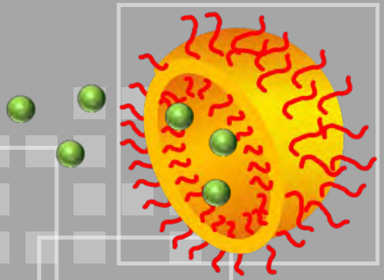
National Taiwan University
Department of Chemical Engineering

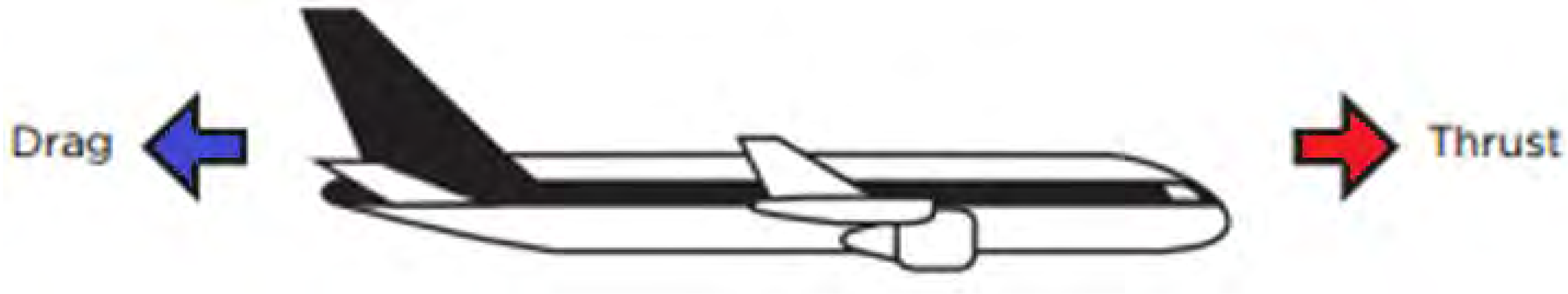


Rectification of a Nano/Micro-Swimmer System : A Dissipative Particle Dynamics Study

Yu-Jane Sheng

Molecular Simulation Laboratory

Introduction : Propulsion / Swimmer

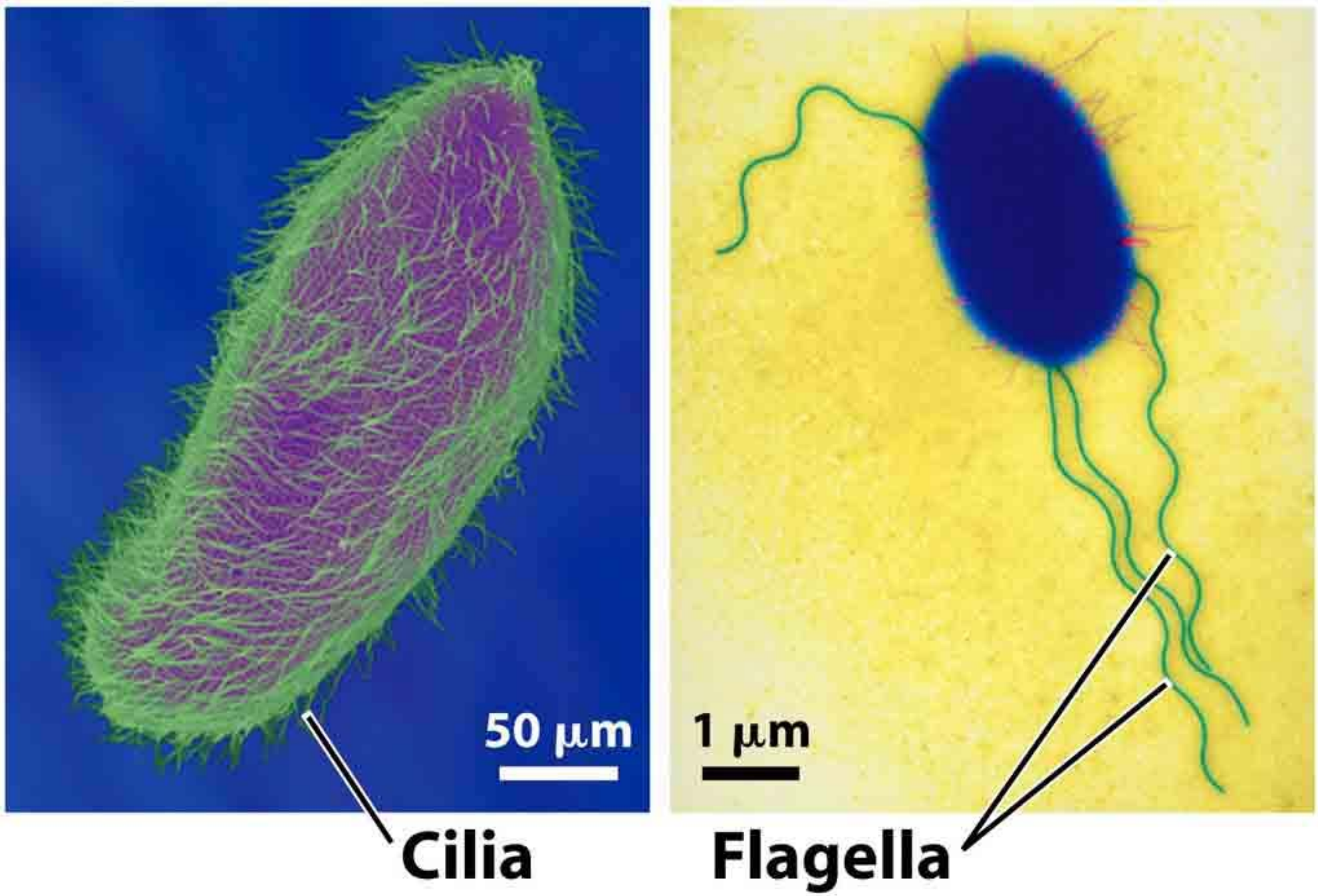


(Swimmer pushes water in the backward direction)

(Water exerts a force on the swimmer)

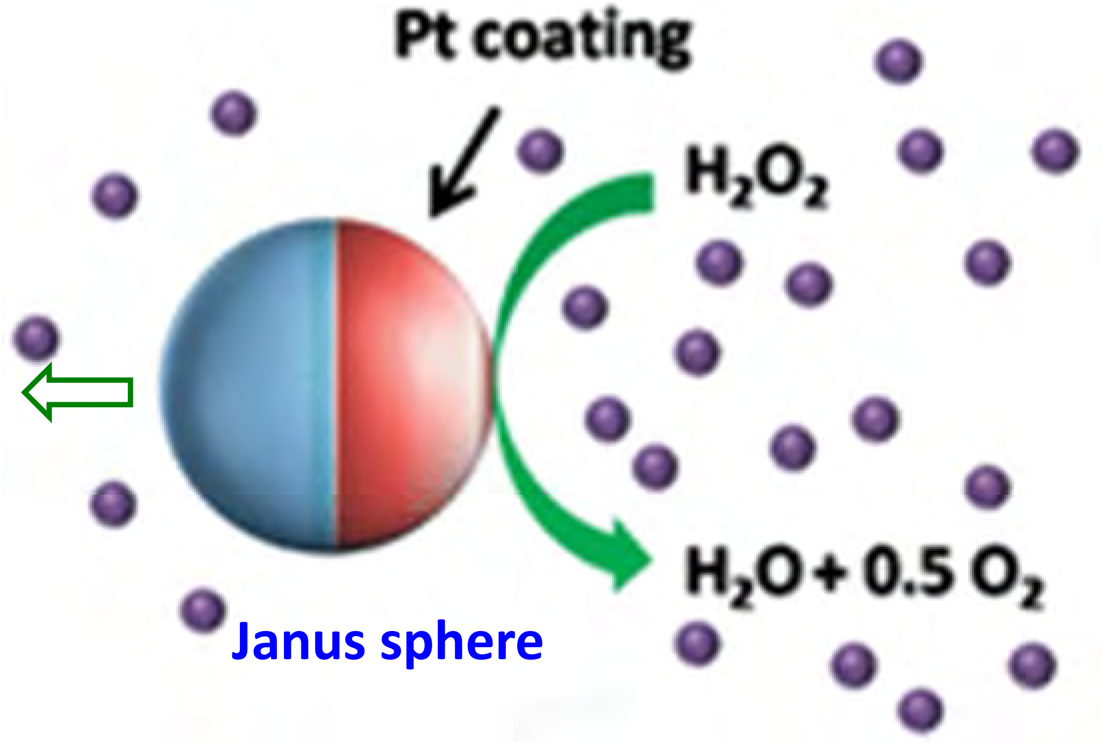
Self-propelled swimmers consume energy from internal or external sources and dissipate it by actively moving through the medium that they inhabit.

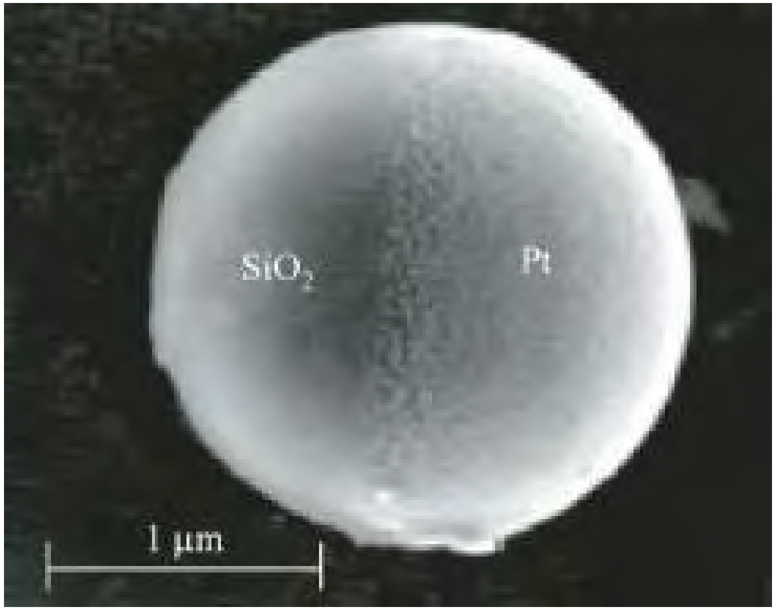
Microswimmer



Microorganisms utilize a wide variety of swimming mechanisms such as beating cilia and flagellar propulsion to propel themselves.

Artificial Swimmer





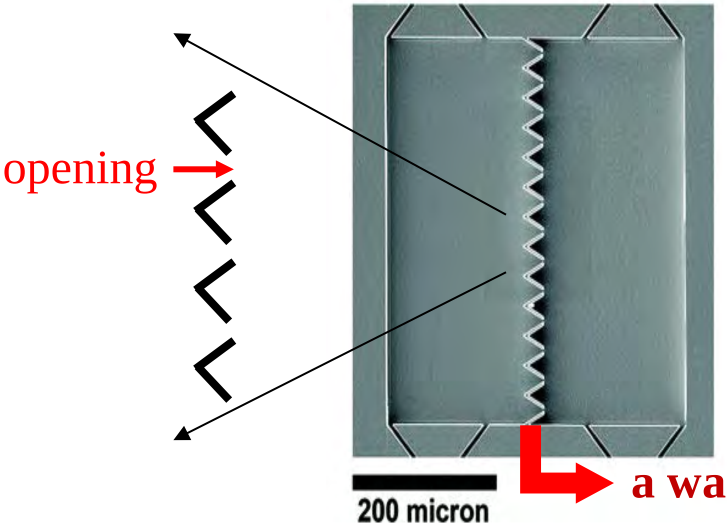
Janus sphere

chemical energy → kinetic energy

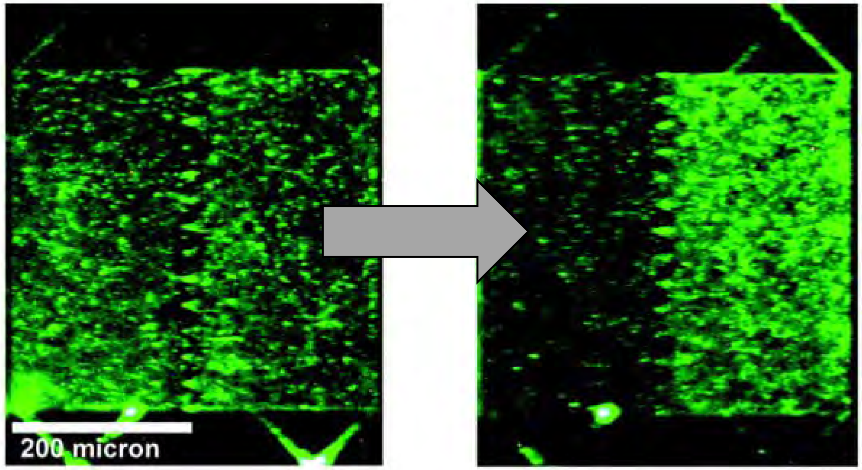
Self-propulsion of a Janus sphere via the asymmetric distribution of reaction products and an accompanying osmotic potential.

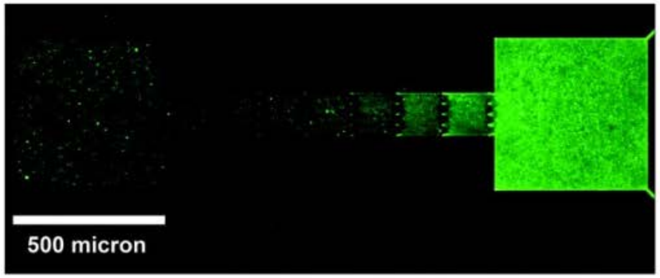
Rectification Phenomenon

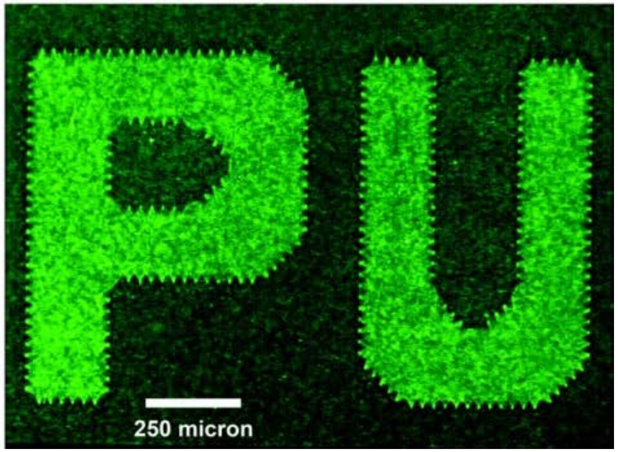
The concentration difference of E. coli occurs through barrier walls.



a wall with barriers

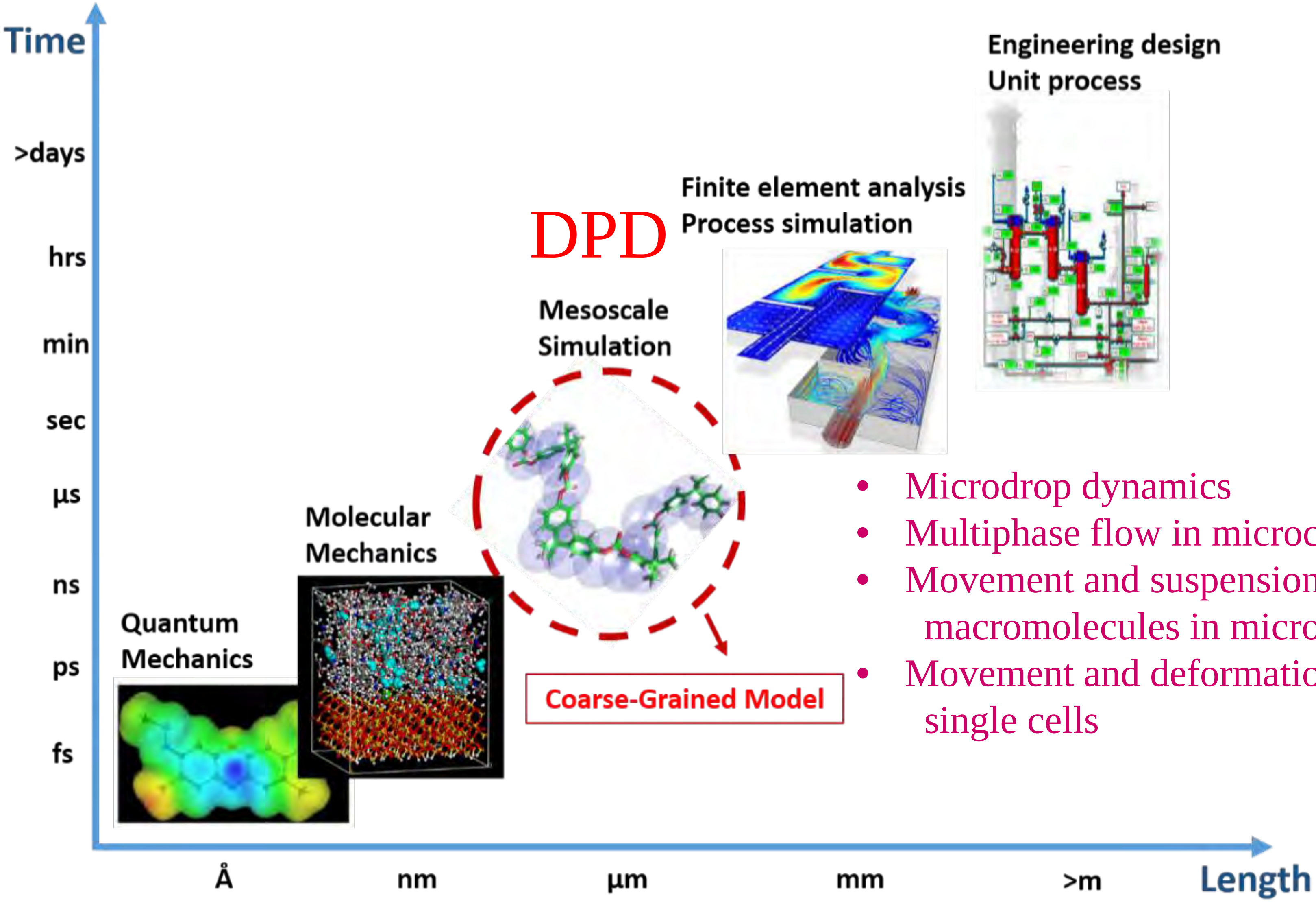






P. Galajda et al, *J. Bacteriol.*, 2007, **189**, 8704.

Simulation Method : Dissipative Particle Dynamics (DPD)



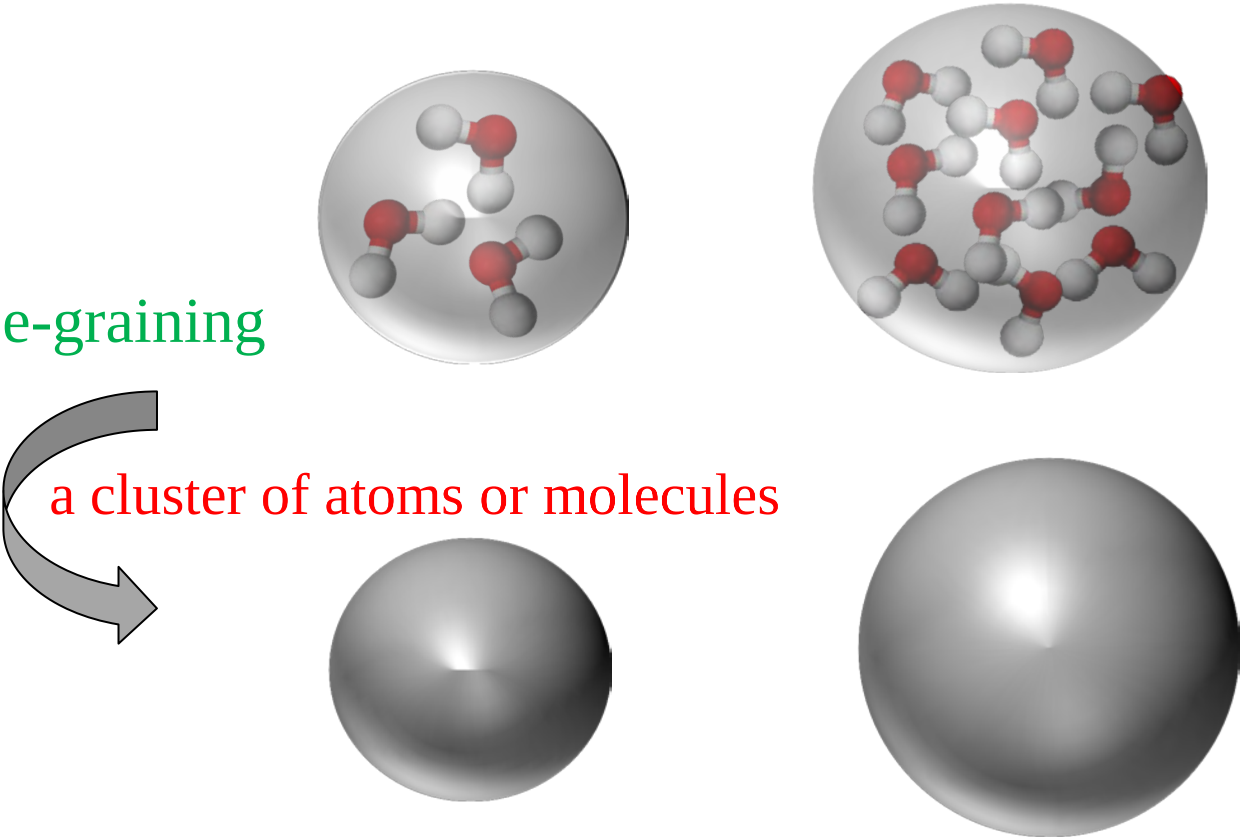
- Microdrop dynamics
- Multiphase flow in microchannels
- Movement and suspension of macromolecules in microchannels
- Movement and deformation of single cells

F. Müller-Plathe, *ChemPhysChem*, 2002, **3**, 754-769.

Coarse-Graining of Small Molecules

DPD is an off-lattice and particle-based simulation method.

- Some trivial molecular details that do not affect the behavior at larger scales can be ignored, while the main features of concerned physics need to be effectively obtained.



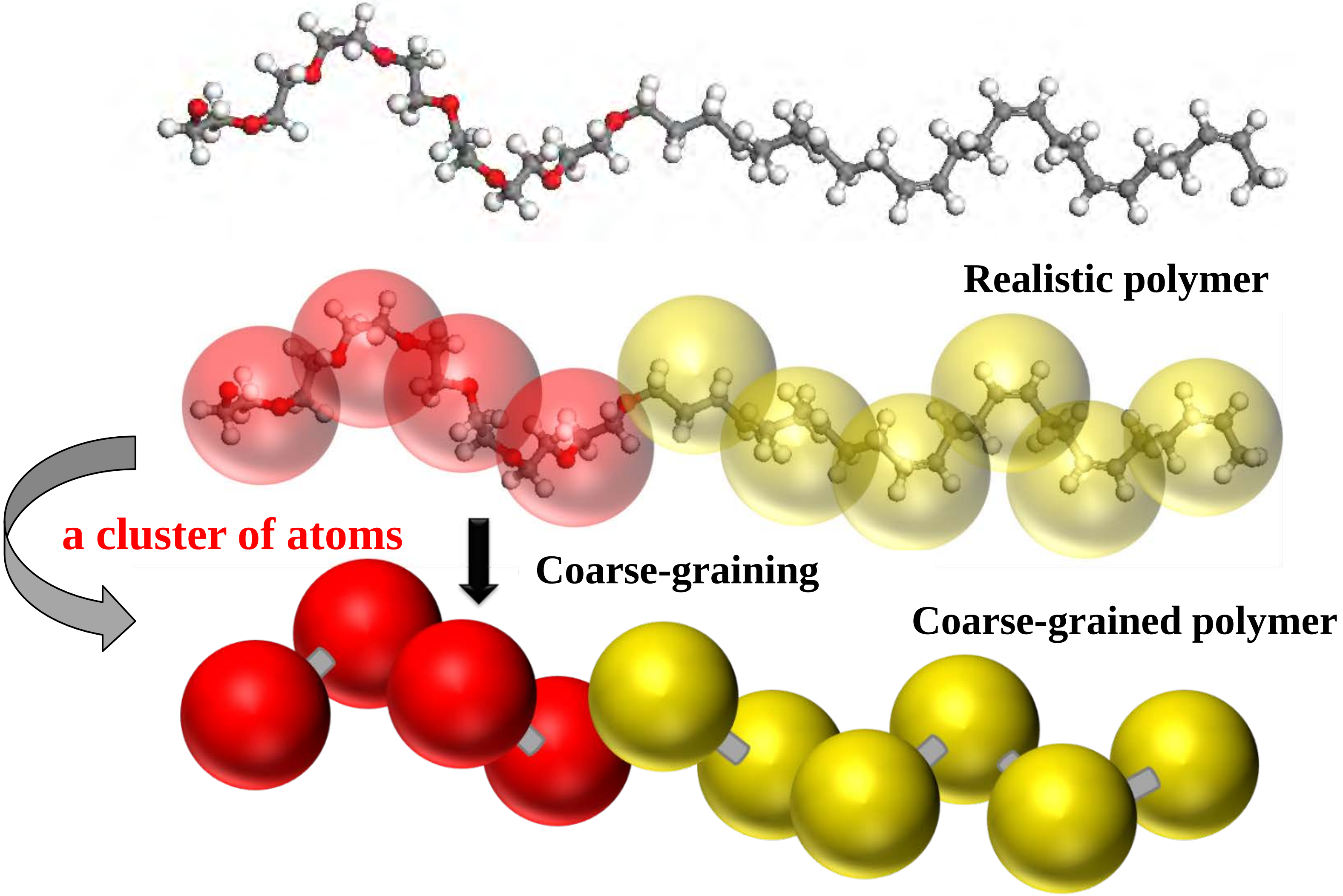
Coarse-graining

a cluster of atoms or molecules

DPD bead :
Nano-sized or
Micro-sized.

Coarse-Graining of a Polymer

poly(ethylene oxide)-block-polybutadiene diblock copolymer (PEO-b-PB)



Realistic polymer

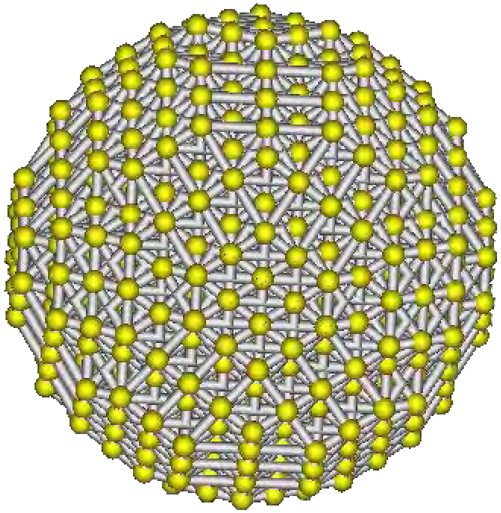
a cluster of atoms

Coarse-graining

Coarse-grained polymer

Coarse-Graining of a Colloidal Particle

Coarse-graining



Colloidal Silica

DPD Microswimmer

DPD : Conservative Force

Time evolution

- **Newton’s law of motion**

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i \,; \quad \frac{d\boldsymbol{v}_i}{dt} = \frac{\boldsymbol{f}_i}{m_i}$$

- **Non-bonded DPD forces**

$$\boldsymbol{f}_i = \sum_{j \neq i} \left(\boldsymbol{F}_{ij}^C + \boldsymbol{F}_{ij}^D + \boldsymbol{F}_{ij}^R \right)$$

1. Conservative force (F_{ij}^C)

2. Dissipative force (F_{ij}^D)

3. Random force (F_{ij}^R)

Conservative Force

Interaction parameter

$$F_{ij}^C = \begin{cases} a_{ij}(r_c - r_{ij})\hat{r}_{ij}, & r_{ij} < r_c \\ 0, & r_{ij} \geq r_c \end{cases}$$

Cutoff radius

- ✓ Soft repulsive force
- ✓ a_{ij} is a maximum repulsion between particles i and j.
- ✓ The conservative force provide beads a chemical identity.

R. D. Groot and P. B. Warren, *JCP*, 1997, **107**, 4423.

DPD : Dissipative Force

Mesoscale simulation

- **Newton's law of motion**

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i \; ; \quad \frac{d\boldsymbol{v}_i}{dt} = \frac{\boldsymbol{f}_i}{m_i}$$

- **Non-bonded DPD forces**

$$\boldsymbol{f}_i = \sum_{j \neq i} \left(\boldsymbol{F}_{ij}^{C} + \boldsymbol{F}_{ij}^{D} + \boldsymbol{F}_{ij}^{R} \right)$$

1. Conservative force (F_{ij}^{C})

2. Dissipative force (F_{ij}^{D})

3. Random force (F_{ij}^{R})

Dissipative Force

Friction coefficient

$$F_{ij}^{D} = -\gamma \omega^{D} (\hat{r}_{ij} \cdot \mathbf{v}_{ij}) \hat{r}_{ij}$$

r-dependent weight function

- ✓ Frictional force
- ✓ Represents viscous resistance within the fluid
- ✓ Reduce the relative velocity of the pair of beads. (leading to energy loss)

$$\omega^{D}(r) = \left(1 - \frac{r_{ij}}{r_c}\right)^2, \qquad r_{ij} < r_c$$

P. Espanol and P. Warren, *EPL*, 1995, **30**, 191.

DPD : Random Force

Mesoscale simulation

Newton’s law of motion

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i\ ; \quad \frac{d\boldsymbol{v}_i}{dt} = \frac{\boldsymbol{f}_i}{m_i}$$

Non-bonded DPD forces

$$\boldsymbol{f}_i = \sum_{j \neq i} \left(\boldsymbol{F}_{ij}^{C} + \boldsymbol{F}_{ij}^{D} + \boldsymbol{F}_{ij}^{R} \right)$$

1. Conservative force (F_{ij}^{C})

2. Dissipative force (F_{ij}^{D})

3. Random force (F_{ij}^{R})

$\sigma = (2\gamma k_B T)^2$

$\omega^R = (\omega^D)^{1/2}$

Random Force

Noise amplitude

$$F_{ij}^{R} = -\sigma \omega^{R} \xi_{ij} \hat{\boldsymbol{r}}_{ij}$$

r-dependent weight function

- ✓ Compensates for lost degrees of freedom eliminated after the coarse-graining.
- ✓ Puts in energy to the system with inducing energy fluctuation.

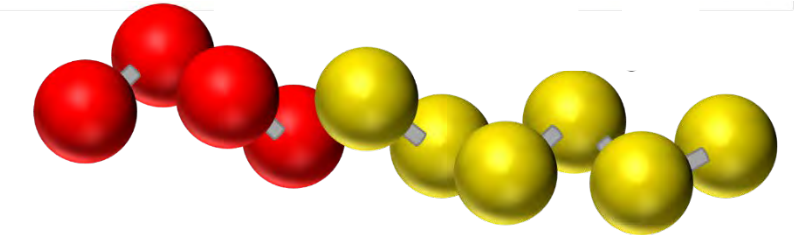
DPD thermostat

- ➢ Constant mean temperature of the system
- ➢ Correct description of hydrodynamics

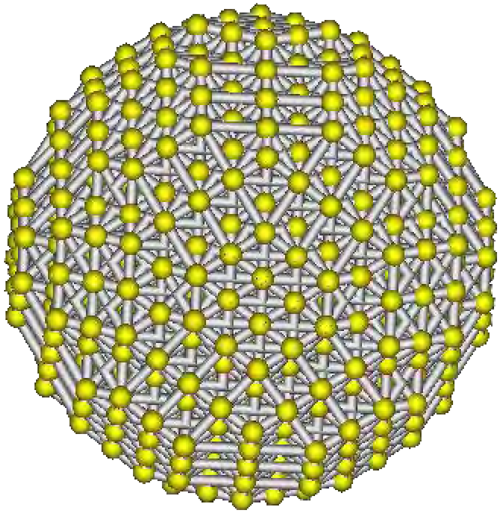
P. Espanol and P. Warren, *EPL*, 1995, **30**, 191.

DPD : Bonded Forces

Model Polymer

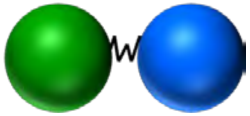


Model Microswimmer



Connectness:

Spring Force

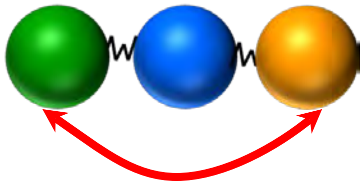


$$F_{ij}^{S} = -\sum_{j} C^{S}(r_{ij} - r_{eq}^{S})\hat{r}_{ij}$$

$$C^{S} = 100 \qquad r_{eq}^{S} = 0.7$$

Rigidity:

Angle Force



$$F_{ij}^{S\theta} = -\sum_{j} C^{\theta}(r_{ij} - r_{eq}^{\theta})\hat{r}_{ij}$$

$$C^{\theta} = 100 \qquad r_{eq}^{\theta} = 2r_{eq}^{S} = 1.4$$

Modified Velocity-Verlet Algorithm

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i \qquad \frac{d\boldsymbol{v}_i}{dt} = \frac{\boldsymbol{f}_i}{m_i}$$

Initial position and velocity for each bead are provided.

To advance the set of positions and velocities, a modified version of the velocity-Verlet algorithm is used,

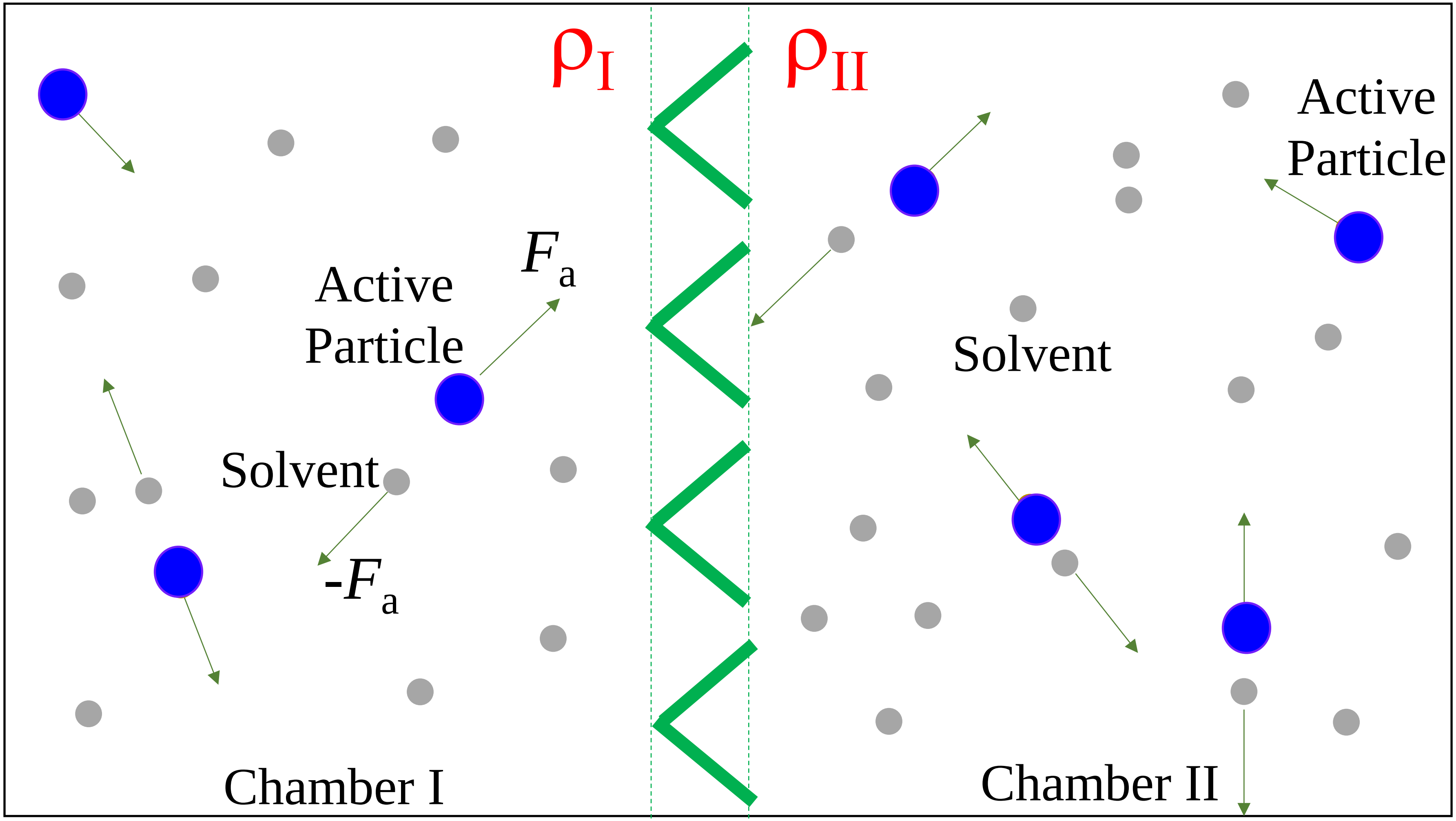
$$\boldsymbol{r}_i(t+\Delta t) = \boldsymbol{r}_i(t) + \Delta t \boldsymbol{v}_i(t) + \frac{1}{2}(\Delta t)^2 \boldsymbol{f}_i(t),$$

$$\tilde{\boldsymbol{v}}_i(t+\Delta t) = \boldsymbol{v}_i(t) + \lambda \Delta t \boldsymbol{f}_i(t),$$

$$\boldsymbol{f}_i(t+\Delta t) = \boldsymbol{f}_i\left(\boldsymbol{r}(t+\Delta t), \tilde{\boldsymbol{v}}(t+\Delta t)\right),$$

$$\boldsymbol{v}_i(t+\Delta t) = \boldsymbol{v}_i(t) + \frac{1}{2}\Delta t\left(\boldsymbol{f}_i(t) + \boldsymbol{f}_i(t+\Delta t)\right).$$

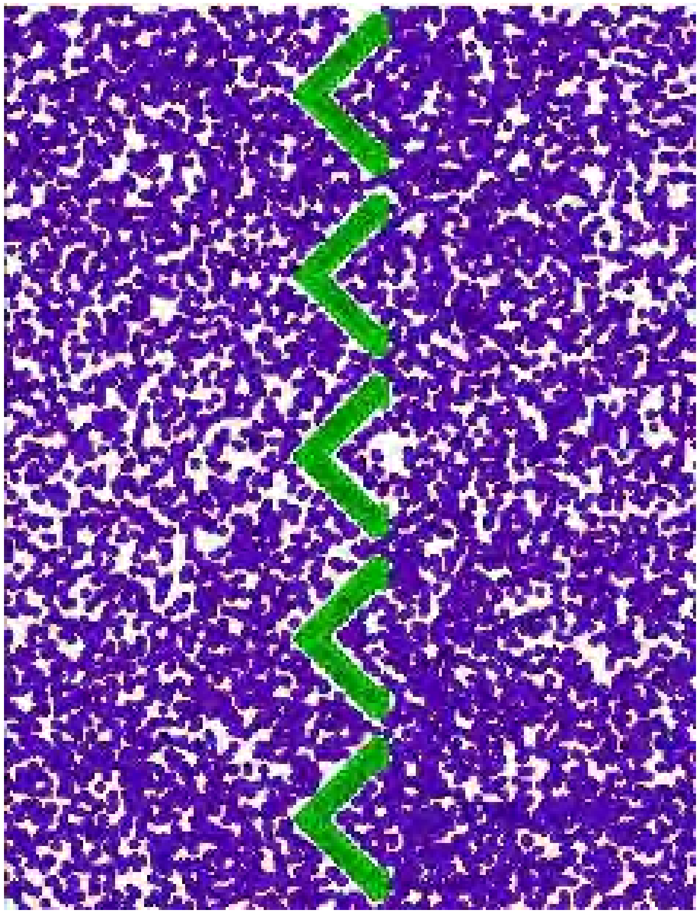
Simulation System



ρ: active particle density

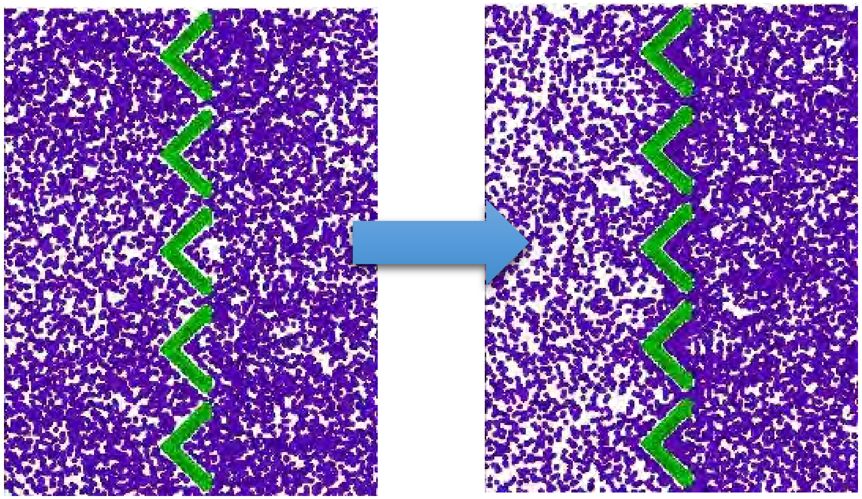
Rectification ratio $A_r\ (= \rho_{II} / \rho_I)$

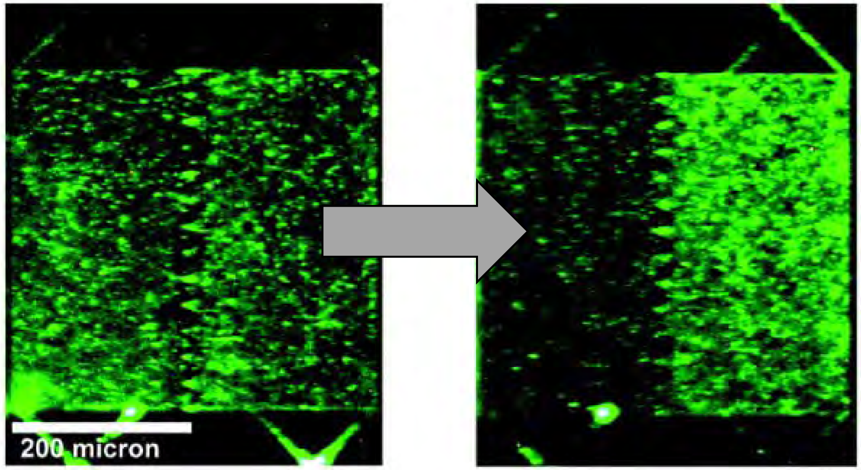
Simulation Movie



$A_r (= \rho_{II} / \rho_I) = 2.2$

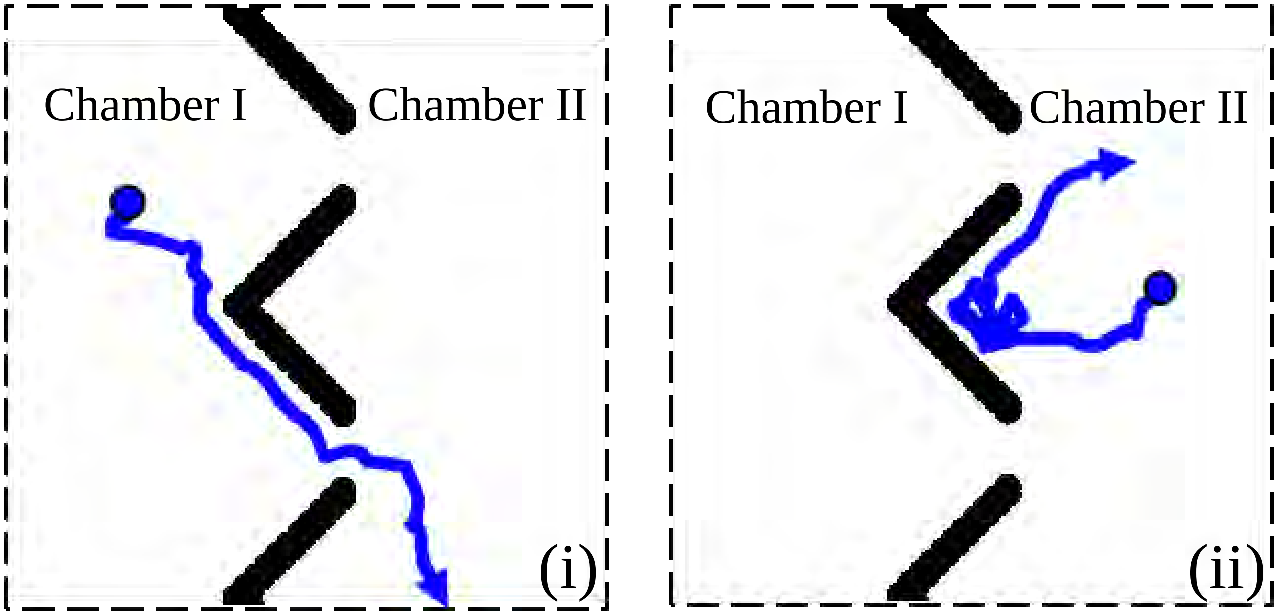
Initial state Final state





- ✓ Only the movements of active particles are shown.

Rectification Mechanism



Geometry-assisted diffusion

Trap-hindered diffusion

The coupling effect leads to the rectification outcome.

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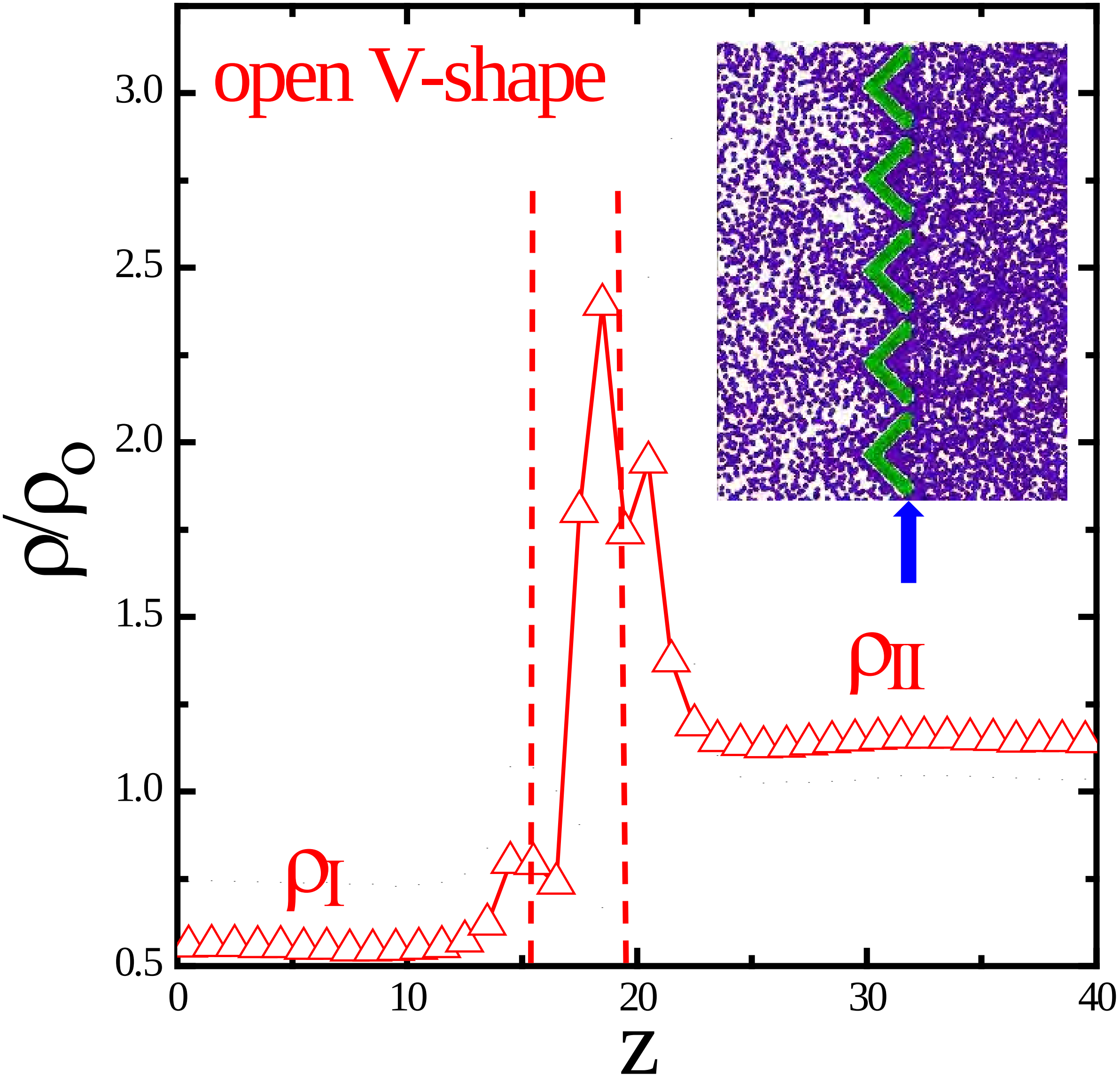
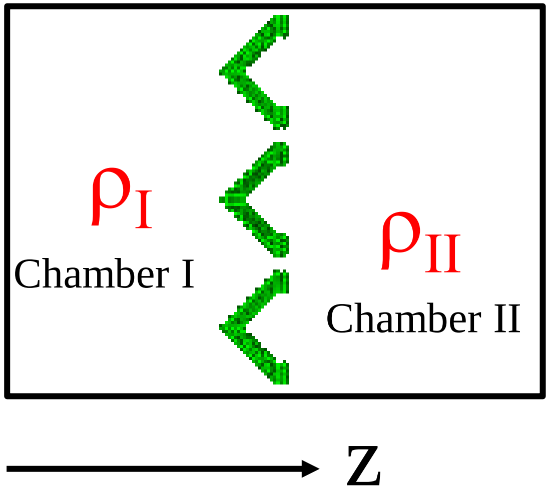
Density Profile

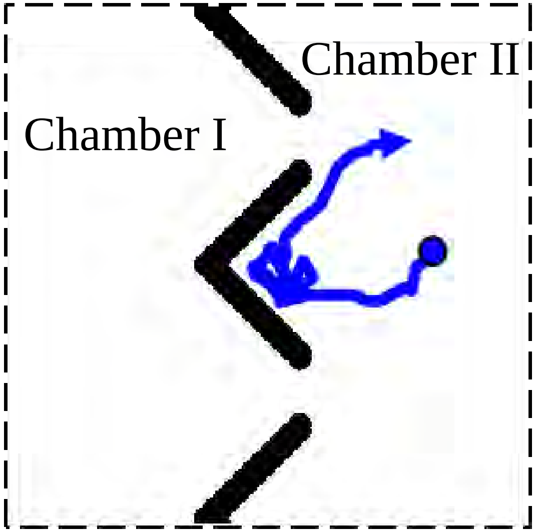




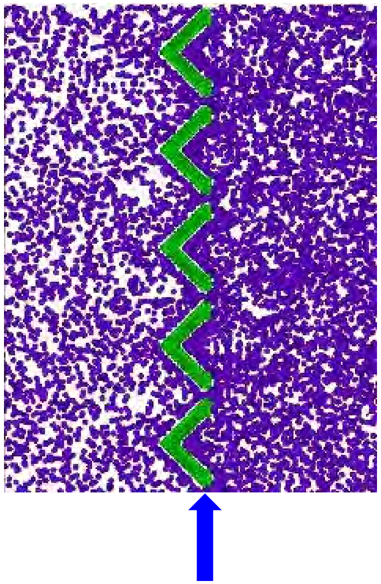
rectification ratio

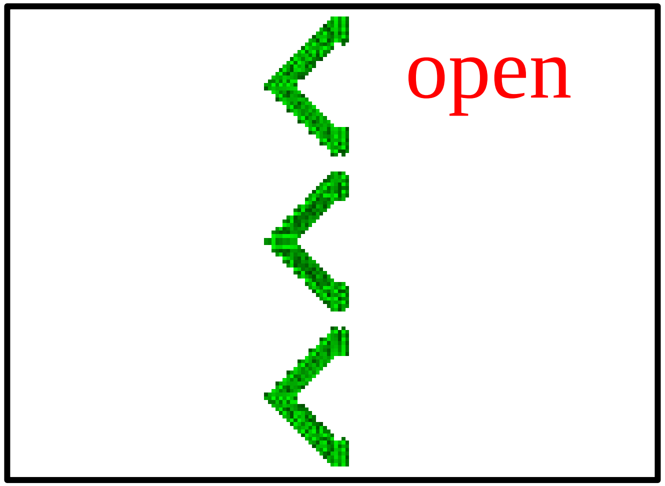
A_r (= ρ_{II} / ρ_{I}) = 2.2

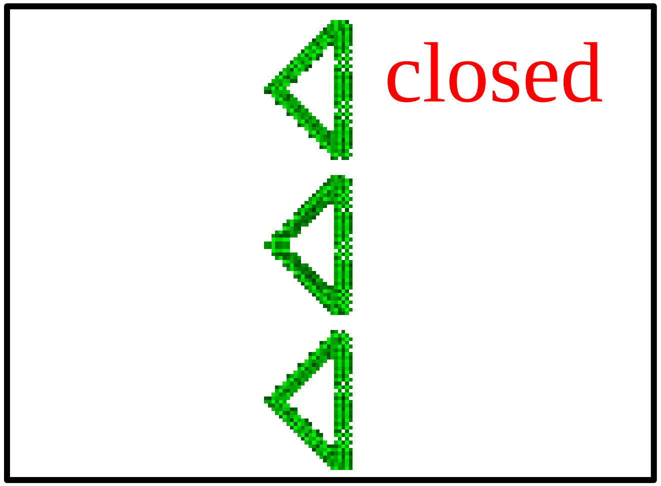
The Effect of the Trap



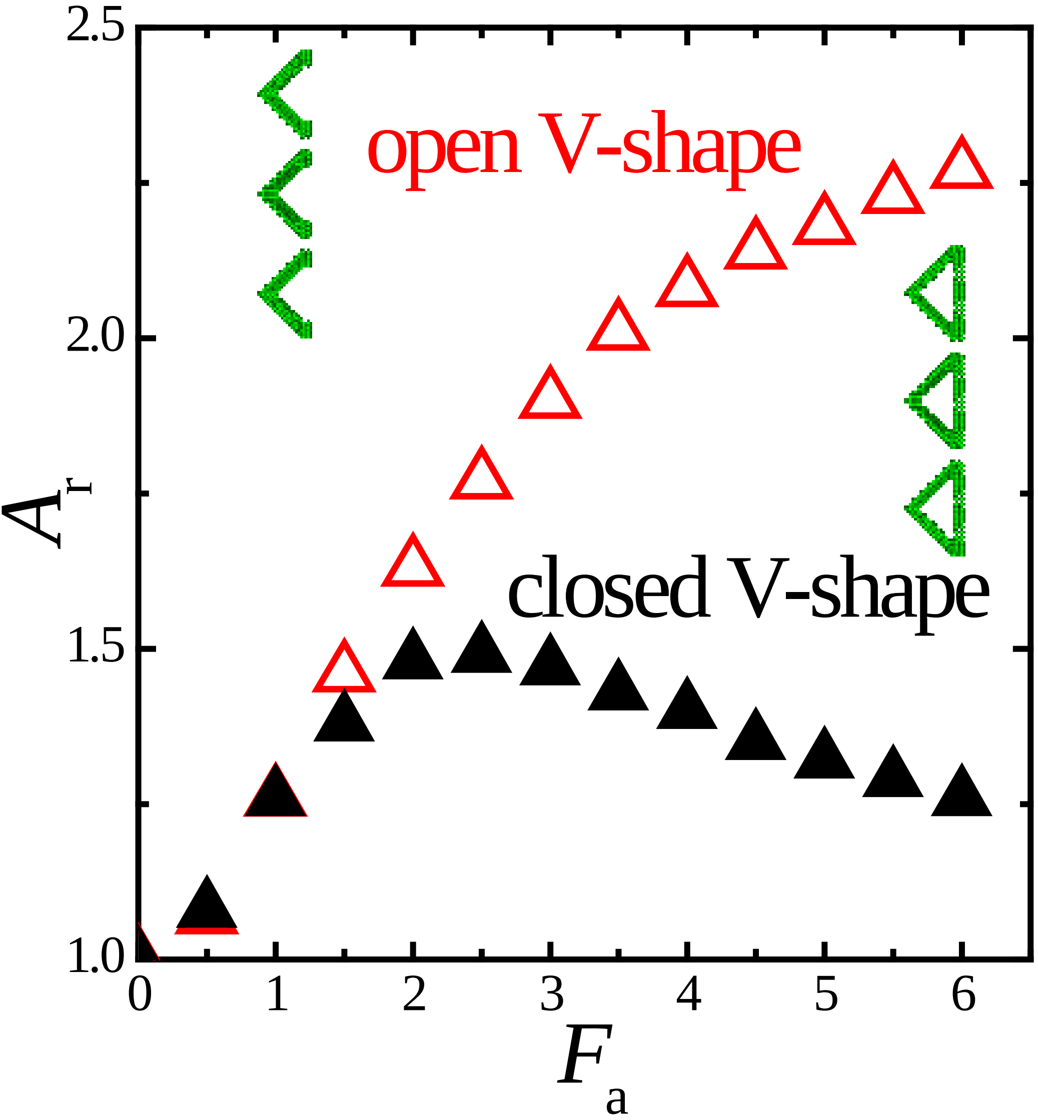
Trap-hindered effect







The Comparison of Rectification Ratio between Open and Closed V-shape Barriers



Open barriers:

$F_a \uparrow$, $A_r \uparrow$

Closed barriers:

A maximum exists for

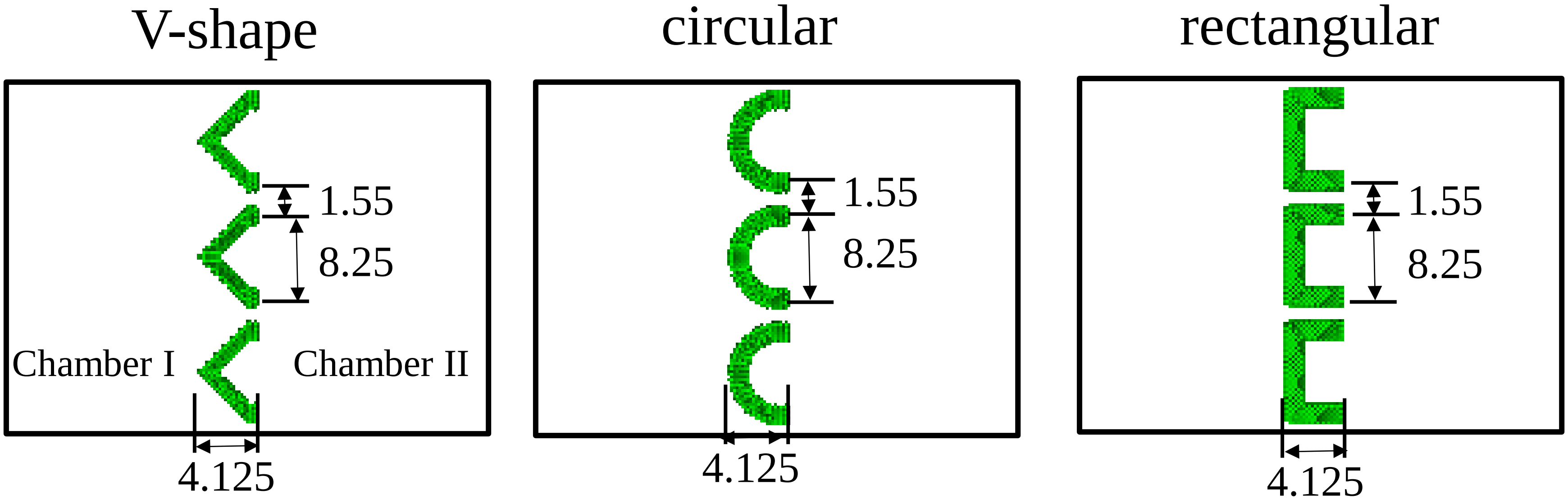
$A_r\ vs\ F_a$

Trap-hindered diffusion is important.

Open barrier > Closed barrier

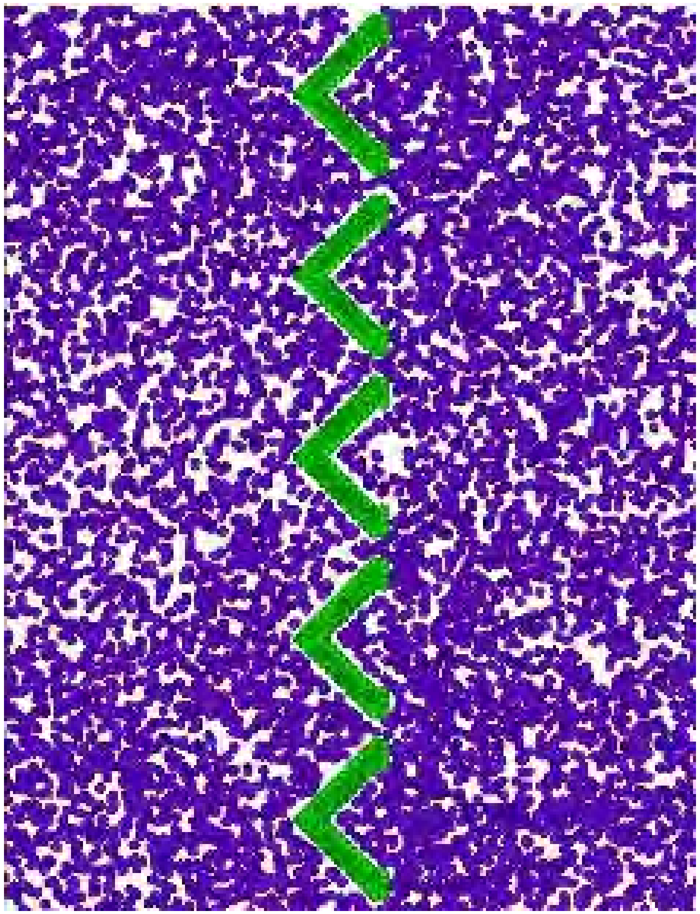
The Effects of Barrier Structures

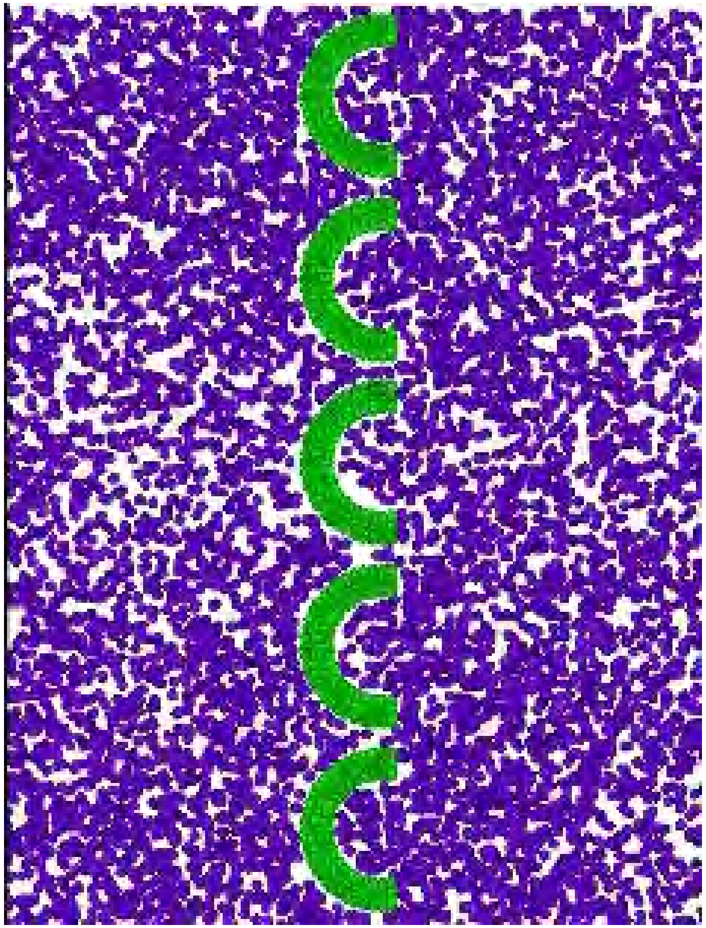
Open barriers



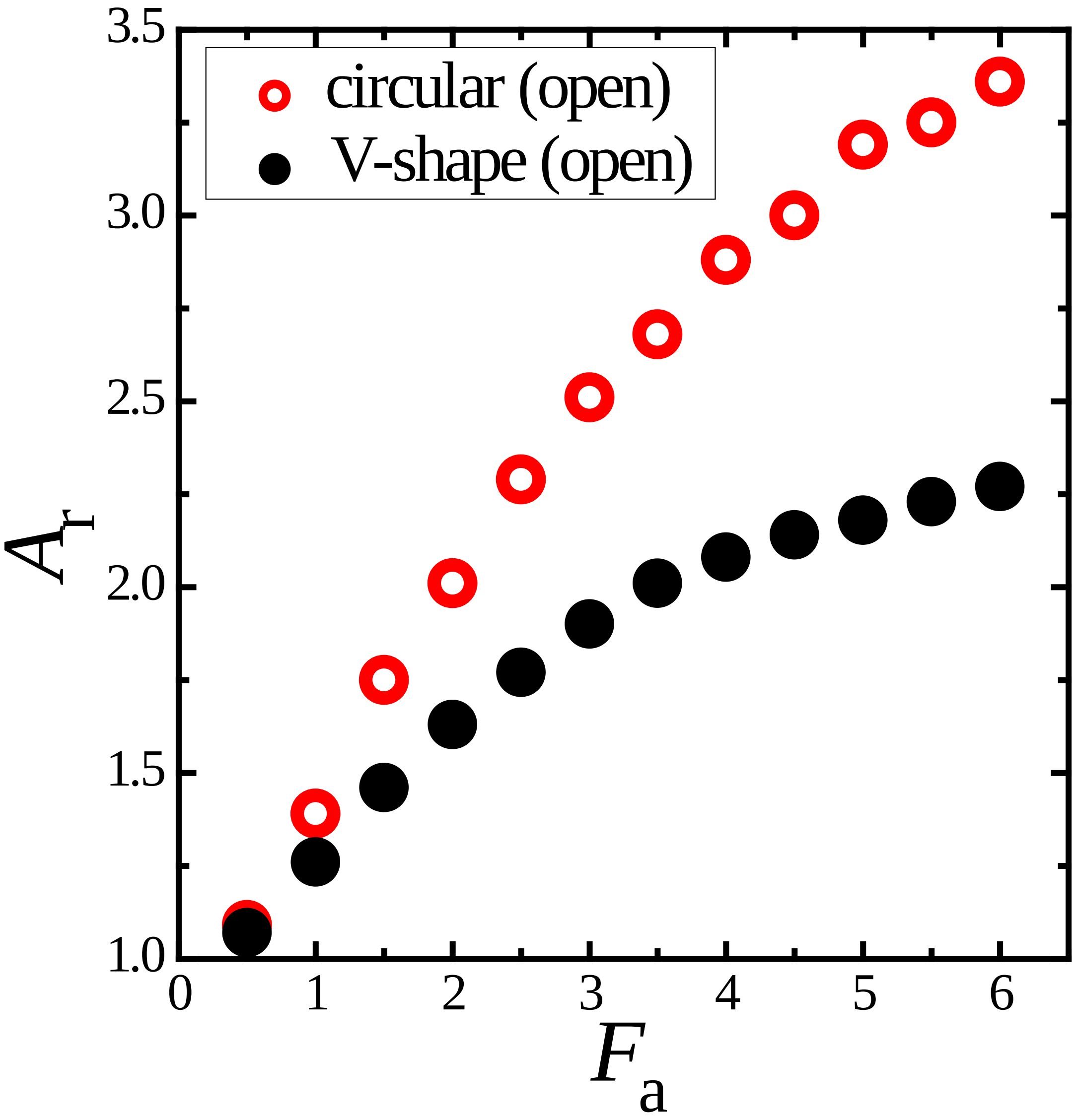
Simulation Movies : Barrier Structures

V-shape, $A_r = 2.2$ Circular, $A_r = 3.4$





The Comparison of Rectification Ratio between Different Barrier Structures



Open barriers:

$F_a \uparrow \;,\; A_r \uparrow$

Circular > Rectangular > V-shape

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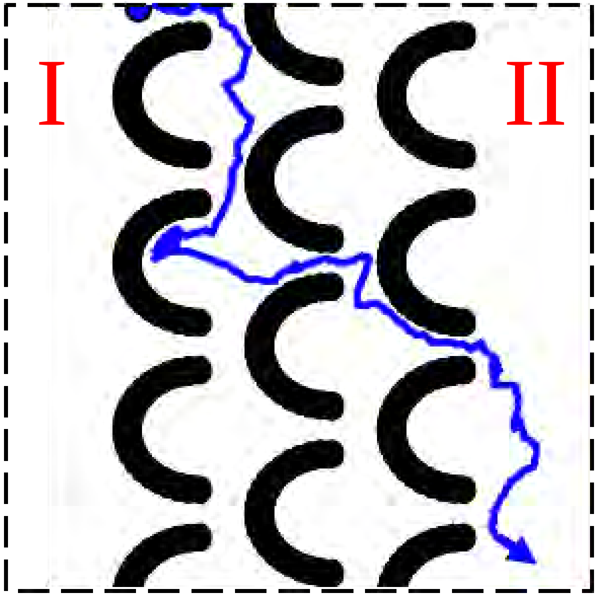
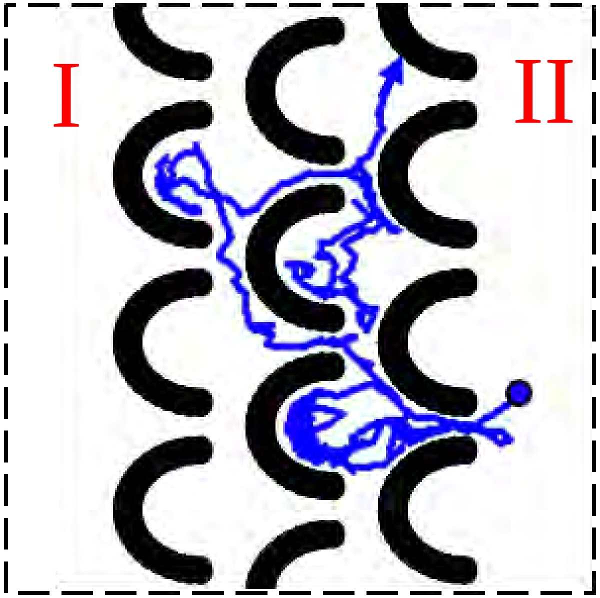
Multilayered Enhancement



Geometry-assisted diffusion

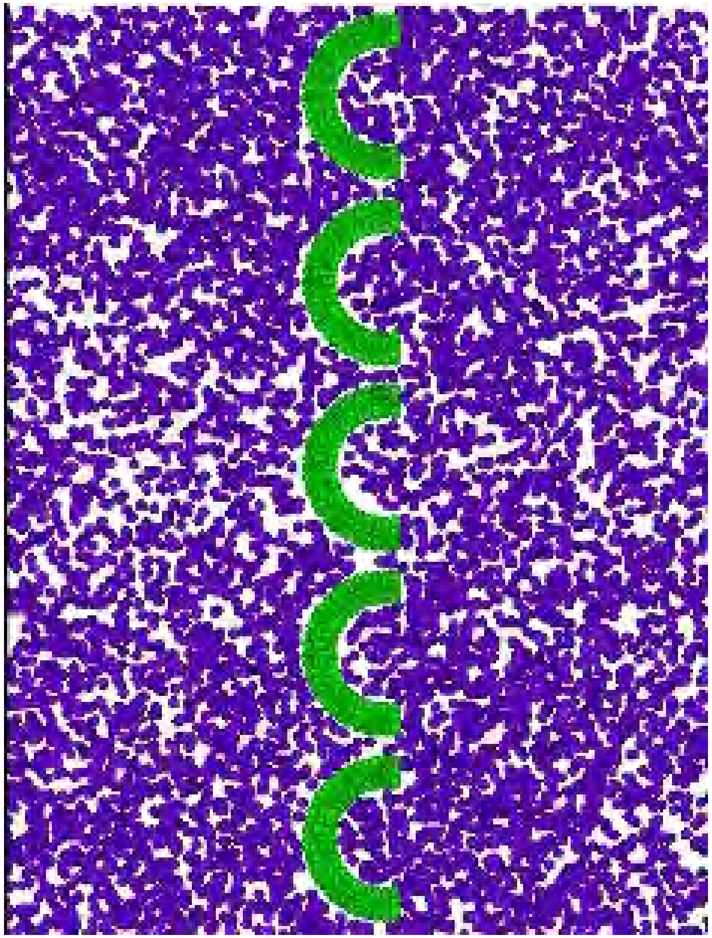


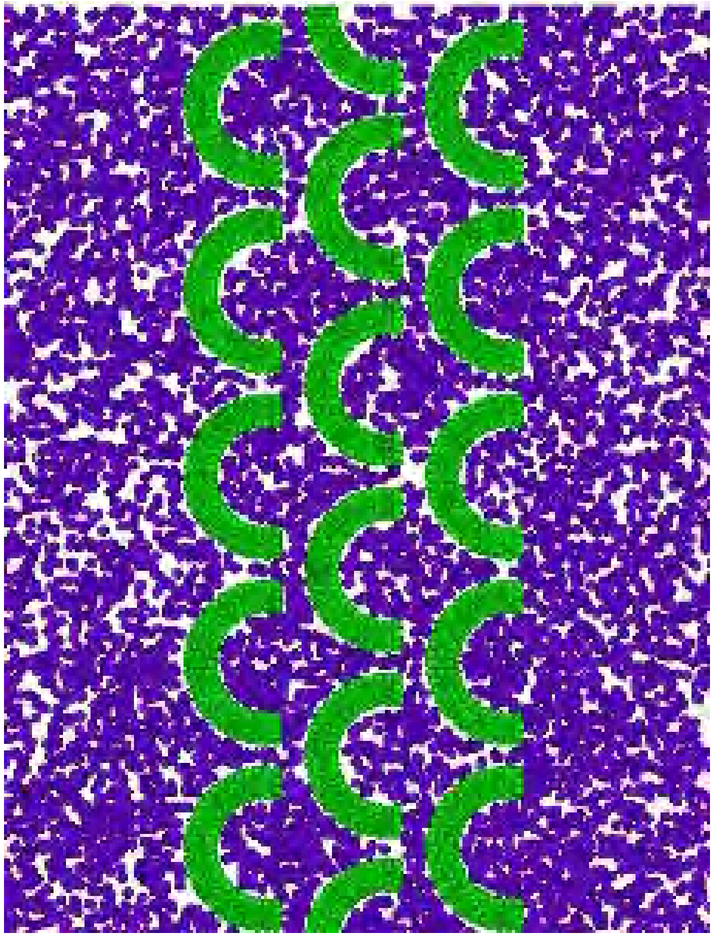
Trap-hindered diffusion

Simulation Movies : Multilayered Enhancement

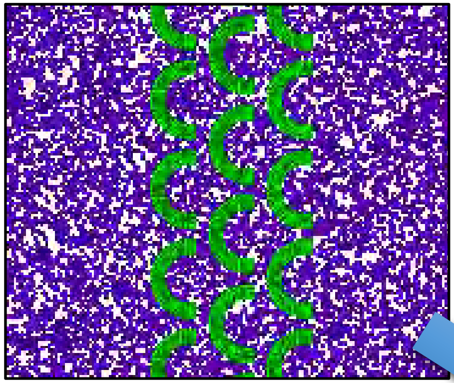
Single, $A_r = 3.4$

Triple, $A_r = 32$

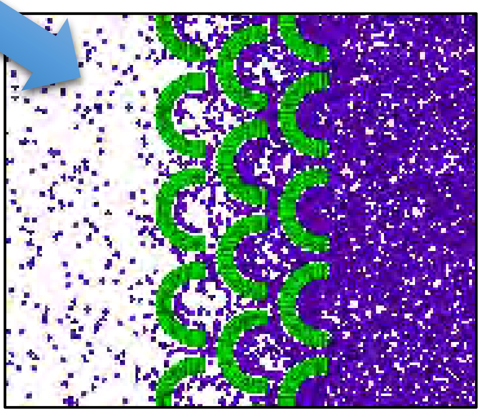




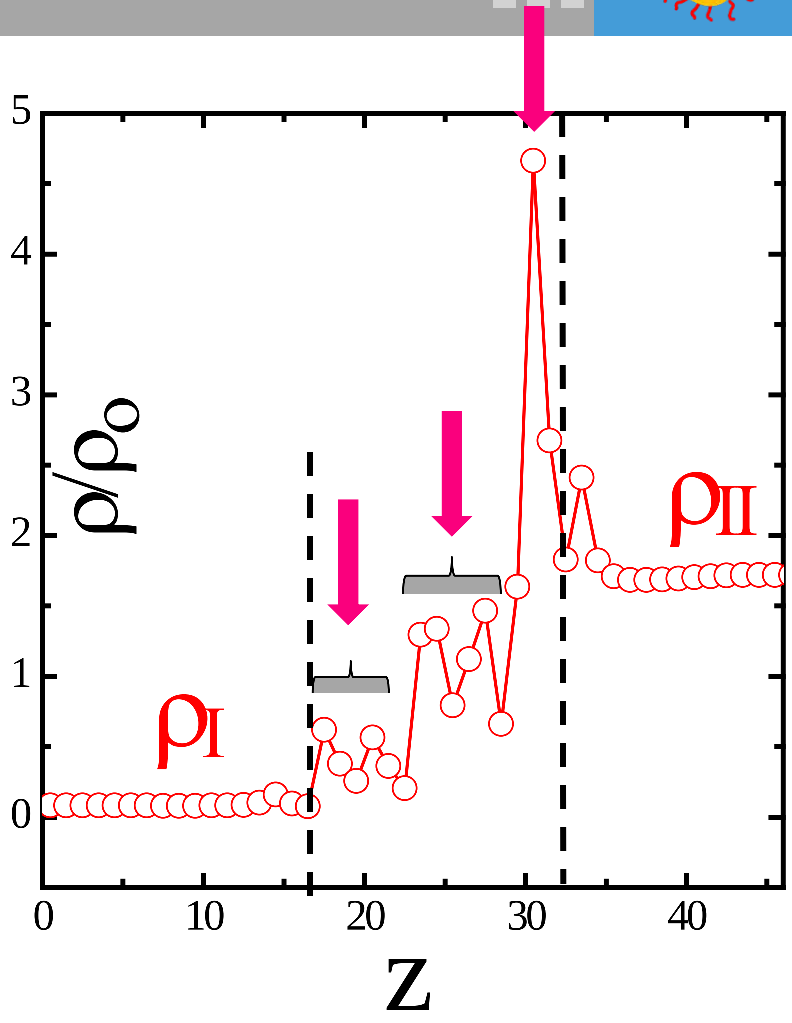
Multilayered Enhancement : Density Profile



Initial state



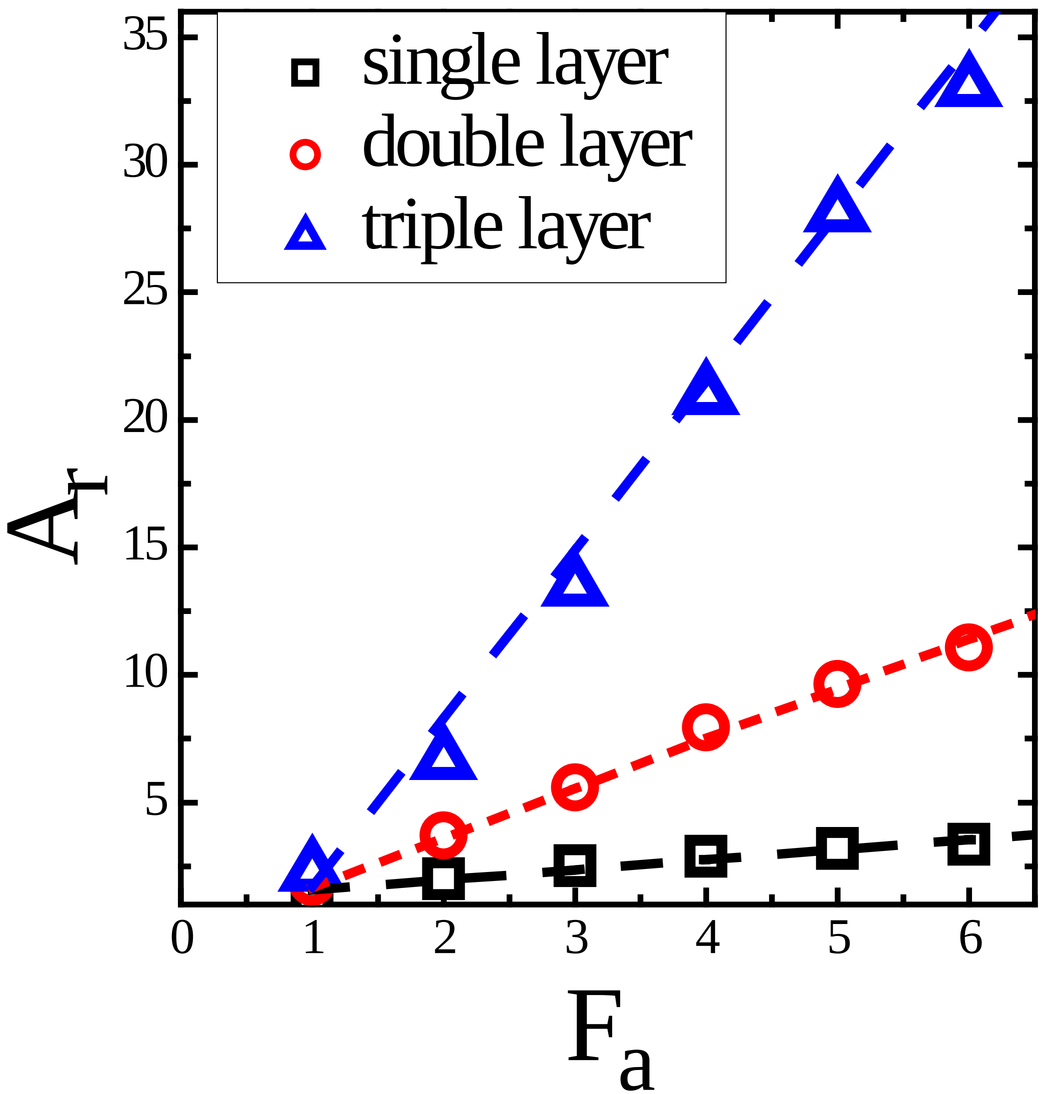
Final state



Rectification ratio

$A_r \; (= \rho_{II} \, / \, \rho_I \,) = 32$

The Comparison of Rectification Ratio between Different Number of Layers Structures



Triple > Double > Single

$$A_r^{(3)} \sim \left[A_r^{(1)}\right]^3$$

Summary

- The rectification of nano/micro-swimmers in a system with asymmetric barriers is investigated by DPD simulations which take into account hydrodynamic effects.

- The rectification mechanism can be clearly identified: geometry-assisted diffusion and trap-hindered diffusion.

- Various barrier shapes are considered and the open circular barrier has the best performance while the V-shape one has the worst.

- Rectification efficiency of nano/microswimmers can be dramatically enhanced by a multi-layers of barriers.