The impact of elongation on transport in shear flow

March 2022
ICTS: Complex Lagrangian Problems of Particles in Flows

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Outline

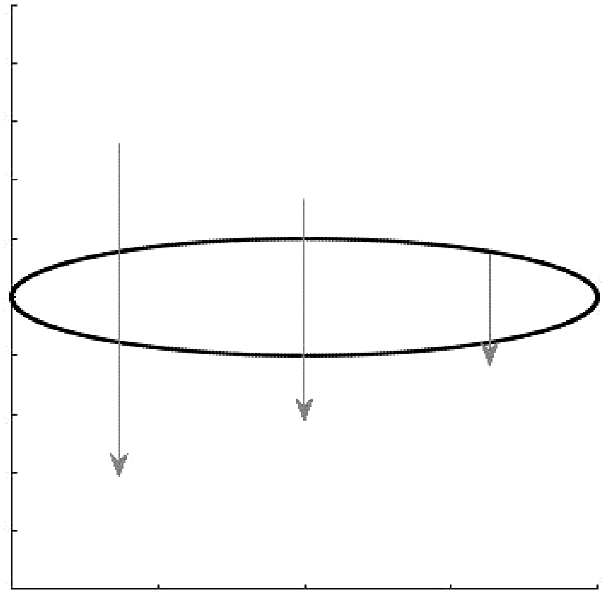
- Elongation enhances migration through hydrodynamic shear

Lovecchio, Climent, Stocker & Durham 2019
Bearon & Durham, *submitted to Phys Rev Fluids*

- Trapping of slender chemotactic bacteria in high shear

Bearon & Hazel, J Fluid Mech 2015
Fung, Bearon & Hwang, J Fluid Mech 2022
Maretvadakethope, Vasiev, Hazel & Bearon, in Prep for Phys Rev Fluids

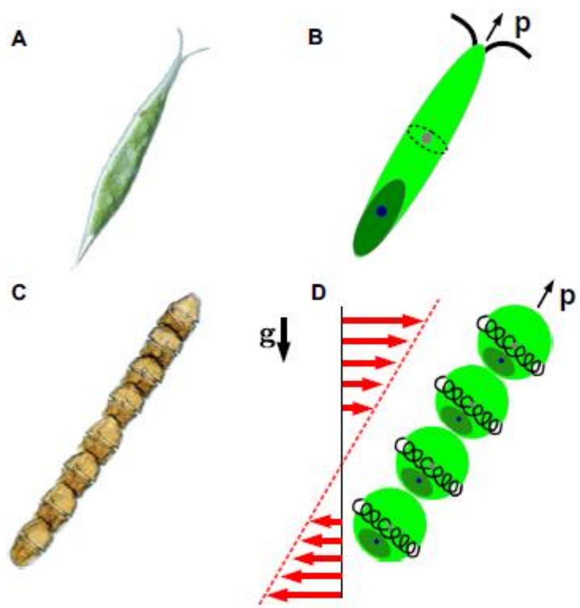
Jeffery orbits



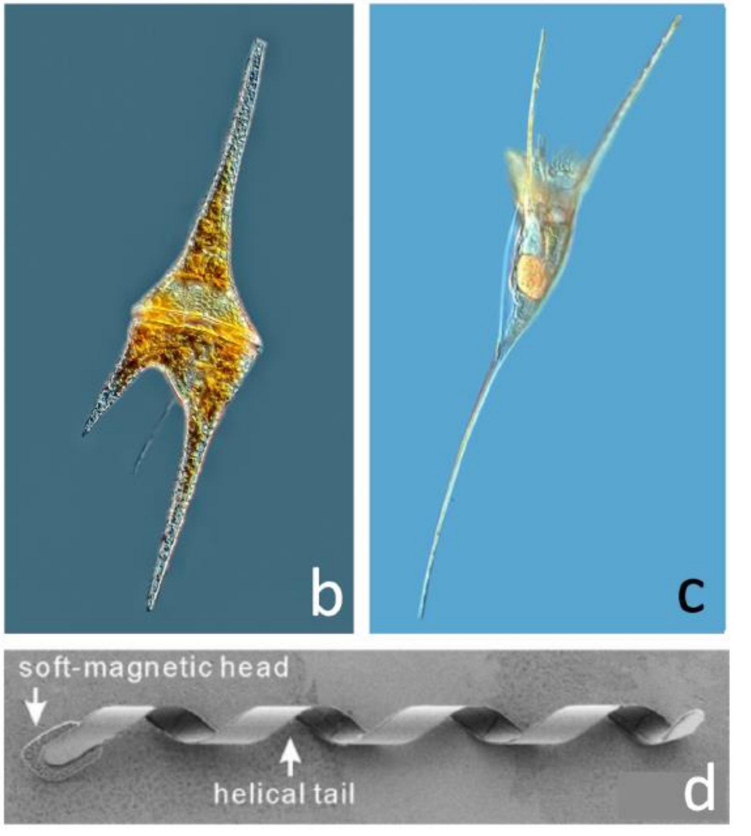
Alignment with flow

$$\frac{d\mathbf{p}}{dt} = \frac{1}{2}\boldsymbol{\omega} \times \mathbf{p} + \alpha(\mathbf{I} - \mathbf{pp}) \cdot \mathbf{E} \cdot \mathbf{p}.$$

How does elongation affect gyrotactic phytoplankton in turbulence?



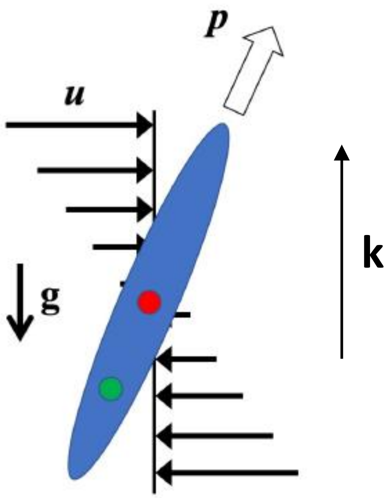
Lovecchio, Climent, Stocker & Durham 2019



Governing equations

$$\frac{d\mathbf{x}}{dt} = \Phi\mathbf{p} + \mathbf{u}$$

$$\frac{d\mathbf{p}}{dt} = \frac{1}{2\Psi}[\mathbf{k} - (\mathbf{k}\cdot\mathbf{p})\mathbf{p}] + \frac{1}{2}\boldsymbol{\omega}\times\mathbf{p} + \alpha(\mathbf{I} - \mathbf{pp})\cdot\mathbf{E}\cdot\mathbf{p}.$$

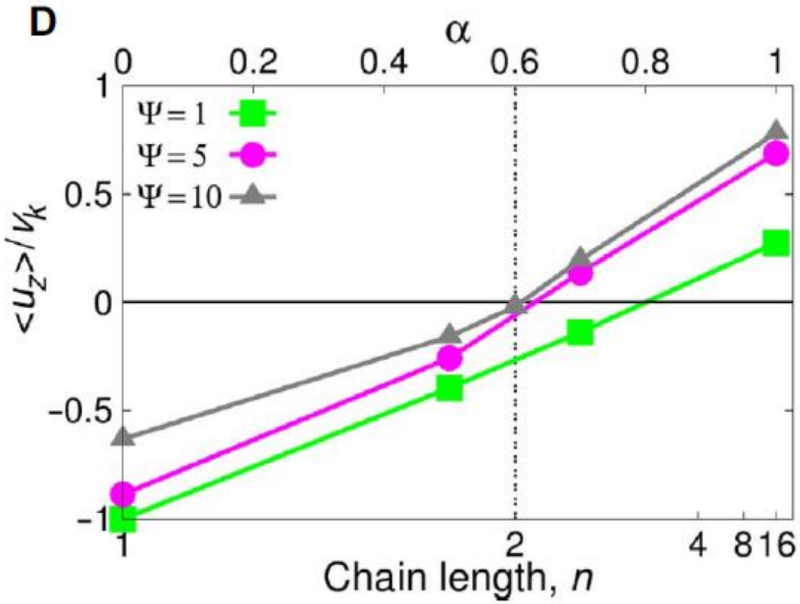


Φ Swimming speed

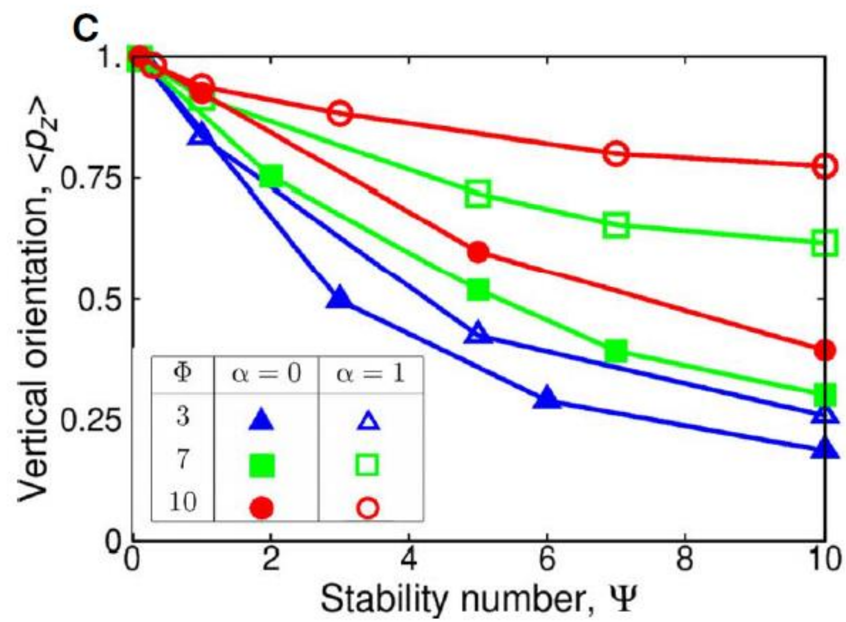
Ψ Stability number

Numerical simulations in DNS

Lovecchio, Climent, Stocker & Durham 2019



Slender cells spend more time in up-welling flow



Slender cells swim up more rapidly

Equilibria in simple shear

Pedley & Kessler (1987)

For flow in x-z plane, $\boldsymbol{\omega} = \omega \mathbf{j}$ $\sigma = \omega \Psi$

$$\mathbf{p} = (p_x, p_y, p_z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

There exists a single stable equilibrium with $\phi = 0, \cos\theta > 0$

Horizontal shear $\mathbf{u} = z\mathbf{i}$

$$\sin\theta = \frac{-1 + \sqrt{1 + 8\sigma^2\alpha(1+\alpha)}}{4\alpha\sigma} \qquad \sigma < (1-\alpha)^{-1}$$

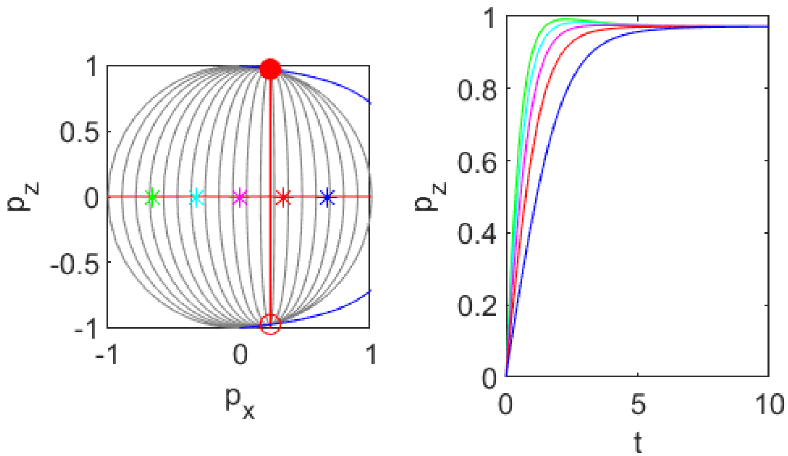
Vertical shear $\mathbf{u} = -x\mathbf{k}$

$$\sin\theta = \frac{1 - \sqrt{1 - 8\sigma^2\alpha(1-\alpha)}}{4\alpha\sigma}$$

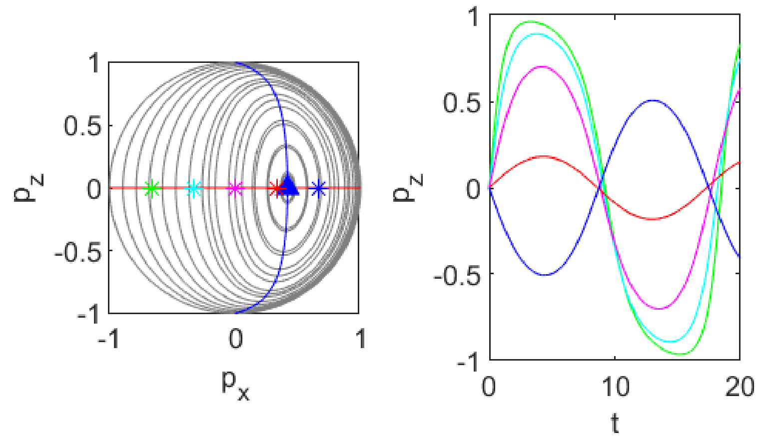
$$\sigma < (1+\alpha)^{-1} \quad \text{for} \quad \alpha < 1/3, \quad \text{and} \quad \sigma < (8\alpha(1-\alpha))^{-1/2} \quad \text{for} \quad \alpha > 1/3$$

At low shear, cells tend to equilibrium, and at high shear they tumble

Vertical shear $\alpha = 0.6$



σ = 0.5

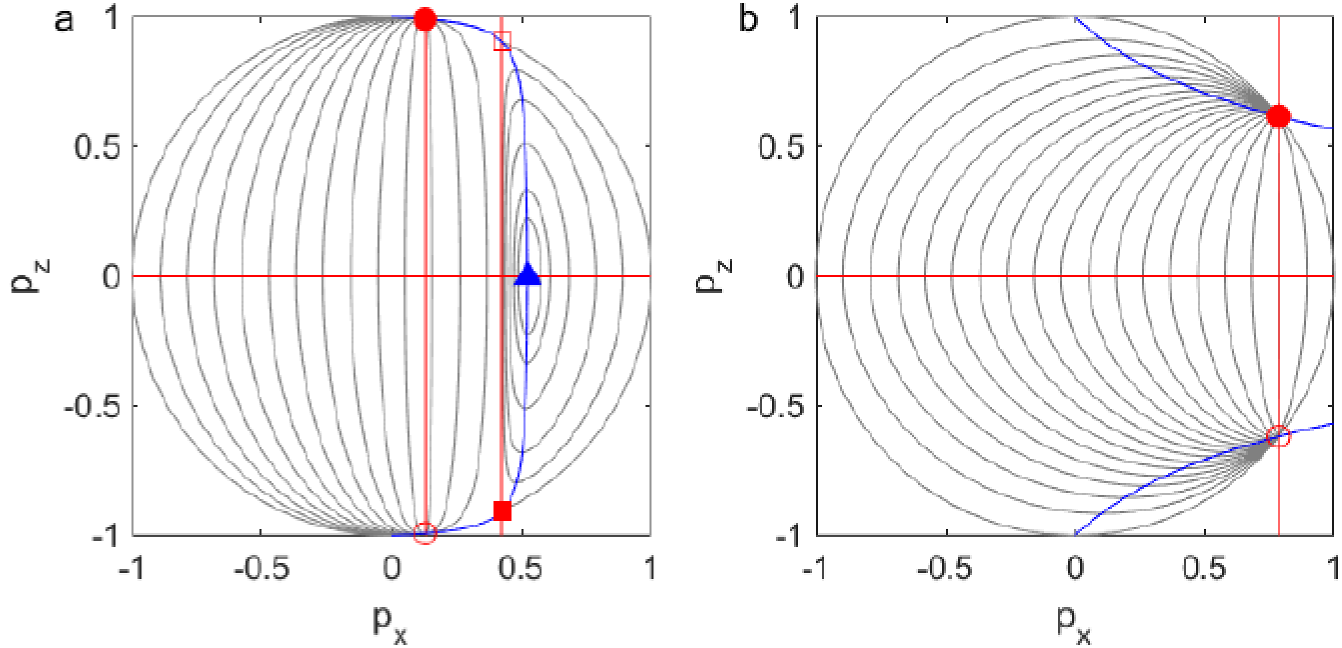


σ = 1.5

$$\dot{p}_z = 0$$

$$\dot{p}_x = 0$$

Equilibrium not necessarily globally attracting



$$\dot{p}_z = 0$$

$$\dot{p}_x = 0$$

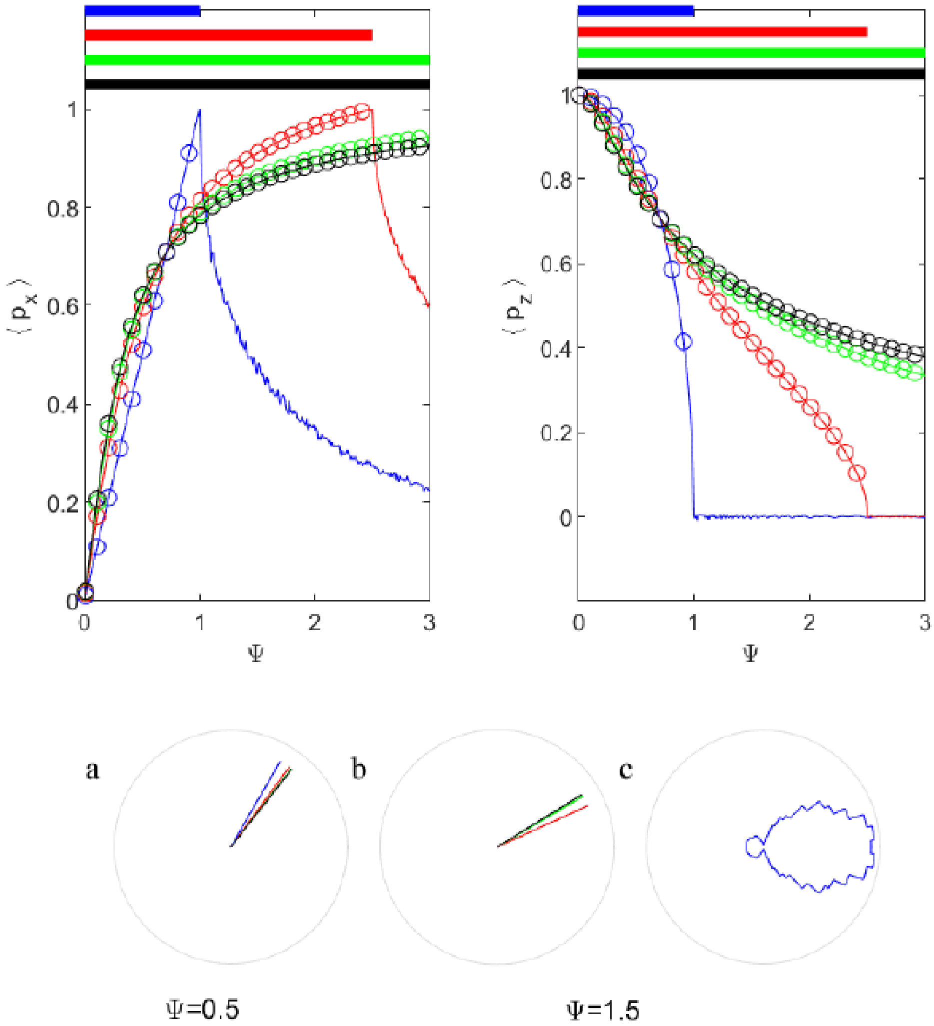
$$\mathbf{u} = -x\mathbf{k} \qquad \mathbf{u} = z\mathbf{i}$$

$\alpha = 0.9$ and $\Psi = 0.7$.

See also Almog & Frankel (1995)

Orientation in horizontal shear

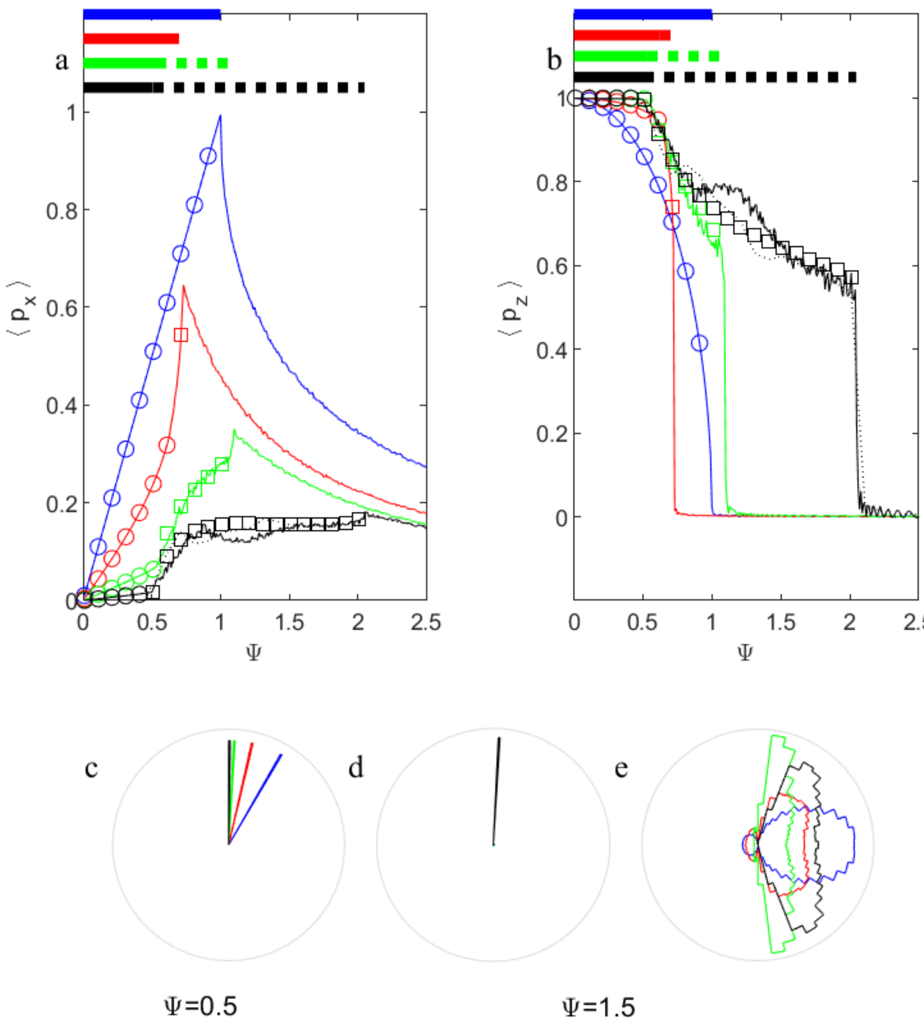
$$\mathbf{u} = z\mathbf{i}$$



n=1 ($\alpha = 0$), blue; n=2 ($\alpha = 0.6$), red; n=4 ($\alpha = 0.8824$), green; n=8 ($\alpha = 0.9692$), black

Orientation in vertical shear

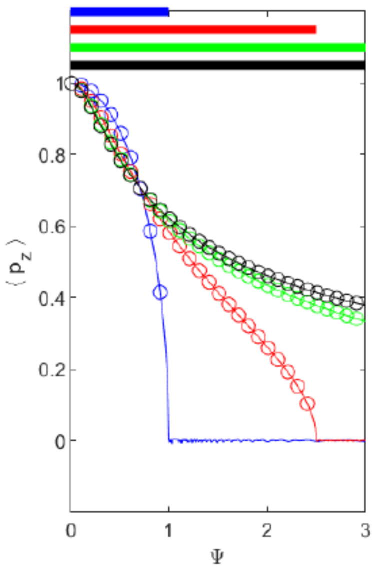
$$\mathbf{u} = -x\mathbf{k}$$



Transport in simple shear

Horizontal shear $\mathbf{u} = z\mathbf{i}$

$$\langle \frac{dz}{dt} \rangle = \Phi \langle p_z \rangle$$

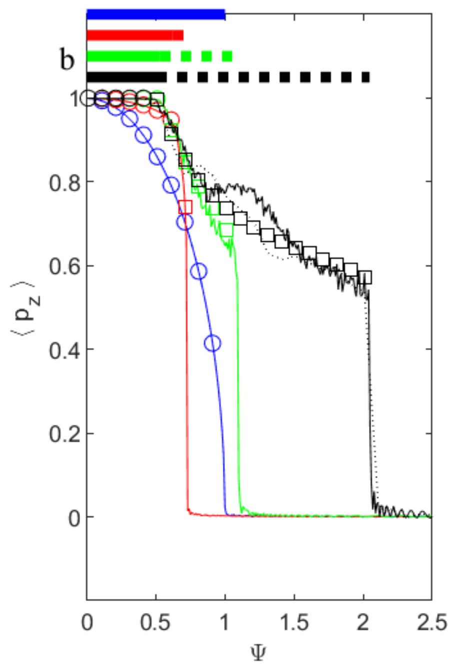


- Elongation generally improves up-swimming (increase p_z)

Transport in simple shear

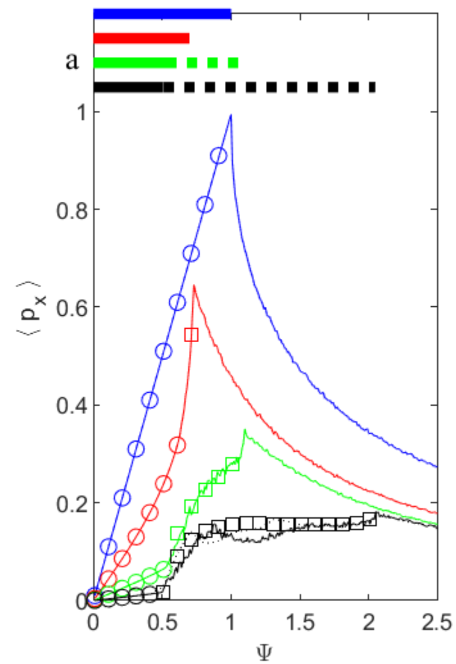
Vertical shear $\mathbf{u} = -x\mathbf{k}$

$$\langle \frac{dz}{dt} \rangle = \Phi \langle p_z \rangle + \langle u_z \rangle$$



tarting from origin, with
quilibrium orientation

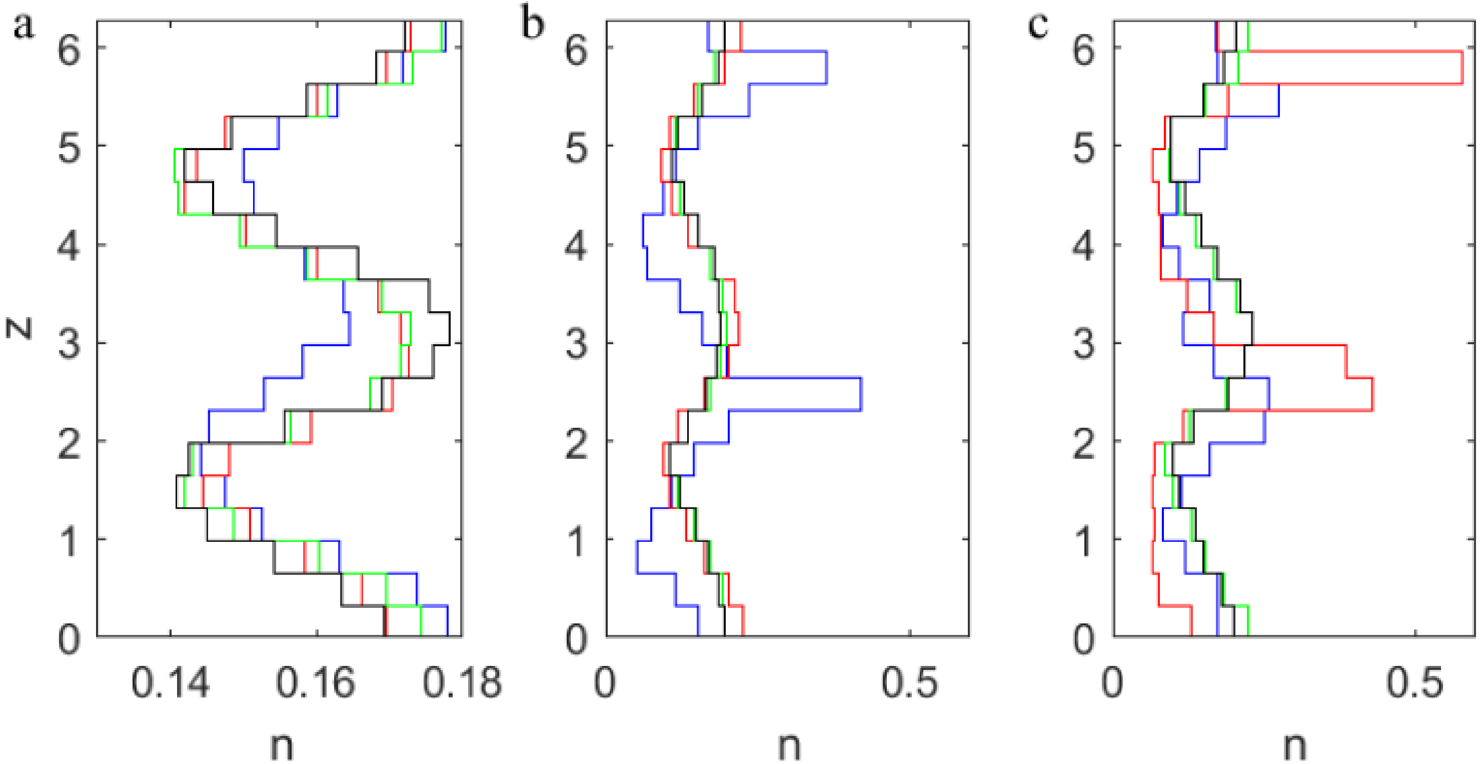
$$u_z = -\Phi p_x t$$



- Elongation generally improves up-swimming (increase p_z)
- Elongation may supress migration into down-welling flow (decrease p_x)

Vertical distribution in Kolmogorov flow

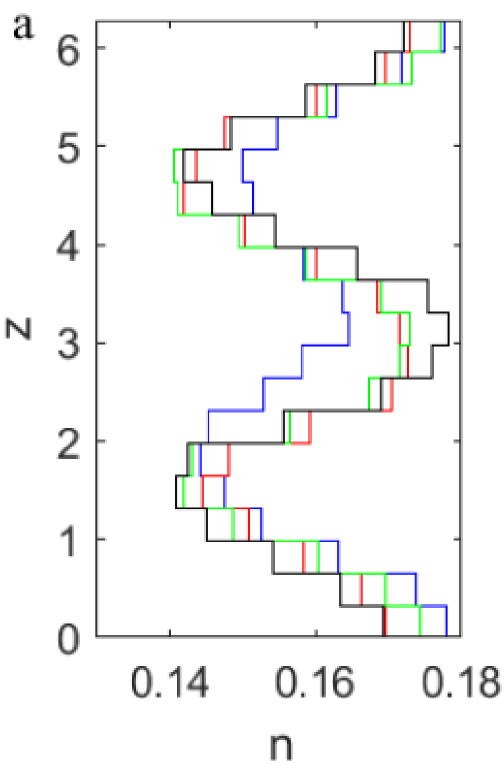
$$\mathbf{u} = \sin(z)\mathbf{i}$$

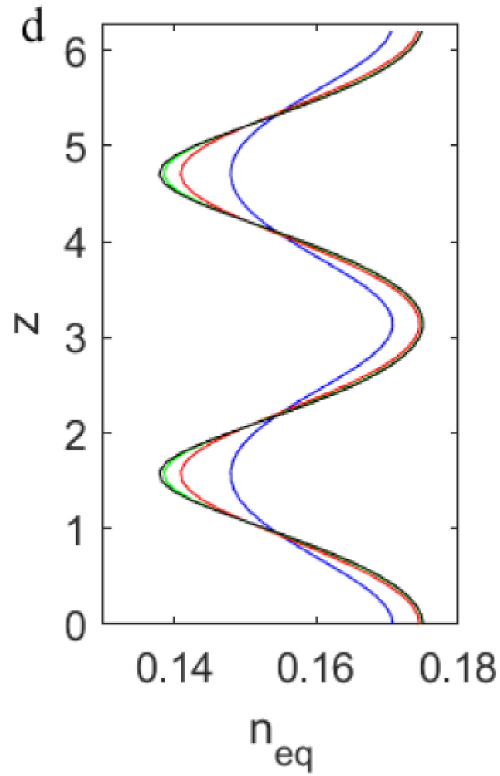


Ψ = 0.5 Ψ = 1.5 Ψ = 3

$\Phi = 0.1$

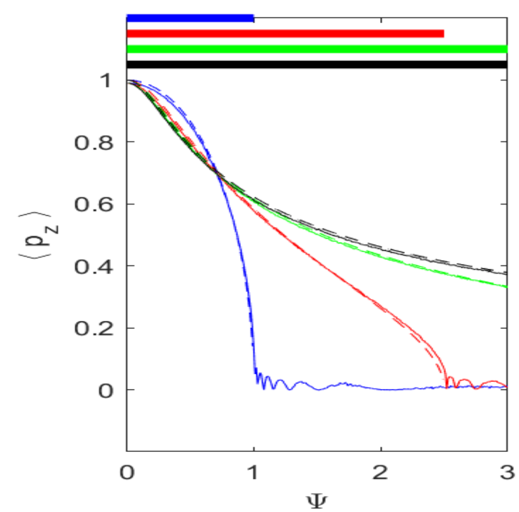
I: Peak due to variation in vertical swimming





$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial z}(\Phi p_z n)$$

$$n_{eq} \propto 1/p_z$$



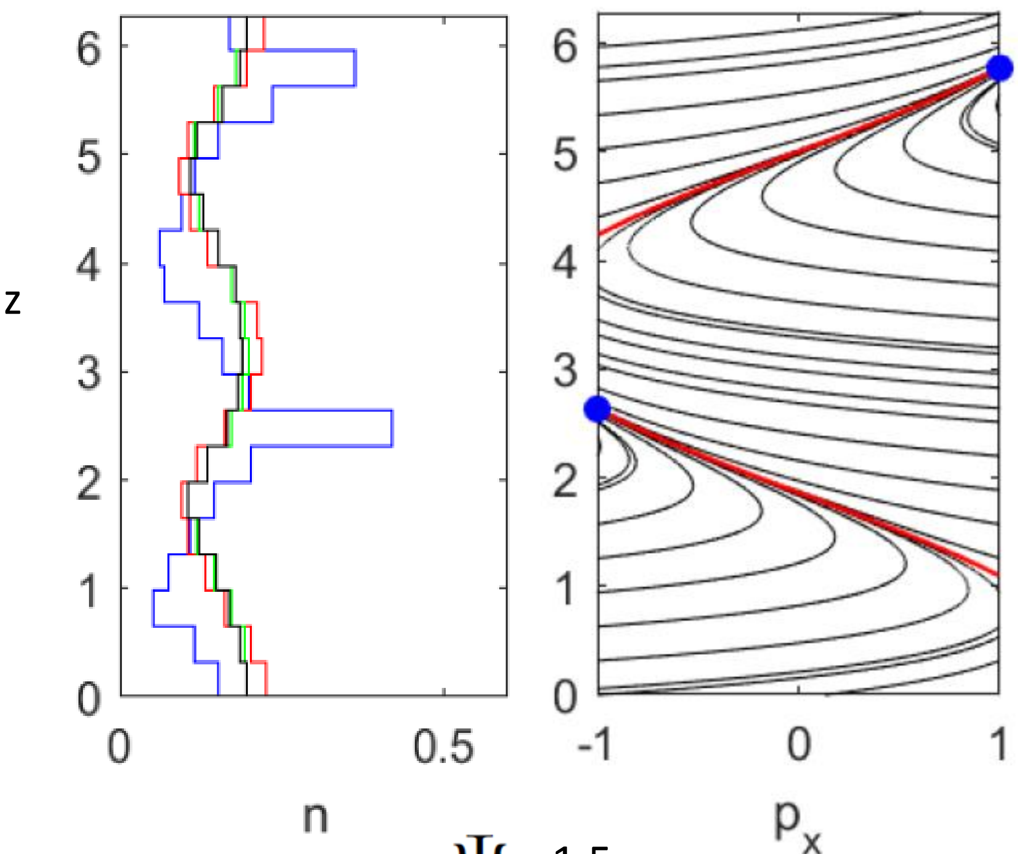
Ψ = 0.5

II: Peak due to tumbling

$\alpha = 0$

$$H(p_x, z) = \Phi \exp(\frac{z}{2\Psi\Phi}) \left(p_x - \frac{\Psi}{1 + 4\Psi^2\Phi^2}(\cos z + 2\Psi\Phi \sin z) \right)$$

Santamaria et al 2014

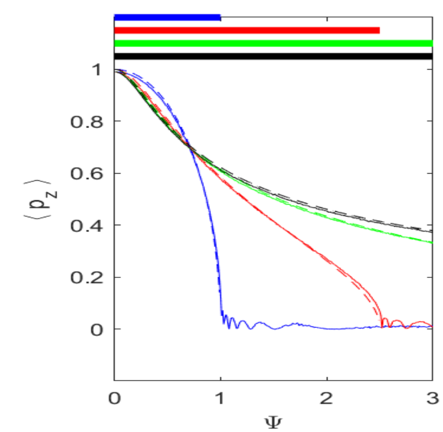


Ψ = 1.5

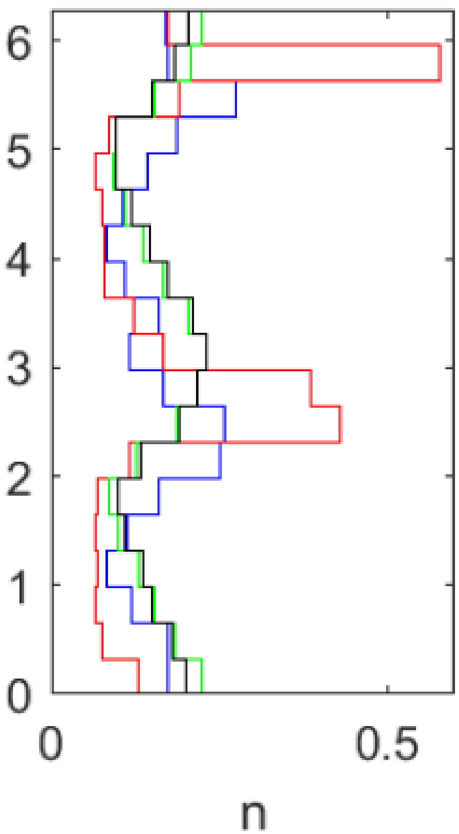
$$p_x = \frac{\Psi}{1 + 4\Psi^2\Phi^2}(\cos z + 2\Psi\Phi \sin z)$$

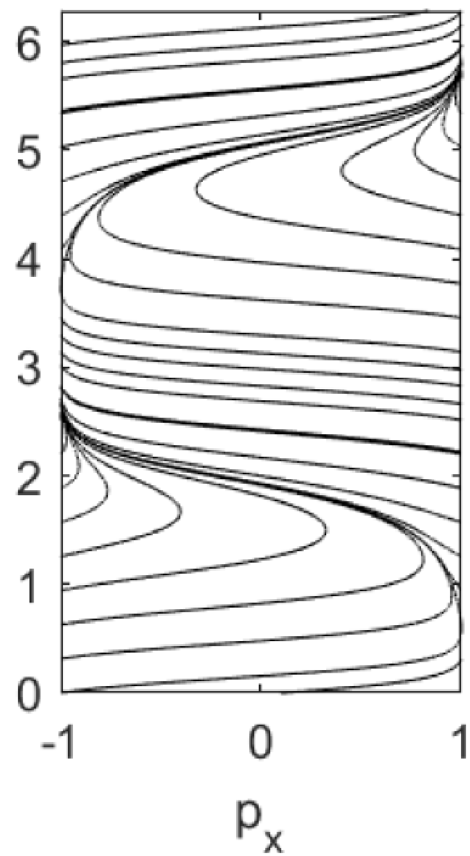
$$p_x = \pm 1$$

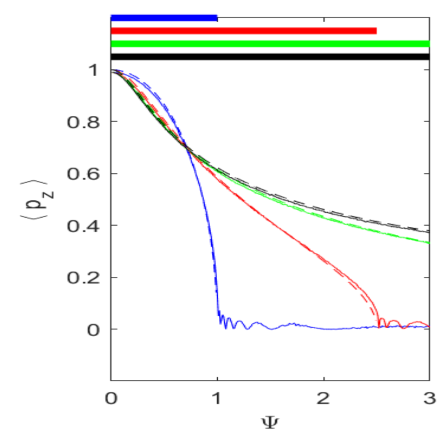
$$z = \arcsin(\frac{\sqrt{1 + 4\Psi^2\Phi^2}}{\Psi}) - \arctan(\frac{1}{2\Psi\Phi})$$



II: Peak due to tumbling dependent on shear & elongation







n=2 $(\alpha = 0.6)$, red

Ψ = 3

Summary Part I

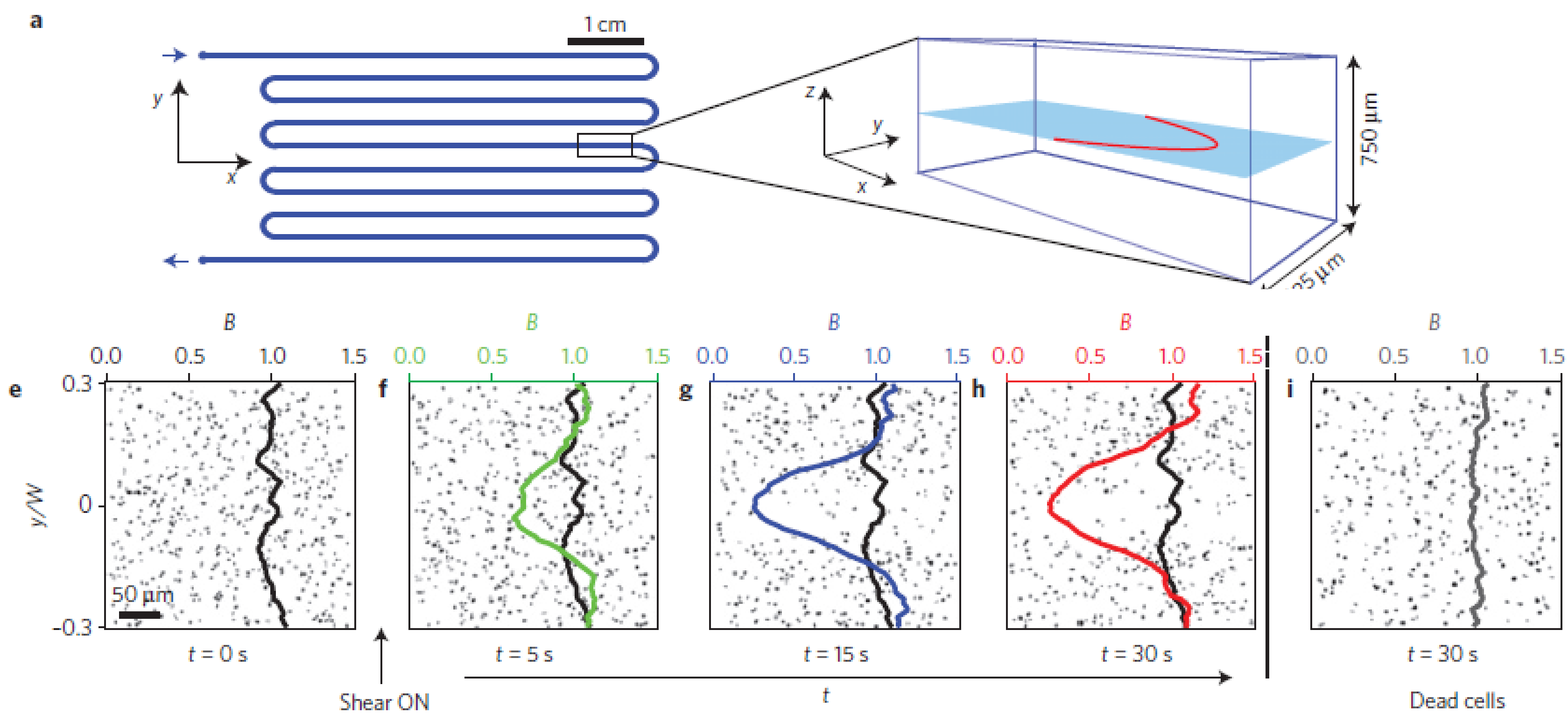
- Many active swimmers are non-spherical
- Elongation generally improves up-swimming (increase p_z)
- Elongation may supress migration into down-welling flow (decrease p_x)
- Shape-dependent horizontal layers can form due to vertical variation in swimming speed & tumbling.

- Note stability ψ & swimming speed Φ also vary with shape ….

LETTERS
PUBLISHED ONLINE: 23 FEBRUARY 2014 | DOI: 10.1038/NPHYS2883
nature physics

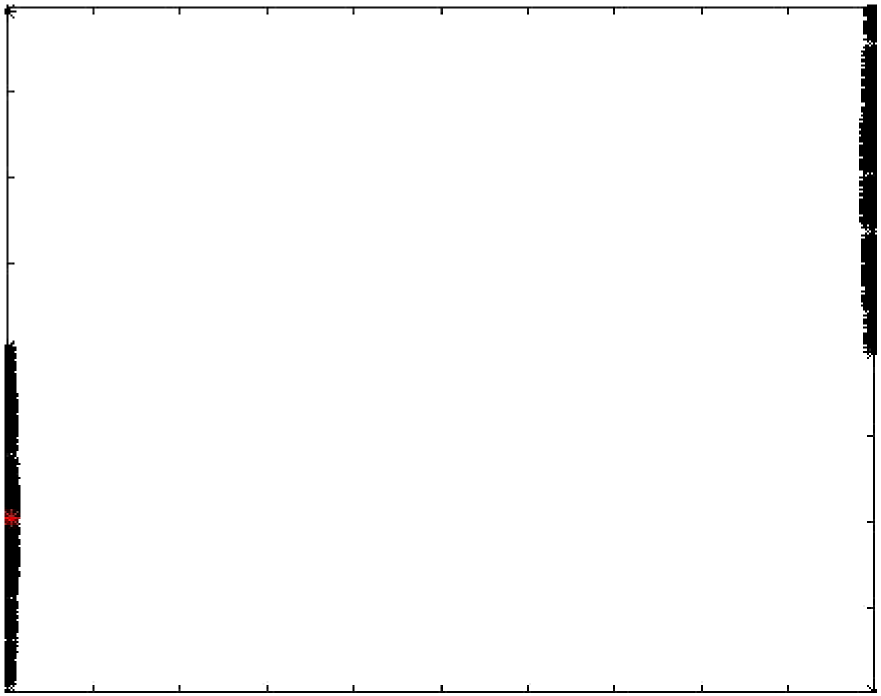
Bacterial transport suppressed by fluid shear

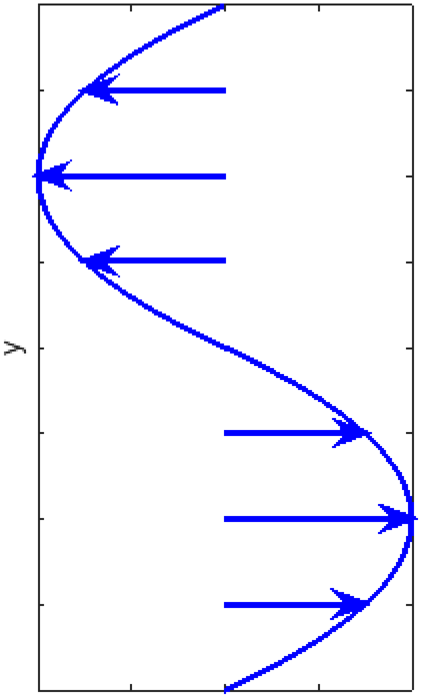
Roberto Rusconi[1], Jeffrey S. Guasto[2] and Roman Stocker[1]*

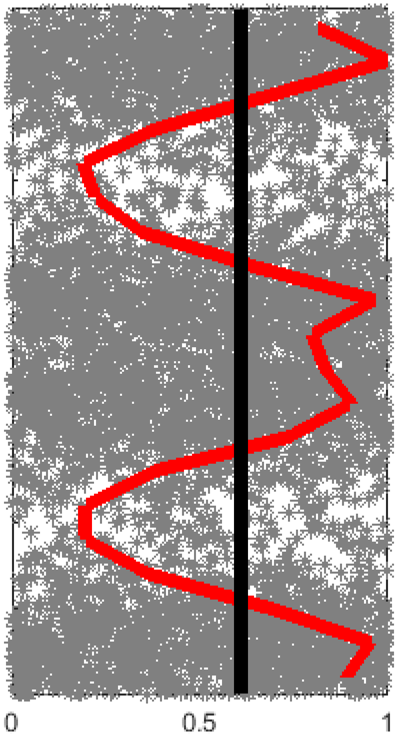


Trapping in high shear is not boundary accumulation

Illustrative IBM simulation of random walk of ellipsoids in periodic Poiseuille flow







Red line: histogram of cell position in shear

$\psi(x,p,t)$: Probability of cell having position *x*, orientation *p* at time *t*

$$\frac{\partial \psi}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\dot{\boldsymbol{x}}\psi) + \nabla_{\boldsymbol{p}} \cdot (\dot{\boldsymbol{p}}\psi)$$
$$+\lambda(\boldsymbol{x},\boldsymbol{p},t)\psi - \int_{\Omega} \lambda(\boldsymbol{x},\boldsymbol{p}',t)K(\boldsymbol{p},\boldsymbol{p}')\psi(\boldsymbol{x},\boldsymbol{p}',t)d\boldsymbol{p}' = 0$$

$$\dot{\boldsymbol{x}} = \boldsymbol{u} + V_s\boldsymbol{p} - D\nabla_{\boldsymbol{x}} \ln \psi$$

swimming velocity, $V_s\mathbf{p}$
fluid velocity, $\mathbf{u}$
translational Brownian diffusion, D

$$\dot{\boldsymbol{p}} = \beta\boldsymbol{p} \cdot E \cdot (I - \boldsymbol{p}\boldsymbol{p}) + \frac{1}{2}\boldsymbol{\omega} \wedge \boldsymbol{p} - d_r\nabla_{\boldsymbol{p}} \ln \psi$$

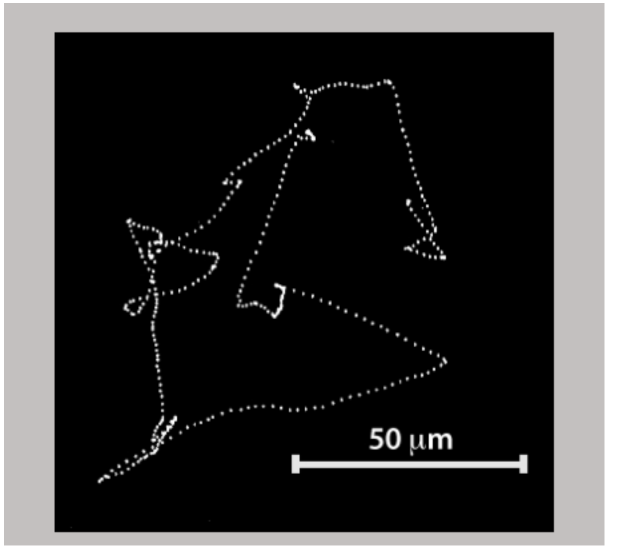
rate-of-strain tensor E and vorticity vector $\boldsymbol{\omega}$

shape factor β rotational diffusion of magnitude d_r

$\lambda(\boldsymbol{x},\boldsymbol{p},t)$ Tumble rate

$K(\boldsymbol{p},\boldsymbol{p}')$ Turning kernel

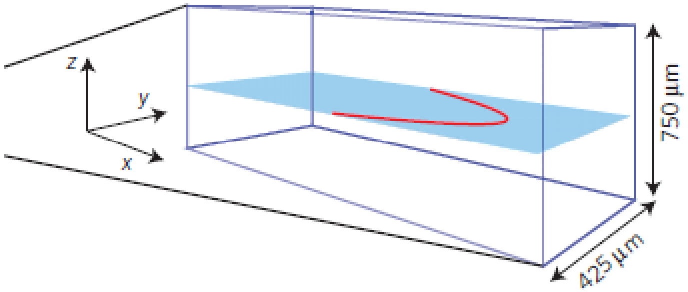
$\lambda(\boldsymbol{p}) = \lambda_0(1 - \zeta V_s\boldsymbol{p} \cdot \nabla s)$ Chemotaxis



Howard Berg's *E. coli* tracks

Steady solution for 2D channel flow

$$\mathbf{u} = U(1-y^2)\mathbf{i}$$



$$\epsilon \frac{\partial}{\partial y}(\sin\theta\,\psi) - \epsilon^2 \mathrm{d}\frac{\partial^2\psi}{\partial y^2} + \frac{\partial}{\partial\theta}\left(yPe(1-\beta\cos 2\theta)\psi - \frac{\partial\psi}{\partial\theta}\right) + (\sigma - \epsilon\chi\sin\theta)\psi - \frac{1}{2\pi}\int_0^{2\pi}(\sigma - \epsilon\chi\sin\theta')\psi(y,\theta')\,\mathrm{d}\theta' = 0,$$

$$\mathbf{p} = \cos\theta\mathbf{i} + \sin\theta\mathbf{j}$$ Swimming direction

$$K(\theta,\theta') = \frac{1}{2\pi}$$ Isotropic tumbles

$$\epsilon = 2V_s/Wd_r$$

$$Pe = 2U/Wd_r$$

$$d = Dd_r/V_s^2$$

$$\sigma = \lambda_0/d_r$$

$$\chi = \lambda_0\zeta\frac{ds}{dy}$$

No flux boundary conditions

Consider the cell concentration

$$n(\boldsymbol{x},t) = \int_{\Omega} \psi(\boldsymbol{x},\boldsymbol{p},t)d\boldsymbol{p}$$

Integrating governing equation gives conservation equation for n and defines cell flux, J

$$\frac{\partial n}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{J} = 0,$$

$$\boldsymbol{J} = \int_{\Omega} \left((\boldsymbol{u} + V_s \boldsymbol{p})\psi - D \boldsymbol{\nabla}_{\boldsymbol{x}} \psi \right) \, d\boldsymbol{p}.$$

For 2D flow, no flux condition at y=+/- 1

$$\int_0^{2\pi} \left(\sin\theta\psi - \epsilon d \frac{\partial \psi}{\partial y} \right) d\theta \bigg|_{y=\pm 1} = 0.$$

Numerical solution not unique, so instead impose

$$\sin\theta\psi - \epsilon d \frac{\partial \psi}{\partial y} = 0$$

But will discuss this more later

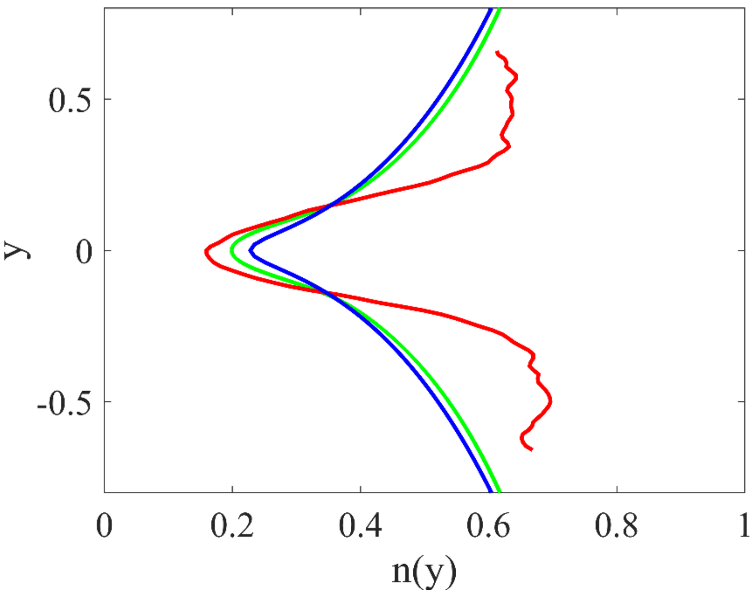
Depletion of cells in central (low shear) region

Green: numerical simulation of

$\psi(x, p, t)$

Red: Experiments

Blue: approximate solution



$$n(y) \propto \frac{e^{\chi y}}{V_{MS}}$$

Mean square cross-channel swim speed

$$V_{MS}(y) = \int_0^{2\pi} \sin^2\theta f(\theta; y) d\theta$$

Approximate solution

Take *d*=0 (neglect translational diffusion) & estimate

$$\psi = n(y) f(\theta; y)$$

$f^{(0)}(\theta; y)$ leading order equilibrium orientation distribution at a given position

$$\frac{\partial}{\partial \theta}\left(yPe(1-\beta\cos 2\theta) f^{(0)} - \frac{\partial f^{(0)}}{\partial \theta}\right) + \sigma(f^{(0)} - \frac{1}{2\pi}) = 0,$$

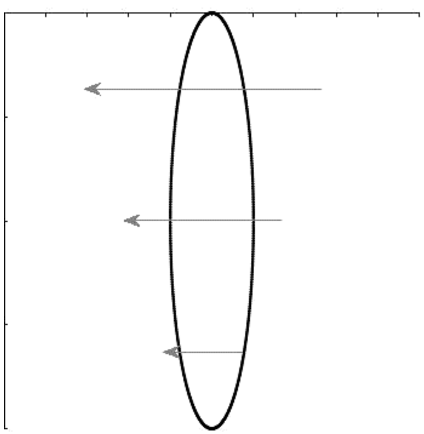
Take first moment of steady governing equation:

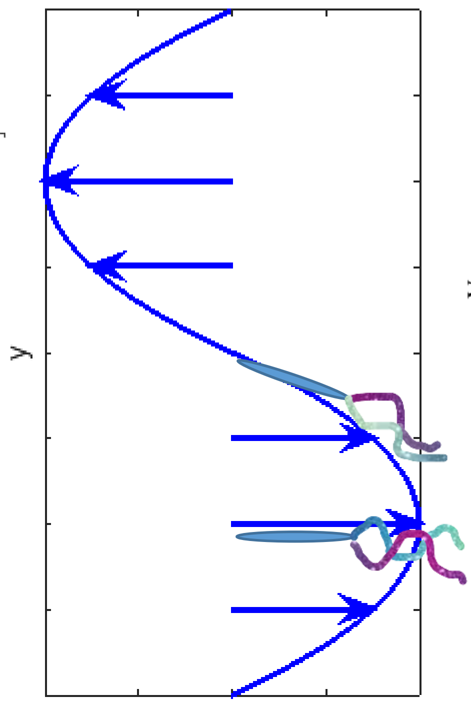
$$\frac{d}{dy}(nV_{MS}) - \chi n V_{MS} = 0 \qquad n(y) \propto \frac{e^{\chi y}}{V_{MS}}$$

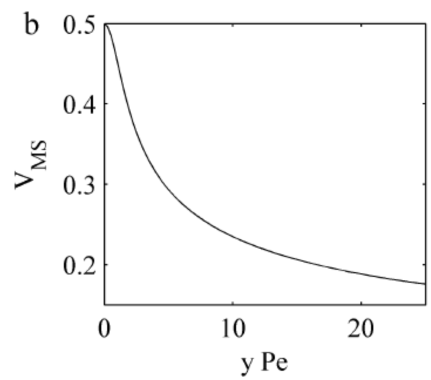
Mean square cross-channel swim speed $V_{MS}(y) = \int_0^{2\pi} \sin^2\theta f(\theta; y) d\theta$

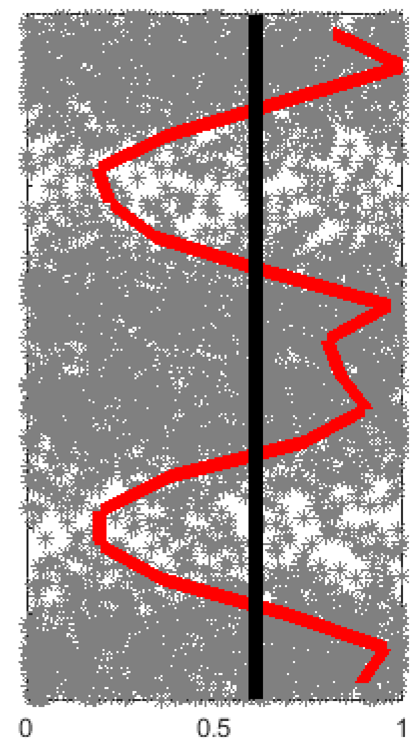
Mechanism for trapping in high shear

- Slender shape leads to non-uniform rotation
- Peak in orientation distribution in stream-wise (x) direction
- Reduction in cross-channel (y) swimming
- Cell accumulation







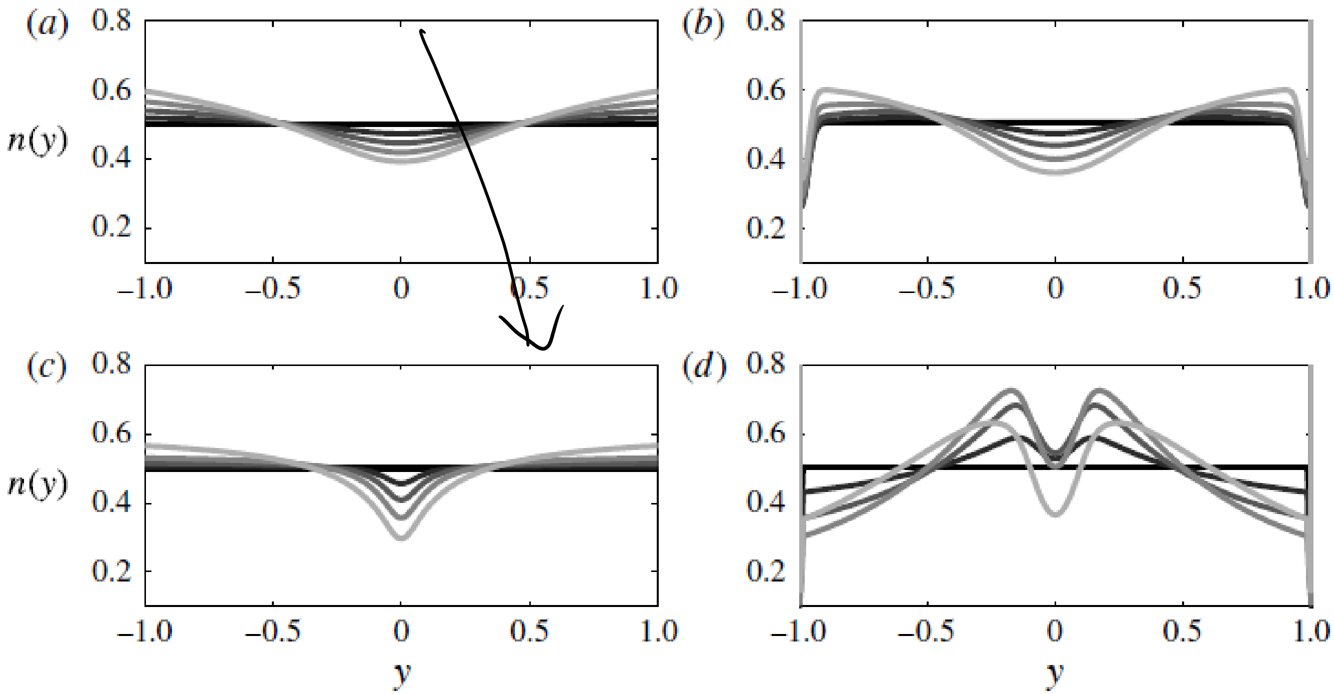


Problem 1: Approximate model doesn't capture effect of shape

$$\beta = [0,\ 0.2,\ 0.4,\ 0.6,\ 0.8],$$

Pe =5

Pe =25



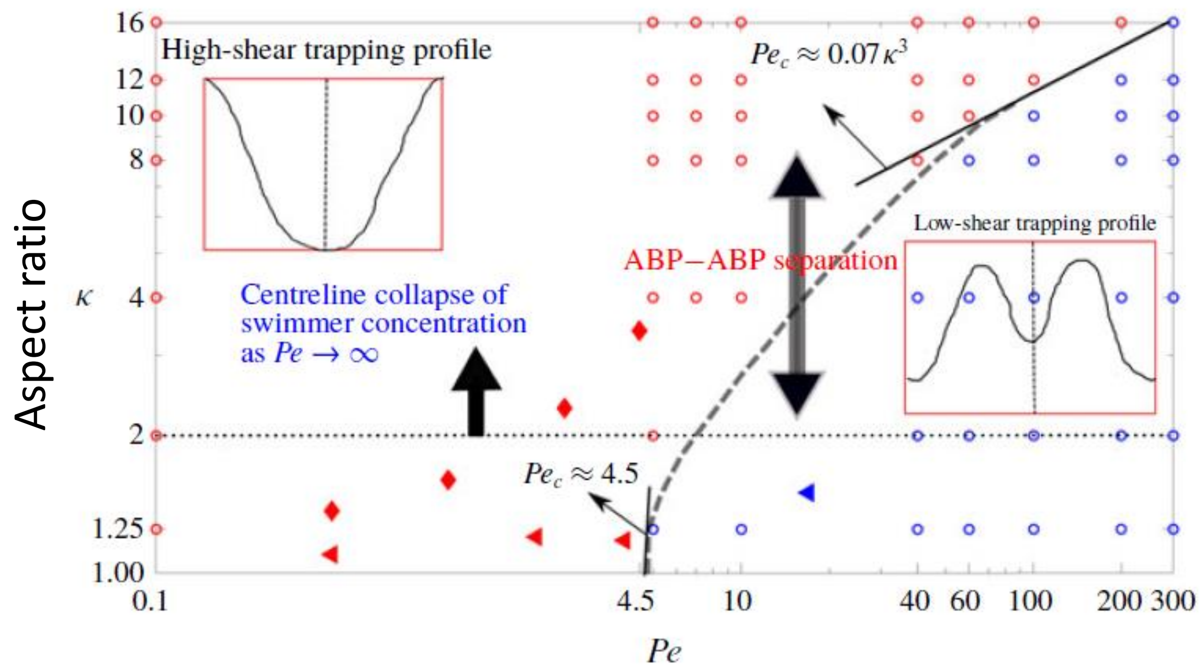
Approximate solution

Full numerical solution

J. Fluid Mech. (2020), vol. 890, A15.
Published by Cambridge University Press
doi:10.1017/jfm.2020.118

Shear-induced migration of microswimmers in pressure-driven channel flow

Laxminarsimharao Vennamneni[1], Sankalp Nambiar[1] and Ganesh Subramanian[1,†]



A local approximation model for macro-scale transport of biased active Brownian particles in a flowing suspension

Lloyd Fung[1] †, Rachel N. Bearon[2] and Yongyun Hwang[1]

J Fluid Mech 2022

Exact expression for cell concentration obtained from Smoluchowski

$$\partial_t n + \nabla_\mathbf{x} \cdot \left[\left(Pe_f \mathbf{u} + Pe_s \left(\langle \mathrm{p} \rangle_g - \mathbf{V}_u - \mathbf{V}_{D_T} - \mathbf{V}_c - \mathbf{V}_{\partial t} \right) \right) n \right]$$
$$= D_T \nabla_x^2 n + Pe_s \nabla_\mathbf{x} \cdot \left(\boldsymbol{D}_{D_T} + \boldsymbol{D}_c \right) \cdot \nabla_\mathbf{x} n.$$

$\langle \mathbf{p} \rangle_g$	Averaged motility of individual particle from the homogeneous solution of $\mathcal{L}_p$
$\mathbf{V}_{\partial t}$	Drift due to interaction between particles' orientational dynamics and the unsteadiness of f in $\mathbf{p}$-space
$\mathbf{V}_u$	Drift due to interaction between particles' orientational dynamics and passive advection of f in $\mathbf{x}$ by the flow field $\mathbf{u}$
$\mathbf{V}_c$	Drift due to interaction between particles' motility and the inhomogeneity of particles' orientational dynamics in $\mathbf{x}$
$\mathbf{V}_{D_T}$	Drift due to interaction between particles' orientational dynamics and translational diffusion of f in $\mathbf{x}$
$\boldsymbol{D}_{D_T}$	Dispersion from interaction between particles' orientational dynamics and the dispersion of n and f due to translational diffusion of f and n
$\boldsymbol{D}_c$	Dispersion due to interaction between particles' motility and orientational dynamics

Vertical 'pipe' flow, steady state, D_T=0

$$\partial_x[(Pe_s\langle p_x\rangle_g - Pe_s V_{x,c})n_{f,s}] = Pe_s\partial_x[D_{xx,c}\partial_x n_{f,s}]$$

Exact (no computational benefit over solving full Smoluchowski)

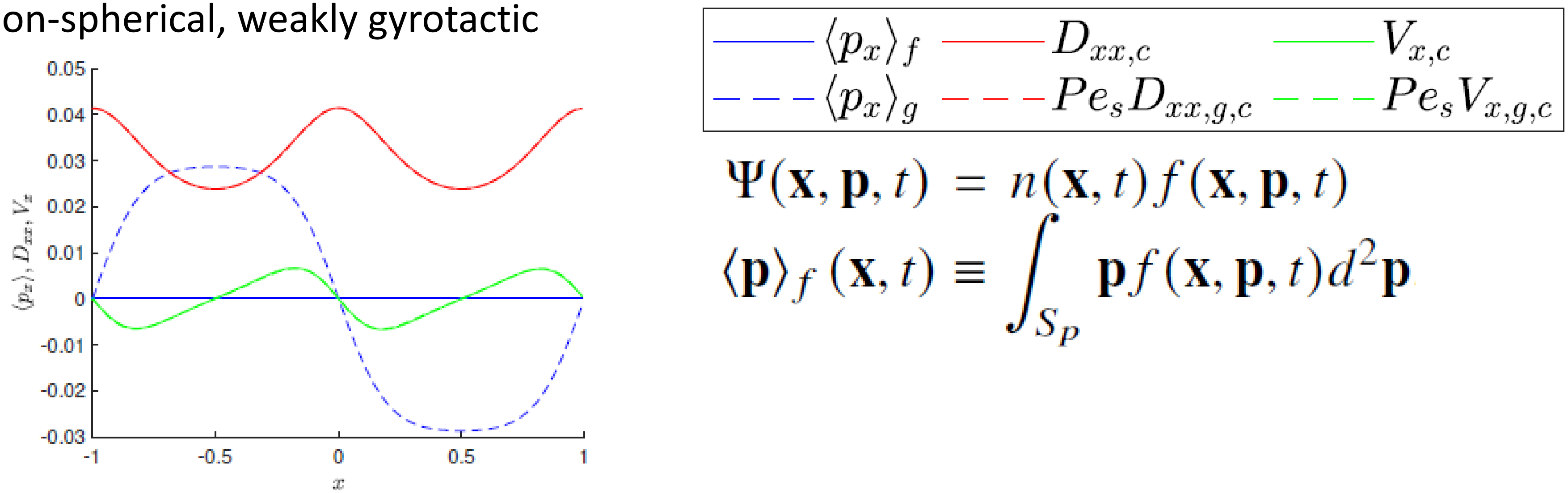
New approximation

$$Pe_s(\equiv \epsilon) \ll 1,\ Pe_f \lesssim O(\epsilon) \text{ and } D_T \lesssim O(\epsilon),$$

Allows for easier computation of drift & diffusion

$$\partial_x[(Pe_s\langle p_x\rangle_g - Pe_s^2 V_{x,g,c})n_{g,s}] = Pe_s^2\partial_x[D_{xx,g,c}\partial_x n_{g,s}]$$

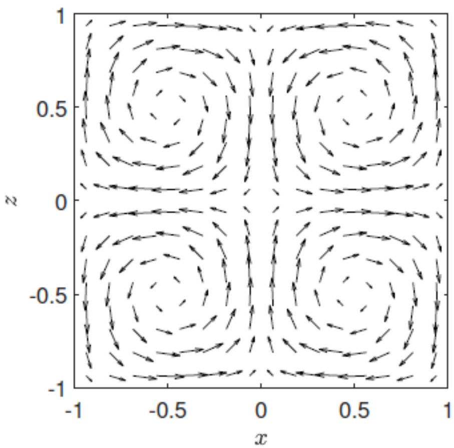
Non-spherical, weakly gyrotactic



$$\Psi(\mathbf{x},\mathbf{p},t) = n(\mathbf{x},t)f(\mathbf{x},\mathbf{p},t)$$

$$\langle\mathbf{p}\rangle_f(\mathbf{x},t) \equiv \int_{S_p}\mathbf{p}f(\mathbf{x},\mathbf{p},t)d^2\mathbf{p}$$

Valid for more complex flows

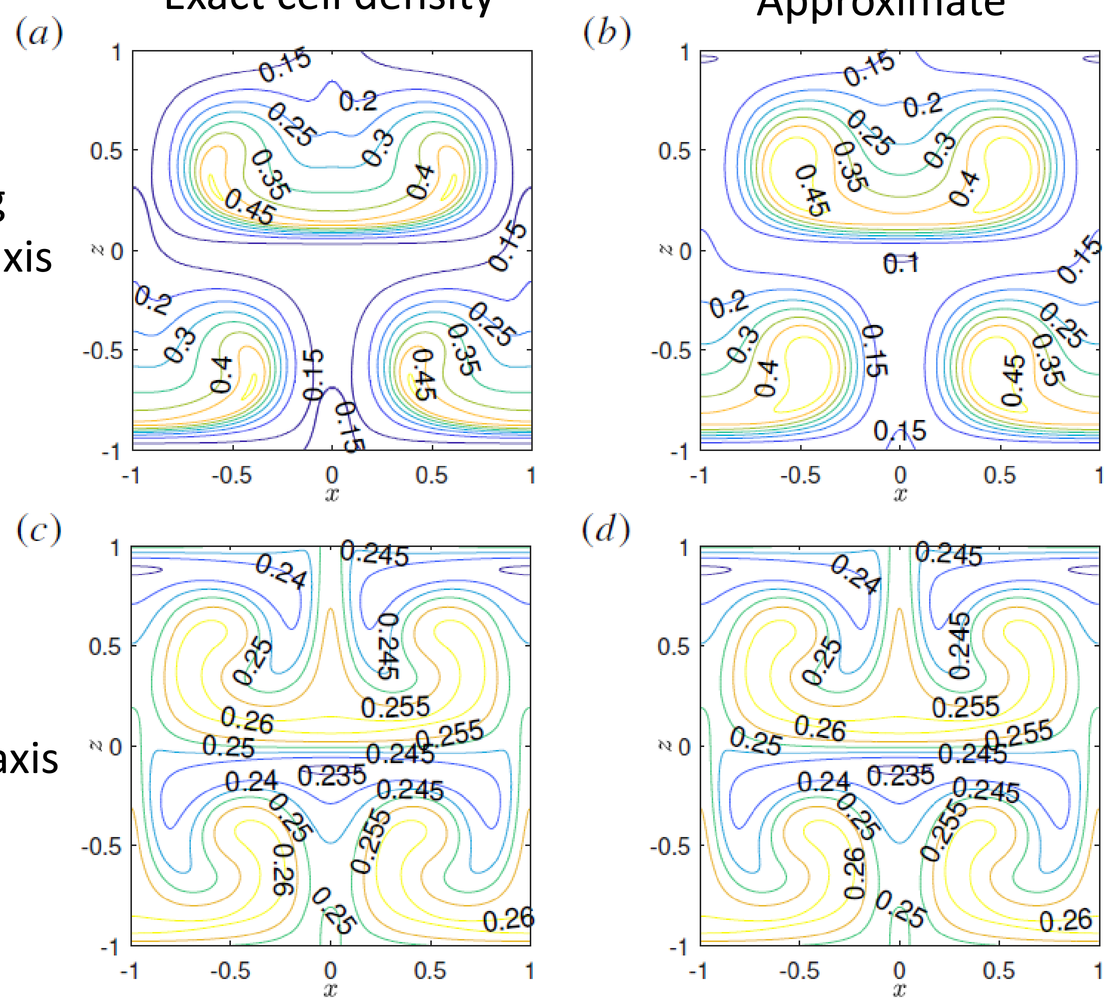


Exact cell density

Approximate

Strong gyrotaxis

Weak gyrotaxis

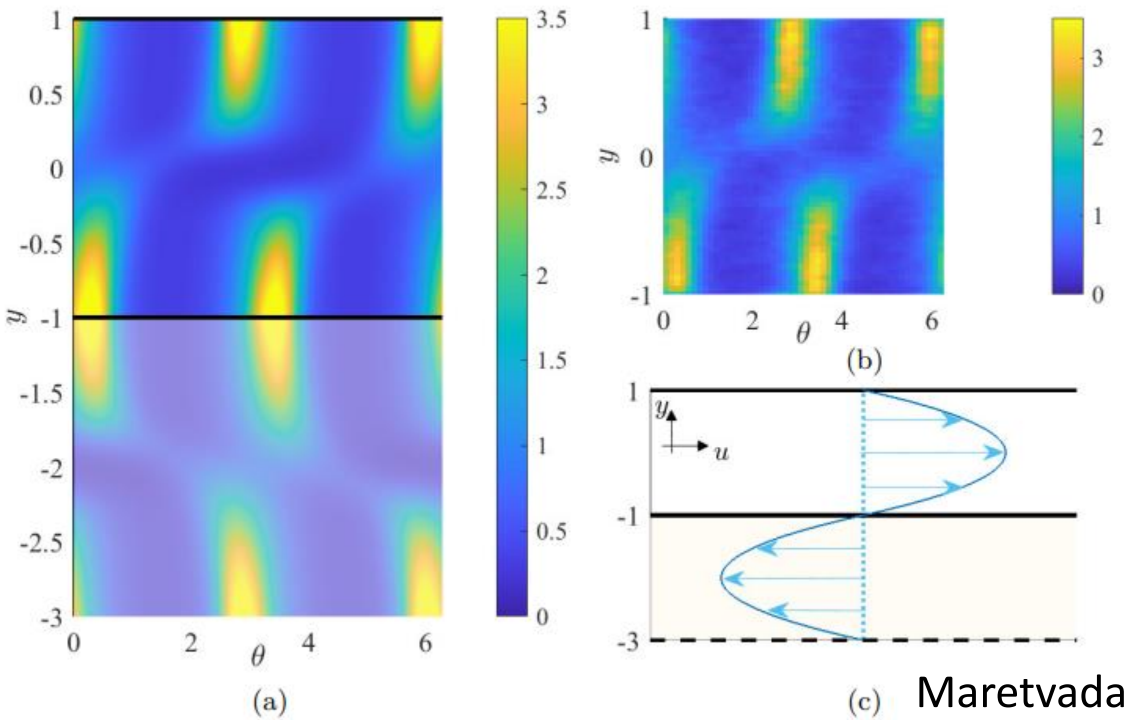


Problem 2: What is the correct boundary condition?

Numerical solution not unique, so instead impose

$$\sin\theta\psi - \epsilon d\frac{\partial\psi}{\partial y} = 0$$

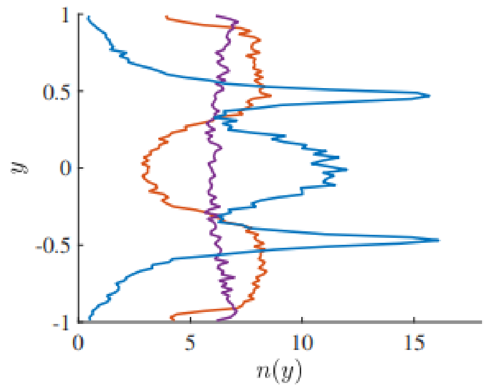
But will discuss this more later



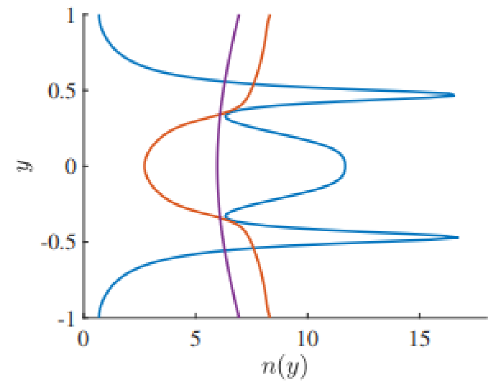
(c)

IBM with specular reflection=doubly periodic Poiseuille

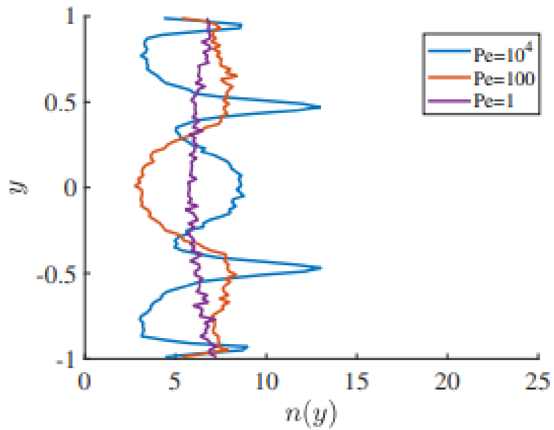
Maretvadakethope, Vasiev, Hazel & Bearon, in Prep for Phys Rev Fluids



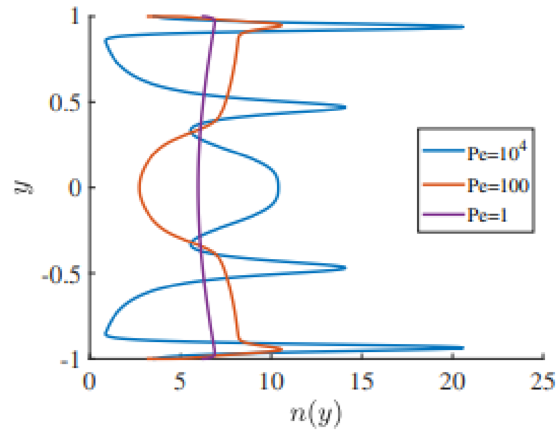
IBM, Specular reflection



Continuum, doubly periodic Poiseuille



IBM, uniform random reflection



Continuum, constant boundary condition

$\beta = 0.99$ with $Pe = 10^4$ (blue), $Pe = 100$ (red) and $Pe = 1$ (purple).

Summary Part II

- Basics of trapping in high shear can be explained:
  Elongated particles undergo non-uniform rotation
  Enhanced peak in orientation distribution in stream-wise (x) direction
  Reduction in cross-channel (y) swimming

- Obtaining correct macro-transport description is non-trivial
- Determining the right boundary conditions is non-trivial
- Progress possible – asymptotic analysis; numerical simulation
- Collaboration!

Conclusions

- Shape matters!
- Curiosity driven research
- Interdisciplinary collaborations can result in fundamental research questions