Passive and Active Colloidal Chemotaxis in a Microfluidic Channel

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CECAM Workshop "Microswimmers, Self-Propelled Particles, and Active Matter" 6-8 March 2017

http://pdebuyl.be/
[arXiv:1701.05020]

Outline

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Bacterial chemotaxis - Chromatium okenii

- Miyoshi (1898) J. Coll. Sci. Imp. Univ. Jap. **10**, 143 (taken from Berg, *E. Coli in Motion*, Springer, 2004)

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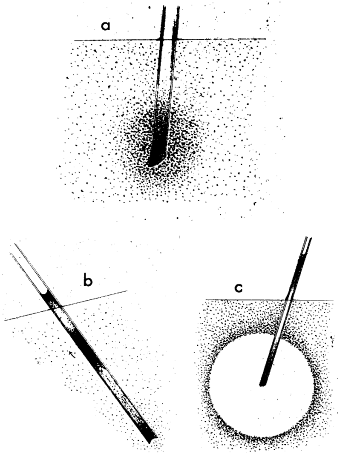

Synthetic chemotaxis

Experiments

- Hong *et al* Phys. Rev. Lett., **99**, 178103 (2007)
- Baraban *et al* Angew. Chem. Int. Ed. **52**, 5552 (2013)

Simulations

- Chen *et al* Soft Matter **12**, 1876 (2016)

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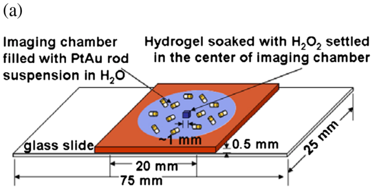

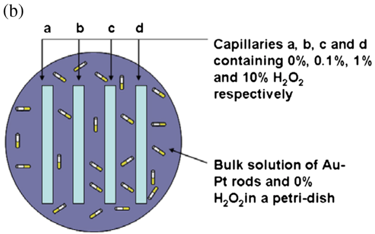

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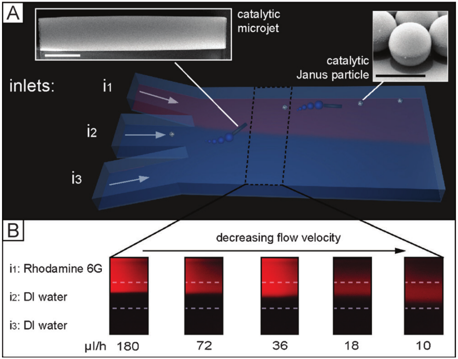

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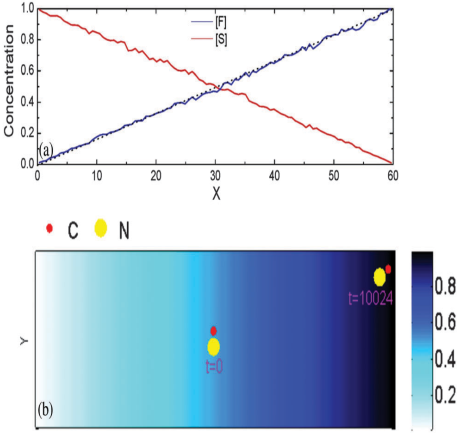

Enzymatic chemotaxis

Experiments

- Sengupta *et al* JACS **135**, 1406 (2013)

Simulations

- ?

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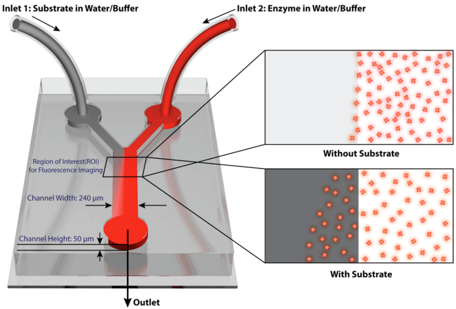

Enzymatic chemotaxis

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Simulations

- ?

Objectives

- Understand the mechanisms for chemotaxis
- Provide simulation models to explore chemotactic behavior
  - "Experimental setup"
  - Chemical activity
  - Surface interaction
- Lay the foundation for later work on enzyme chemotaxis

Outline

Mesoscopic simulation

Microfluidic channel

- MPCD fluid.
- Flow: constant acceleration for the solvent, bounce-back BC and ghost particles in z.
- Gradient device: two inlets for the different chemical species.
- For the colloids: Molecular Dynamics.
- Activity:

$$A + C \rightarrow B + C$$

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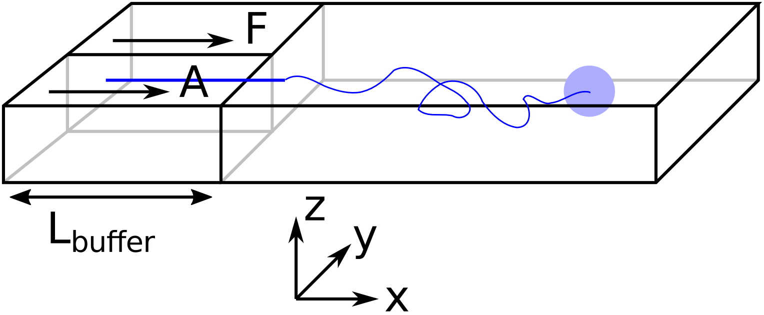
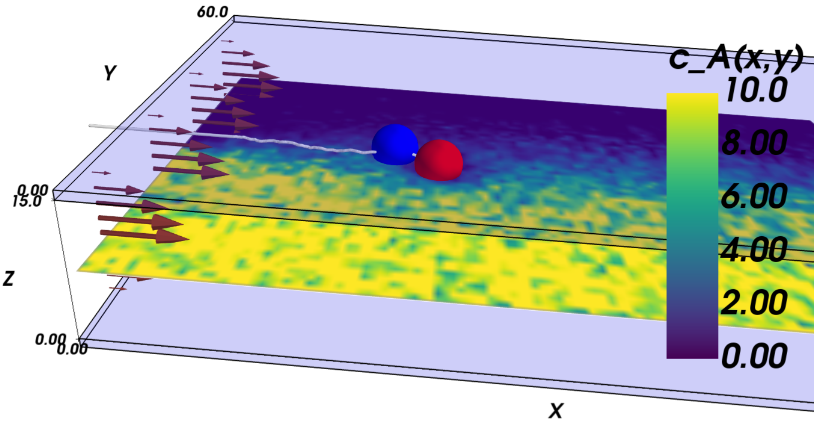
Software

- All simulations were performed with RMPCDMD http://lab.pdebuyl.be/rmpcdmd/ & de Buyl *et al* J. Open Res. Software **5**, 3 (2017)

Mesoscopic simulation



Mesoscopic simulation



Chemical concentration

- For high Pe, at the center of the channel $z = L_z/2$

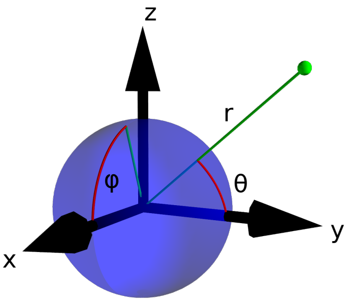
$$v_{\mathrm{flow}} \partial_x c_\alpha(x, y) = D \partial_y^2 c_\alpha(x, y)$$

Spherical coordinates

$$\begin{cases} x &= r \cos\varphi \sin\theta \\ y &= r \cos\theta \\ z &= r \sin\varphi \sin\theta \end{cases}$$

$$c_A = c_0 + c_1 \frac{R}{r} + c_2 \left(\frac{R}{r}\right)^2 \cos\theta + \lambda r \cos\theta$$

with $\lambda = \partial_y c_A(x, y)$



Surface interaction

- Methodology used in Rückner and Kapral, Phys. Rev. Lett. **98**, 150603 (2007)
- Explicit expression for the surface force

$$\vec{F} = \frac{2}{\beta} \sum_{\alpha} \Lambda_{\kappa,\alpha} \int_{r=R} d\mathbf{r} c_{\alpha}(R\hat{r}) \vec{1}_r \ ,$$

where we have defined

$$\Lambda_{\kappa,\alpha} = \int_0^R drr \left(e^{-\beta V_{\kappa,\alpha}(r)} - 1 \right) \ .$$

- c_{α} is the concentration of chemical species α.
- $V_{\kappa,\alpha}$ is the interaction potential between colloid κ and fluid species α.
- $\beta = (k_B T)^{-1}$

Stochastic simulation

Passive and active spheres

$$\dot{x} = v_{\mathrm{flow}} + \sqrt{2D}\xi_x$$
$$\dot{y} = \frac{F_y(x/v_{\mathrm{flow}}, y)}{\gamma} + \sqrt{2D}\xi_y$$

Nanomotor

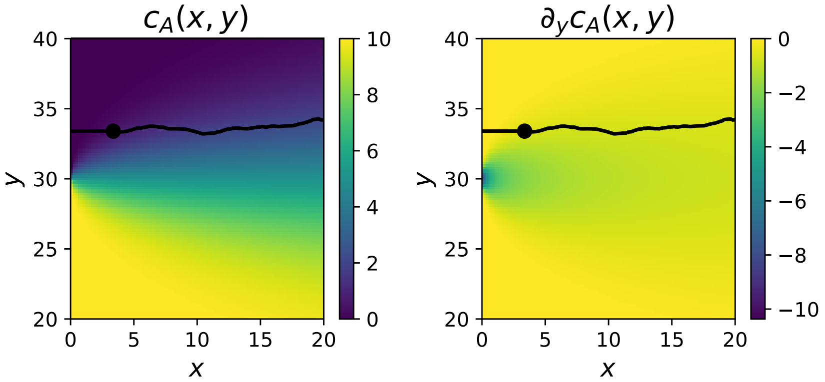
$$\begin{pmatrix} \dot{x} - v_{\mathrm{flow}} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} \frac{F_{\parallel}}{\gamma_{\parallel}} + \sqrt{2D_{\parallel}}\xi_{\parallel} \\ \frac{F_{\perp}}{\gamma_{\perp}} + \sqrt{2D_{\perp}}\xi_{\perp} \end{pmatrix}$$
$$\dot{\phi} = \mathcal{T}/\gamma_r + \sqrt{2D_r}\xi_{\phi}$$

where $F_{\parallel}$ and $F_{\perp}$ are the projected forces and $\mathcal{T}$ is the torque on the nanomotor.

Outline

Results

Pseudocolor represents the magnitude of the gradient

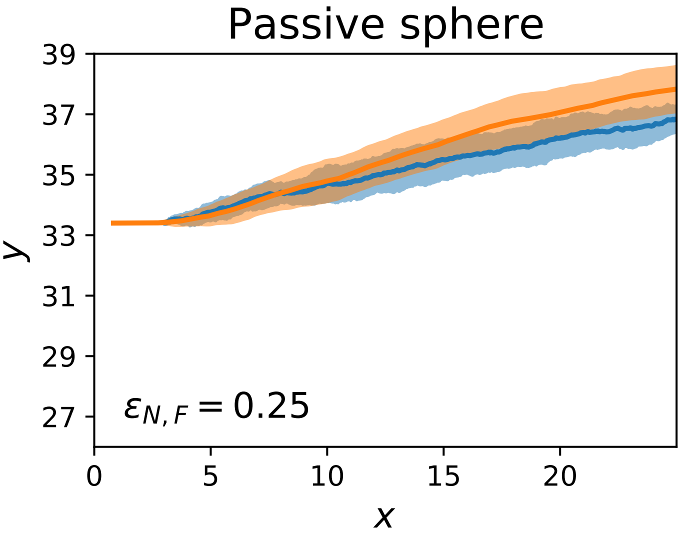


Passive sphere

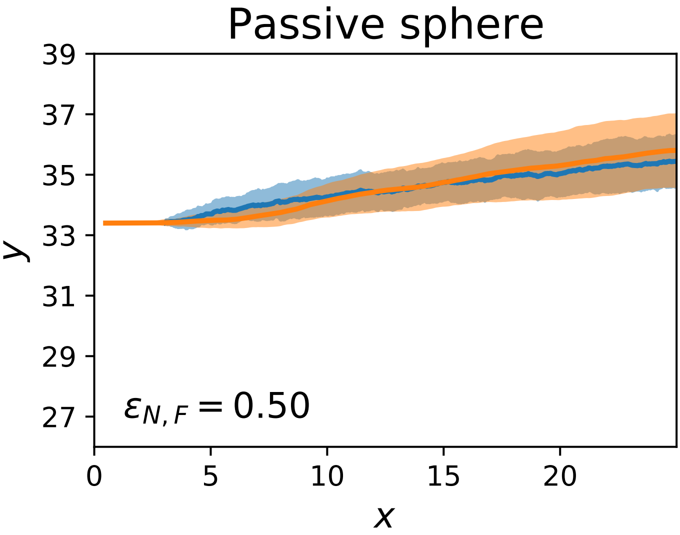
Parameters

- $\epsilon_{N,A} = 1$
- $\epsilon_{N,F}$ is varied
- There is no B

Passive sphere



Passive sphere



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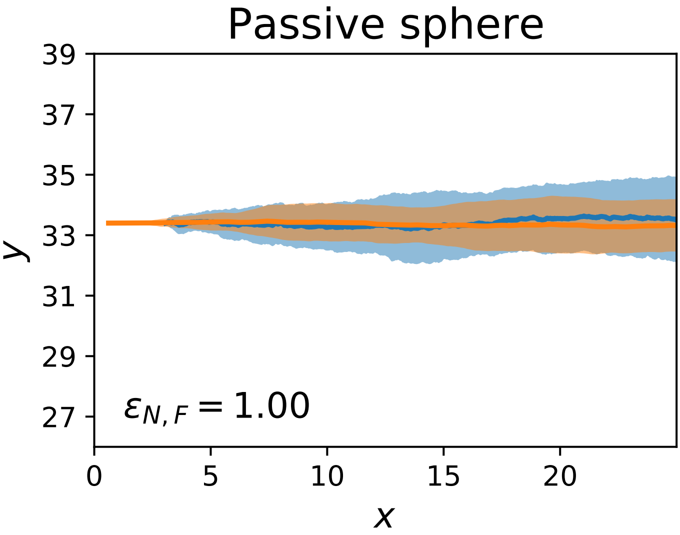

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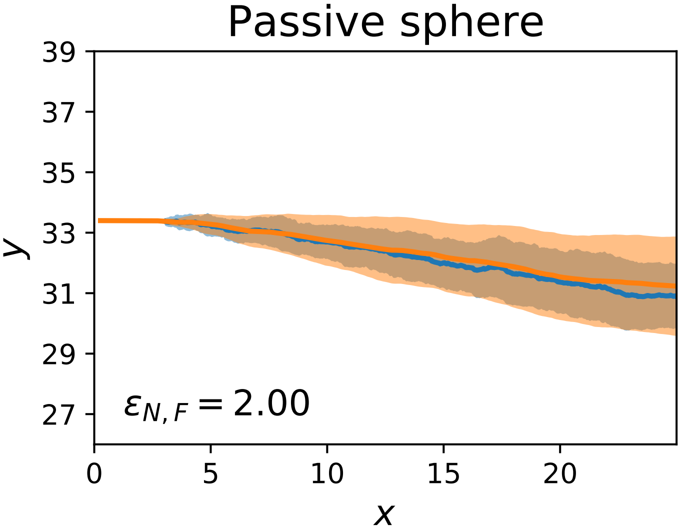

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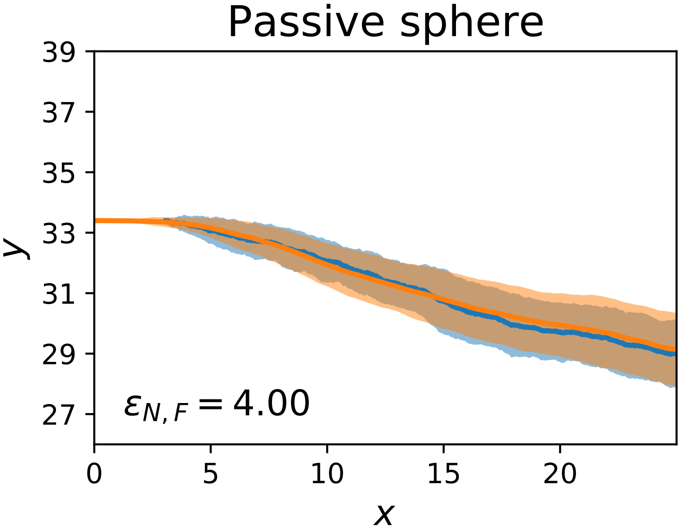
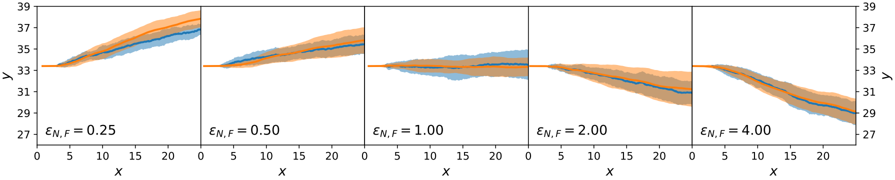


Passive sphere - summary

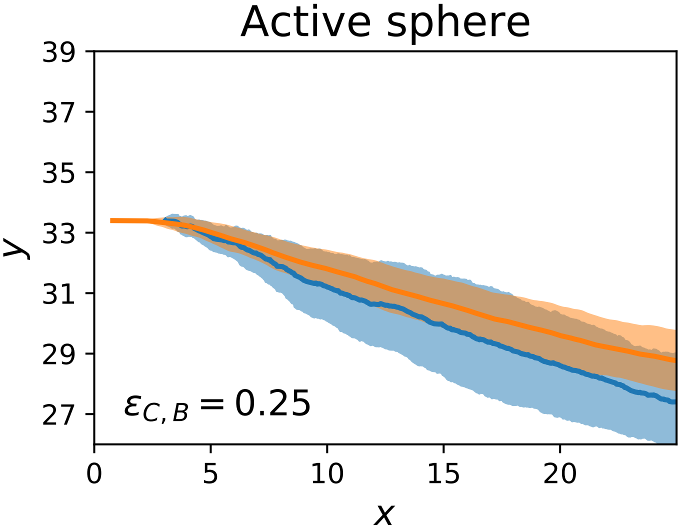


Active sphere

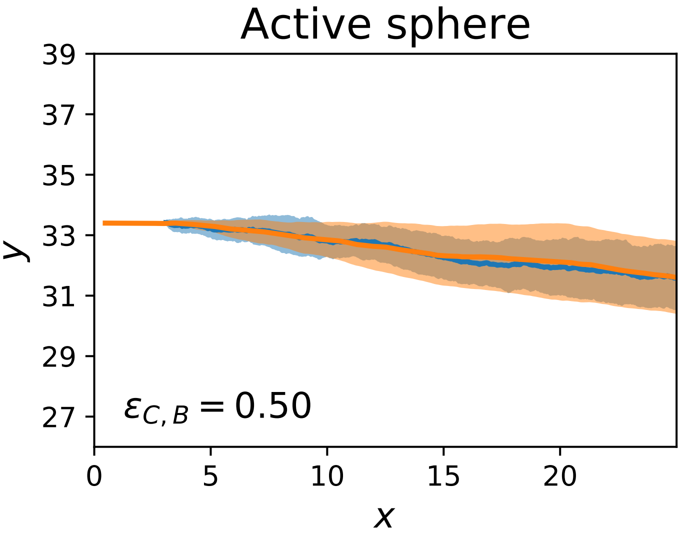
Parameters

- $\epsilon_{C,A} = 1$
- $\epsilon_{C,F} = 1$
- $\epsilon_{C,B}$ is varied

Active sphere



Active sphere



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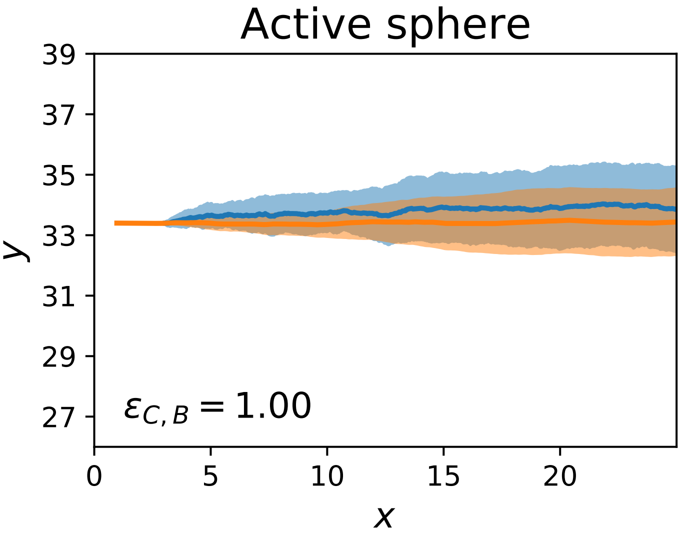
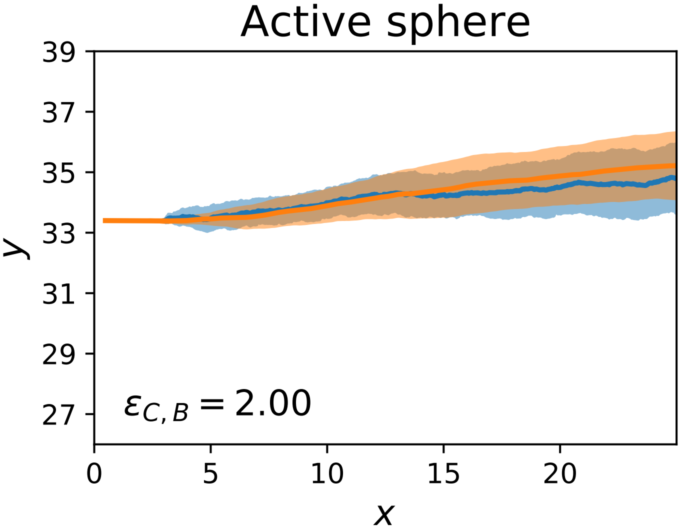


Active sphere



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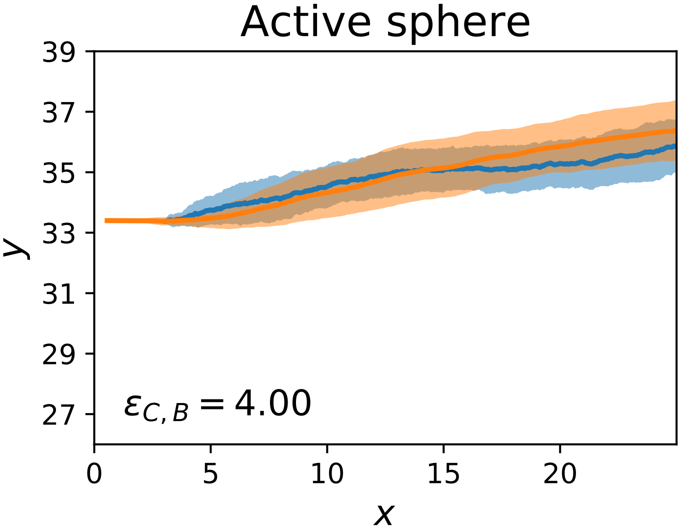

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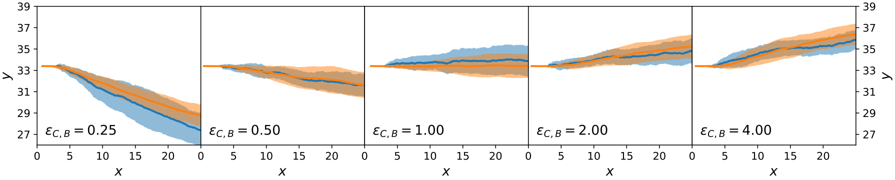

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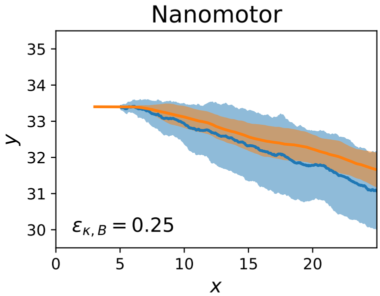
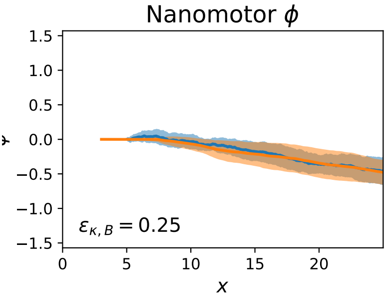
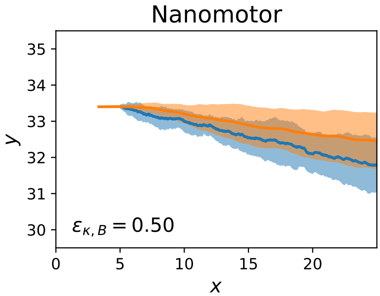
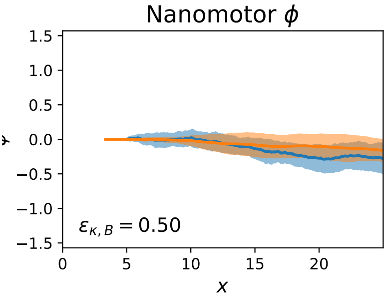
Nanomotor


Nanomotor
y
x
$\epsilon_{\kappa,B} = 0.25$
35
34
33
32
31
30
0
5
10
15
20

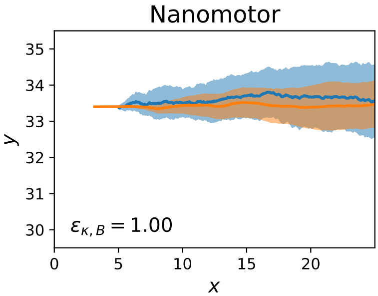

Nanomotor ϕ
x
$\epsilon_{\kappa,B} = 0.25$
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
5
10
15
20

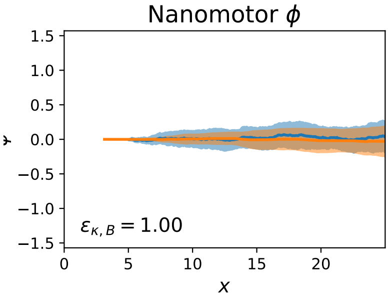
Nanomotor


Nanomotor
35
34
33
32
31
30
y
$\varepsilon_{\kappa,B} = 0.50$
0
5
10
15
20
x

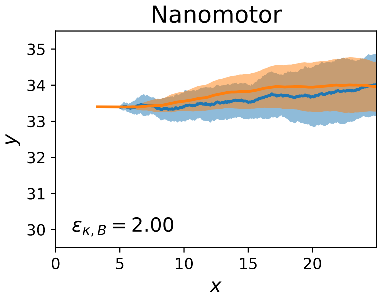

Nanomotor ϕ
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
$\varepsilon_{\kappa,B} = 0.50$
0
5
10
15
20
x

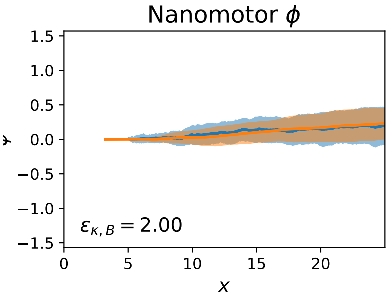
Nanomotor


Nanomotor
y
35
34
33
32
31
30
$\varepsilon_{\kappa,B} = 1.00$
0
5
10
15
20
x


Nanomotor ϕ
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
$\varepsilon_{\kappa,B} = 1.00$
0
5
10
15
20
x

Nanomotor


Nanomotor
y
x
$\varepsilon_{\kappa,B} = 2.00$
35
34
33
32
31
30
0
5
10
15
20


Nanomotor ϕ
x
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1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
5
10
15
20

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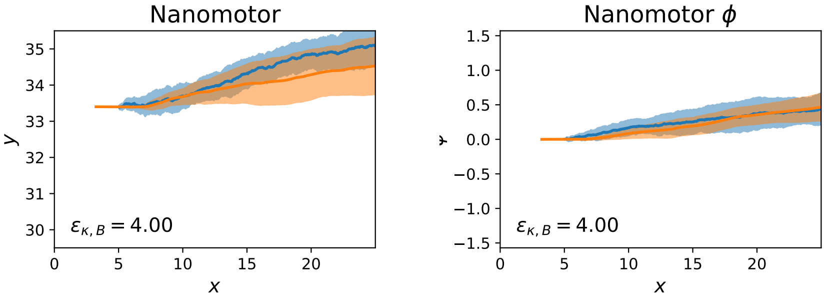
Nanomotor
35
34
33
32
31
30
y
$\varepsilon_{\kappa,B} = 4.00$
0
5
10
15
20
x
Nanomotor ϕ
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
$\varepsilon_{\kappa,B} = 4.00$
0
5
10
15
20
x

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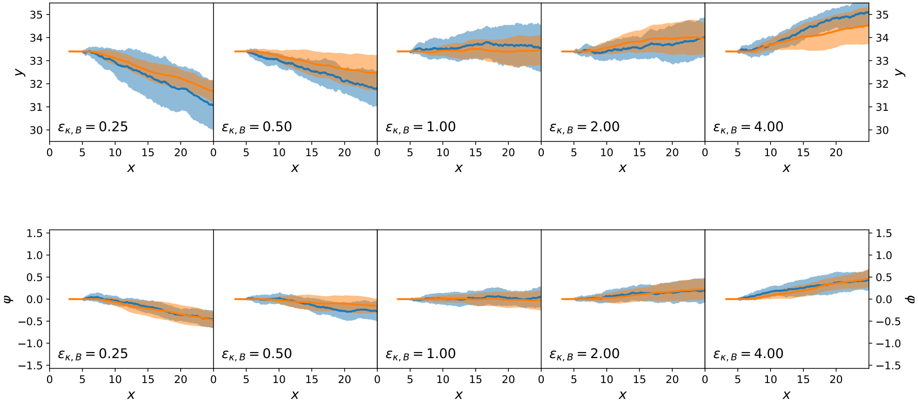

Comparison to "constant gradient"

In Chen *et al* Soft Matter **12**, 1876 (2016)

- The average orientation of the dimer nanomotor is against the gradient.
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Comparison to our *stochastic model*

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  - The distribution of orientation
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  - The overal histogram of position
- Orientation is matched.
- Chemotactic behavior: it depends.

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  - Passive and active chemotaxis

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- Perspectives:
  - Other motors
  - Integration with enzyme chemo-mechanical models
- Thank you!

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