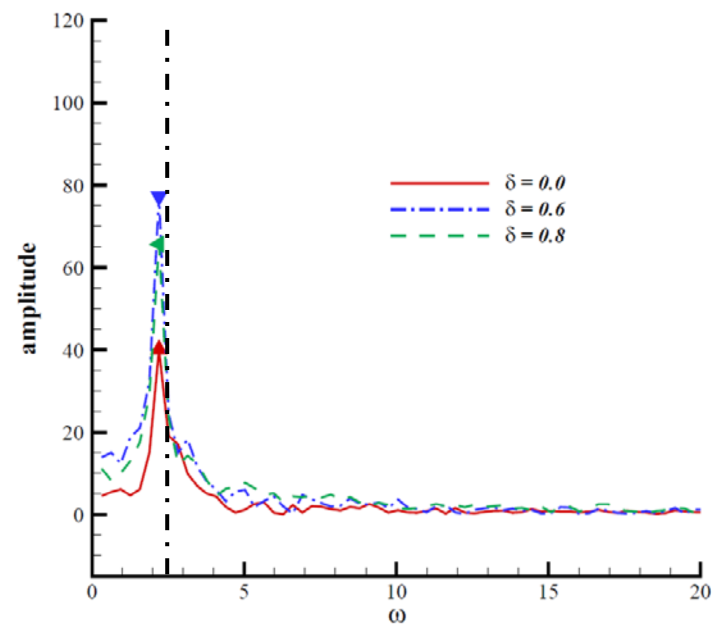


Microbubble oscillation

- Bubble Dynamics
  - Natural frequency from **Rayleigh – Plesset** Equation
    (C. E. Brennen, *Cavitation and Bubble Dynamics*, 2013)

$$\omega_N = \frac{1}{R_0}\sqrt{\frac{1}{\rho_l}\left(3kP_{g0} - \frac{2S}{R_0}\right)},\ \ P_g(R) = P_{g0}\left(\frac{R_0}{R}\right)^{3k}$$



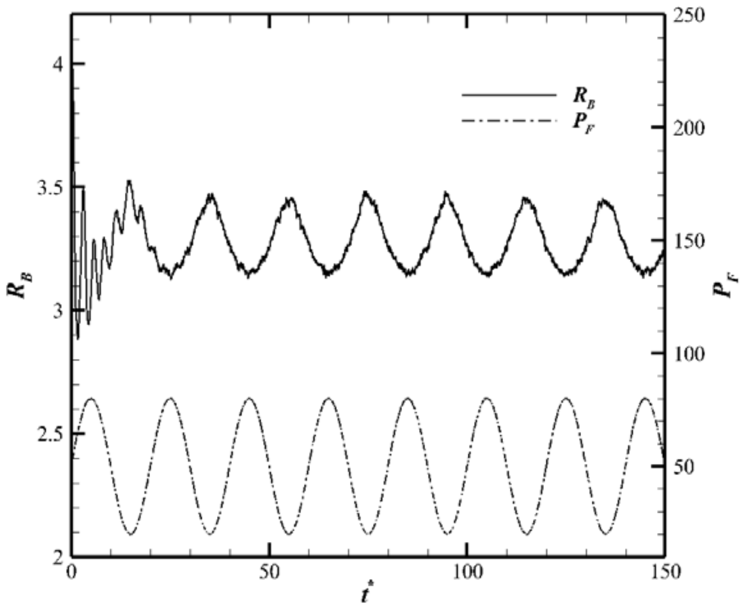


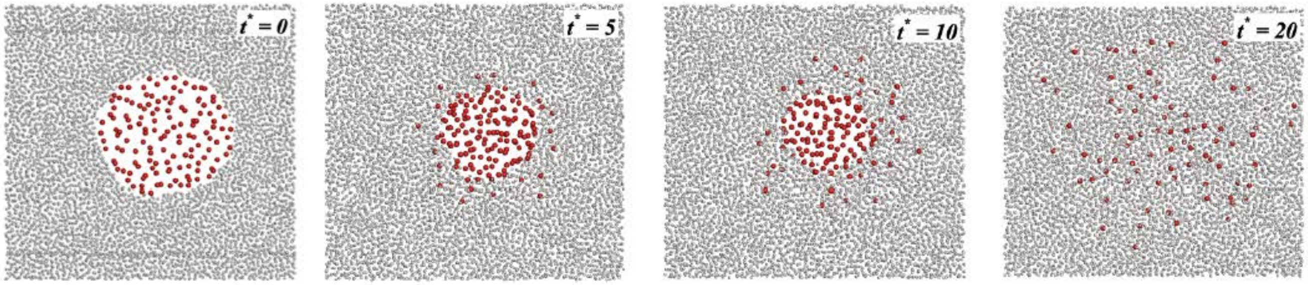
Bubble oscillation and collapse

- Control the surrounding fluid pressure become the fluctuating value $P_0{}^*$.

$$P_0^* = P_0 + P_a sin(2\pi f \cdot t^*)$$

- Partial Berendsen barostat could be good barostat in nonequilibrium dynamics.





Summary

- The original **Berendsen barostat** works well in the (M)DPD simulation of the single-component system under **constant pressure** condition and **nonequilibrium dynamic** process;
- **A partial** Berendsen barostat is proposed to study the **multi-component** system in (M)DPD simulation;
- **The partial** Berendsen barostat could be a good candidate for the study on single or few droplets/bubbles under certain pressure control in **nonequilibrium dynamics**.

Thanks.

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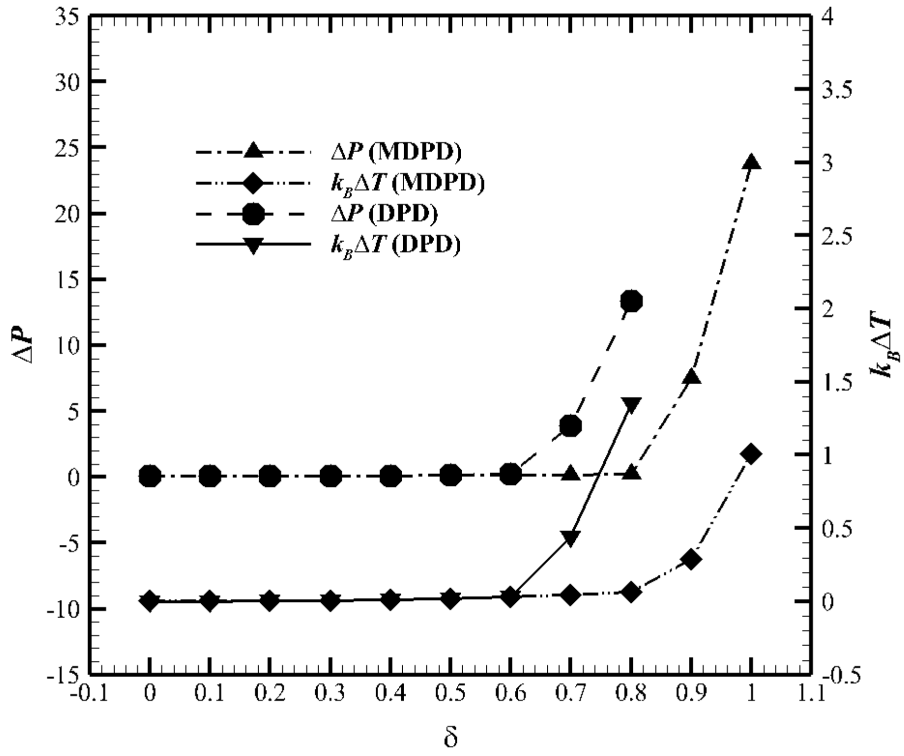
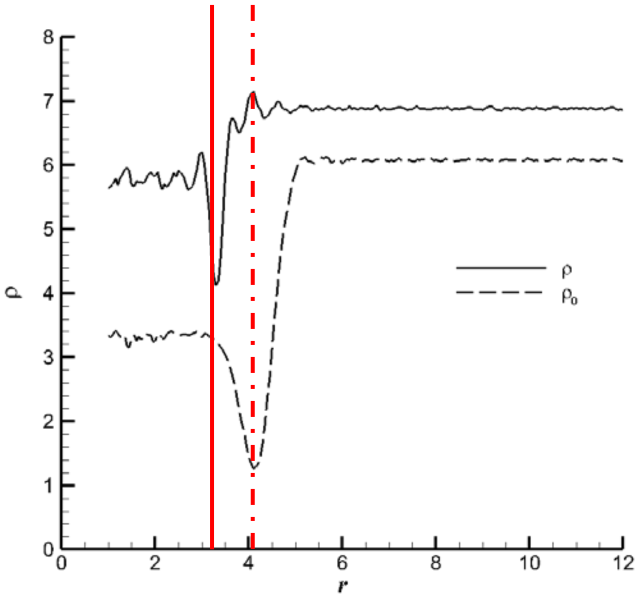
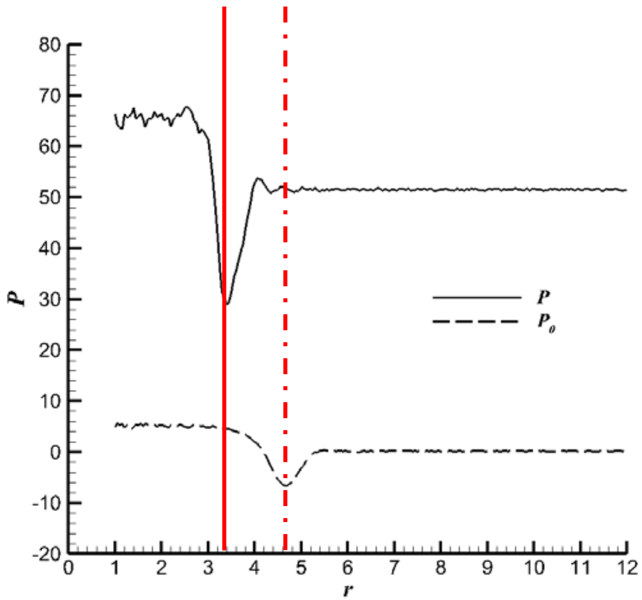
Partial Berendsen barostat

- Applys in (M)DPD Single-component system
  - A critical value of δ exist, when it smaller than the value, the barostat will work well.
  - Too great partial degree(greater than the critical value of δ) will lead to invalid the thermostat.



Gaseous bubble





- Improving the surrounding fluid pressure by the partial Berendsen barostat.
- Bubble shrink and become smaller, but the inside pressure improve with the outside fluid pressure.
- The surface tension increased because that the size of bubble dereased.