Passive and Active Colloidal Chemotaxis in a Microfluidic Channel

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http://pdebuyl.be/

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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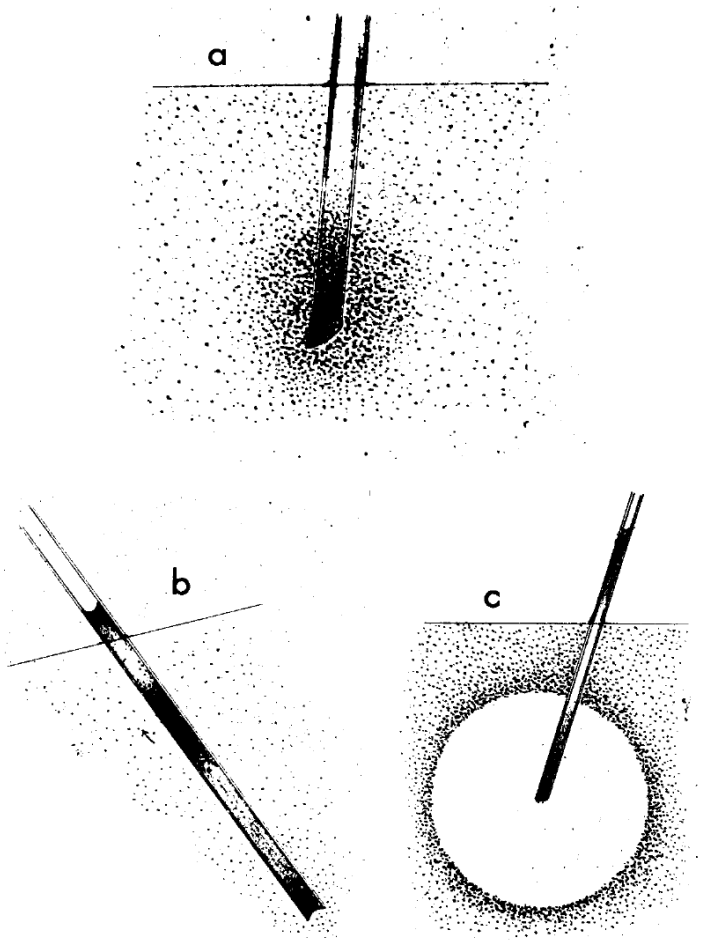

Synthetic chemotaxis

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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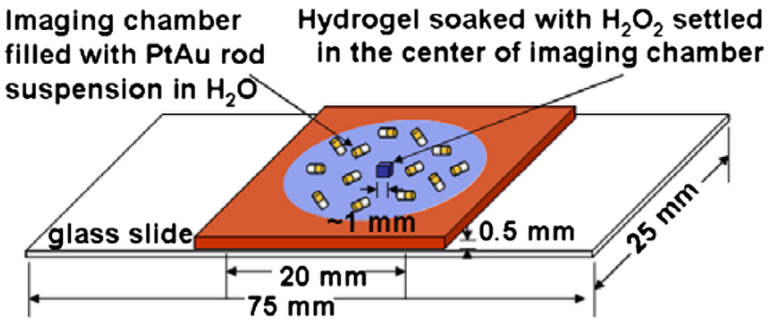
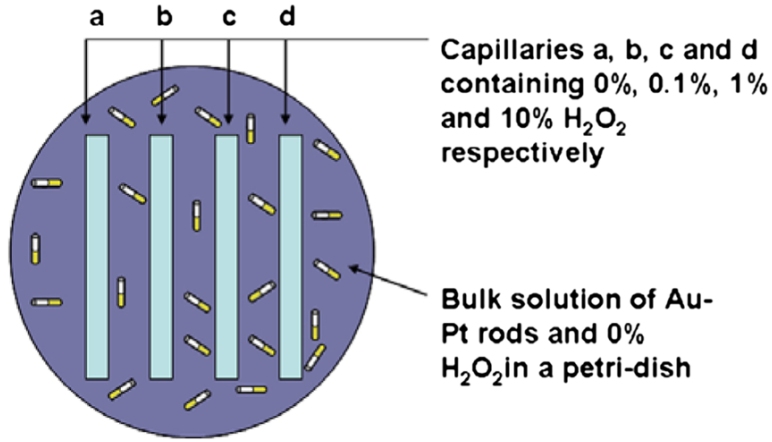
(a)



(b)



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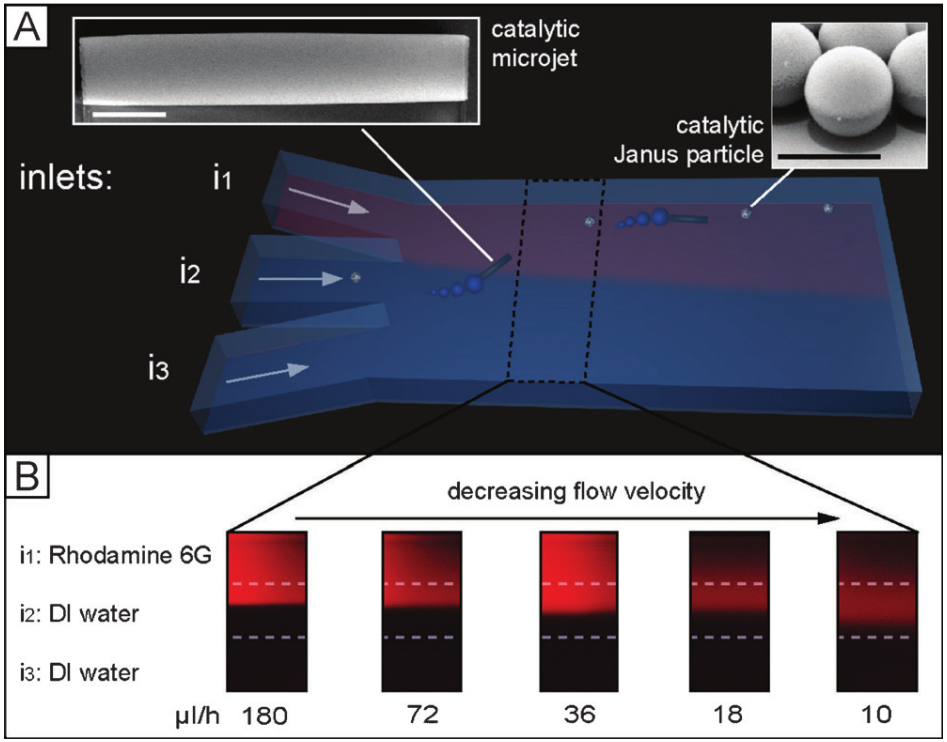

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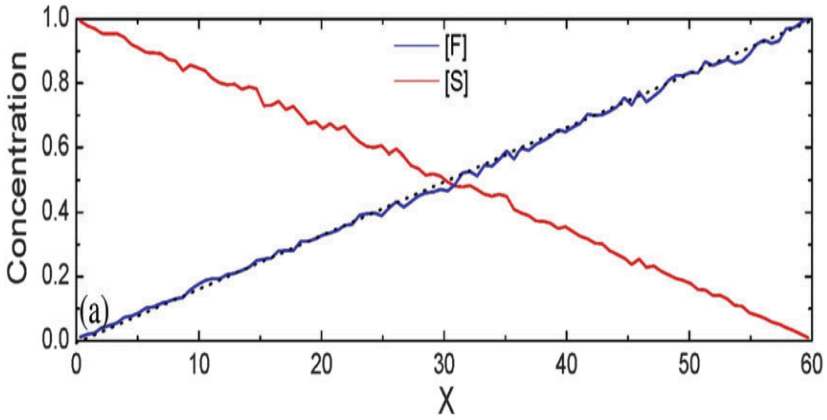

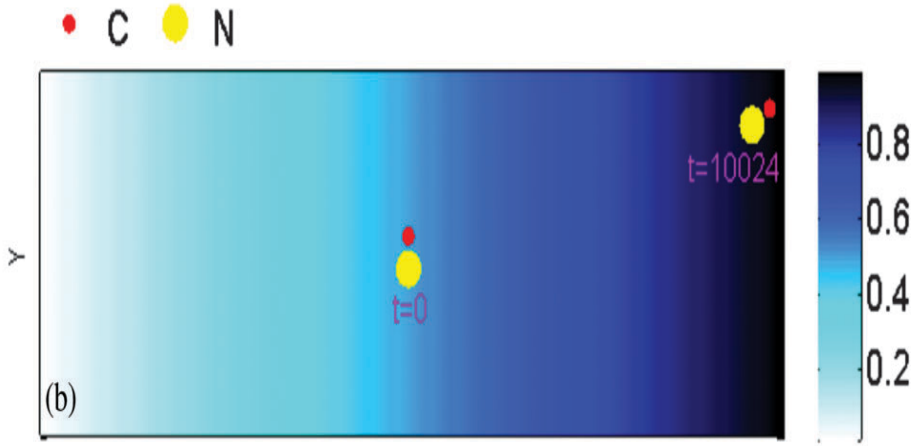

Enzymatic chemotaxis

Experiments

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

Simulations

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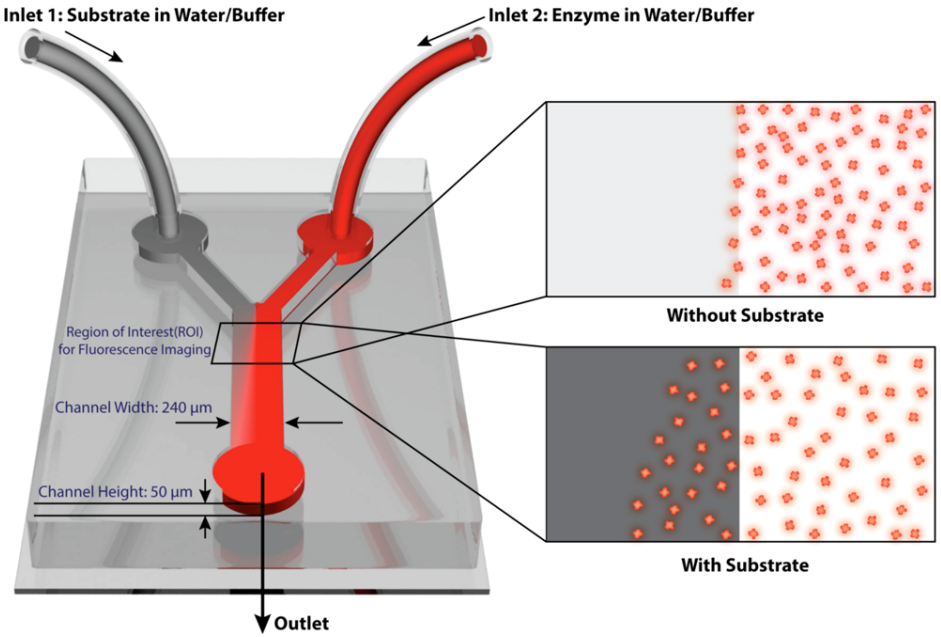

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Objectives

- Understand the mechanism for chemotaxis
  - For passive and active colloids
  - Under a flow
- 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 (here, close to 1M particles).
- 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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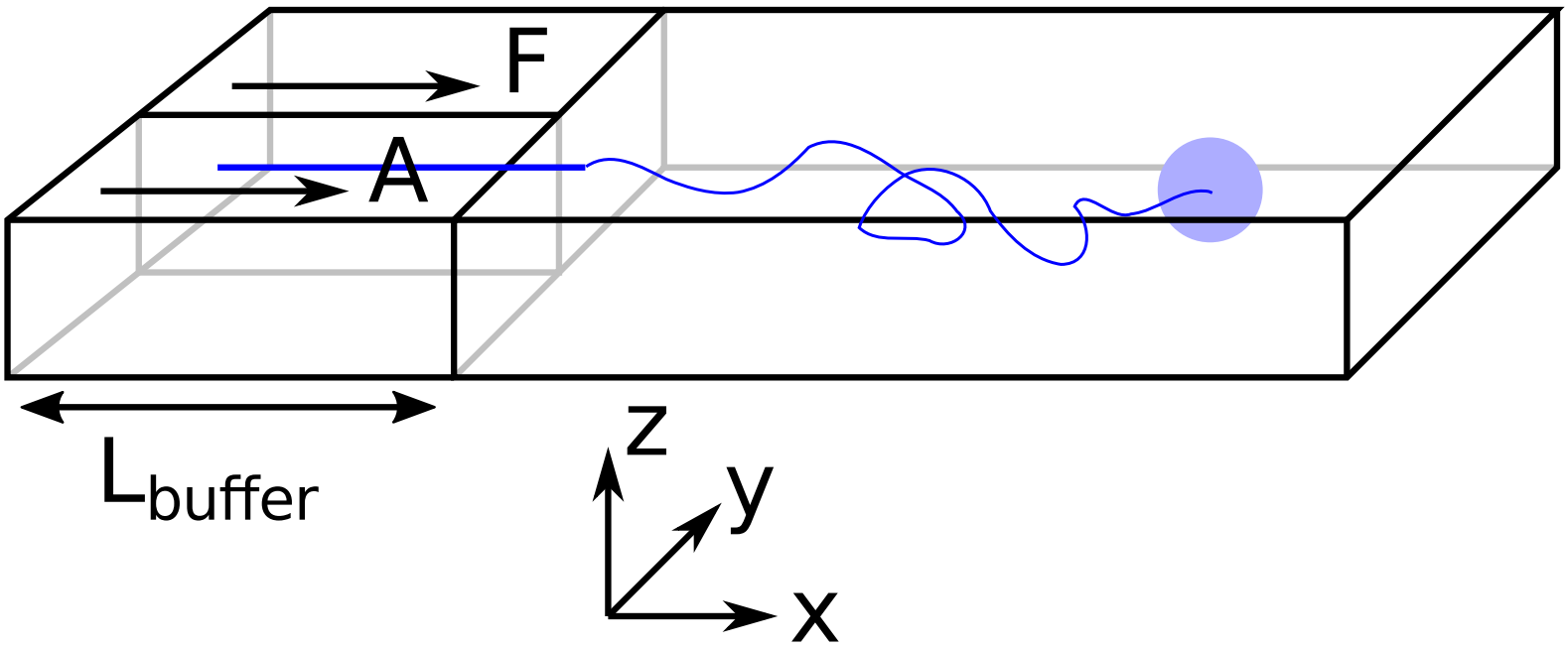
Software

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

Mesoscopic simulation



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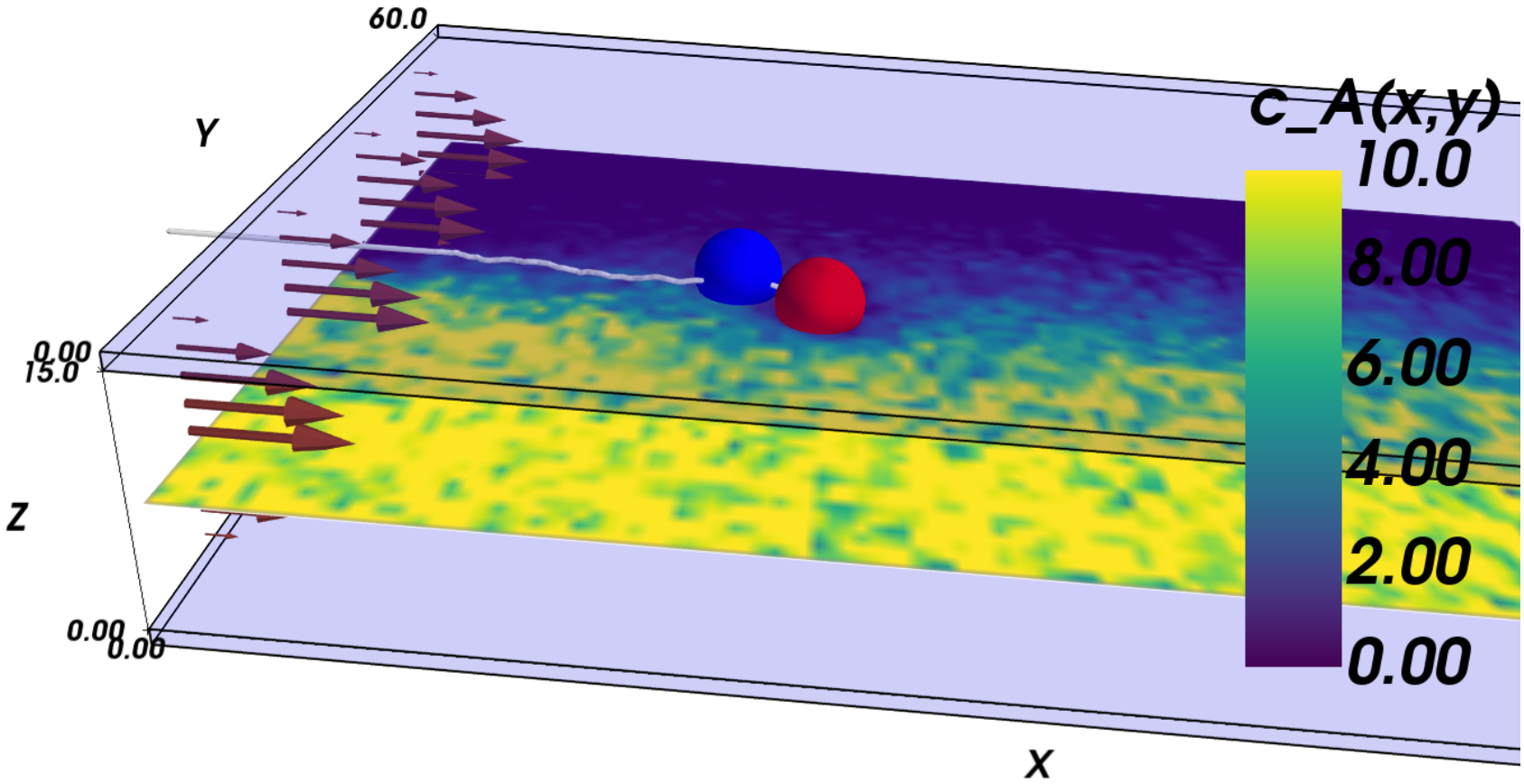


Stochastic simulation

Langevin equation for the sphere

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

Langevin equation for the dimer nanomotor

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

$F_\parallel$ & $F_\perp$: forces on the axes of the dimer. $\mathcal{T}$: torque on the dimer.

Chemical concentration

- For high Pe, at the center of the channel $z = L_z/2$
  Ismagilov *et al*, Appl. Phys. Lett. **76**, 2376 (2000)

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

- Solution:

$$c_A(x,y) = c_0 \left(1 - \frac{1}{2}\,\mathrm{erfc}\left(\frac{L_y/2 - y}{\sqrt{4Dx/v_{\mathrm{flow}}}}\right)\right)$$

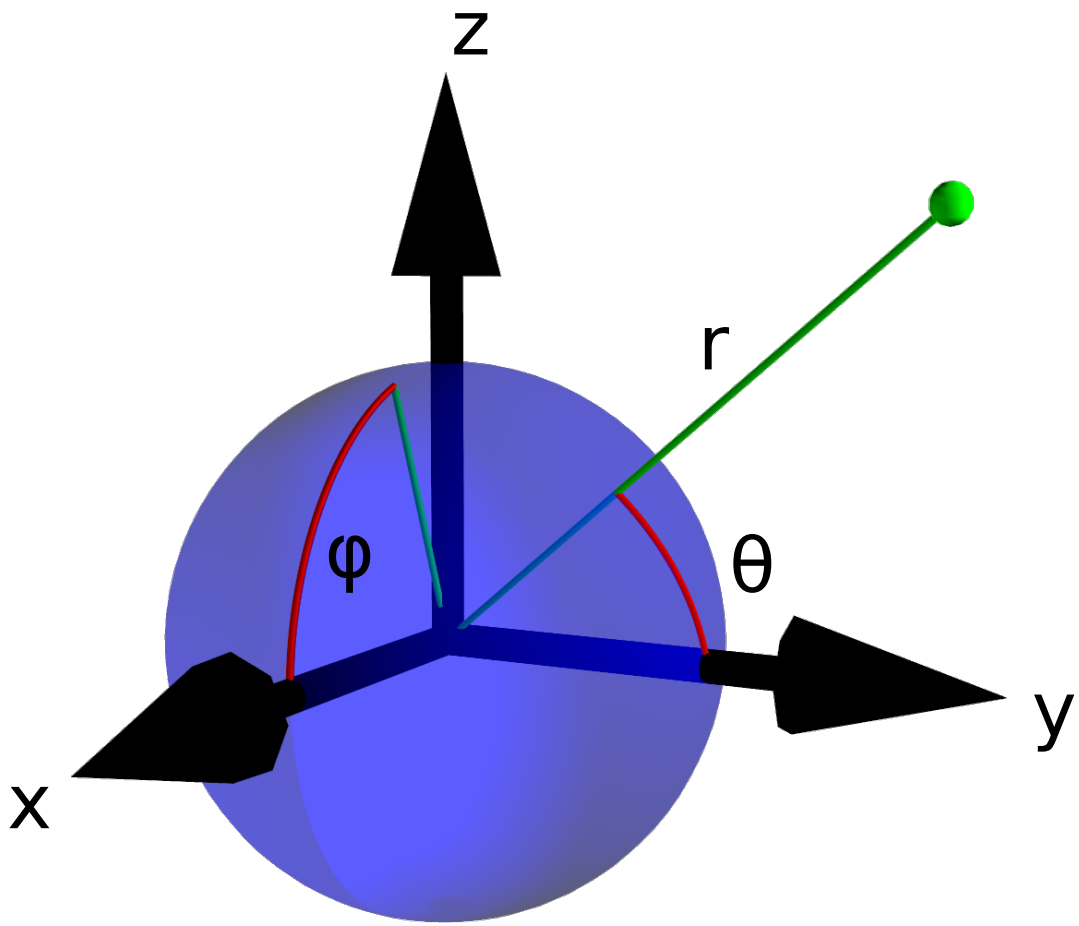
$$c_F(x,y) = c_0 - c_A(x,y)$$

$$c_B(x,y) = 0$$

Chemical concentration

Spherical coordinates

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



Chemical concentration

Ansatz for $c_A(x, y)$

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

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- $$\begin{cases} c_0 &= c_A(x, y) \\ c_1 &= -\frac{k_0}{k_0 + k_D} c_0 \\ c_2 &= -\frac{k_0}{k_0 + 2k_D} \lambda R \end{cases}$$

Surface interaction

- Methodology used in Rückner and Kapral, Phys. Rev. Lett. **98**, 150603 (2007)
- Integrating the force over the surface gives

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

where we have defined

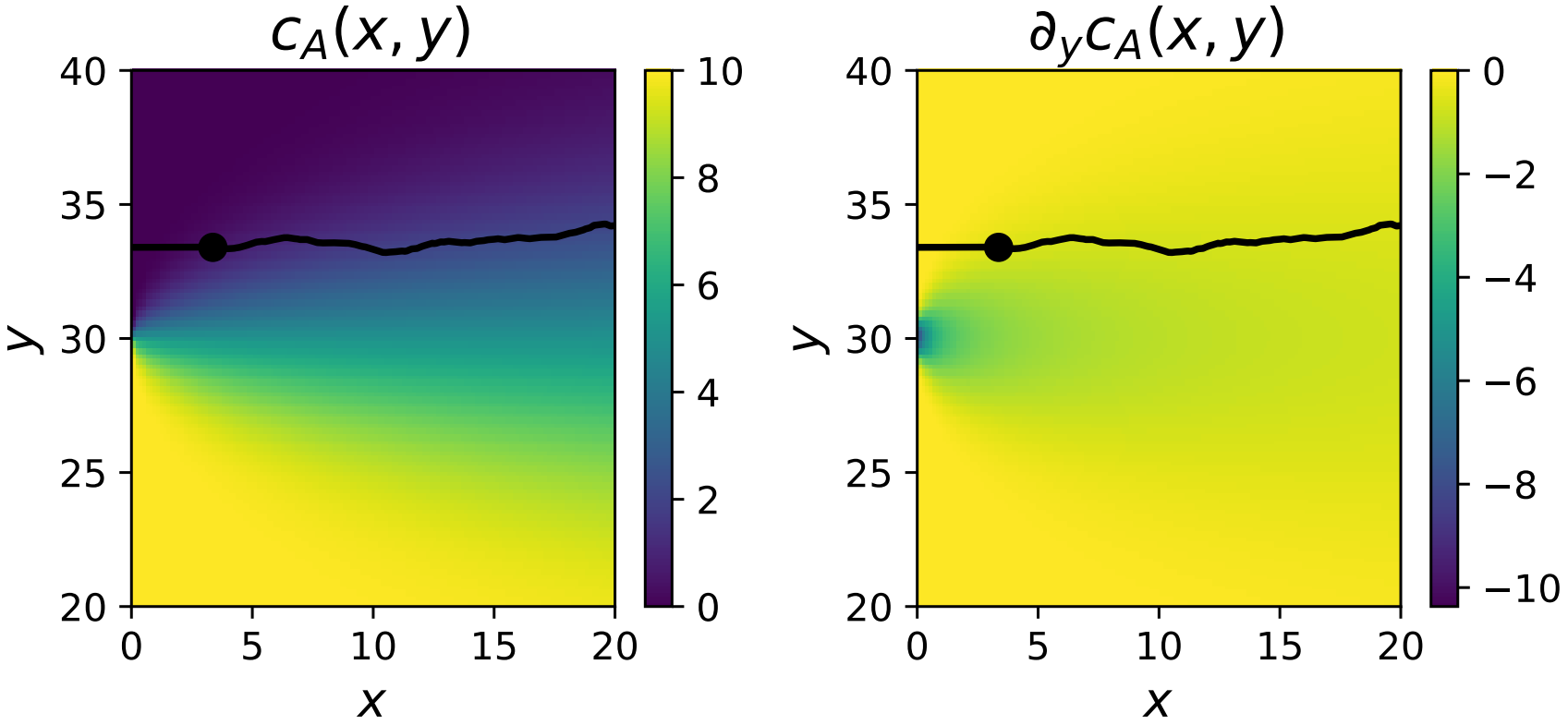
$$\Lambda_{\kappa,\alpha} = \int_0^R dr r \left(e^{-\beta V_{\kappa,\alpha}(r)} - 1 \right) \ .$$

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

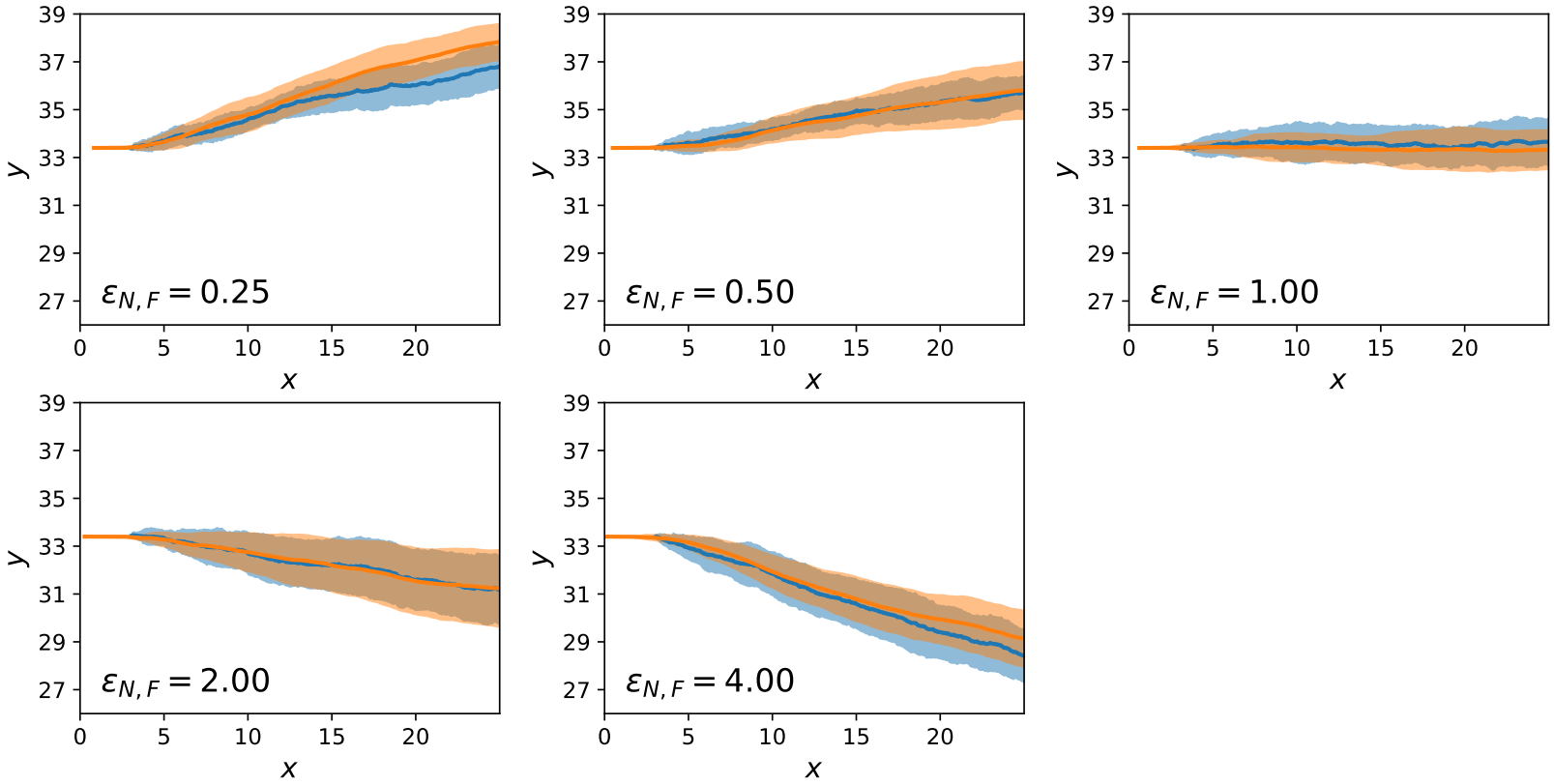
Outline

Results

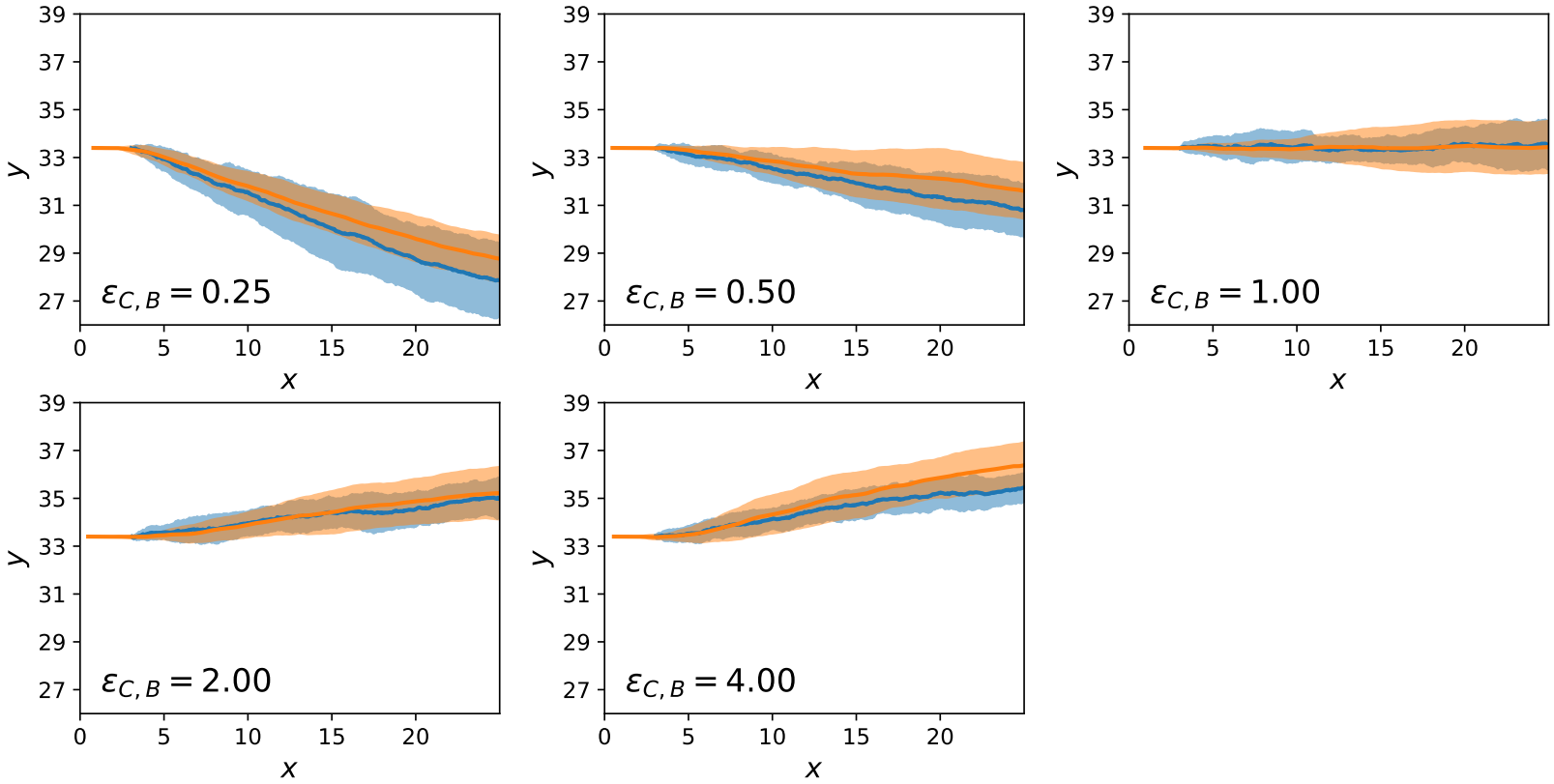
Pseudocolor represents the concentration (left) and the magnitude of the gradient (right).



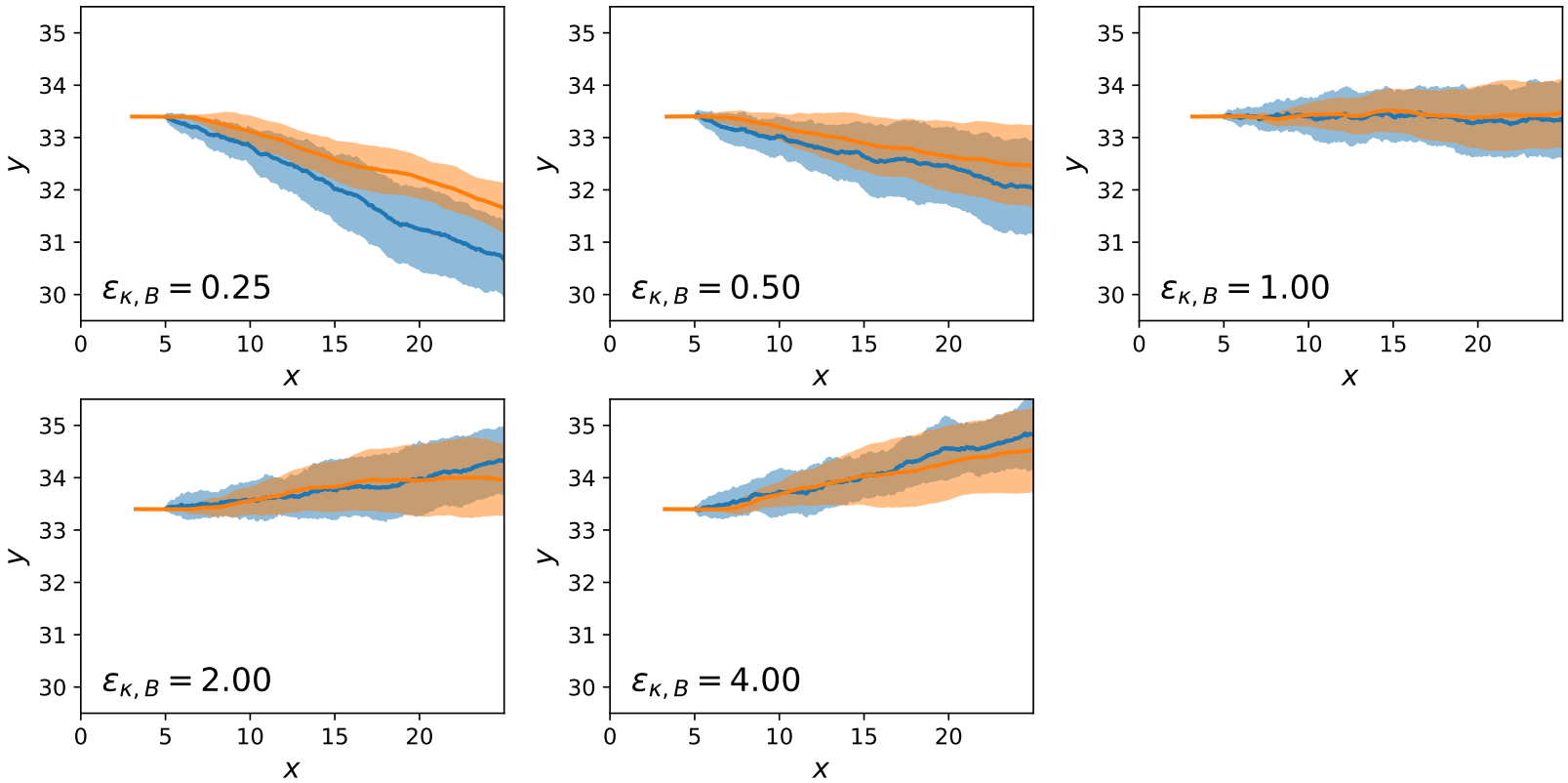
Passive sphere - only A and F, $\epsilon_A = 1$



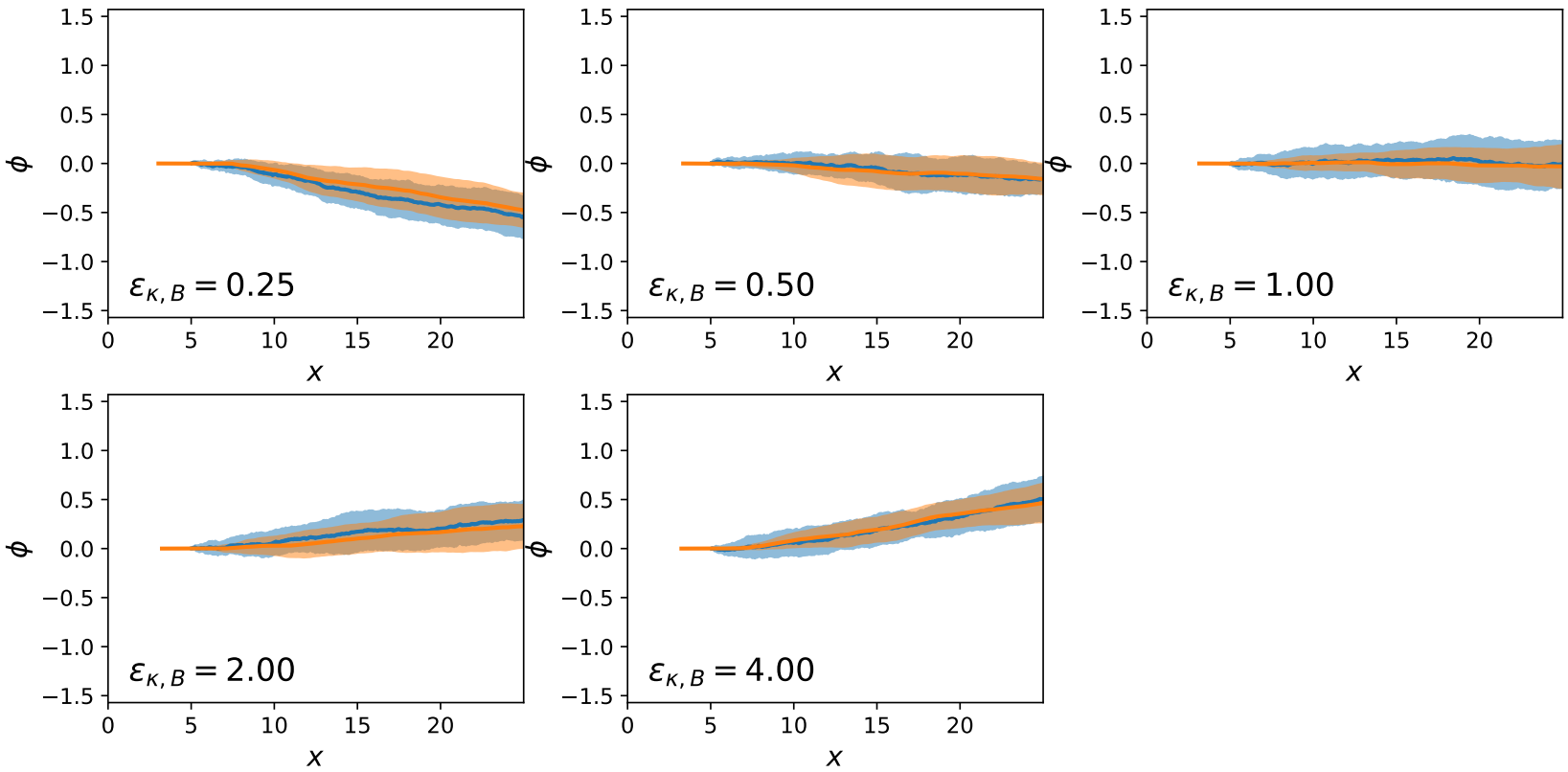
Active sphere - $A + C \rightarrow B + C$, $\epsilon_A = 1$



Nanomotor - $A + C \rightarrow B + C$, $\epsilon_A = 1$, $\epsilon_{\kappa,B}$ is varied



Nanomotor angle - $A + C \rightarrow B + C$, $\epsilon_A = 1$, $\epsilon_{\kappa,B}$ is varied



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

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