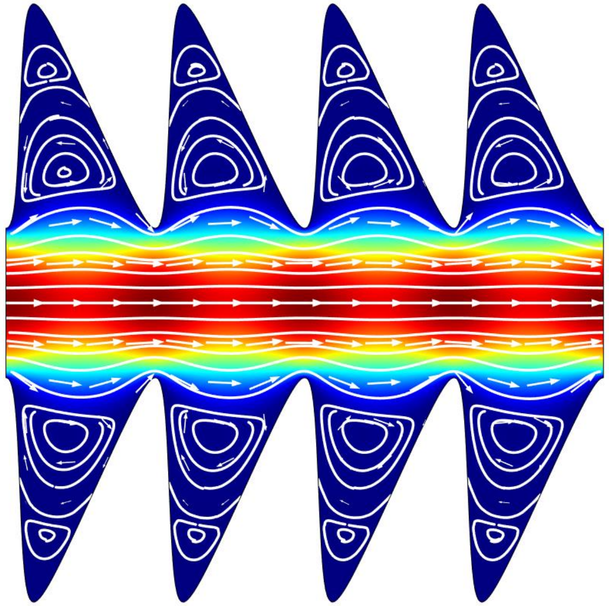
Effective description of Taylor dispersion in strongly corrugated channels



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École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.
[3] SIB Swiss Institute of Bioinformatics, CH-1015 Lausanne, Switzerland

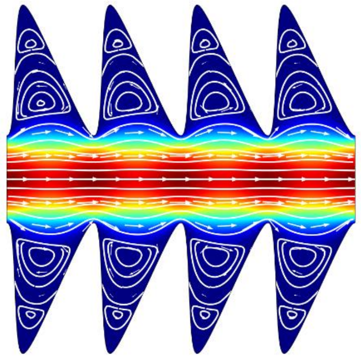
Background

2019-2022: PhD, LOMA, University of Bordeaux, France

Supervisors: David. S. Dean, Thomas Guérin

Title: Dispersion in heterogeneous media: a study of hydrodynamic effects and surface-mediated diffusion

- Model of surface mediated diffusion [PRL 2022]
- Taylor dispersion in channels [Physics of Fluids 2021; Preprint 2025]
- Non Gaussian diffusion near surfaces [PRL 2022]
- Active matter: self phoretic motion [PRE 2024]



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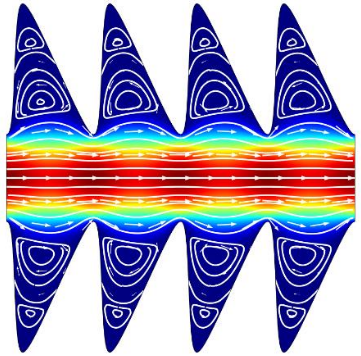

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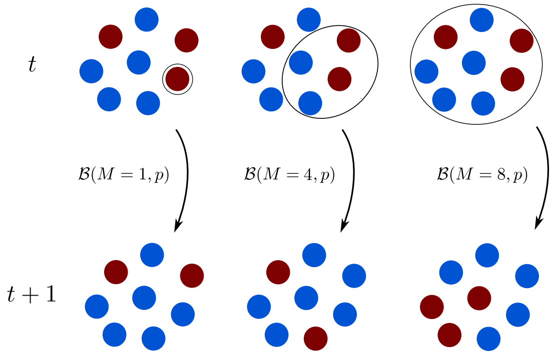
Since 2022: Postdoc, Bitbol lab, EPFL, Switzerland

Supervisor: Anne-Florence Bitbol, collaboration with Claude Loverdo (CNRS, LJP, Sorbonne Université, Paris)

Title: Modeling evolution of population

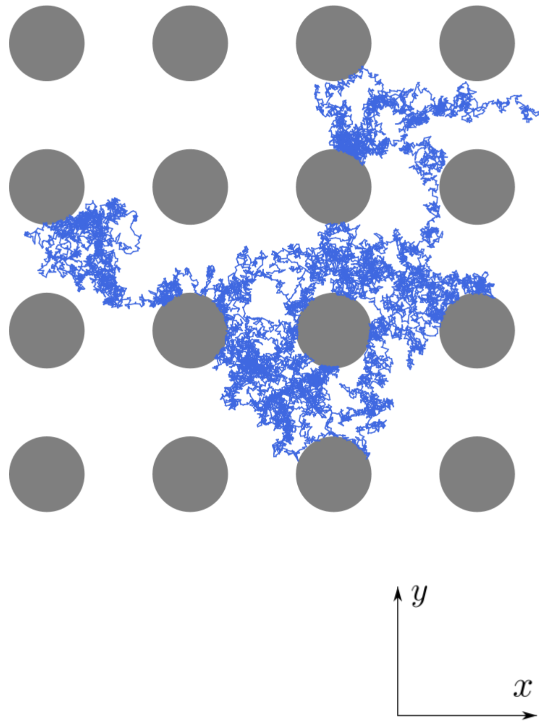


- Modeling expanding population, application to bacterial population in the gut
- Models of non expanding population, evolutionary graph theory [Evolution (in press) 2025; JTB 2025]

Context

Transport properties are crucial quantities to evaluate in **heterogeneous media**

- Chemical engineering [Aminian et al., Science, 2016]
- Biochannels and nanopores [Marbach et. al., Nature Physics, 2018]
- Porous structures [Putzel et al., PRL, 2014]



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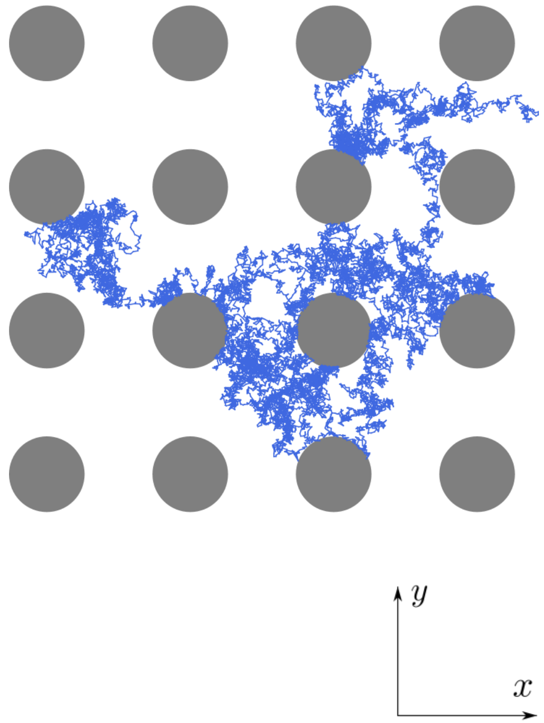

Transport properties can be quantified at large time with an effective drift and **effective diffusivity**

$$v_e = \frac{\overline{[x(t) - x(0)]}}{t}$$

$$D_e \underset{t \to \infty}{\simeq} \frac{\overline{[x(t) - x(0) - v_e t]^2}}{2t}$$

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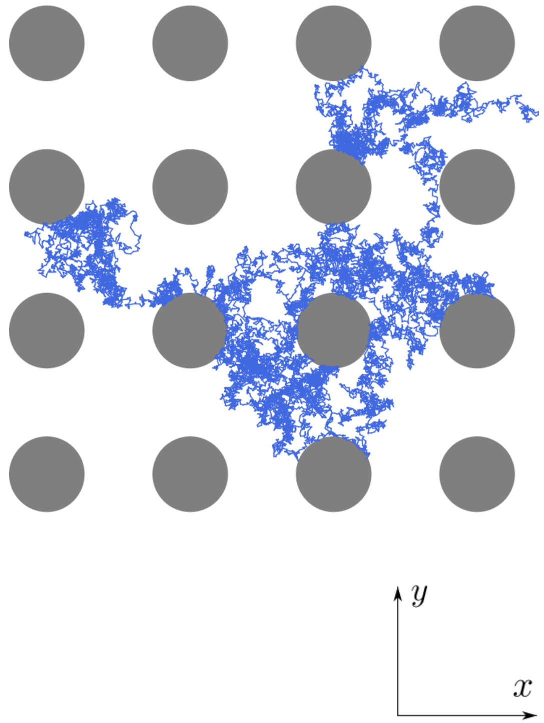

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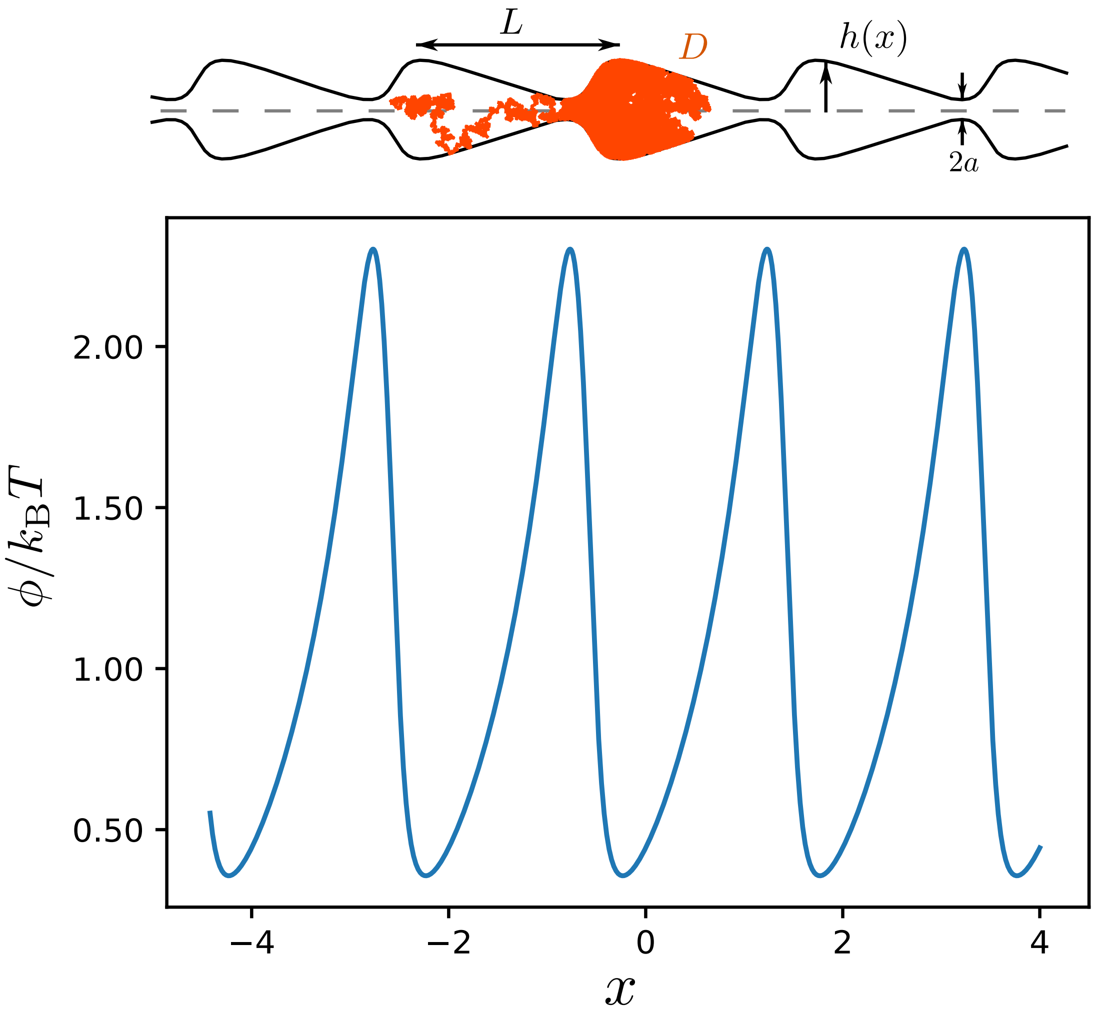
The effective diffusivity can **significantly** differ from the microscopic one (e.g. spatial heterogeneities, flow...)

Context

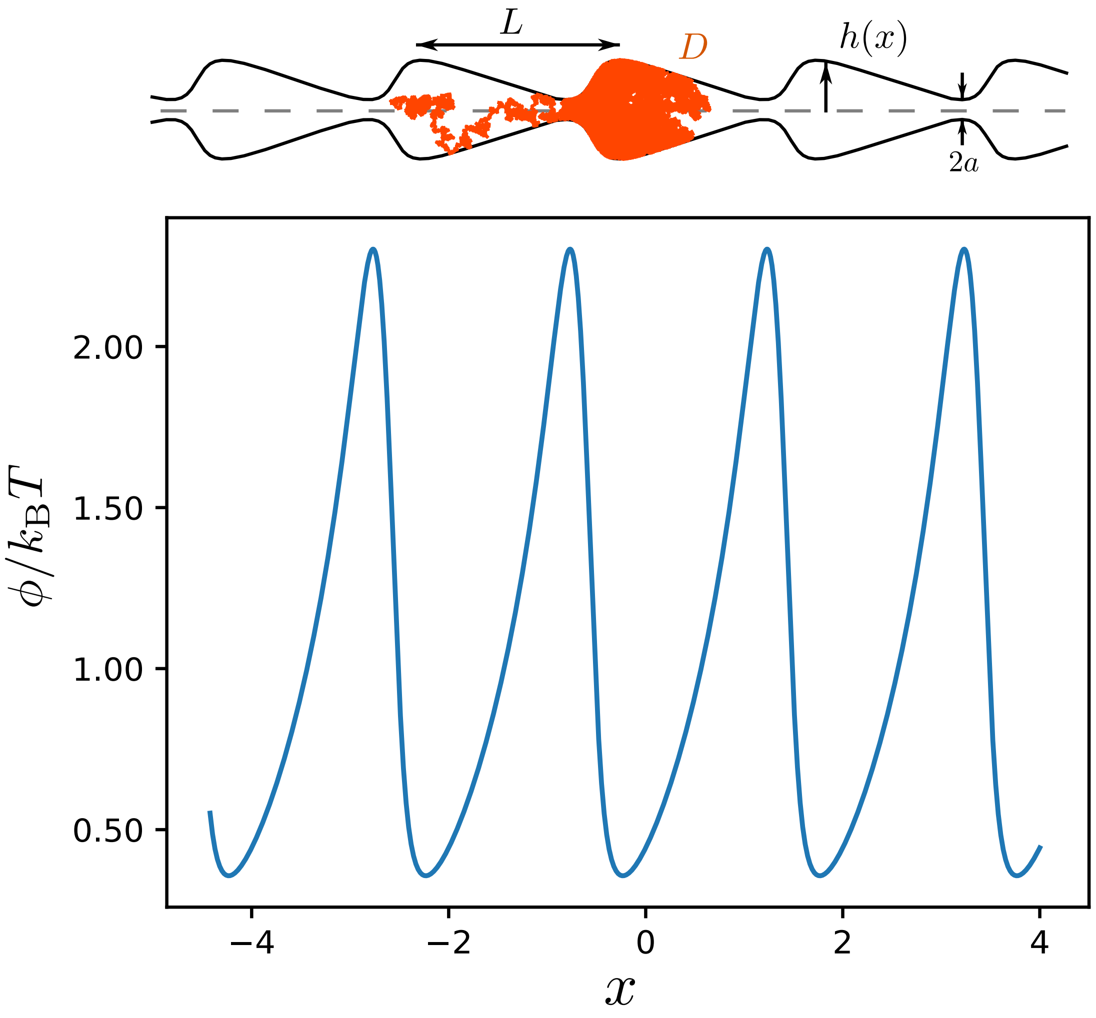


Example 1: Slowly undulated channel

Fick-Jacobs approximation: fast equilibrium in the transverse direction to the channel

Approximation valid in the limit $L \gg a$

Context



Example 1: Slowly undulated channel

Fick-Jacobs approximation: fast equilibrium in the transverse direction to the channel

Approximation valid in the limit $L \gg a$

Effective potential $\phi(x) = -TS(x) = -k_{\mathrm{B}}T \log\left[h(x)\right]$

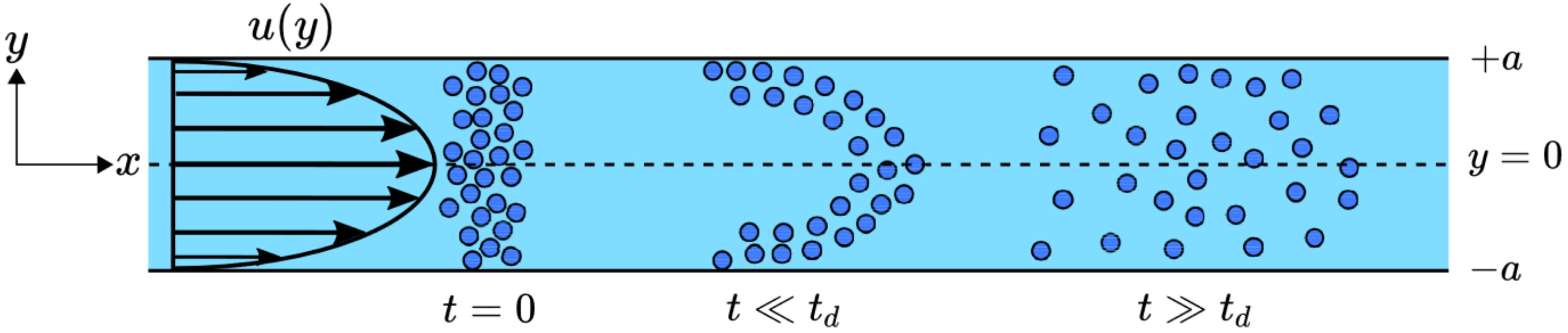
$$D_e = \frac{D}{\left\langle e^{-\phi/k_{\mathrm{B}}T}\right\rangle \left\langle e^{+\phi/k_{\mathrm{B}}T}\right\rangle} = \frac{D}{\langle h\rangle \langle h^{-1}\rangle} \leq D$$

[Jacobs 1935; Lifson, & Jackson, JCP, 1962]

Reduction of diffusivity resulting from entropic trapping

Context

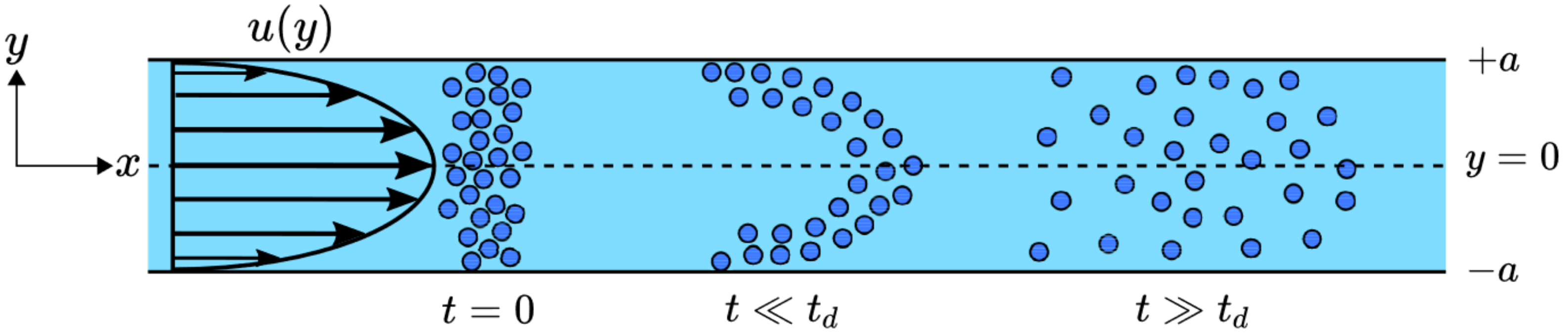
Example 2: Taylor dispersion



[Kumar et al., PRF, 2021]

Context

Example 2: Taylor dispersion



[Kumar et al., PRF, 2021]

$\overline{u}$	Averaged flow velocity
D	Local diffusion coefficient
$\mathrm{Pe} = \dfrac{\text{advection}}{\text{diffusion}} = \dfrac{a\overline{u}}{D}$	Péclet number

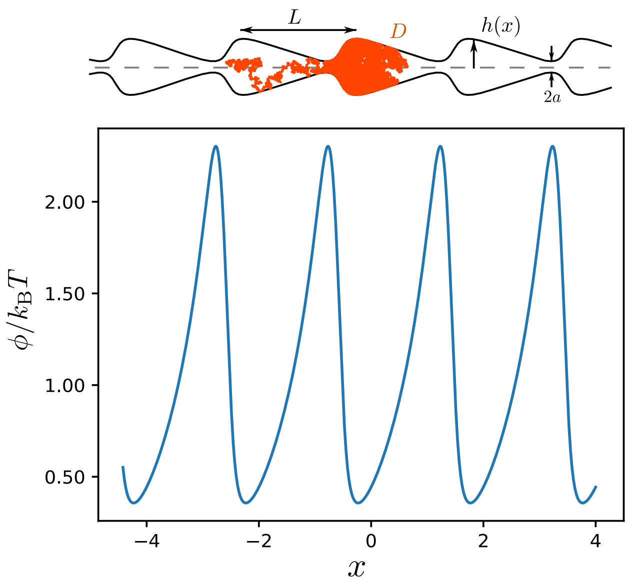
Effective diffusivity $$D_e = D\left(1 + \frac{2}{105}\mathrm{Pe}^2\right) > D$$

[Taylor 1953, Aris 1956]

Enhanced diffusivity
due to the gradient of velocity

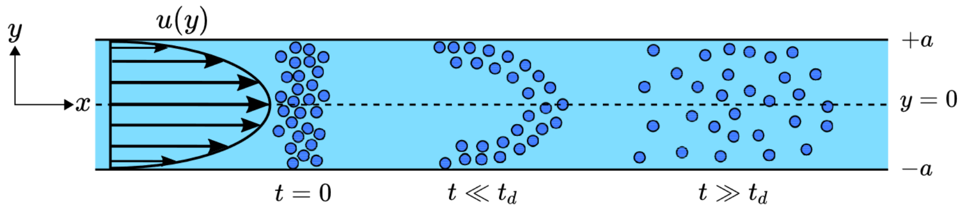
Context

Slowly undulated channel



$$D_e = \frac{D}{\langle h \rangle \langle h^{-1} \rangle} \leq D$$

Taylor dispersion



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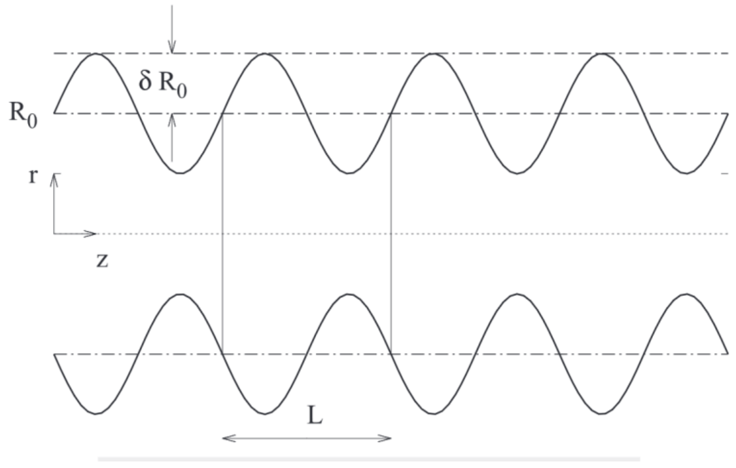
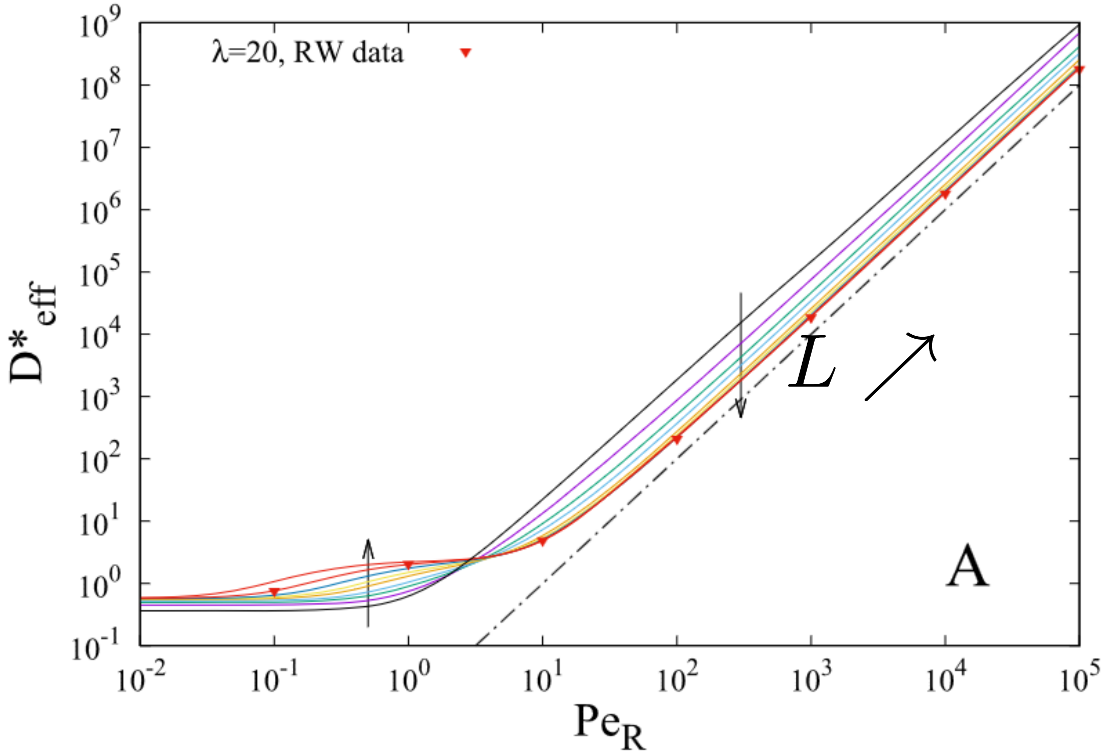
Context

Taylor dispersion in slowly undulated channel



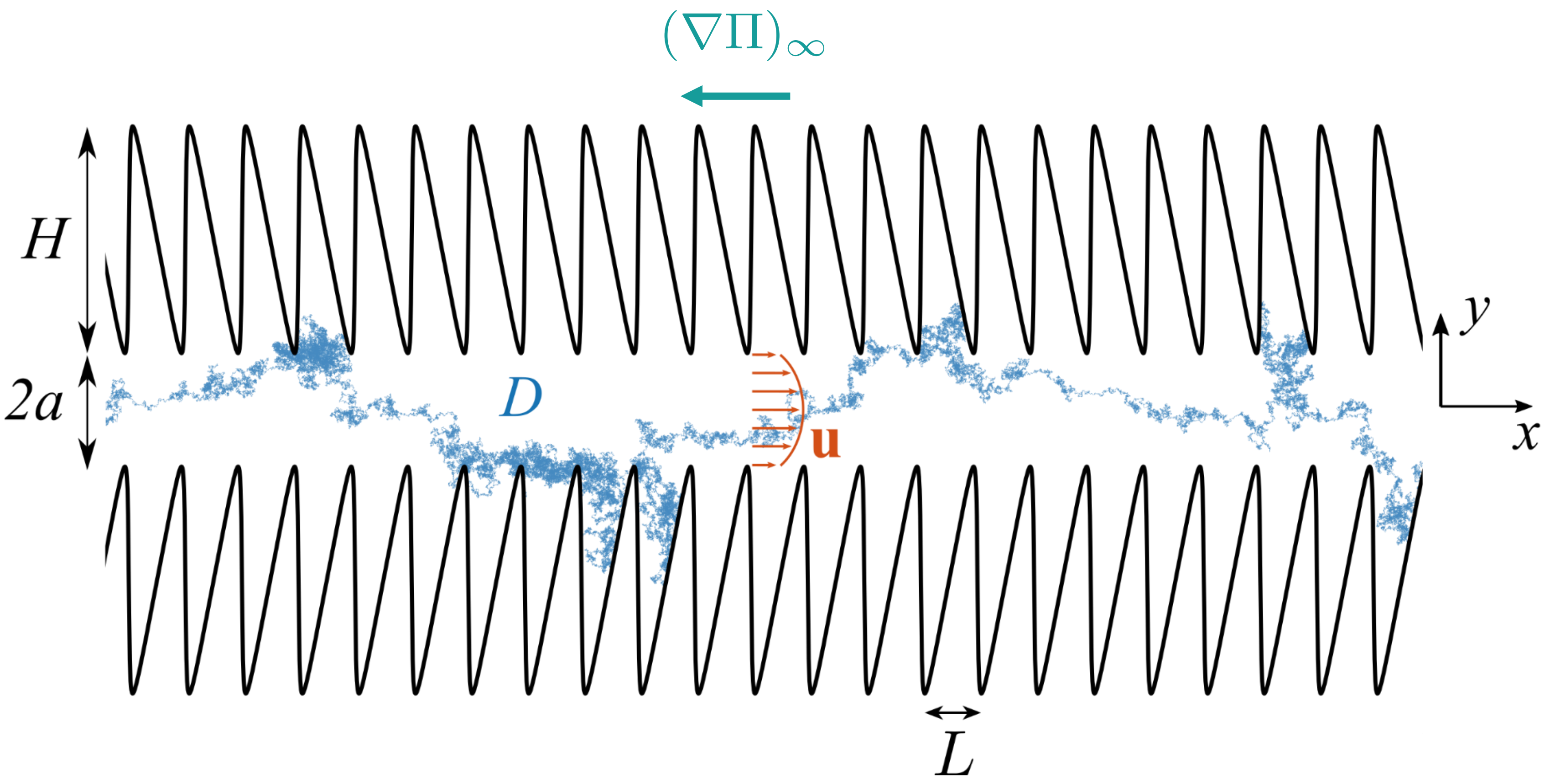
Flow determined in the **lubrication approximation**

[Adrover et al., Laminar dispersion at low and high Peclet numbers in finite-length patterned microtubes. Physics of Fluids, 2017]



Interplay between advection and entropic effects in slowly undulated channels

Question



What happens in highly corrugated channel?
Does any effective description exist for this problem?

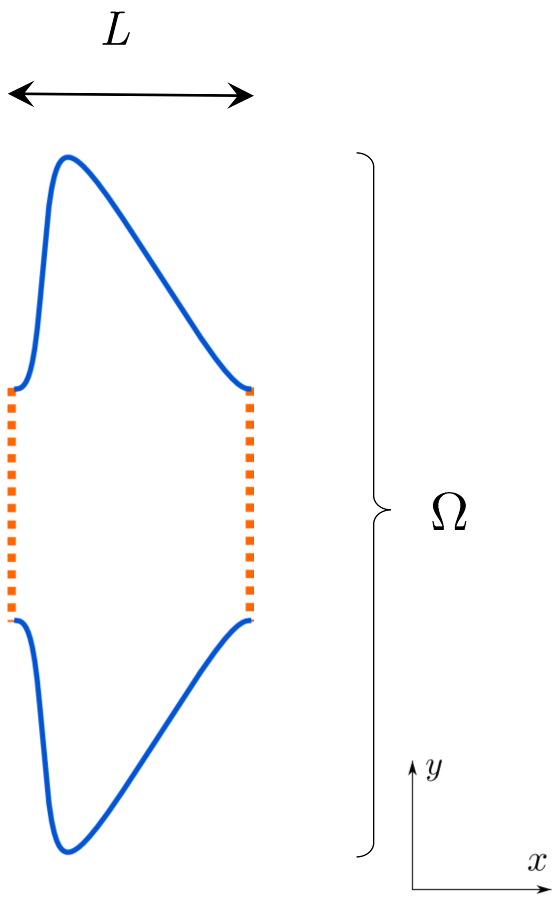
Effective diffusivity in the limit $L \to 0$

General expression

$$D_e = D + \frac{1}{\Omega} \int_{\Omega} \mathrm{d}\mathbf{r} \; (u_x f - D \partial_x f)$$

Incompressible flow $\mathbf{u}$

Auxiliary field f



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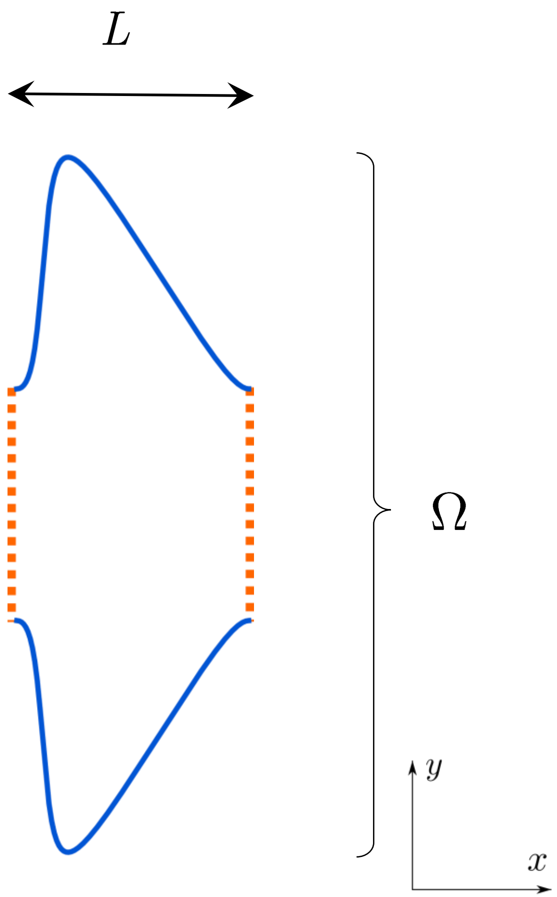

	Incompressible flow $\mathbf{u}$	Auxiliary field f
Bulk equation	$\nabla \cdot \mathbf{u} = 0$ $\eta\ \nabla^2\mathbf{u} - \nabla\Pi = 0$	$D\nabla^2 f - \mathbf{u}\cdot\nabla f = \langle u_x\rangle - u_x$

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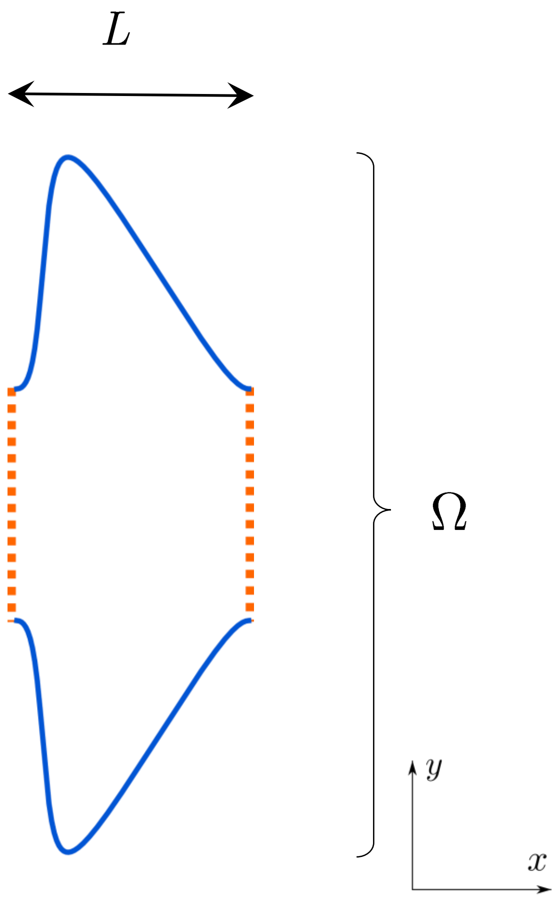
Boundary conditions	$\mathbf{u} = 0$ $\mathbf{u}(\mathbf{r} + L\,\mathbf{e}_x) = \mathbf{u}(\mathbf{r})$	$\mathbf{n}\cdot\nabla f = \mathbf{n}\cdot\mathbf{e}_x$ $f(\mathbf{r} + L\,\mathbf{e}_x) = f(\mathbf{r})$



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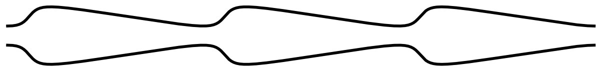

✓ Fick-Jacobs approximation

✓ Lubrication theory

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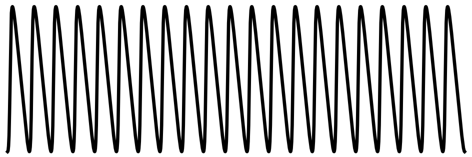
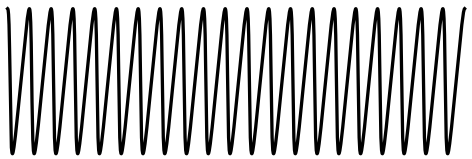




✗ Fick-Jacobs approximation

✗ Lubrication theory

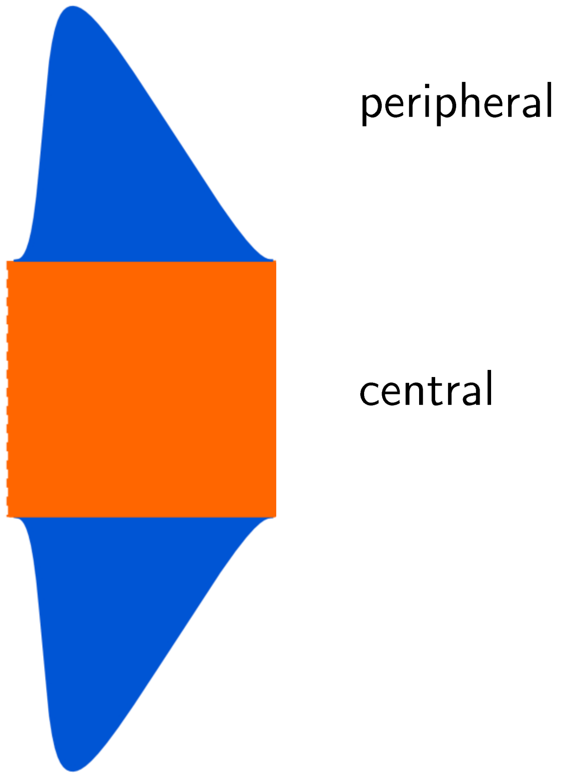
Problem: lubrication and Fick-Jacobs approximations break down in the limit $L \to 0$!

Effective diffusivity in the limit $L \to 0$

$\to$ Use matching asymptotics method!

Auxiliary field $$f = \begin{cases} f_0^p(X,y) + L f_1^p(X,y) + \ldots & (|y| > a) \\ f_0^c(X,y) + L f_1^c(X,y) + \ldots & (|y| < a) \end{cases}$$

$$X = x/L$$

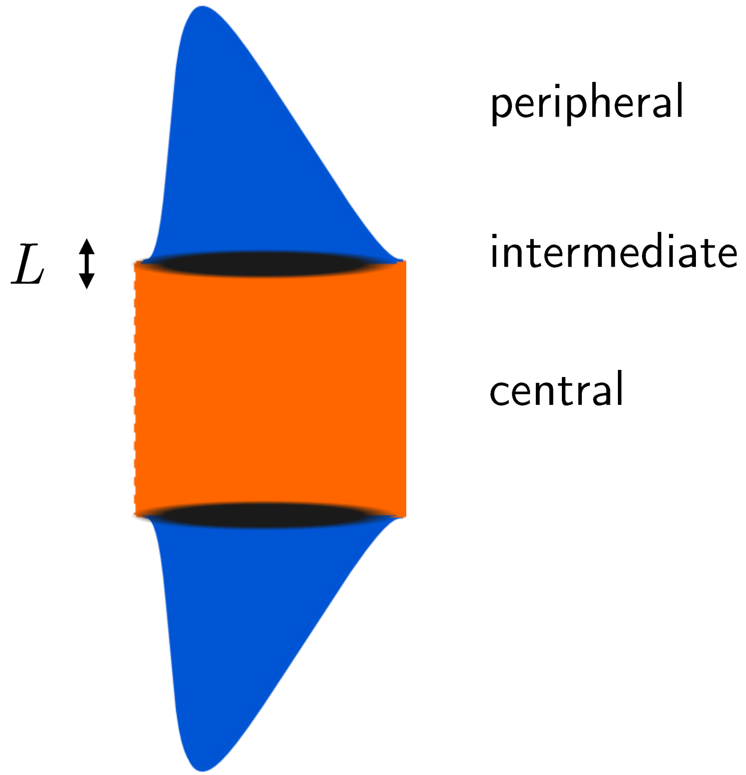


Effective diffusivity in the limit $L \to 0$

$\to$ Use matching asymptotics method!

Auxiliary field
$$f = \begin{cases} f_0^p(X,y) + L f_1^p(X,y) + \ldots & (|y| > a) \\ f_0^*(X,Y) + L f_1^*(X,Y) + \ldots & (|y| \sim a) \\ f_0^c(X,y) + L f_1^c(X,y) + \ldots & (|y| < a) \end{cases}$$

$$X = x/L \qquad Y = (y-a)/L$$



Effective diffusivity in the limit $L \to 0$

$\to$ Use matching asymptotics method!

$$\text{Flow} \qquad \mathbf{u} \underset{L \to 0}{\simeq} \begin{cases} 0 & (|y| > a) \\ L\ \mathbf{u}^*(X, Y) + \ldots & (|y| \sim a) \\ \mathbf{u}_0(X, y) + L\mathbf{u}_1(X, y) + \ldots & (|y| < a) \end{cases}$$

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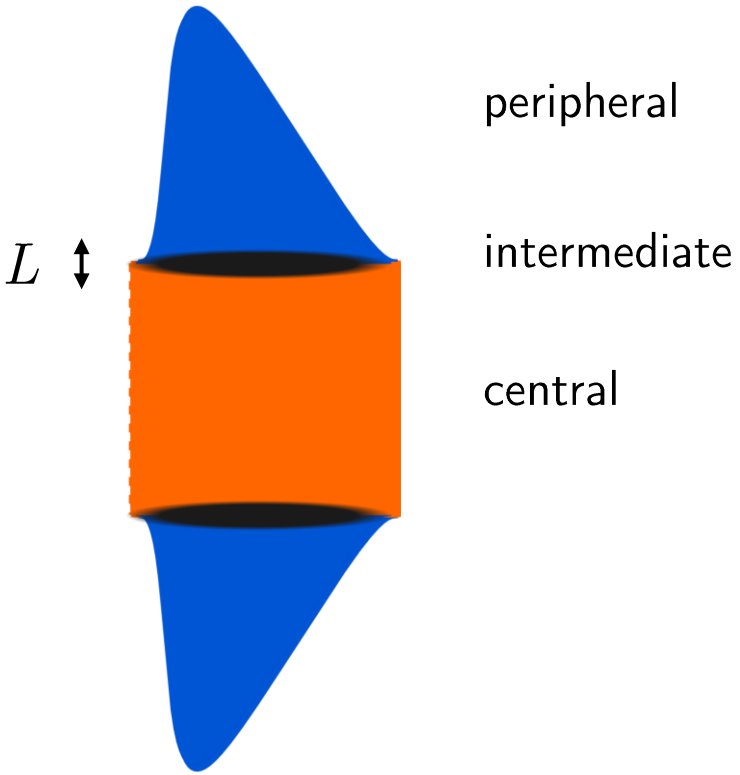
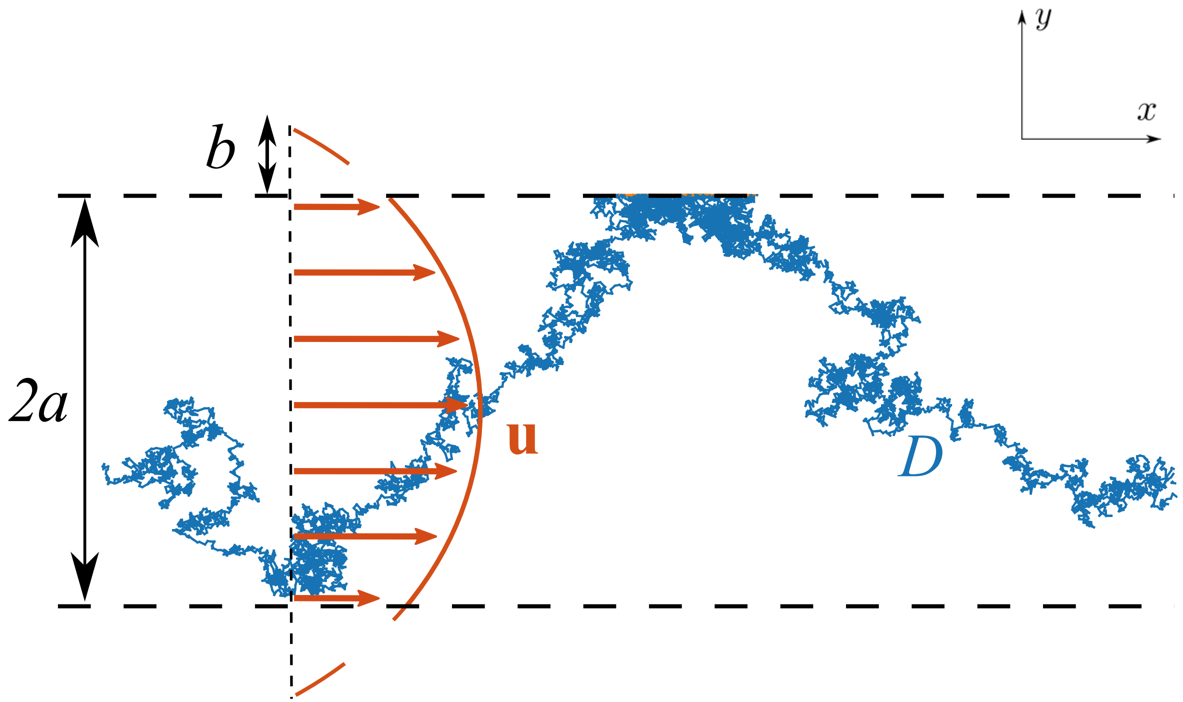


Effective diffusivity in the limit $L \to 0$

Flow in the central region $\mathbf{u} = \mathbf{u}_0 + u_s \mathbf{e}_x$

Leading order $\mathbf{u}_0 = U\left(1 - \frac{y^2}{a^2}\right)\mathbf{e}_x$

First order correction $u_s = UL\beta/a$

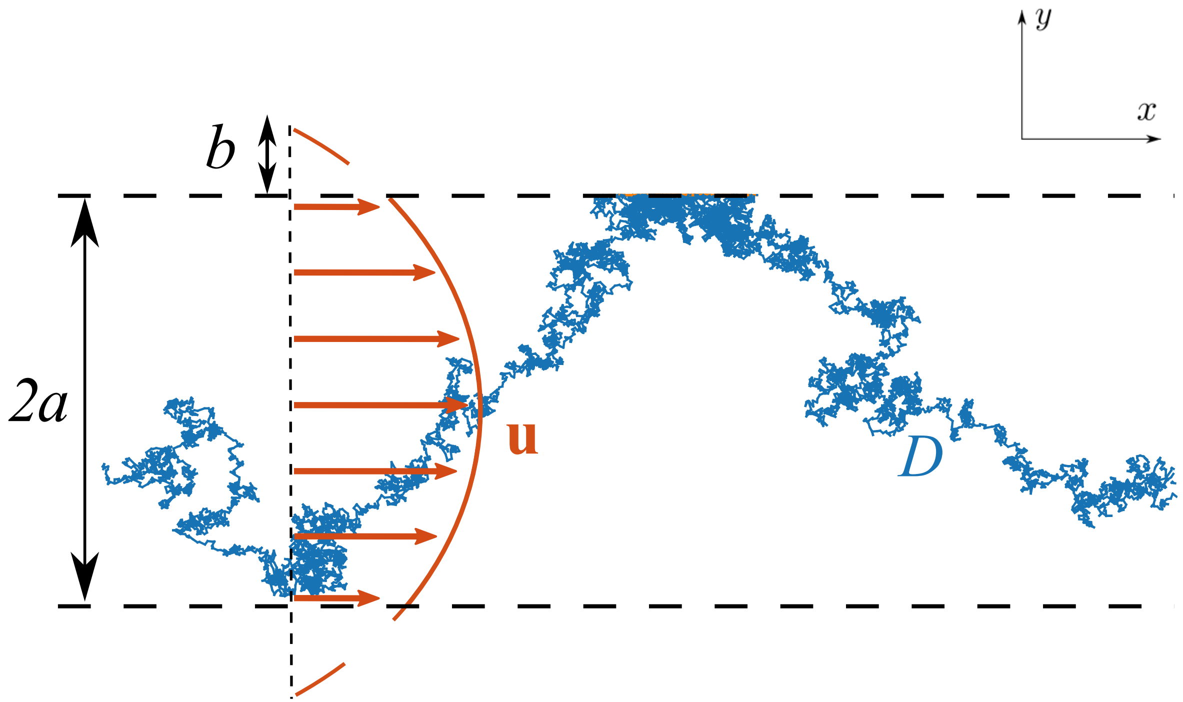


$$U = -\frac{a^2(\nabla\Pi)_\infty}{2\eta}$$

$$\beta \simeq 0.1772$$

[Luchini, J. Fluid. Mech., 1991;
Jeong, Phys. Fluids, 2001]

Effective diffusivity in the limit $L \to 0$



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→ Effective slip length

$$b = \frac{u_s}{|\partial_y u_x|_{y=a}} = \frac{\beta L}{2}$$

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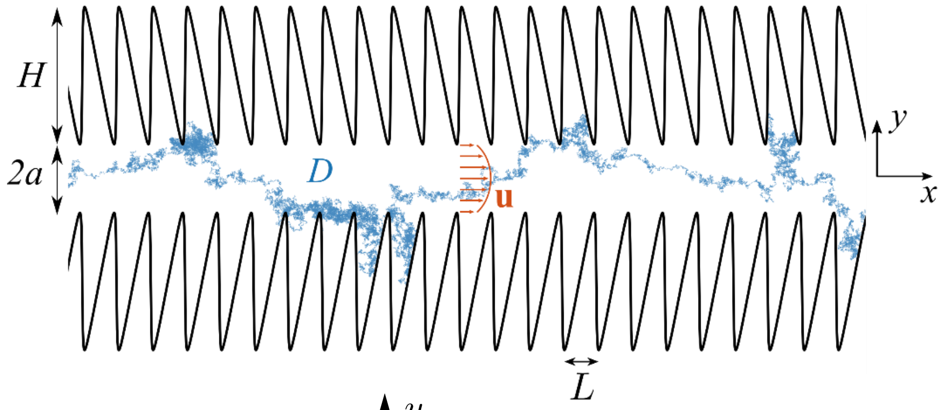
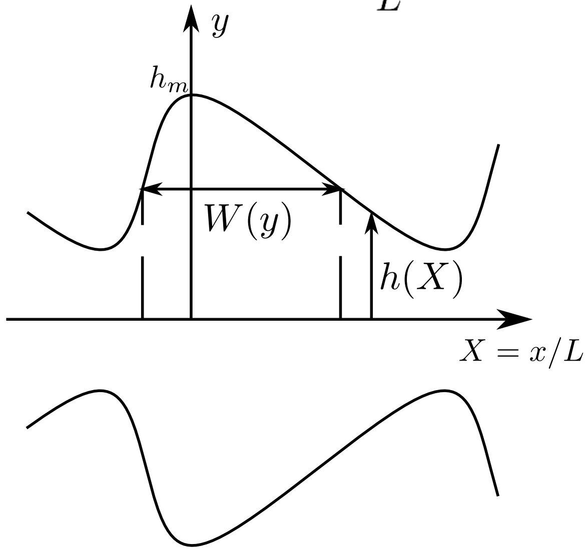
Effective diffusivity in the limit $L \to 0$

Highly corrugated channel with reflecting boundaries



$$D_e = \frac{Da + DL(\ln 2)/\pi}{a+\delta} + \frac{4U^2a^2}{9D(a+\delta)^3}\left\{\frac{17a\delta^2}{35} + \frac{6a^2\delta}{35} + \frac{2a^3}{105} + \tau D\delta\right\} + \frac{4a^2Uu_s}{45D(a+\delta)^3}\left\{6a\delta^2 + a^2\delta + 15D\tau\delta\right\}$$



$$\delta = \langle h - a \rangle$$

$$\tau = \int_a^{h_m} \frac{dy}{\delta D W(y)}\left[\int_y^{h_m} dy' W(y')\right]^2$$

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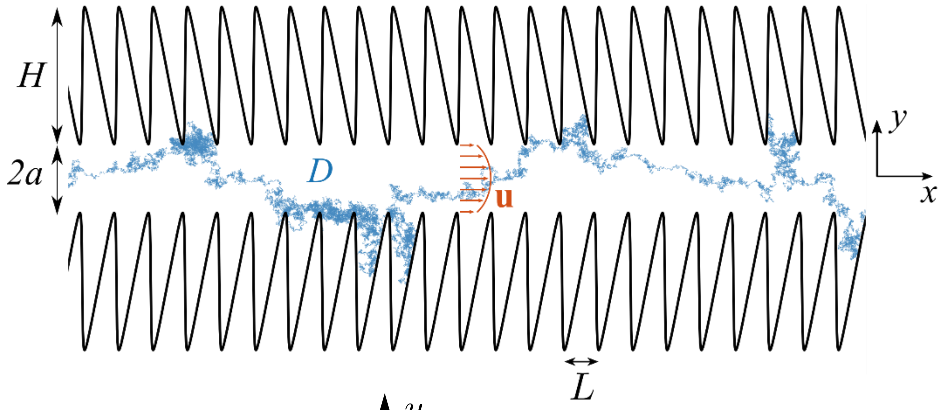

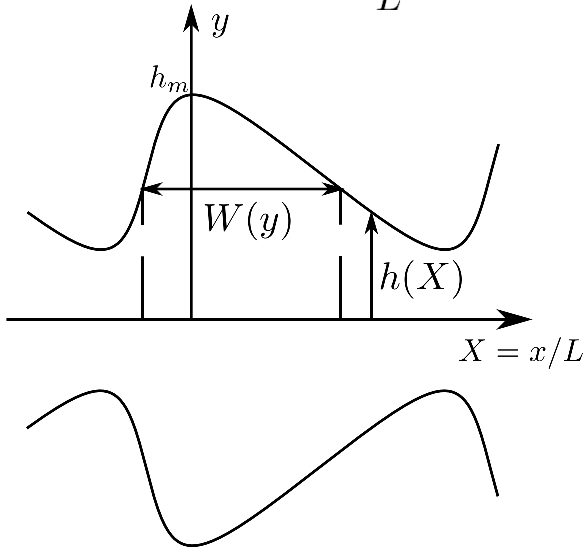

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[Mangeat et al., EPL, 2017]

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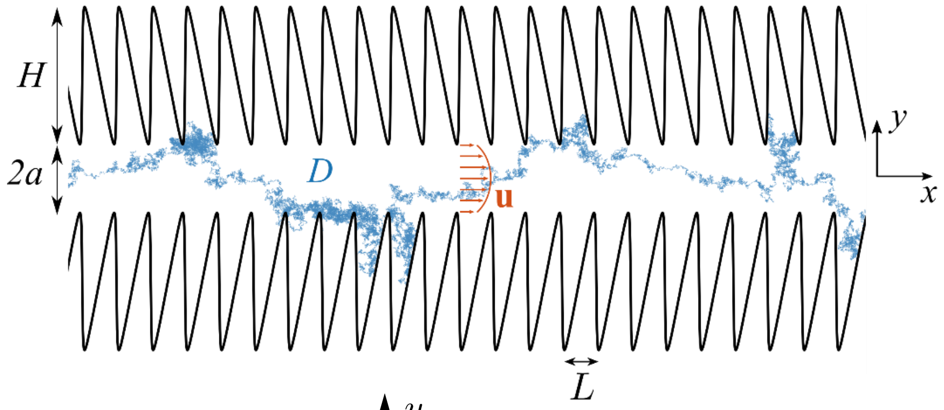

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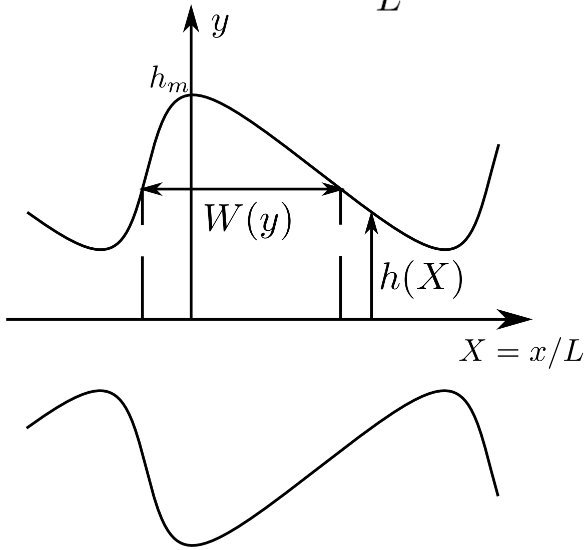

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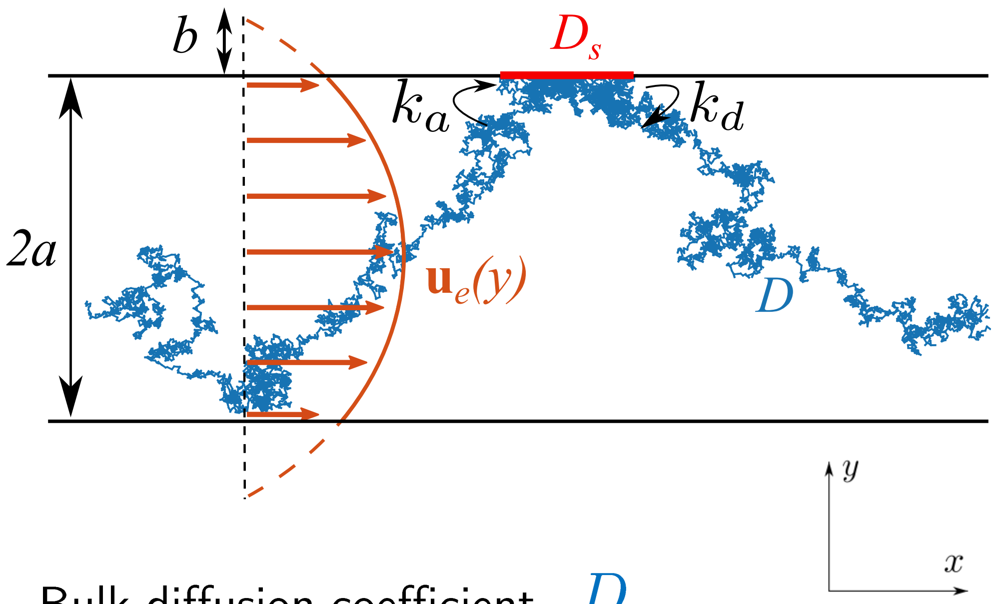
Analogy with surface-mediated diffusion

Flat channel with sticky boundaries



Bulk diffusion coefficient D

Surface diffusion coefficient D_s

Attachment rate k_a

Detachment rate k_d

Fokker–Planck equation

$$\partial_t p_b = -u_e(y)\partial_x p_b + D(\partial_x^2 + \partial_y^2)p_b \qquad (|y| < a)$$

$$\partial_t p_s = D_s \partial_x^2 p_s - k_d p_s + k_a p_b, \qquad (|y| = a)$$

Analogy with surface-mediated diffusion

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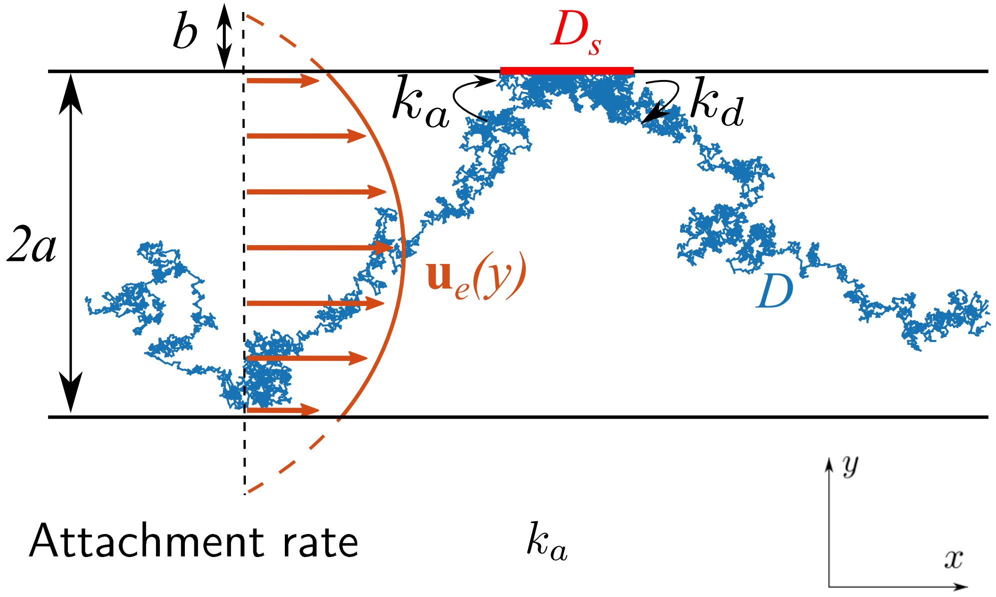

Attachment rate	k_a
Detachment rate	k_d
Adsorption length	$\delta = \frac{k_a}{k_d}$
Characteristic detachment time	$\tau = k_d^{-1}$

Fokker–Planck equation

$$\partial_t p_b = -u_e(y)\partial_x p_b + D(\partial_x^2 + \partial_y^2)p_b \qquad (|y| < a)$$
$$\partial_t p_s = D_s \partial_x^2 p_s - k_d p_s + k_a p_b, \qquad (|y| = a)$$

By taking $u_e(y) = U\left(1 - \frac{y^2}{a^2}\right) + u_s$

$$D_e = \frac{Da + D_s\delta}{a+\delta} + \frac{4U^2a^2}{9D(a+\delta)^3}\left\{\frac{17a\delta^2}{35} + \frac{6a^2\delta}{35} + \frac{2a^3}{105} + \tau D\delta\right\} + \frac{4a^2Uu_s}{45D(a+\delta)^3}\left\{6a\delta^2 + a^2\delta + 15D\tau\delta\right\}$$

[Levesque et al., PRE, 2012; Berezhkovskii, JCP, 2013]

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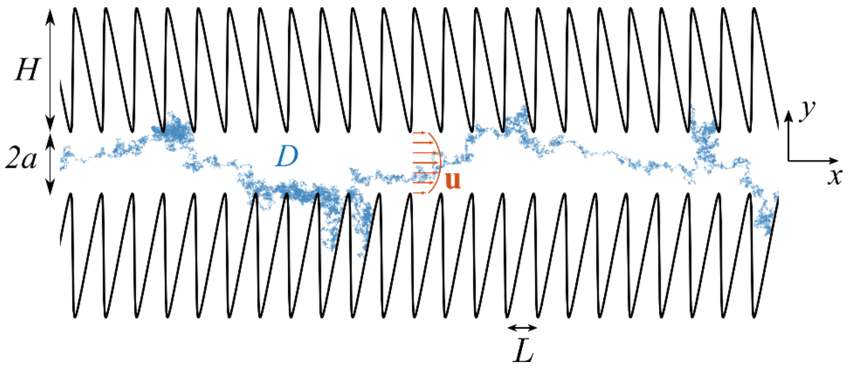
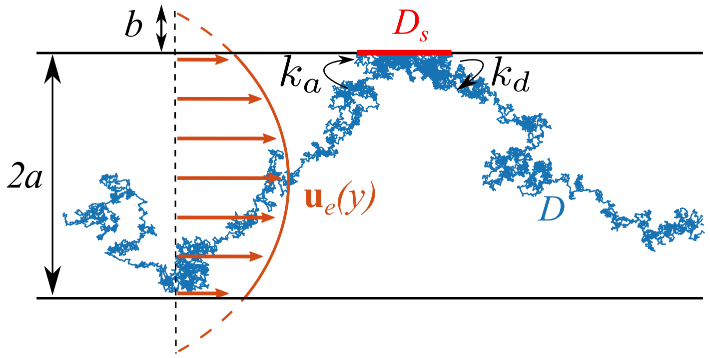


Flat channel with sticky boundaries

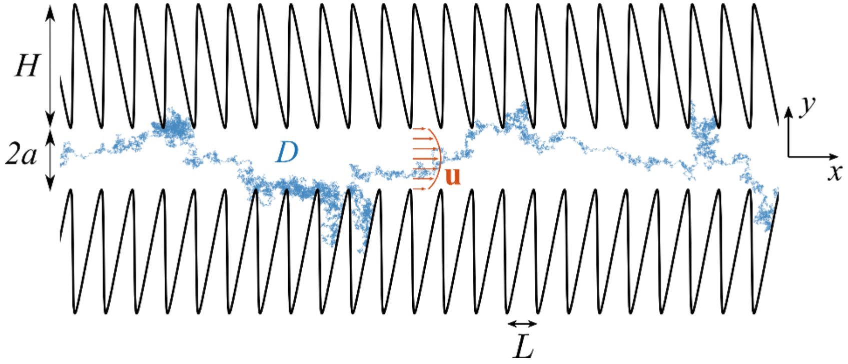


	Highly corrugated channel with reflecting boundaries	Flat channel with sticky boundaries
Adsorption length	$\delta = \langle h - a \rangle$	$\delta = \frac{k_a}{k_d}$
Mean escape time	$\tau = \int_a^{h_m} \frac{dy}{\delta D W(y)} \left[\int_y^{h_m} dy' W(y') \right]^2$	$\tau = k_d^{-1}$
Surface diffusion	$D_s = \frac{D L \ln 2}{\pi \delta}$	D_s

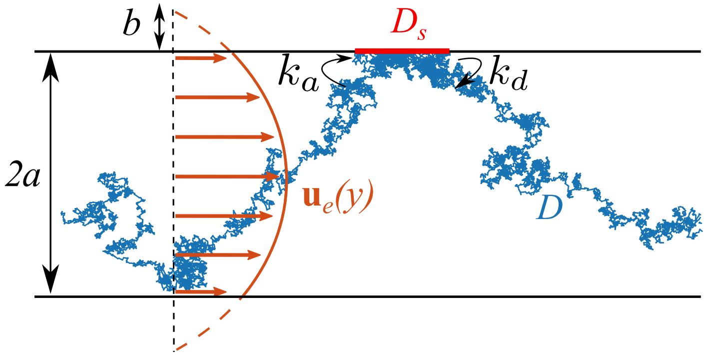
Analogy with surface-mediated diffusion

Highly corrugated channel with reflecting boundaries		Flat channel with sticky boundaries

Highly corrugated channel with reflecting boundaries



Flat channel with sticky boundaries



	Highly corrugated channel	Flat channel
Adsorption length	$\delta = \langle h - a \rangle$	$\delta = \frac{k_a}{k_d}$
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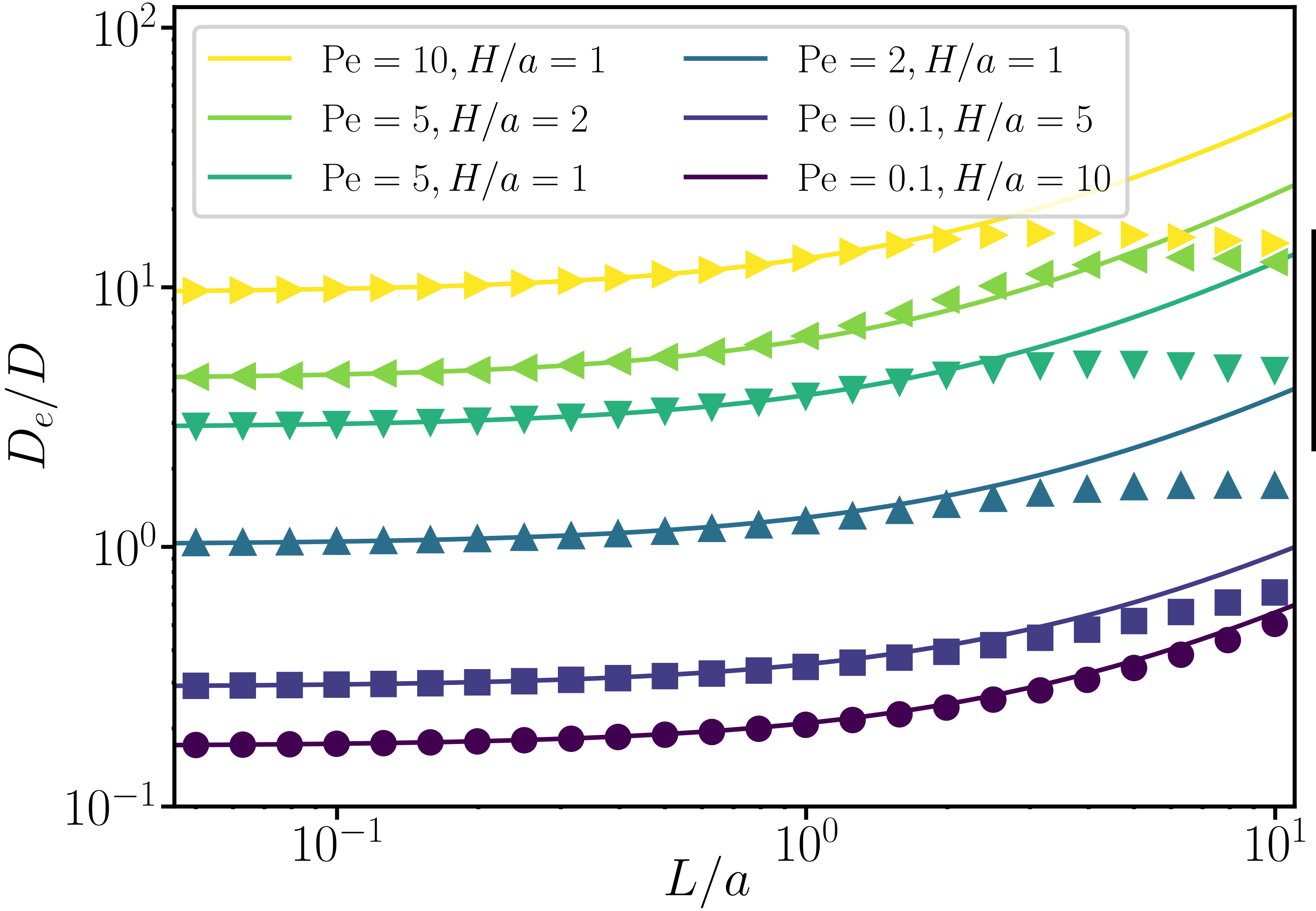
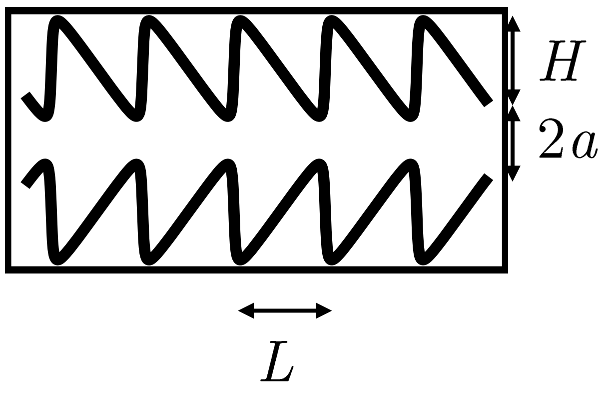
Surface diffusion	$D_s = \frac{DL \ln 2}{\pi \delta}$	D_s

→ Diffusive incursion length

$$\ell = L \ln 2 / \pi$$

Effective diffusivity in the limit $L \to 0$





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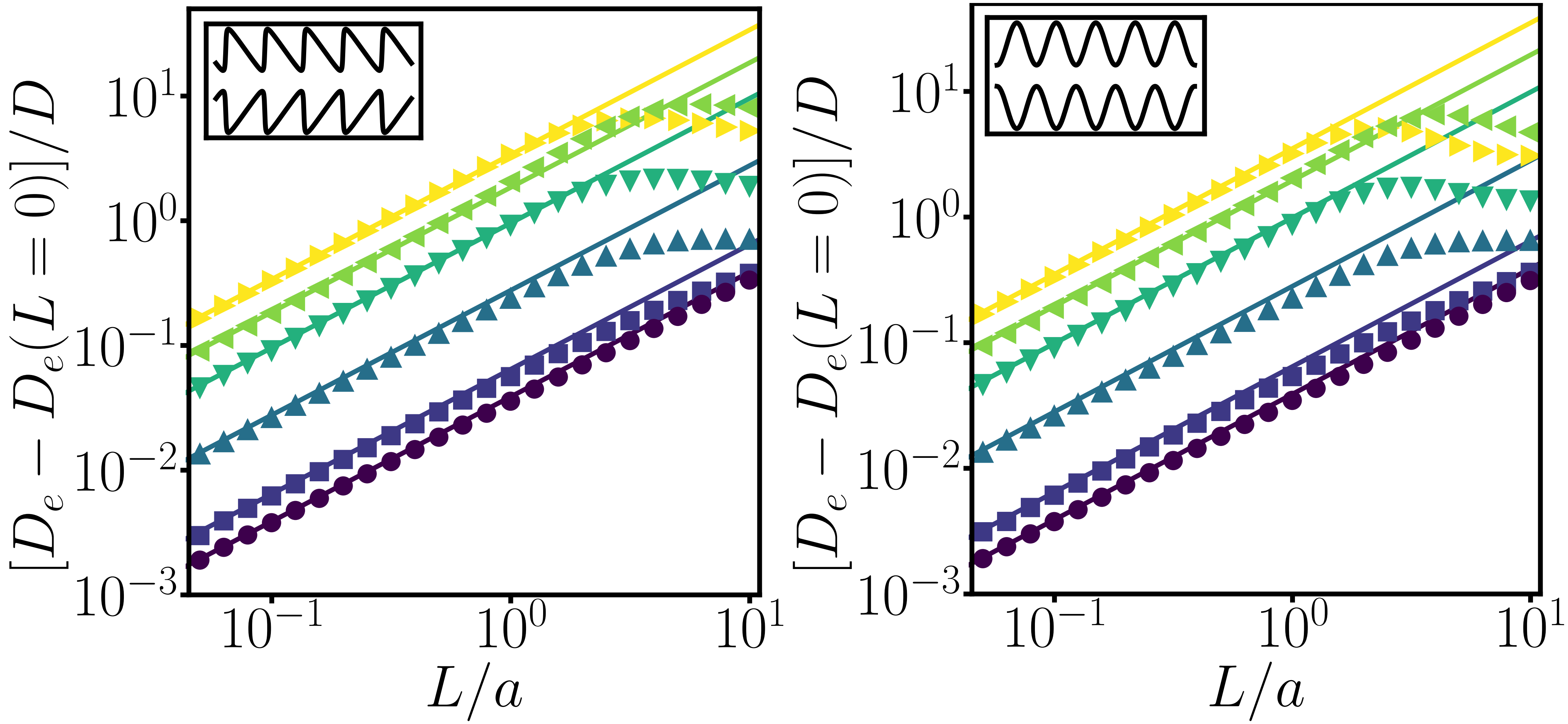

Conclusion

Effective description of **Taylor dispersion** in a corrugated channel in the limit $L \to 0$ using matching asymptotics technique

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Two phenomena near the entrance of protrusions:

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- diffusion along the channel axis is not completely suppressed

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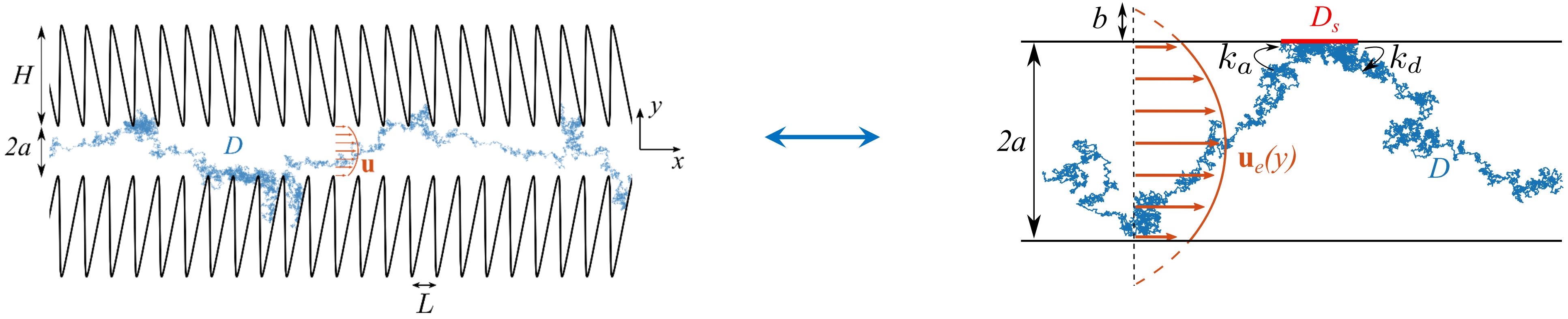
Mapping with a model of **surface-mediated diffusion** with flow, determination of effective attachment and detachment rates, and effective surface diffusion coefficient



Conclusion

Effective description of **Taylor dispersion** in a corrugated channel in the limit $L \to 0$ using matching asymptotics technique

[Alexandre, Guérin, & Dean (2025). Effective description of Taylor dispersion in strongly corrugated channels. *arXiv preprint arXiv:2502.07464*]

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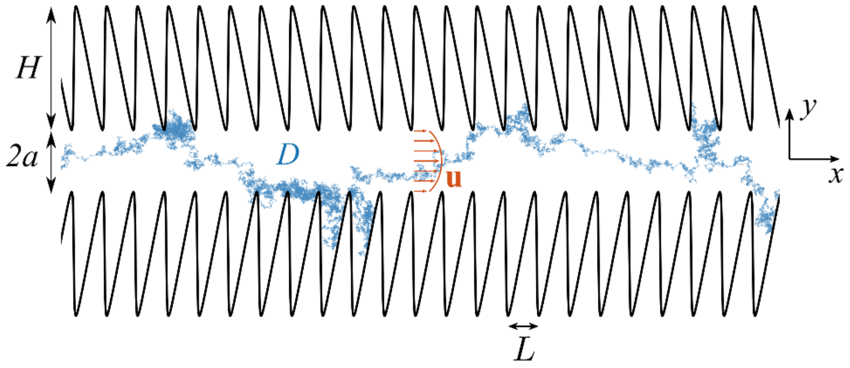

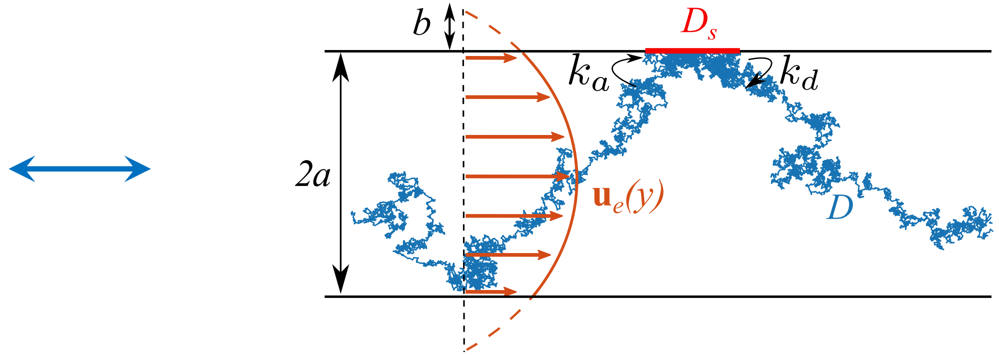

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Kubo formula

General expression
$$D_e = D - \int_0^\infty \mathrm{d}t \; \overline{[V_x(\mathbf{r}(t)) - \overline{V_x}][V_x^*(\mathbf{r}(0)) - \overline{V_x^*}]}$$

$$\mathbf{V} = \mathbf{u} + D\,\mathbf{n}\,\delta_s(\mathbf{r})$$

$$\mathbf{V}^* = -\mathbf{u}(\mathbf{r}) + D\,\delta_s(\mathbf{r})\,\mathbf{n}$$

Auxiliary function
$$f(\mathbf{r}) = -\int_0^\infty \mathrm{d}t \int_\Omega \mathrm{d}\mathbf{r}_0 \; P(\mathbf{r}, t|\mathbf{r}_0)[V_x^*(\mathbf{r}_0) - \overline{V_x^*}]$$

$$\Rightarrow \qquad D_e = D + \frac{1}{\Omega}\int_\Omega \mathrm{d}\mathbf{r} \; (u_x f - D\partial_x f)$$