Motion of suspended nanoparticles in a field of periodic obstacles*

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* From Herrmann, John, Michael Karweit, and German Drazer, "Separation of suspended particles in microfluidic systems by directional locking in periodic fields", Phys. Rev. E, **79** (2009)

GCB celebration

50 years of fluid mechanics research
= 50 years of celebrating

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Nanoparticle manipulation and separation

Manipulation

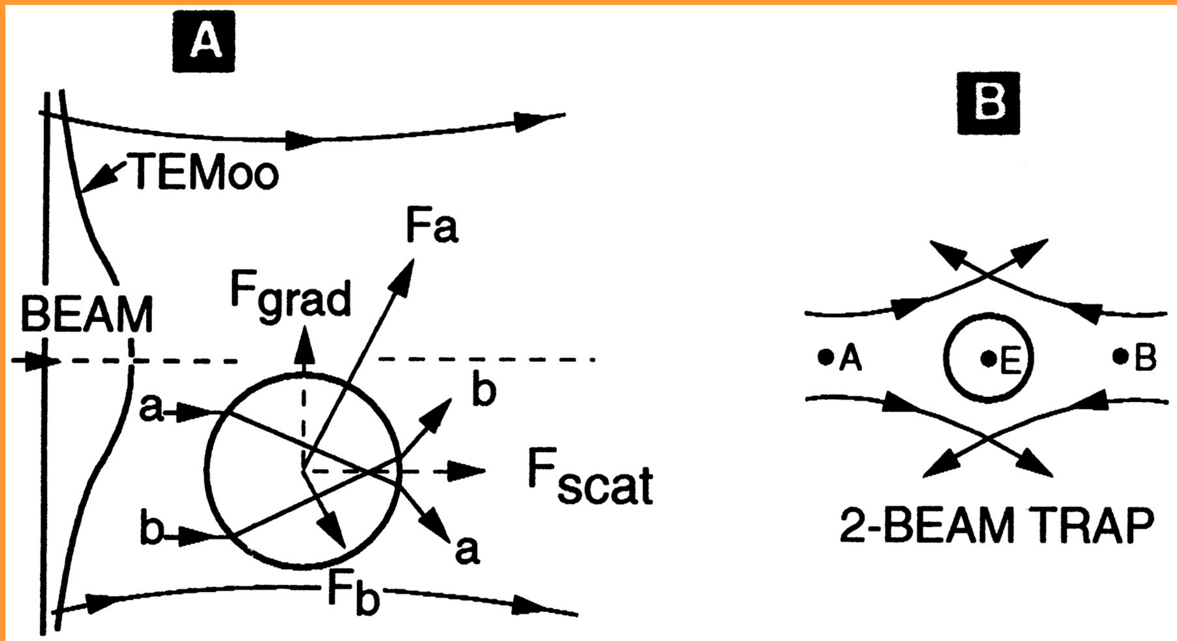
- **Optical tweezers**
- **Acoustic tweezers**

Separation

- **Magnetic (link nanomagnets to organic molecules)**
- **Electrophoresis**
- **Capillary electrophoresis (separates species based on size to charge ratio)**
- **Size**
  - **Wedge**
  - **Periodic lattice**
    - **hard obstacles**
    - **potential wells**

Optical tweezers

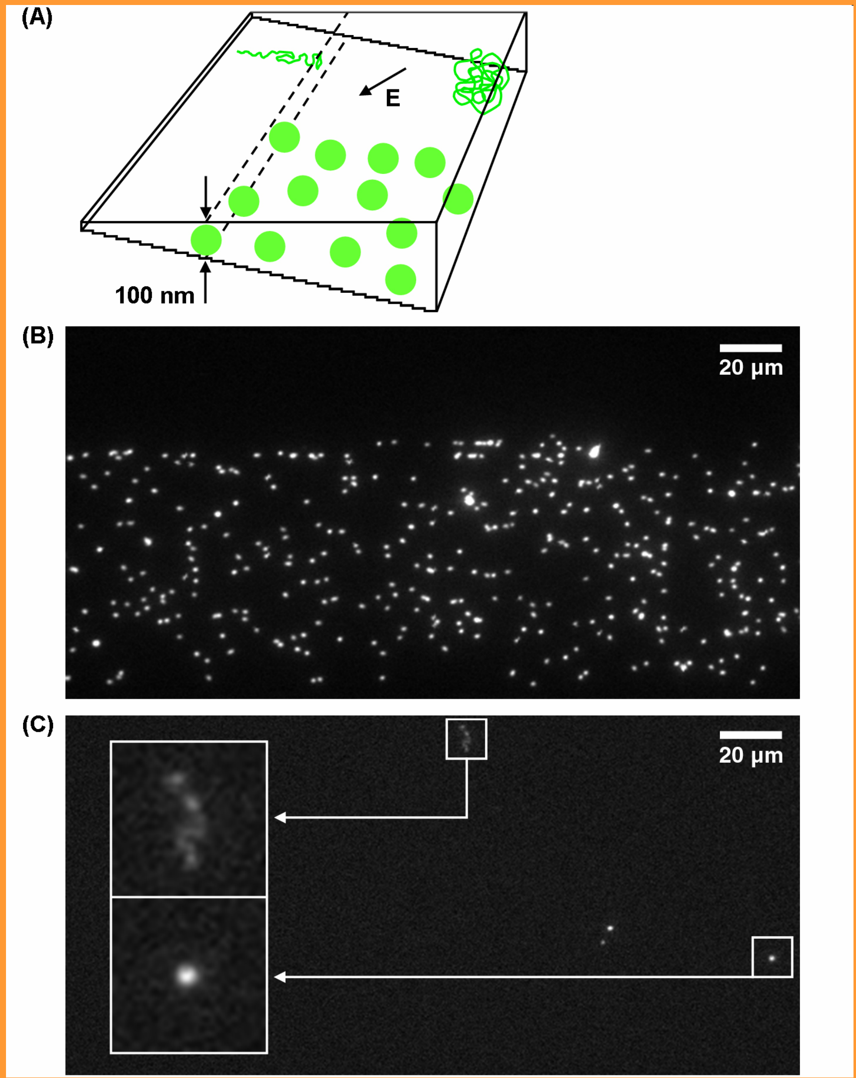
(A) Origin of Fscat and Fgrad for high index sphere displaced from TEM00 beam axis



Ashkin A PNAS 1997;94:4853-4860

“Coin sorter” separator:

An electric field E drives nanoparticles through a multi-step wedge.
Wedge thickness restricts motion.
Green spheres are 100nm diameter.
Spherical coil is a strand of DNA.
Elongated coil is stretched DNA.



* S.M. Stavis, E.A. Strychalski and M.Gaitan. Nanofluidic structures with complex three-dimensional surfaces. *Nanotechnology* Vol. 20, Issue 16 (online March 31, 2009; in print April 22, 2009)

Continuous Particle Separation Through Deterministic Lateral Displacement

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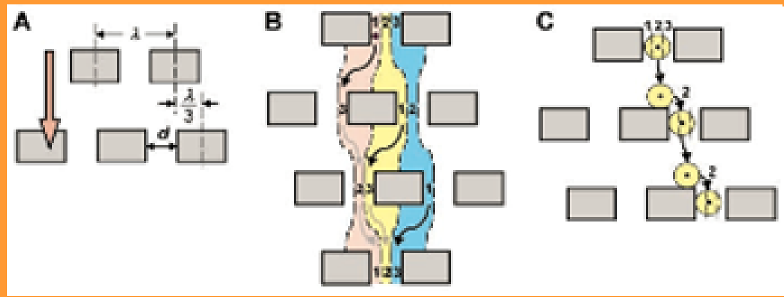
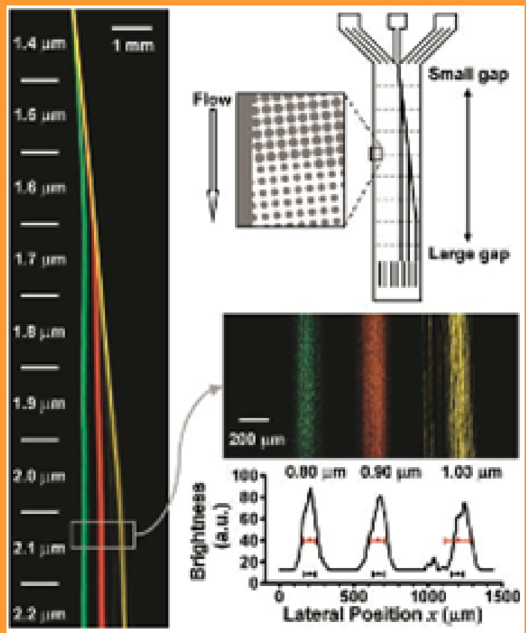
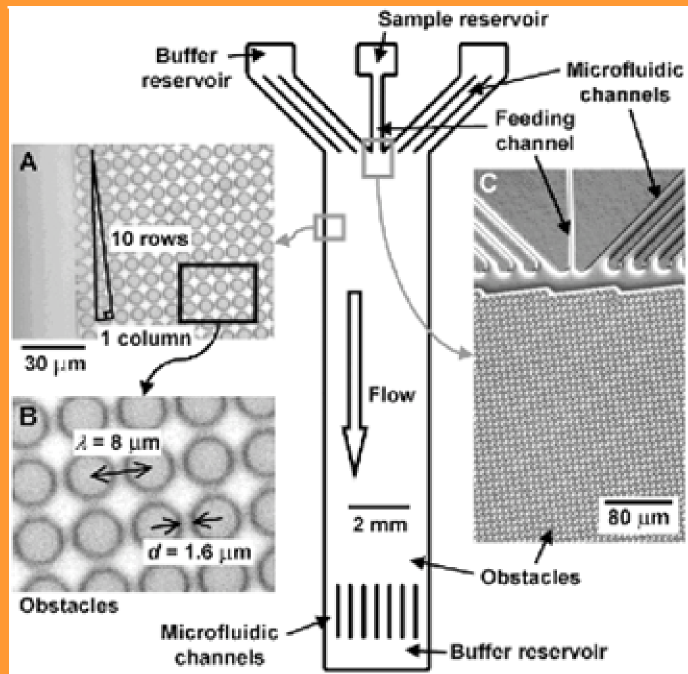
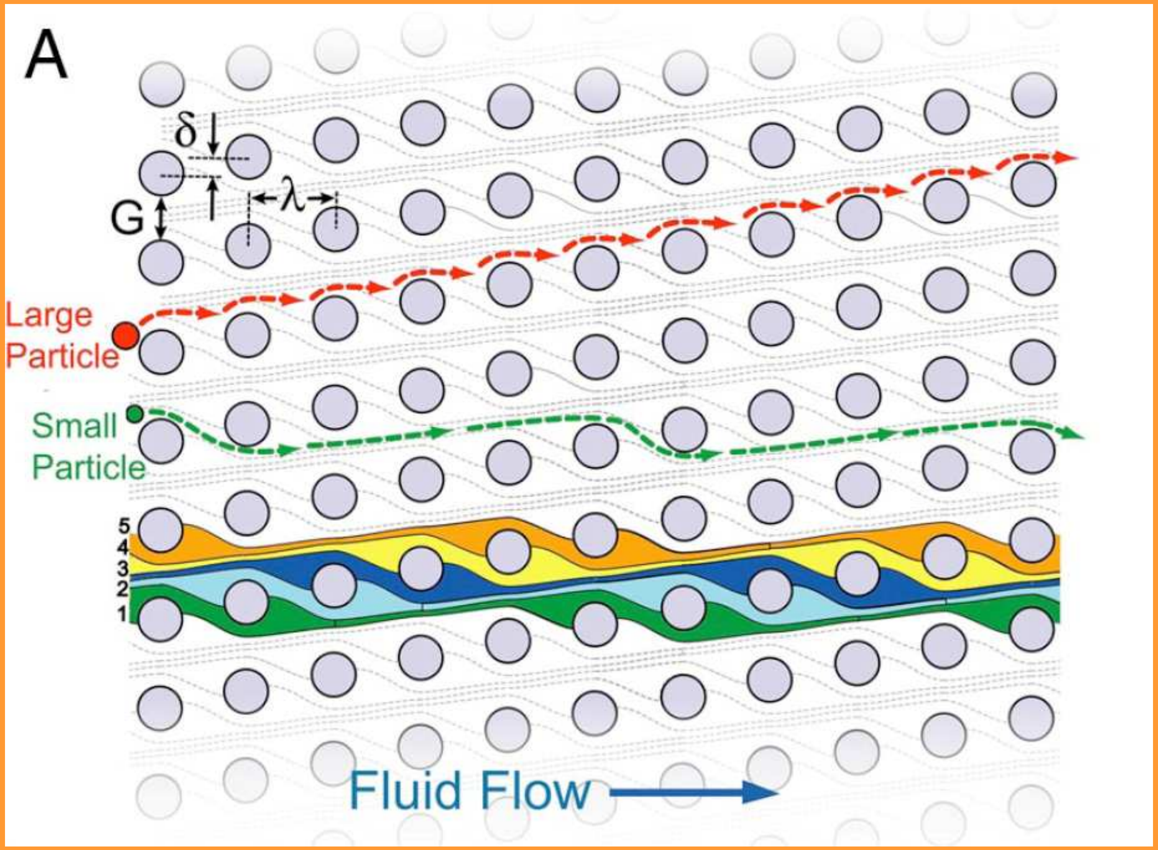


Fig. 1. (A) Geometric parameters defining the obstacle matrix. A fluid flow is applied in the vertical direction (orange arrow). (B) Three fluid streams (red, yellow, and blue) in a gap do not mix as they flow through the matrix. Lane 1 at the first obstacle row becomes lane 3 at the second row, lane 3 becomes lane 2 at the third row, and so on. Small particles following streamlines will thus stay in the same lane. (C) A particle with a radius that is larger than lane 1 follows a streamline passing through the particle's center (black dot), moving toward lane 1. The particle is physically displaced as it enters the next gap. Black dotted lines mark the lanes.

Fig. 3. High-resolution separation of fluorescent microspheres with diameters of 0.80 μm (green), 0.90 μm (red), and 1.03 μm (yellow), with a matrix of varying gap size. Whereas the shift in registry and the lattice constants of the matrix remain the same, the obstacle diameters are changed to create gaps (d) of different sizes, which are labeled on the left side of the fluorescent image. The red bars on the fluorescence profile represent the width of the peaks (FWHM), and the black bars label the 1% inhomogeneity in the bead population. a.u., arbitrary units.







Morton, Keith J., et al, "Hydrodynamic metamaterials: Microfabricated arrays to steer, refract, and focus streams of biomaterials", PNAS**, 105** -21, May 27, 2008**.**

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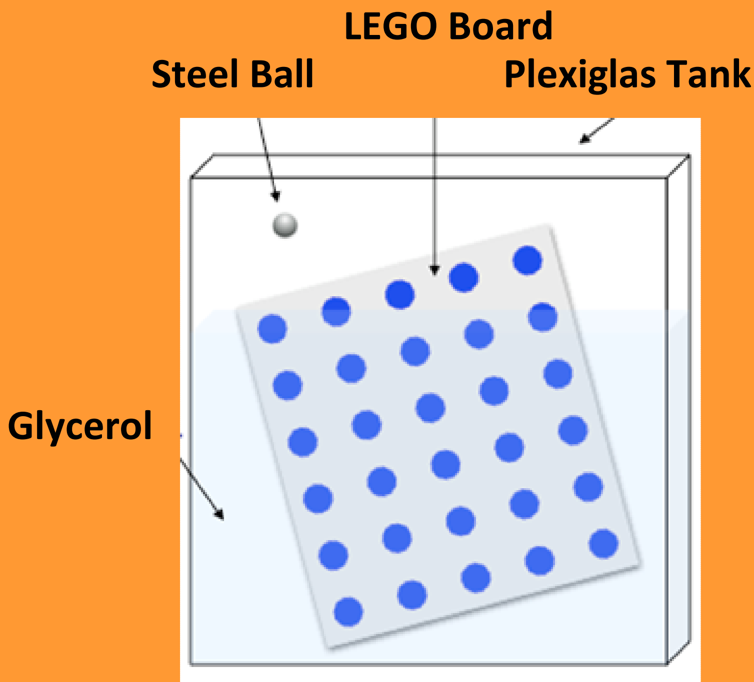

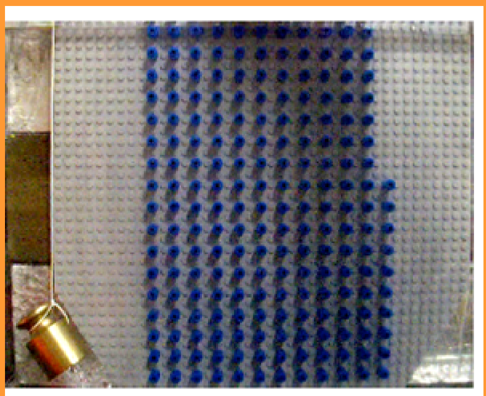

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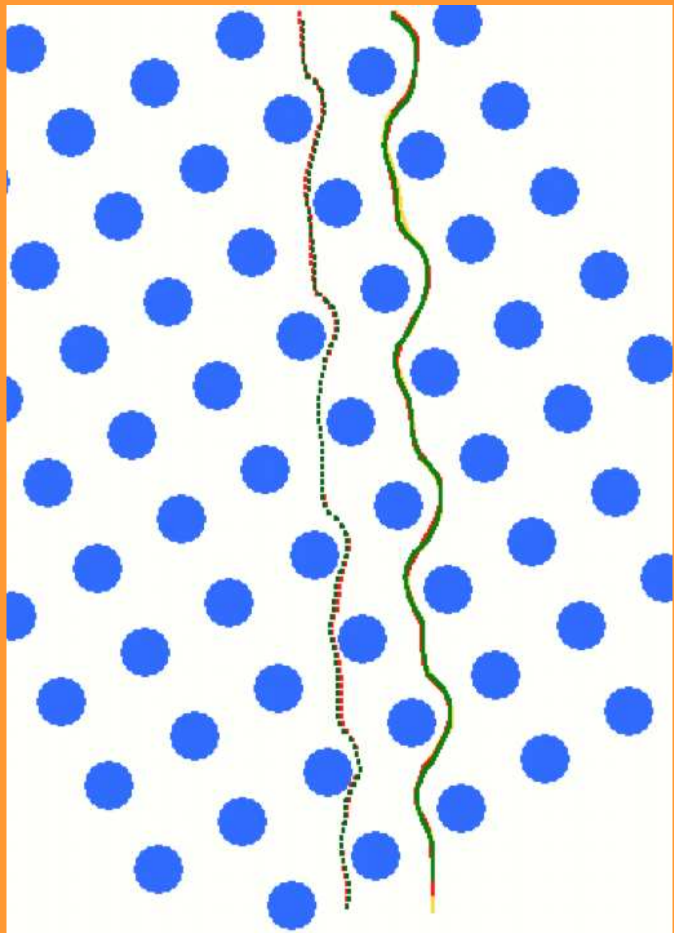
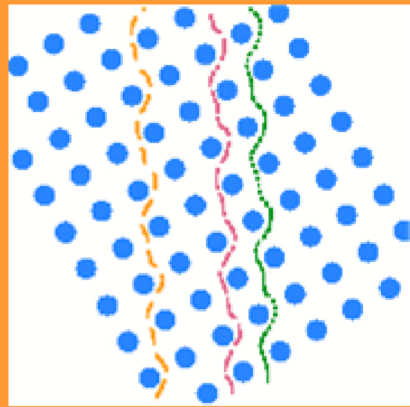
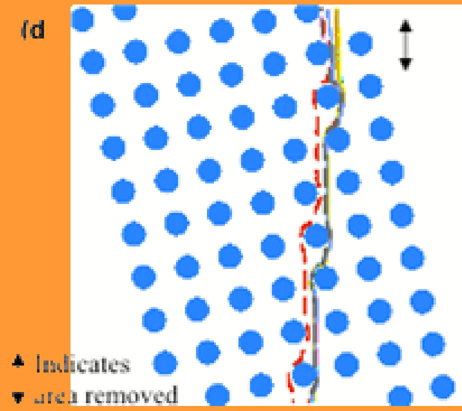
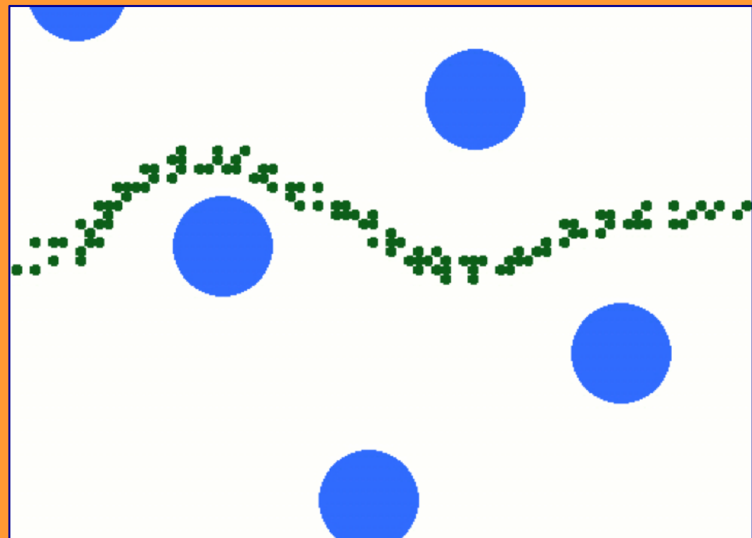


Trajectories for 3mm and 6mm spheres showing their directional locking in the [1,2] at a forcing angle of 30.0º







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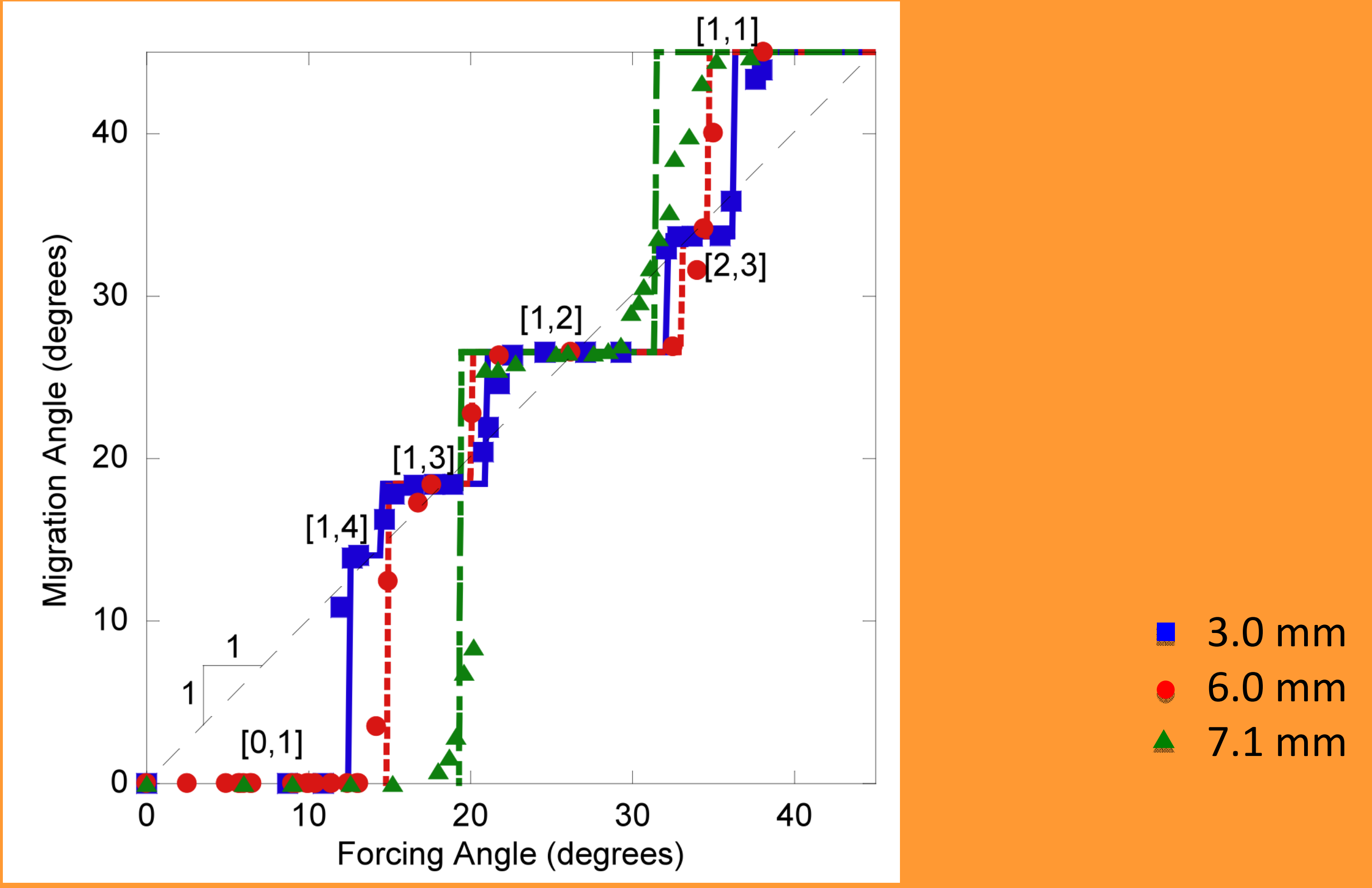
Directional Locking (Devil's Staircase) and Separation
LEGO Experiments



Motion of a Brownian particle traversing a periodic force field is the Langevin equation, which in the limit of high friction is

$$\gamma \frac{d\vec{x}}{dt} = \vec{F}(\vec{x}) + \vec{F}_0(\vec{x}) + \vec{\xi}(t)$$

$\vec{F}(\vec{x})$ is the periodic force field

$\vec{F}_0(\vec{x}) \equiv \vec{F}_0$ is the external driving force (in this case, constant)

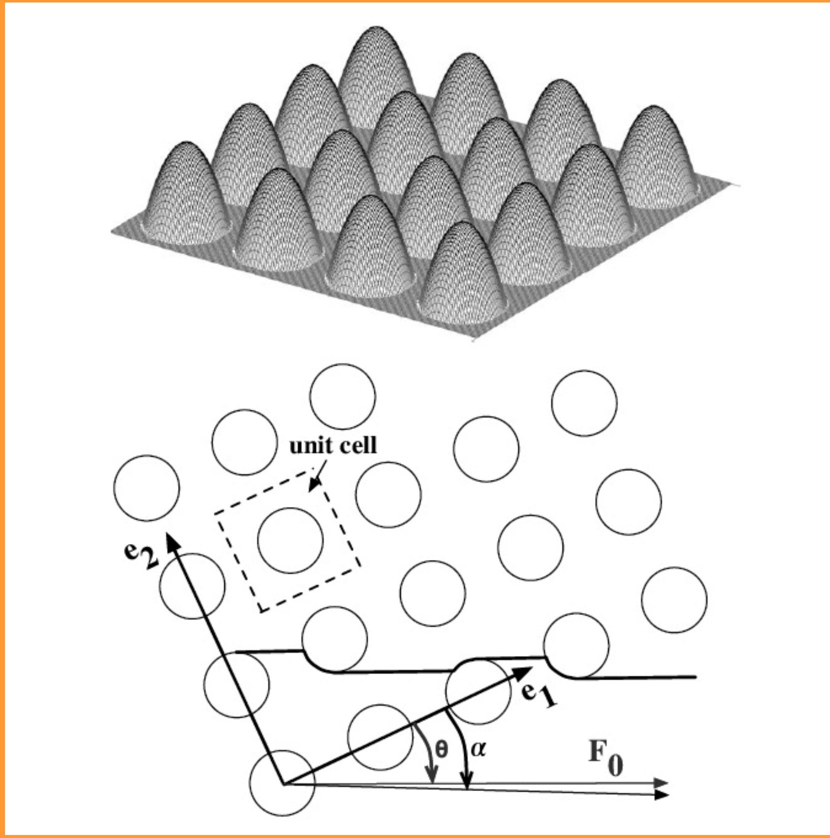
$\vec{\xi}(t)$ is a fluctuating, Gaussian Langevin force exerted by the fluid on the particle with $\left\langle \vec{\xi}(t) \right\rangle = 0$ $\left\langle \xi_i(t)\xi_j(s) \right\rangle = 2\gamma kT\delta(t-s)\delta_{ij}$

$\gamma = 6\pi\mu a$ is the friction constant, where *a* is the particle diameter, and μ is the viscosity

Periodic force defined from a potential field

$$\mathbf{F}(\mathbf{x}) = -\nabla V(\mathbf{x})$$

Piecewise smooth potential composed of repulsive centers of size R with lattice spacing L>2R



$$V(x,y) = -\frac{F_{\max}}{2R}(x^2 + y^2 - R^2) \quad r \le R$$
$$= 0 \quad r > R$$

Deterministic transport: exact solutions

Outside parabolic obstacles: uniform flow

Inside parabolic obstacles (in dimensionless form):

$$\dot{x} = -\frac{\partial V}{\partial x} + f = x + f \qquad r < 1$$

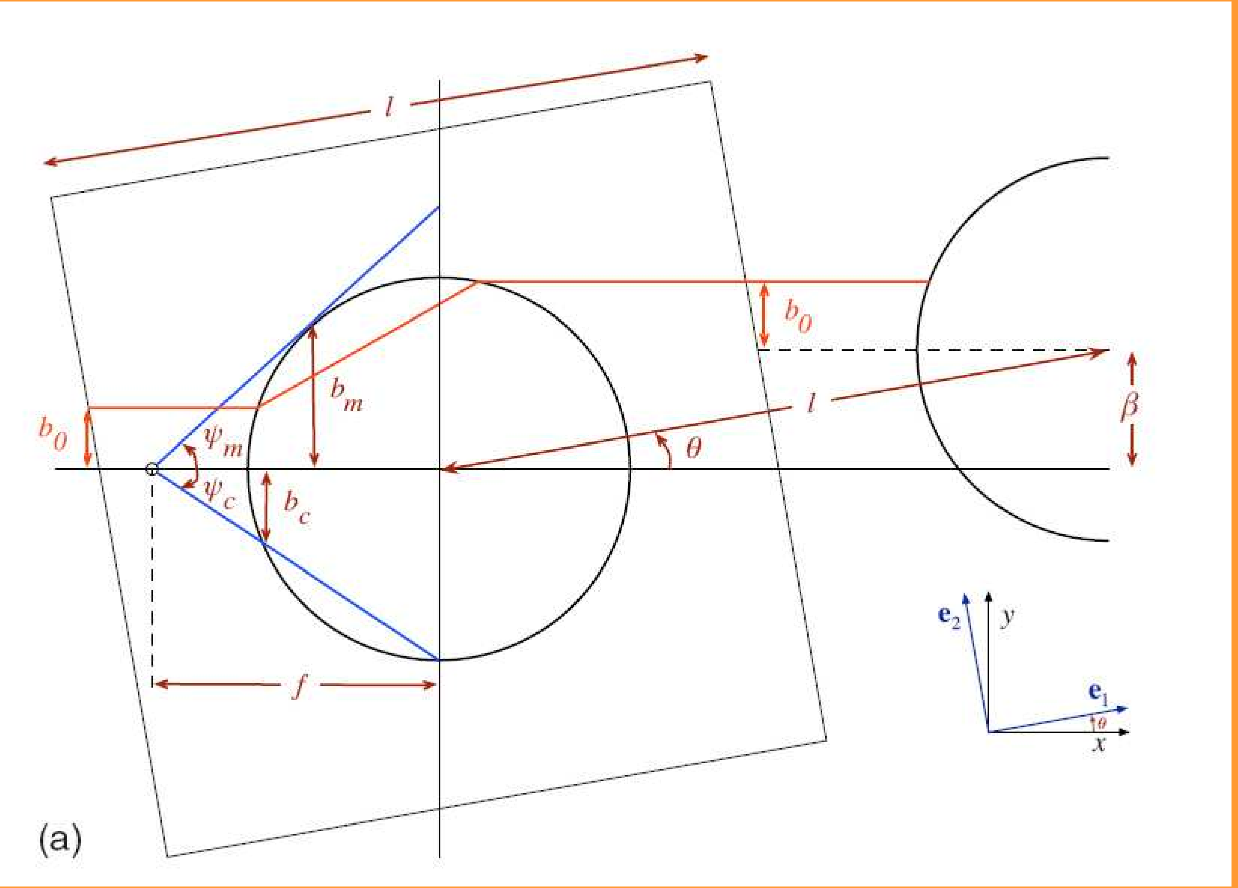
$$\dot{y} = -\frac{\partial V}{\partial y} = y \qquad r < 1$$

$$\textit{with} \quad f = F_0 / F_{\max} \quad = \textit{driving force/maximum repulsive force}$$

Dimensionless variables

$$u_c = F_{max} / \gamma = \textit{characteristic velocity}$$

$$\dot{\mathbf{x}} = \dot{\mathbf{x}}\gamma / F_{\max}, \quad \mathbf{x}' = \mathbf{x}/R, \quad r' = r/R \quad l = L/R$$



b_0 = y coord when particle enters cell
b_m= y coord where particle skirts parabolic region
b_c= y coord where particle enters parabolic region, exits before x = 0, and skirts region up to x = 0.

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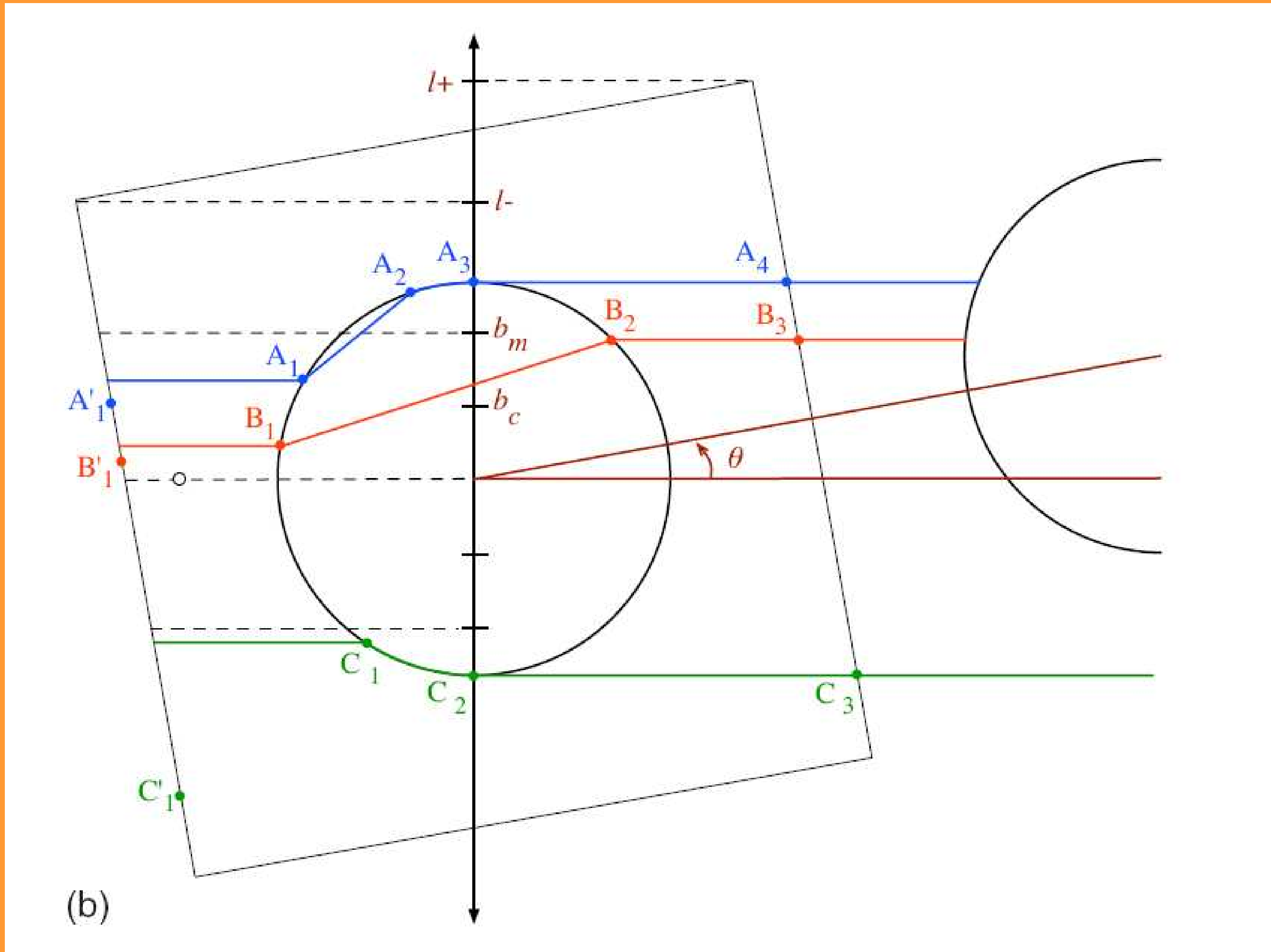

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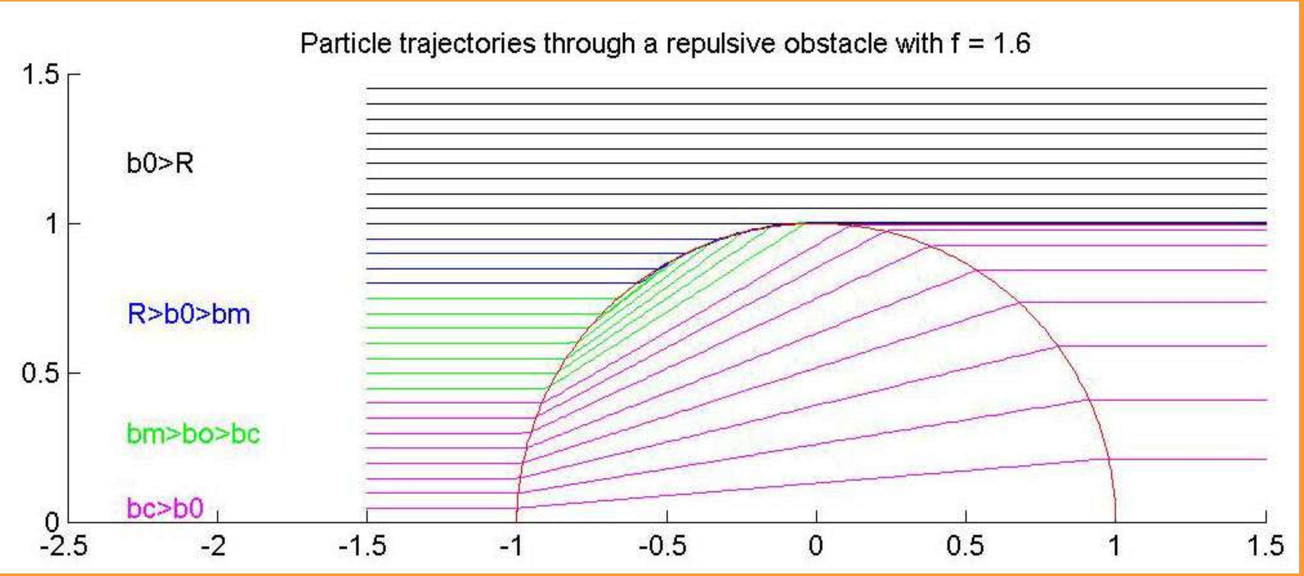
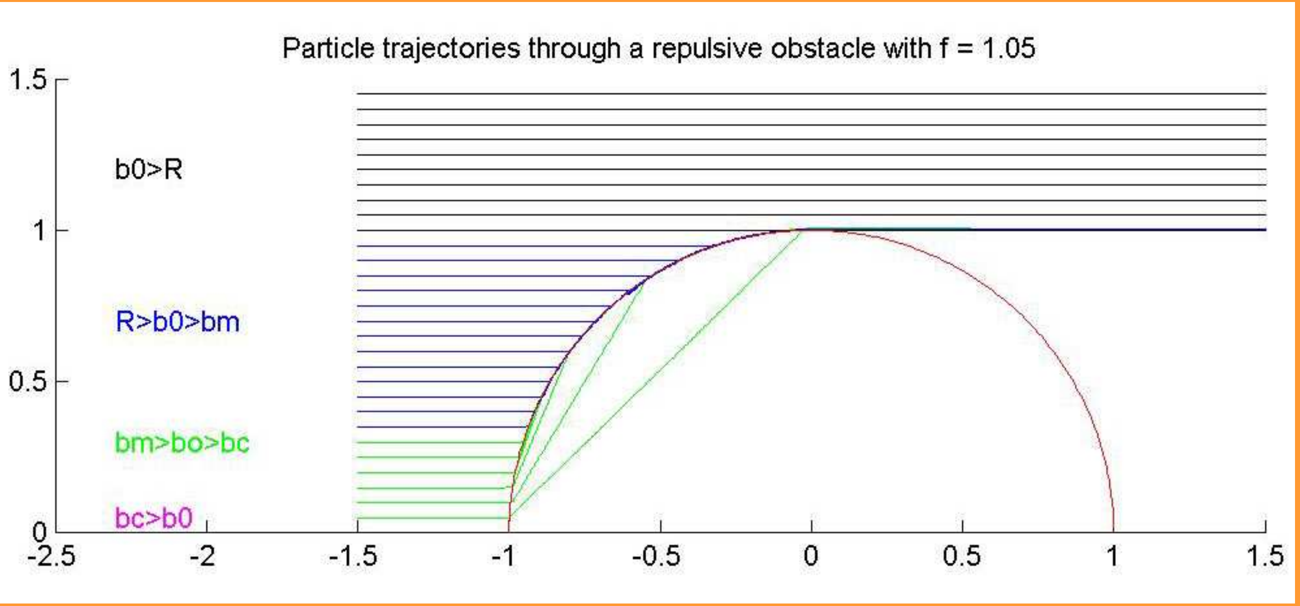
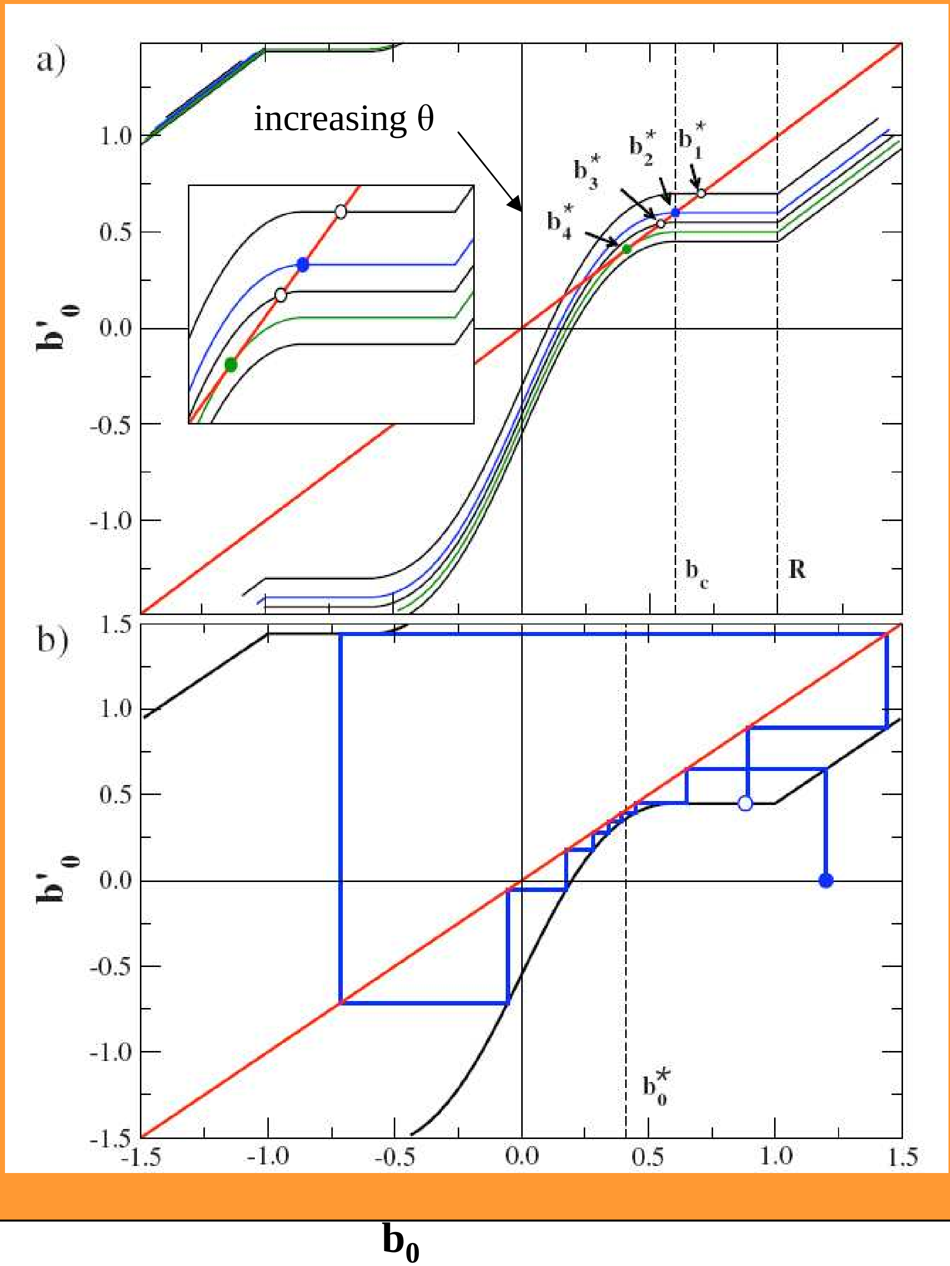




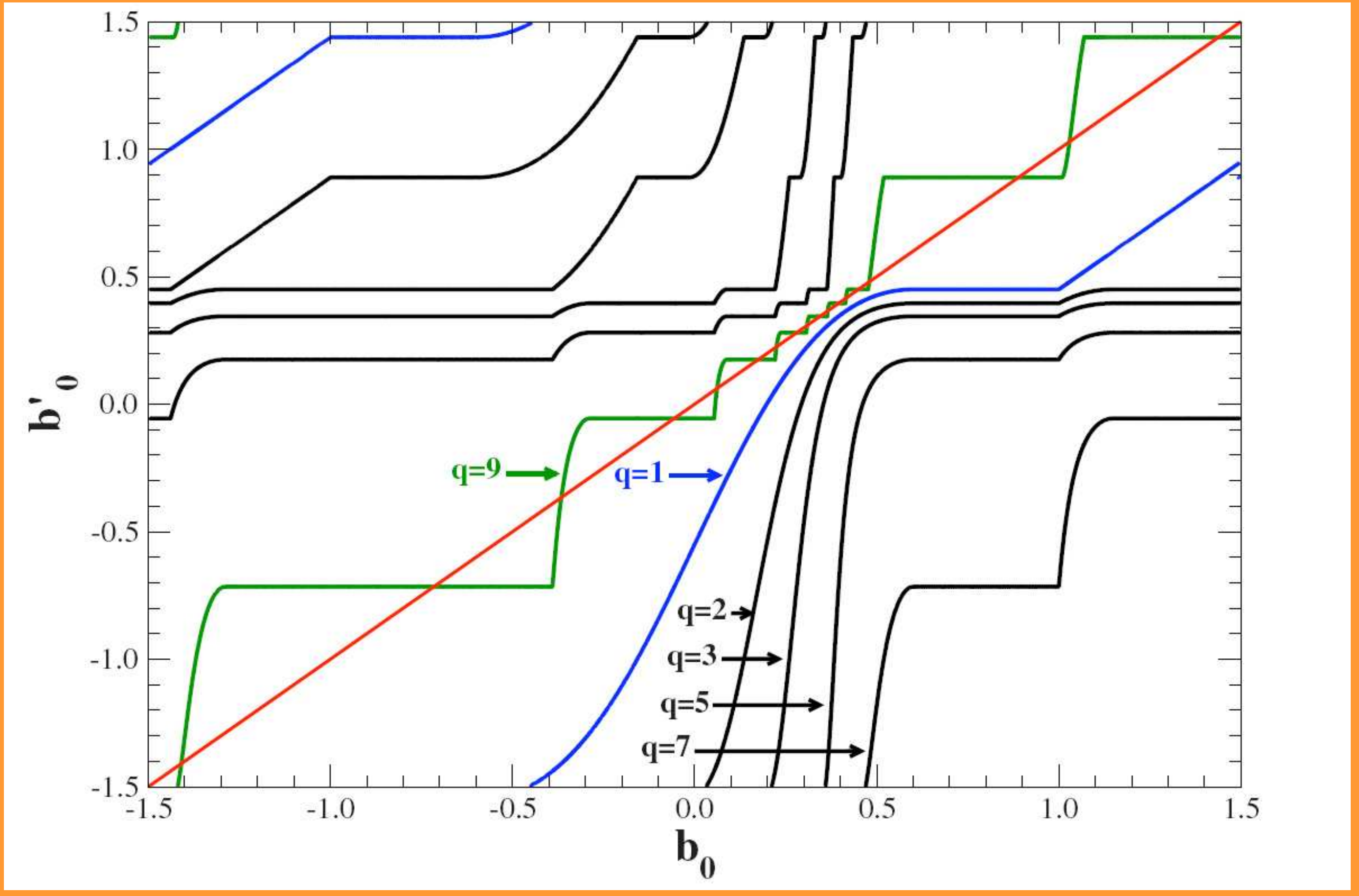


Poincare map of the incoming collision parameter onto itself for different forcing angles

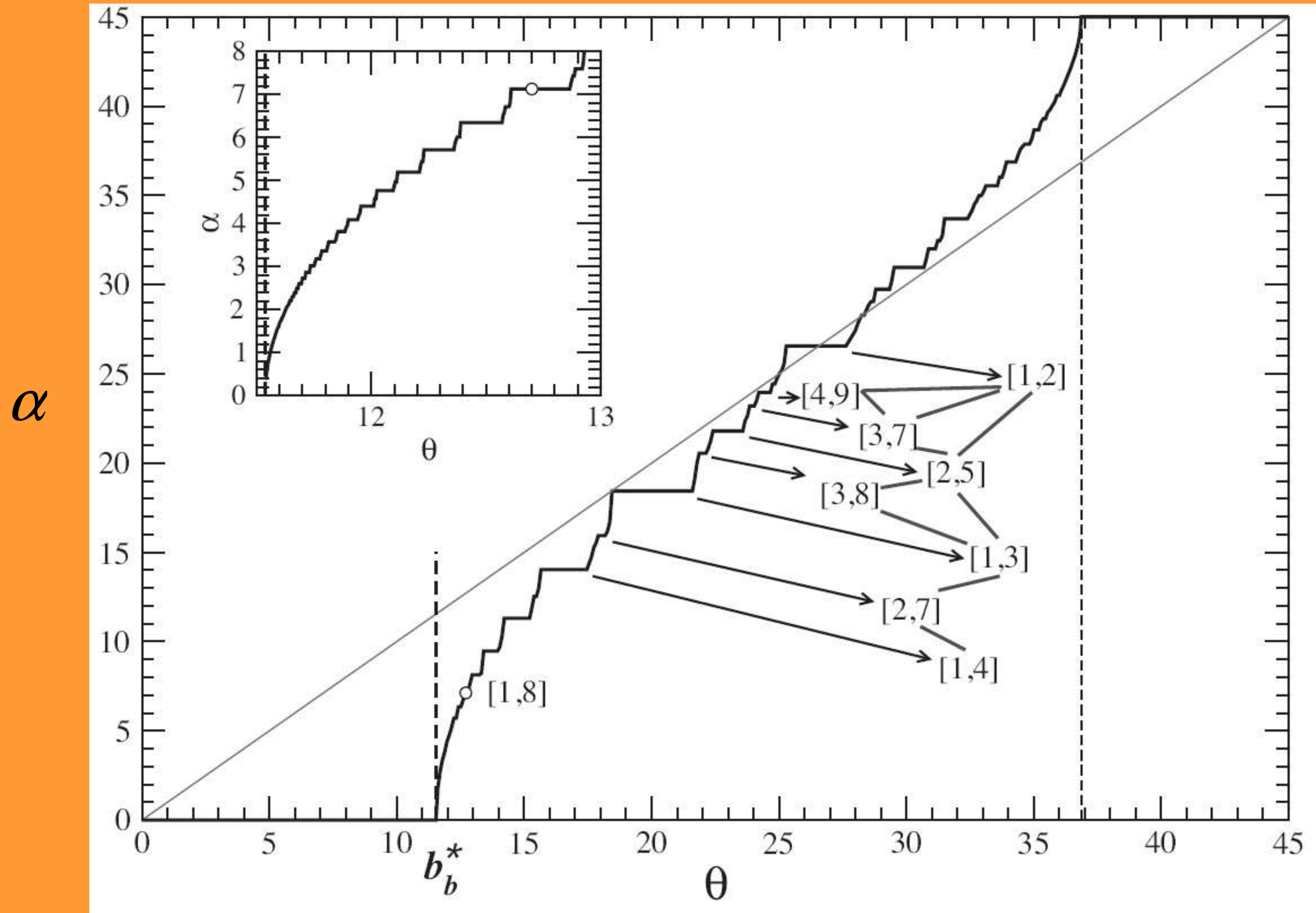
b_1^*= region of irreversible collisions
b_2^*= fixed point with $b_0=b_c$
b_3^*= region of reversible collisions
b_4^*= fixed point at bifurcation angle
$\theta = \theta_b = \sin^{-1}(R/(f\,L))$

(l = 2.5; f = 2.0; $b_m = \sqrt{3}/2$; b_c = 0.6; β_b = 0.5; θ_b = 11.54°)

Trajectory with a periodicity of q = 9.



Poincare map of the incoming collision parameter b_0 onto itself after passing through q unit cells. ($\beta = 0.55 > \beta_b$; $l = 2.5$; $f = 2.0$; $b_m = \sqrt{3}/2$; $b_c = 0.6$; $\beta_b = 0.5$; $\theta_b = 11.54^o$)



Migration angle α as a function of forcing angle θ.
Critical forcing angle causing tangent bifurcation is b_b^*

Stochastic transport: High Peclet number

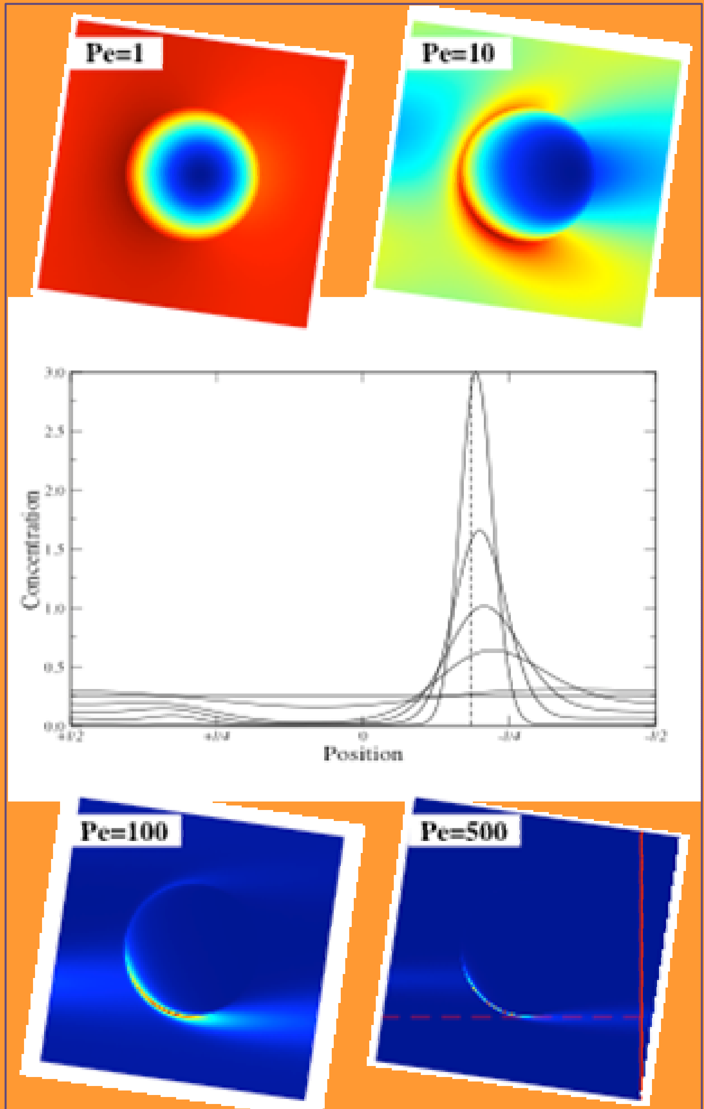
Fokker-Planck equation for probability density
for stochastic motion of colloidal particles

$$\frac{\partial}{\partial t}P(\mathbf{x},t)+f\frac{\partial}{\partial x}P(\mathbf{x},t)-\frac{1}{Pe}\nabla^2 P(\mathbf{x},t)=0, \quad r>1$$

$$where\ Pe=\frac{F_{\max}}{D\gamma}R$$

Average migration angle α

$$\tan(\alpha)=\frac{\langle U_y\rangle}{\langle U_x\rangle}\left\{\int_0^l dx\left[-D\frac{\partial}{\partial y}\mathbf{P}_\infty(\mathbf{x})\right]\right\}*\left\{\int_0^l dy\left[f\,\mathbf{P}_\infty(\mathbf{x})-D\frac{\partial}{\partial x}\mathbf{P}_\infty(\mathbf{x})\right]\right\}^{-1}$$



Steady-state solution $P_\infty(X)$ of Fokker-Planck equation on a unit cell

$l = 4.0$
$f = 1.0$
$\theta = 8.53^o$

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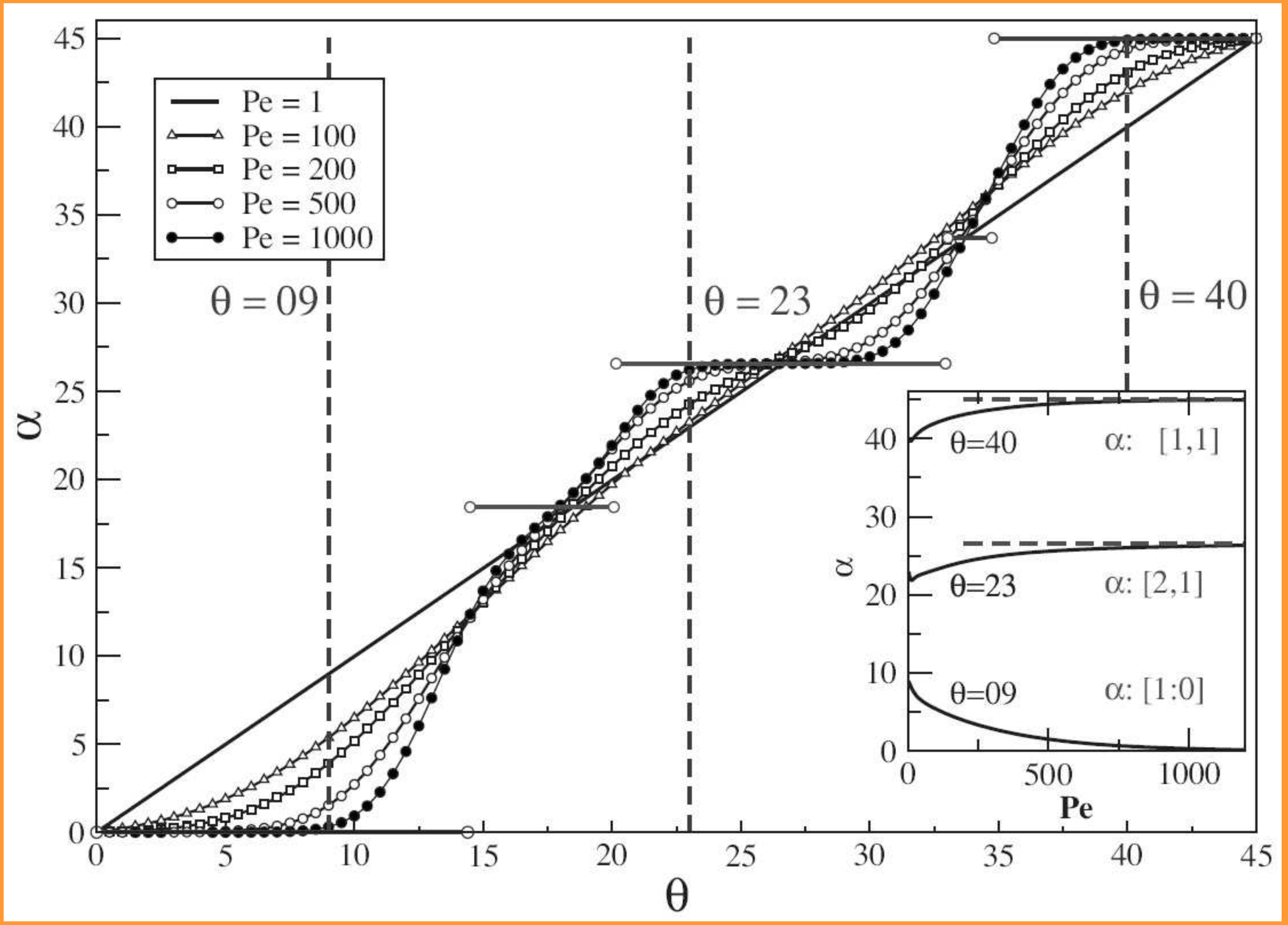
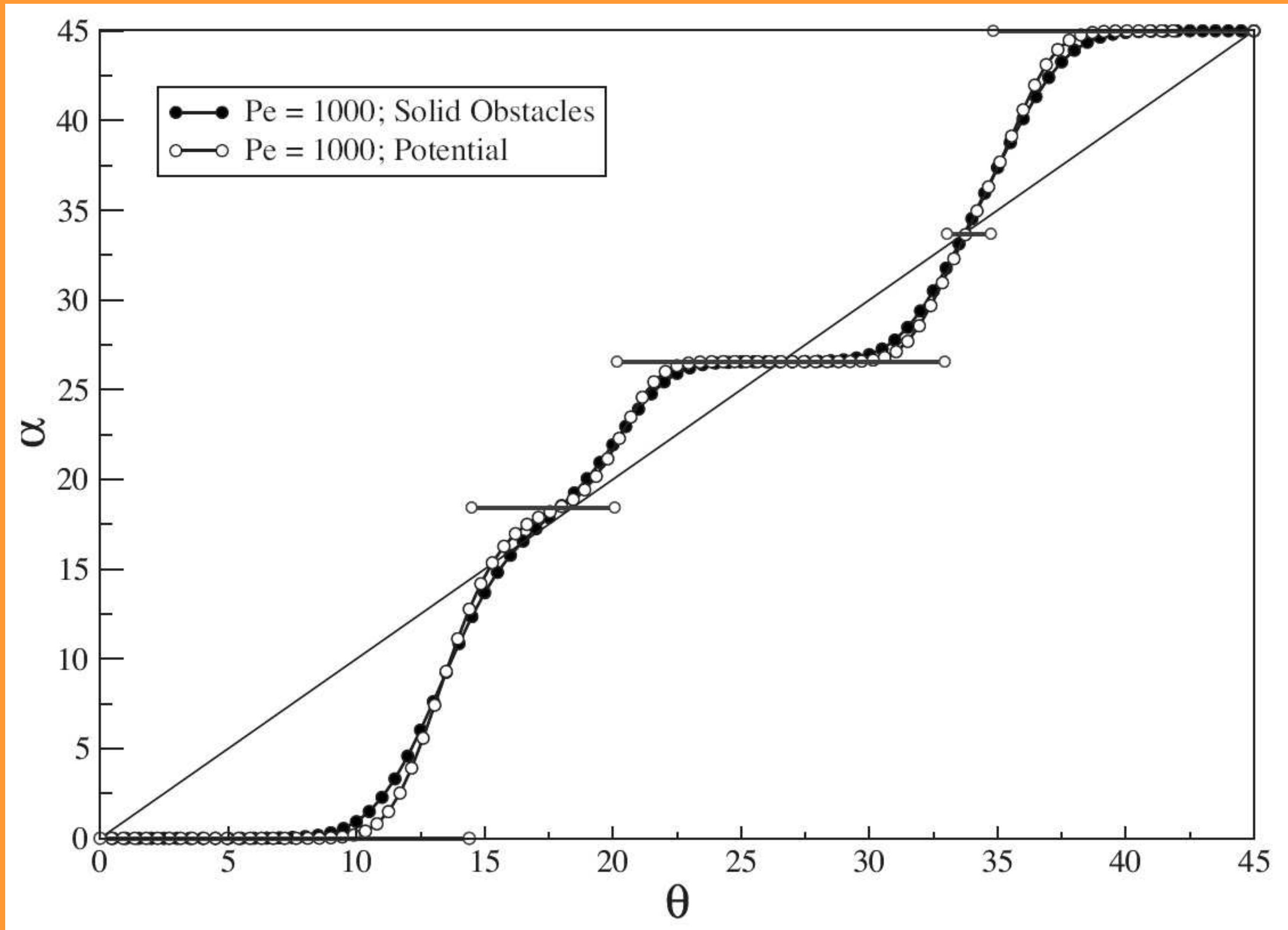


Average migration angles α for different forcing angles θ



Migration angle α as a function of forcing angle θ.
(l = 4, f = 1)

Application to microfluidic devices

Example of particle separation

Bifurcation angle is $\theta_b = \sin^{-1}(R/(fL))$

Particle size affects $R = R_0 + a$

R_0 = radius of the obstacle
a = radius of the particle

For $a_1 = 4\mu m$ $a_2 = 6\mu m$
$R_0 = 5\mu m$ $L = 25\mu m$
$U \approx 10\mu m/s$ $f \sim 1$

Bifurcation angles are $\theta_{b1} = 21.1^o$ $\theta_{b2} = 26.1^o$

Therefore for $\theta_{b1} < \theta < \theta_{b2}$ particles will separate with
$\alpha_1 = 26.56^o$ (lattice direction [2,1]) and $\alpha_2 = 0^o$