Understanding colloidal particle dynamics in microfluidic obstacle arrays with symbolic dynamics

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NORDITA Soft Matter Seminar
September 1, 2020

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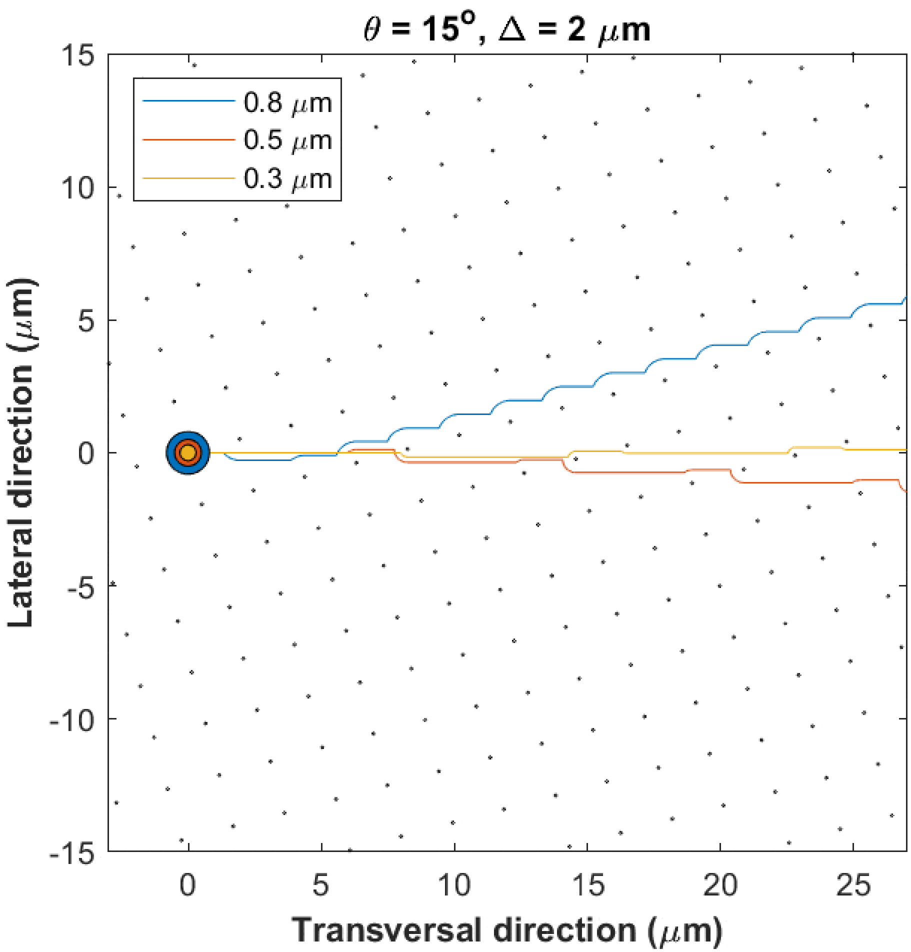
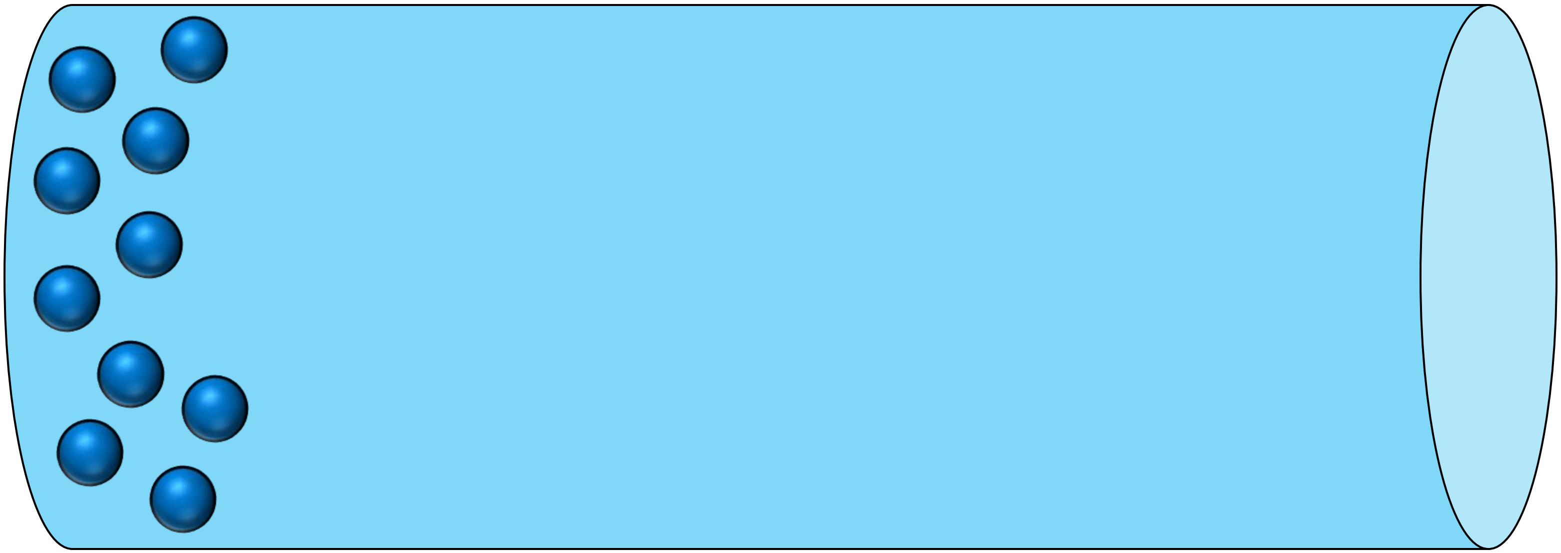


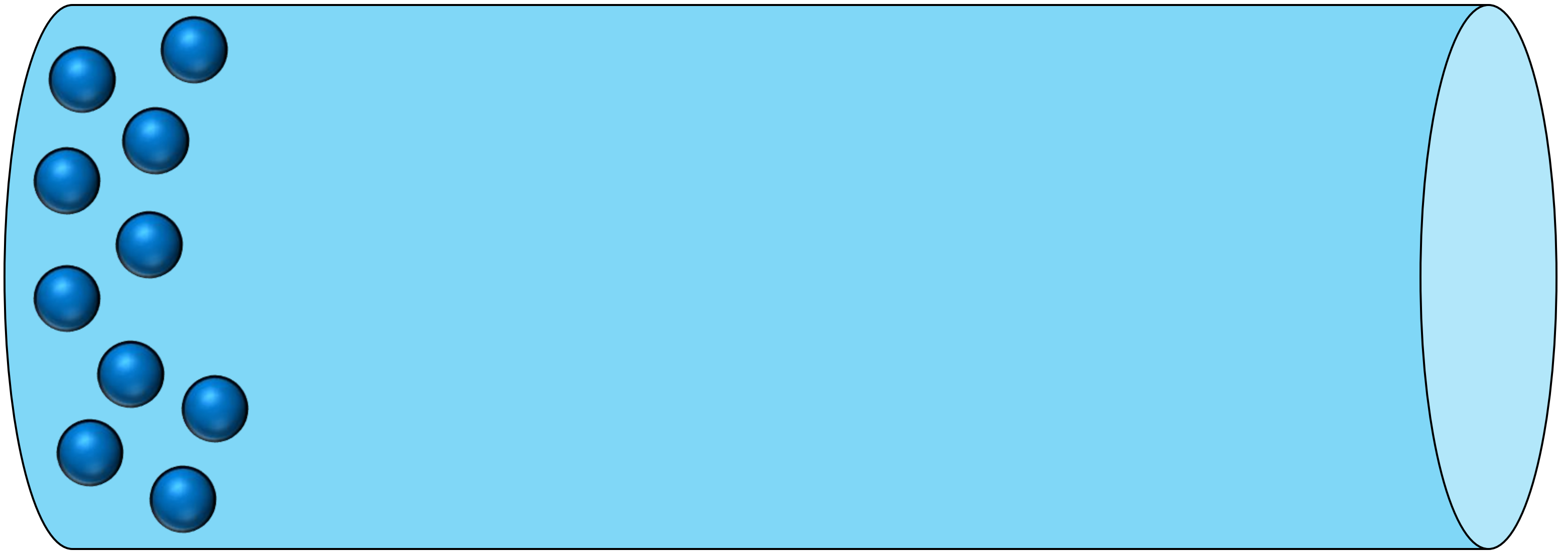
Prelude: laminar flow of colloidal particles through a long pipe should be straightforward



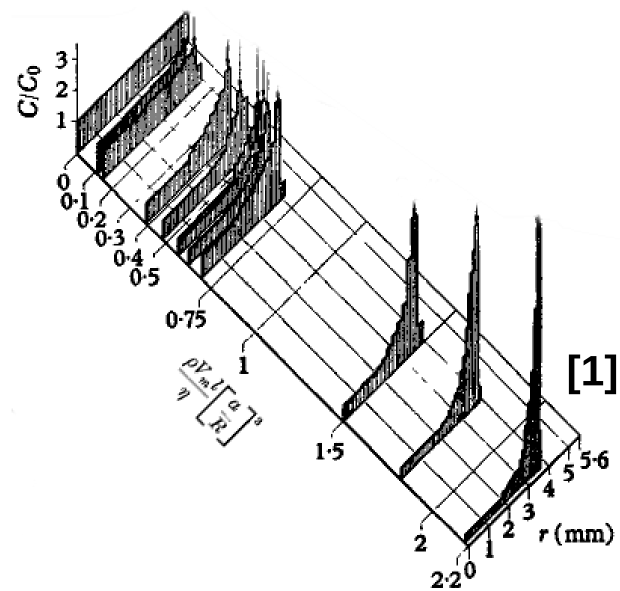
Laminar & fully developed flow → no nonlinearities in the Navier-Stokes equations.

$$\mu \nabla^2 \vec{\mathbf{u}} = \nabla \mathbf{p}$$

Prelude: laminar flow of colloidal particles through a long pipe should be straightforward, but isn't

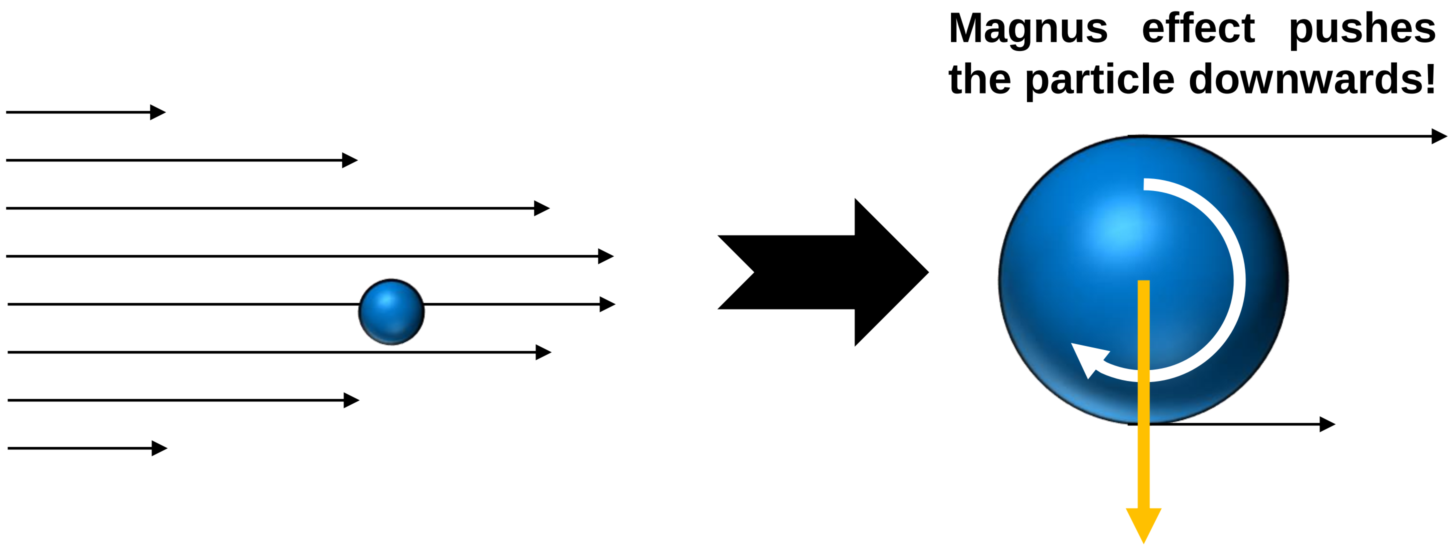


Particles laterally and *irreversibly* flow into a specific annular region within the pipe (Segré-Silberberg effect)!



[1]

Inertial effects can play a significant role even in low Reynolds number systems



Moral of the story:
Particle inertia + colloidal dispersion = macroscale inertial effects even in low-Re systems!

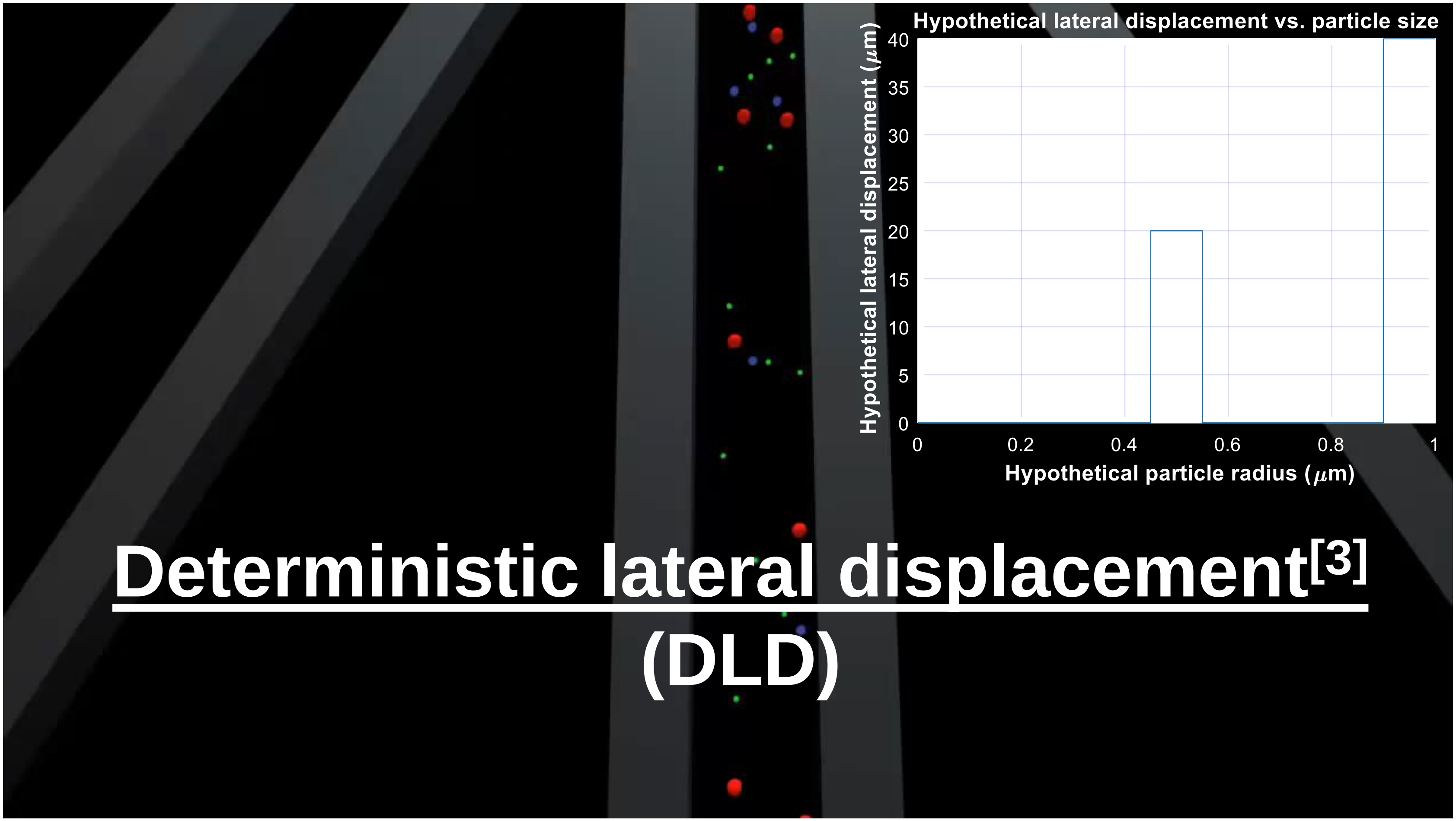
Colloidal particles flowing through a channel will displace laterally when interacting with an obstacle

Expectation for low Reynolds number

What usually happens

Colloidal particles flowing through an obstacle-patterned channel show size-dependent dynamics

[2]



The dynamics of a colloidal particle in a fluid are very complicated

The Maxey-Riley (or Basset-Boussinesq-Oseen) equation[4]:

Particle acceleration **Local fluid acceleration** **Added-mass effect (accounts for fluid mass displaced by particle)**

$$m_p \dot{\mathbf{v}} = m_f \frac{D}{Dt}\mathbf{u}(\mathbf{r}(t),t) - \frac{1}{2} m_f \left(\dot{\mathbf{v}} - \frac{D}{Dt}\left[\mathbf{u}(\mathbf{r}(t),t) + \frac{1}{10} a^2 \nabla^2 \mathbf{u}(\mathbf{r}(t),t)\right]\right)$$

$$-6\pi a \rho_f \nu \mathbf{q}(t) + \left(m_p - m_f\right)\mathbf{g} + \boldsymbol{\delta}\big(\mathbf{r}(t)\big) - 6\pi a^2 \rho_f \nu \int_0^t d\tau \frac{d\mathbf{q}(\tau)/d\tau}{\sqrt{\pi\nu(t-\tau)}}$$

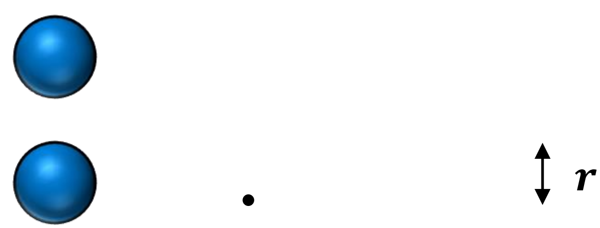
Drag (Stokesian) **Buoyancy** **Particle-obstacle contact force** **Basset force (accounts for time-lag in boundary layer development lag)**

$$\mathbf{q}(t) \equiv \mathbf{v}(t) - \mathbf{u}(\mathbf{r}(t),t) - \frac{1}{6} a^2 \nabla^2 \mathbf{u}$$

We have taken complicated analyses of particle motion through these lattices and simplified it into a dynamical sequence

- **Assumptions we make:**
  - **Peclét number is large**
  - **Obstacles are negligibly small**
  - **Particle-particle interactions are negligible**
  - **Particle-obstacle interactions are modeled as hard-sphere repulsion forces[5]**

- **With these assumptions, trajectories can be approximated as purely streamwise advection plus a sequence of lateral displacements from collisions!**



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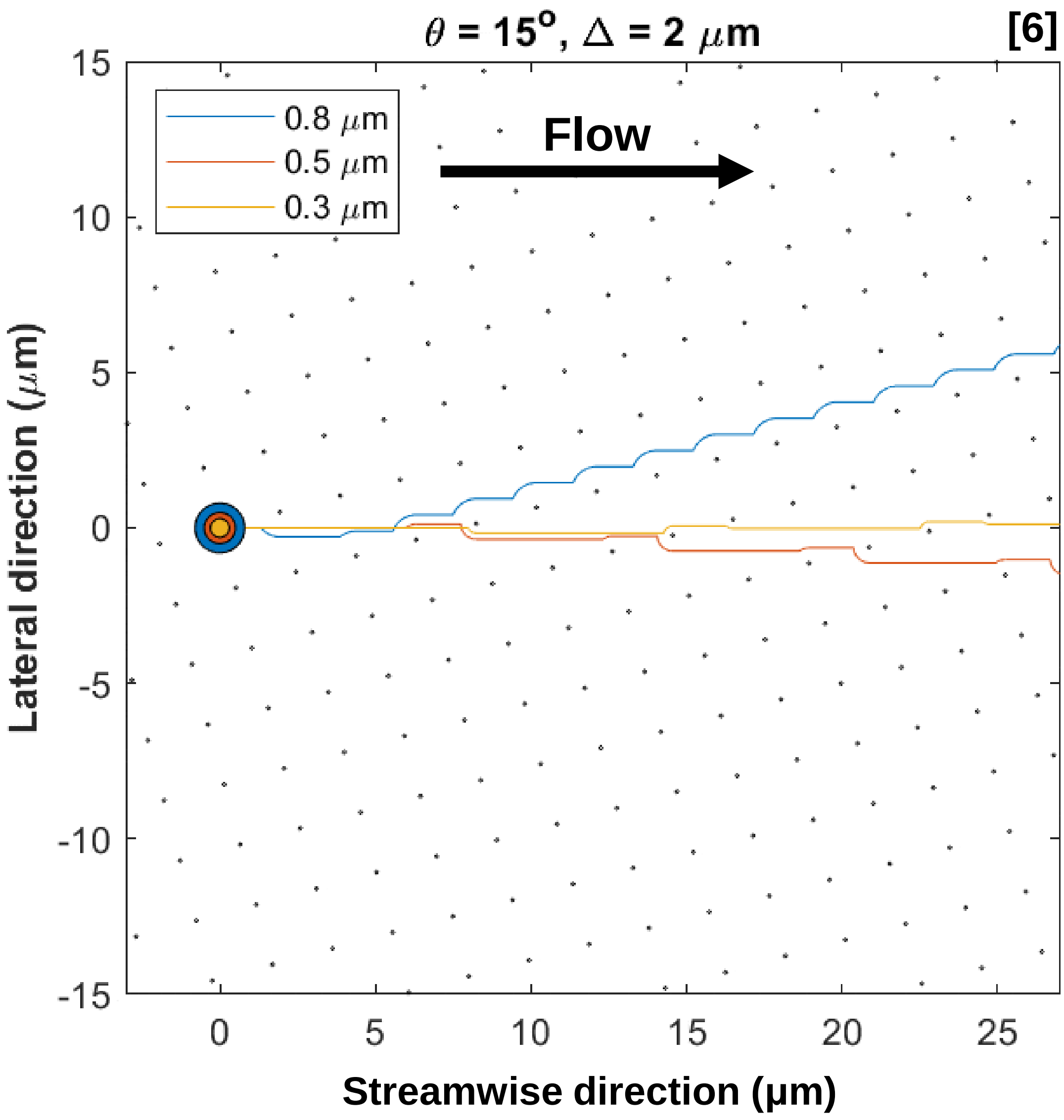
This simplified dynamical model reproduces deterministic lateral displacement



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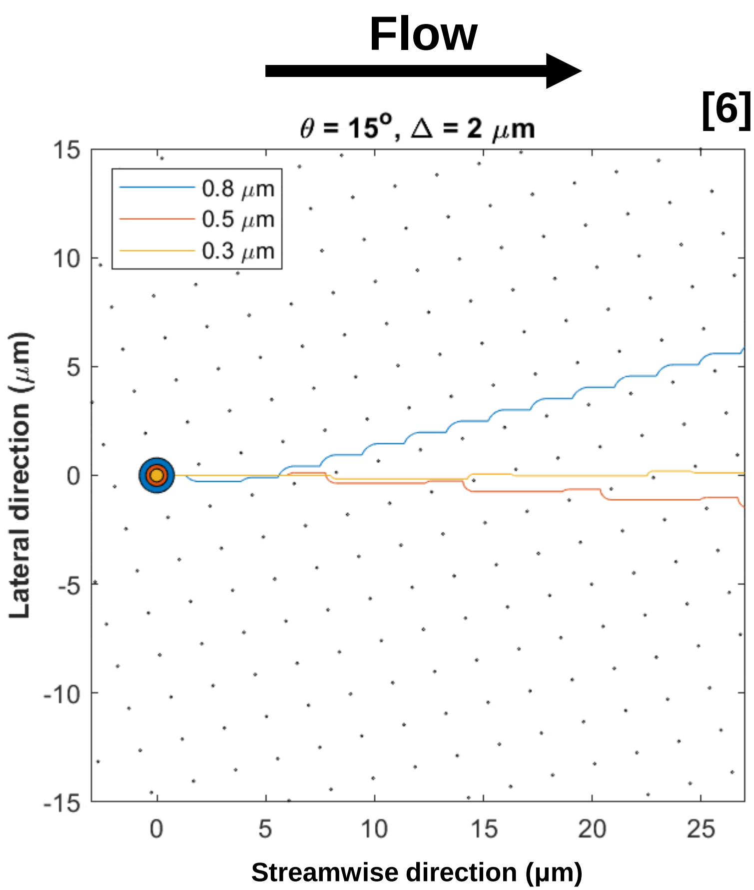
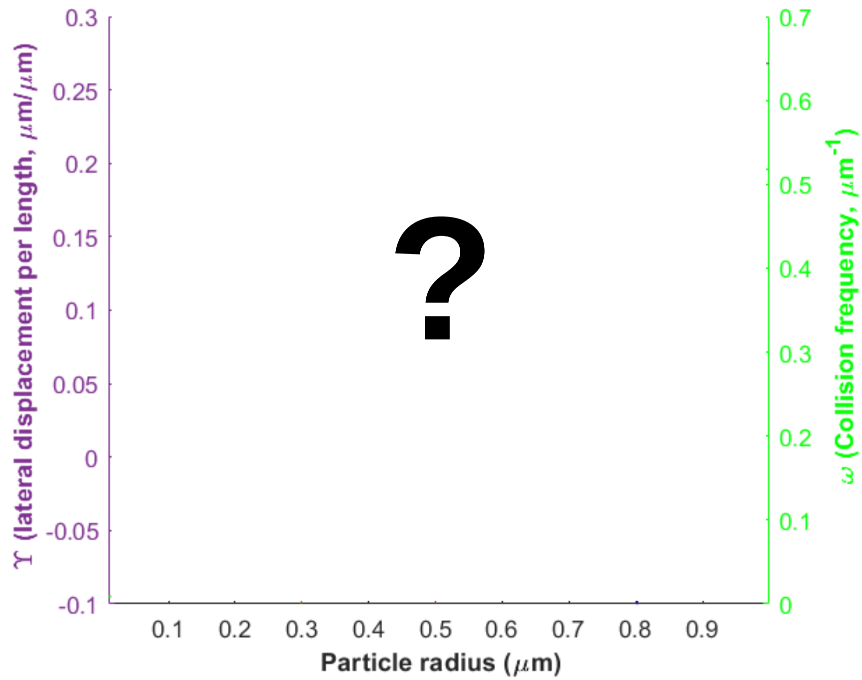
Our goal was to construct a theory that allowed us to obtain key dynamical readouts as a function of particle size & lattice geometry





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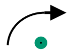
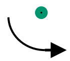
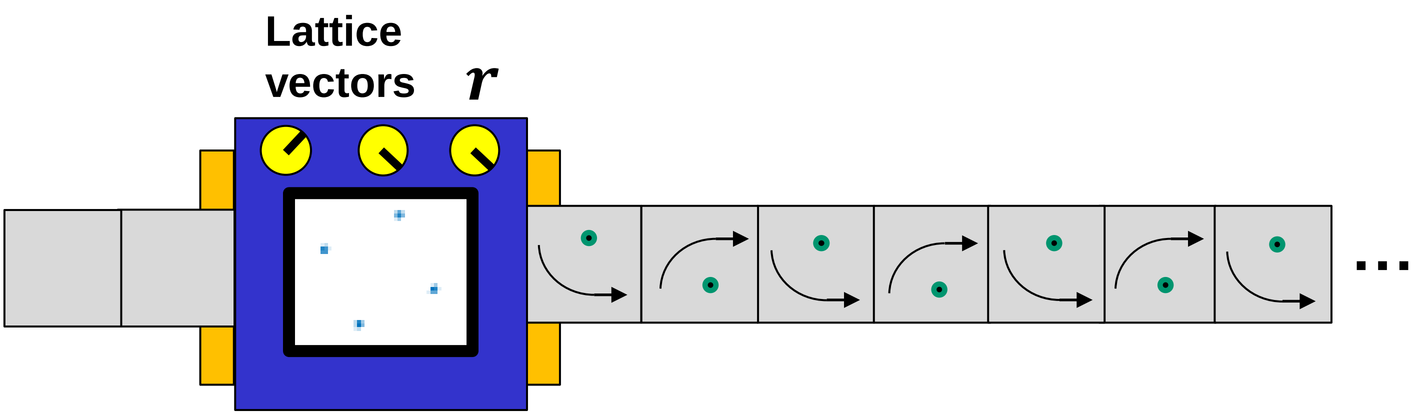
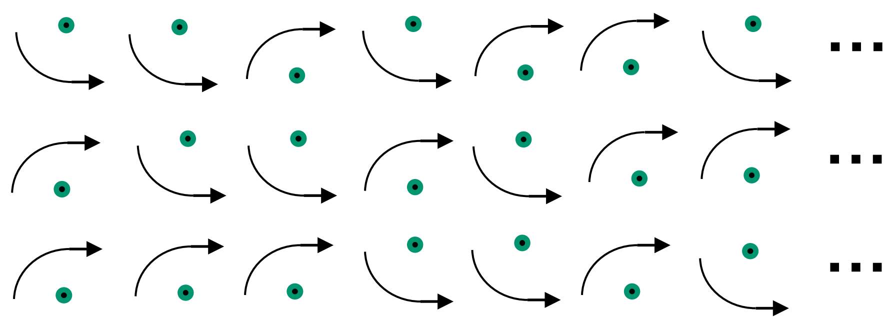
Our model describes colloidal particle advection through lattices as a discrete sequence of collision outcomes using symbols

- After colliding with an obstacle, the particle displaces either up or down a distance of r from the obstacle it collided with.
  -  or 



What sequences can occur?



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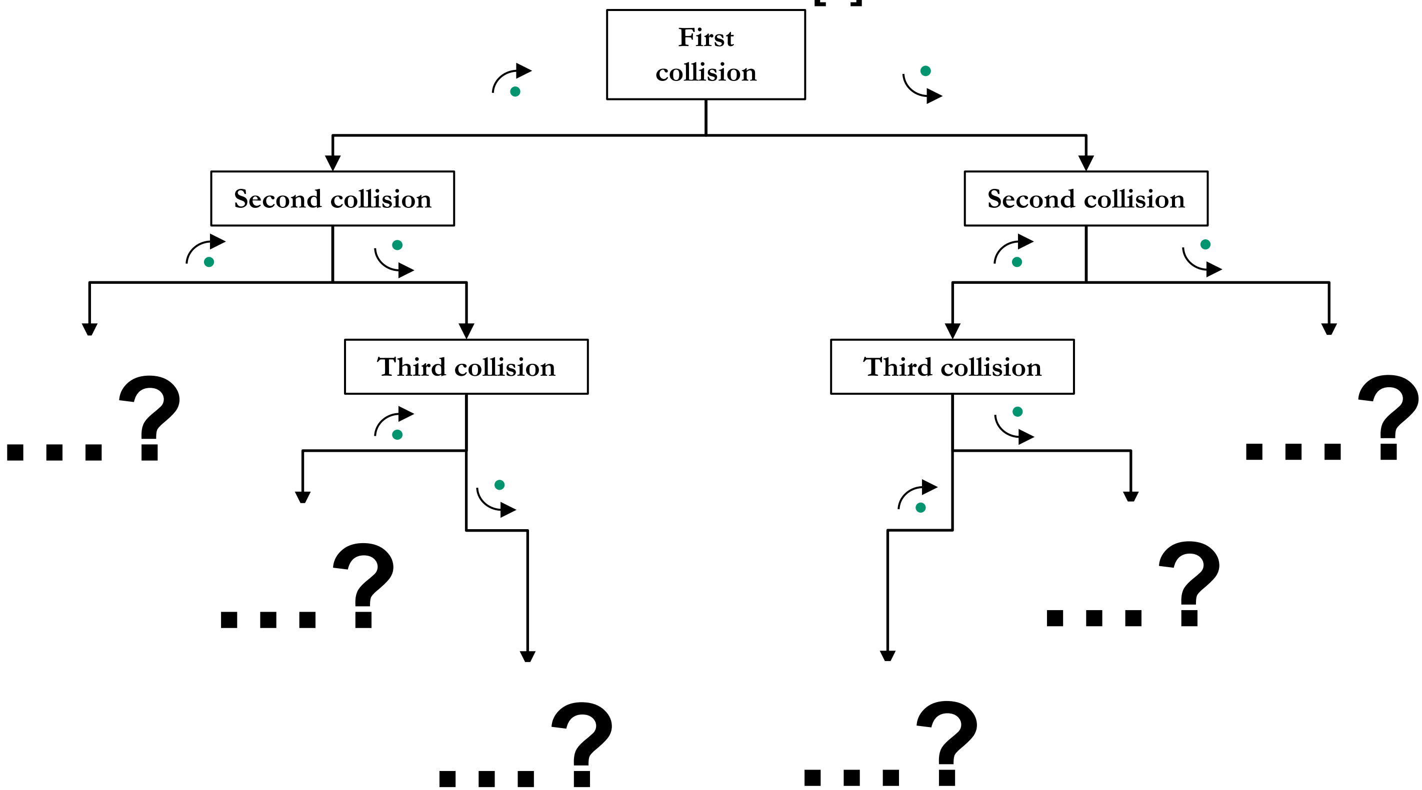
The spatial symmetry of the collisions heavily restricts the kinds of paths the particles can take

[6]



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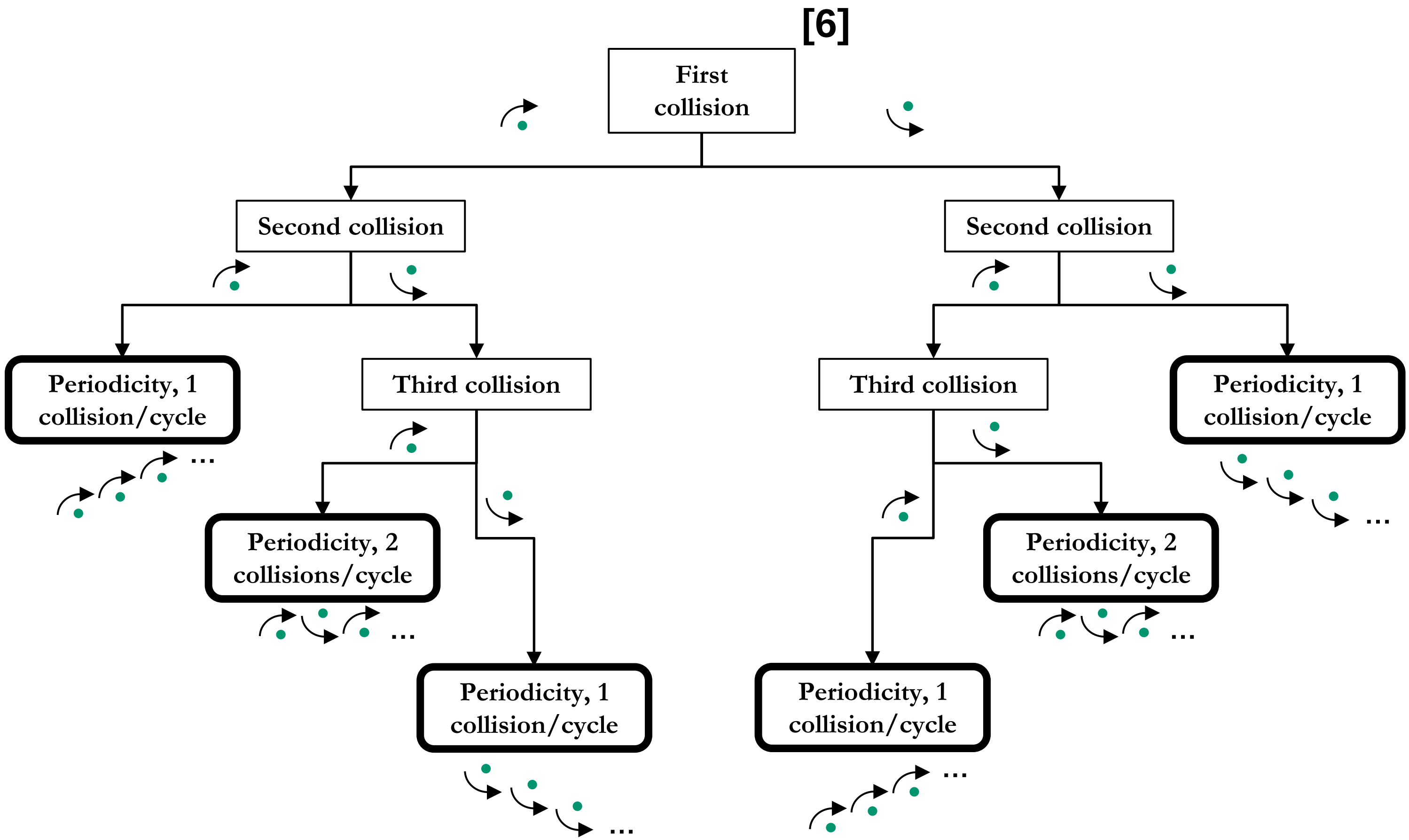

First observed in [7], we term the general phenomenon "symmetry-induced cyclical dynamics"

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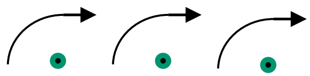
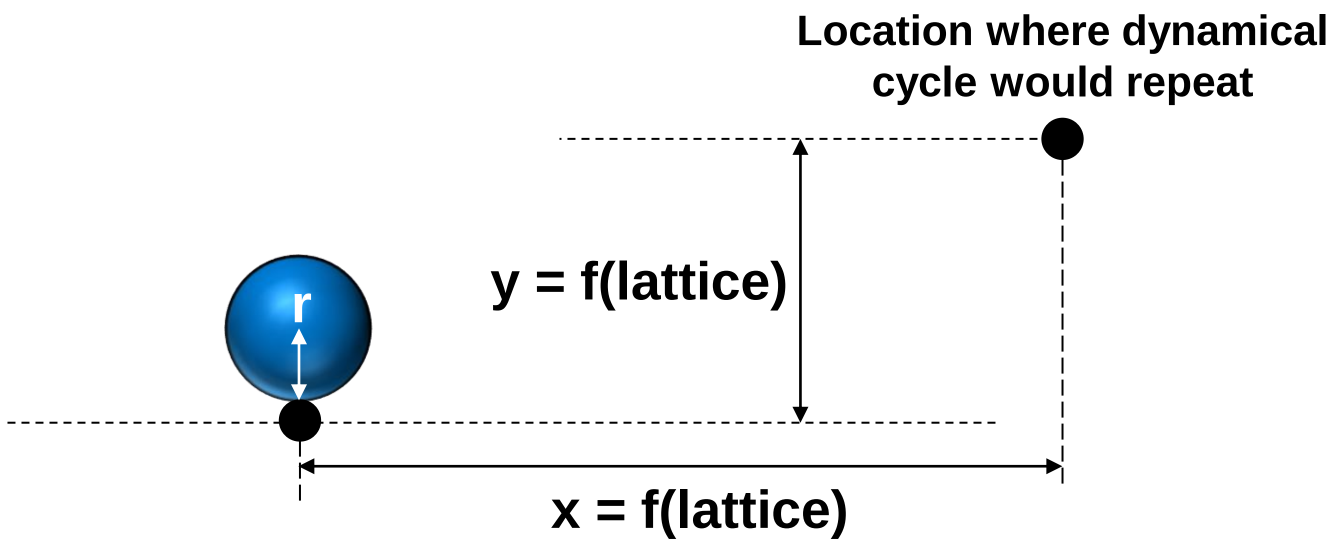
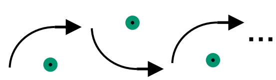
After determining which orbits are possible, we can determine the conditions needed for each to occur

- **Under what conditions does a particle follow a  … orbit?**



$r \geq |y|$

True of  as well!

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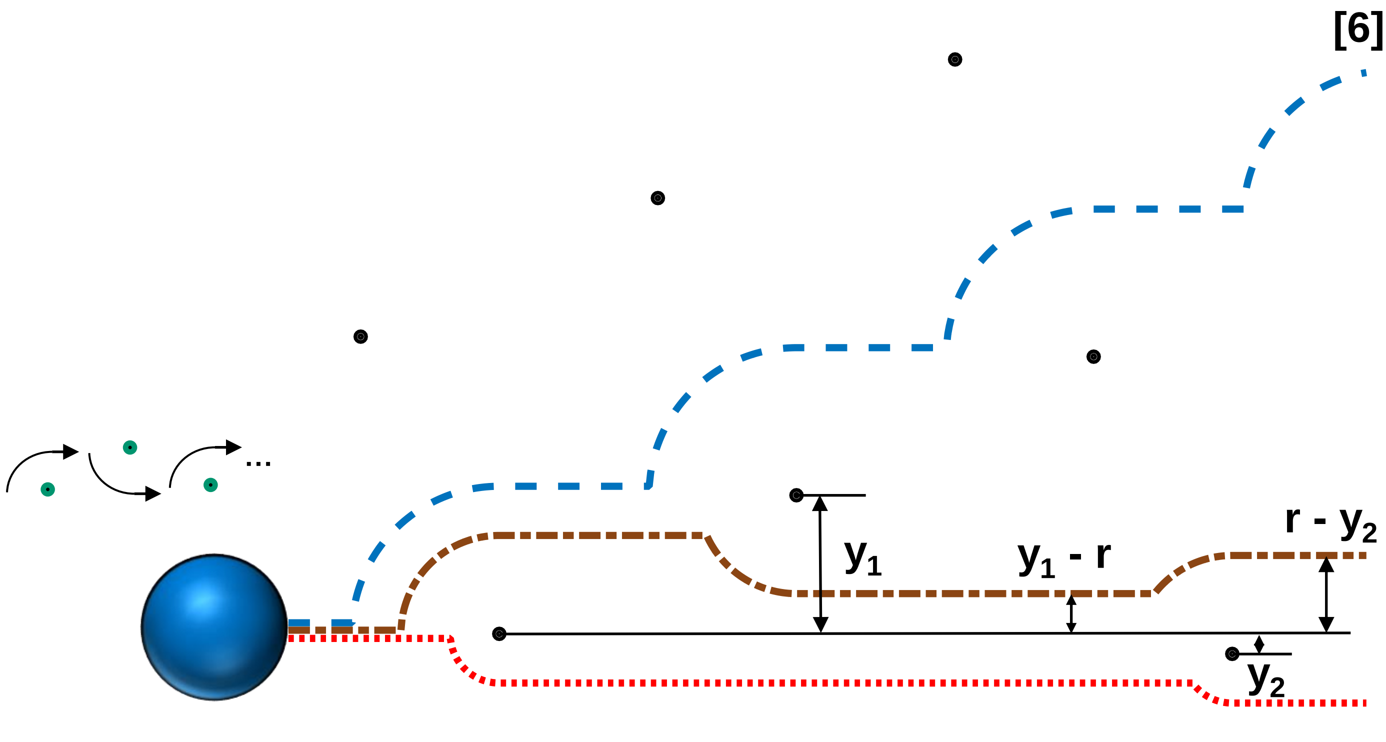
After determining which orbits are possible, we characterized trajectories that were previously not fully understood



Period-2 orbit occurs if $y_1 - r \leq r - y_2$ or

$$y_1 \geq r \geq \frac{y_1 + y_2}{2}$$

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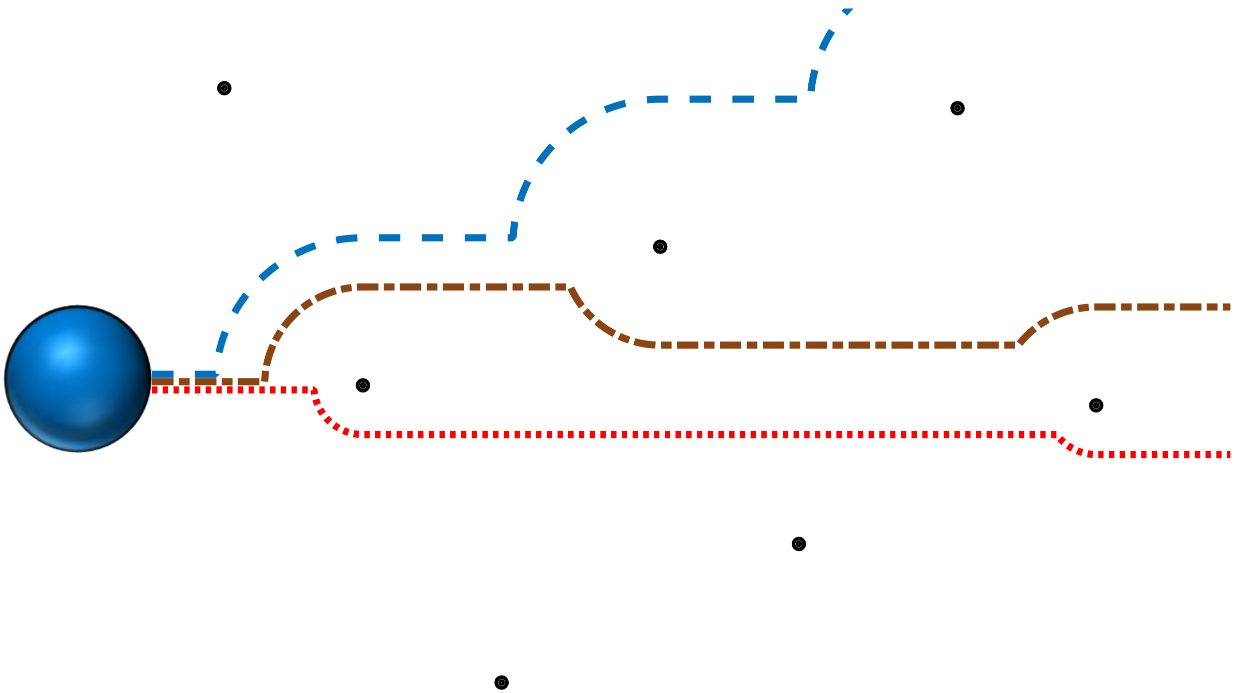
After determining which orbits are possible, we characterized trajectories that were previously not fully understood

[6]

As a function of particle radius, there is always a period-2 orbit sandwiched between period-1 orbits <u>for all obstacle lattice geometries</u>!



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We can determine the lattice coordinate where a trajectory repeats its dynamical cycle

Sort lattice coords. (x,y) by increasing x value
r = biggest possible value, y_{prev} = y of first obst. on list
For increasing x > 0,
    if r ≥ |y|
        if $r \geq \frac{|y|+|y_{prev}|}{2}$
            mode is period-2 (g = 2)
            next mode is period-1 on same (x,y)
        else
            mode is period-1 (g = 1)
    $y = y_{prev}$
    decrease r enough to not satisfy inequality
    else
        proceed to next (x,y) pair in sequence
end

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We can now obtain key dynamical readouts for particles displacing through lattices of this type

- **If we average the lateral displacement and collision frequency over a single dynamical cycle:**
  - **Lateral displacement per length =** $\frac{y}{x}$
  - **Spatial collision frequency =** $\frac{g}{x}$

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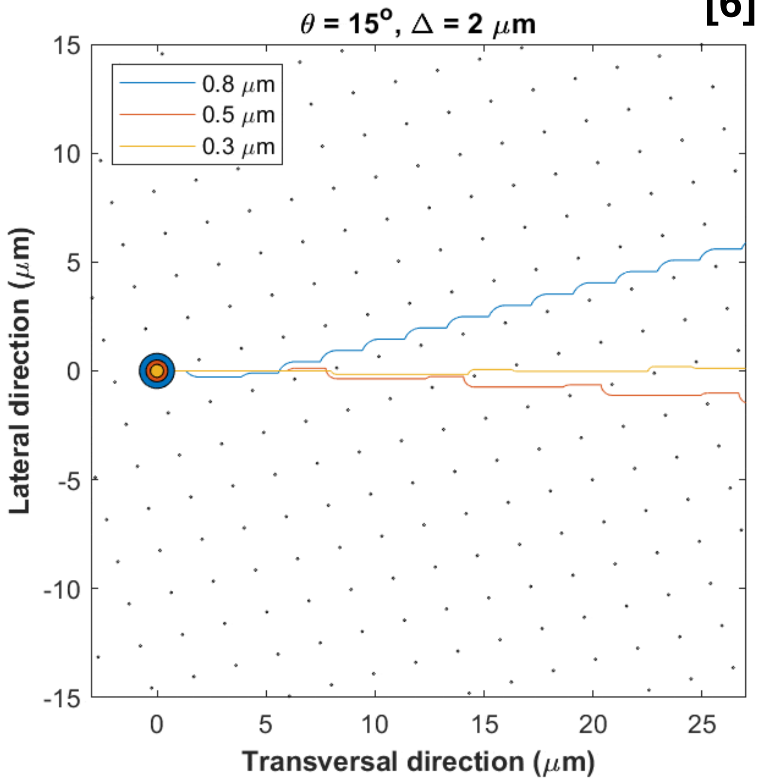
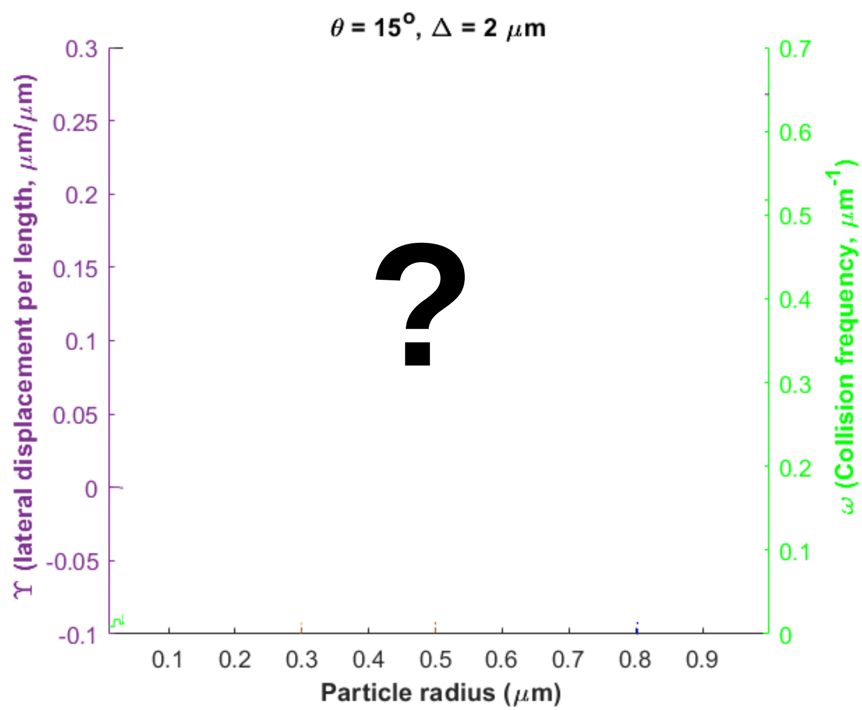
We've used this framework to predict all possible particle trajectories through the microchannel

- **Thanks to this theoretical framework, we can fully predict the trajectories a particle can take through the microfluidic lattice.**

[6]





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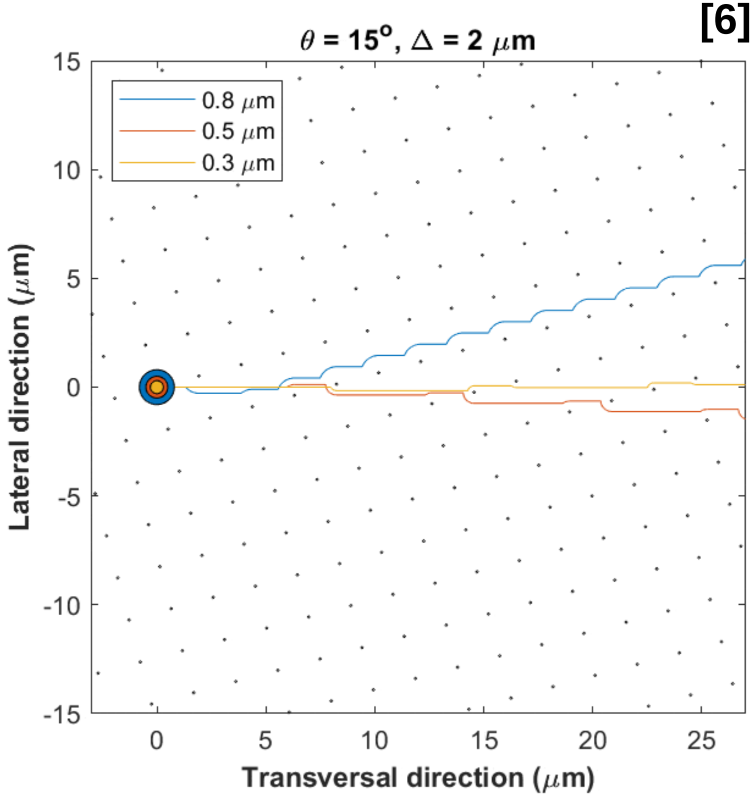
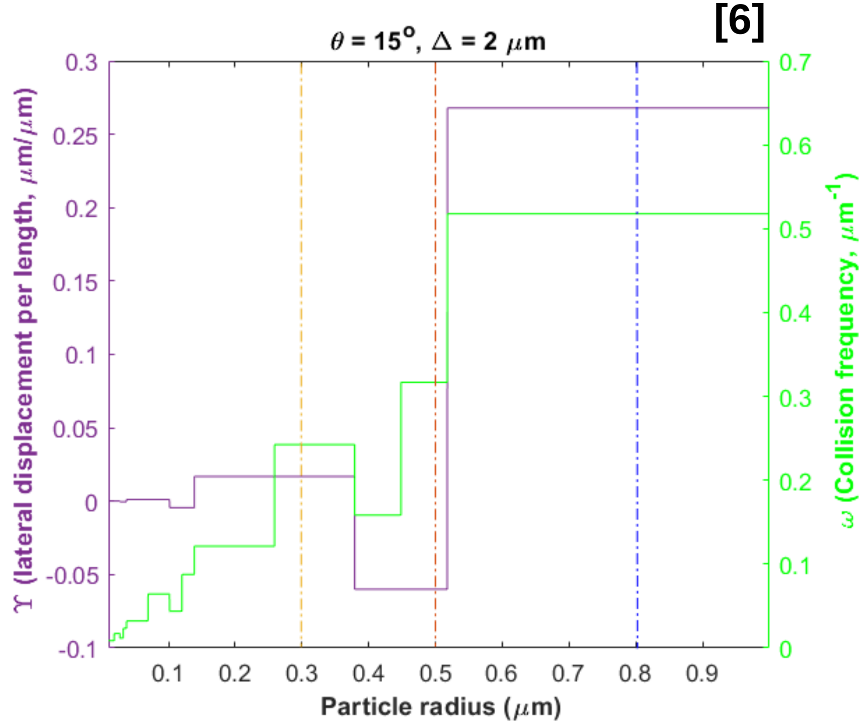


[6]



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Work in the literature validates that we have captured the dominant physics and that the theory is extendable

- **Our results are in good qualitative & quantitative agreement with what's been described in the literature ([3][7][8][9] among many others).**

- **Particularly, [9] discusses the existence of a parameter describing the irreversible displacement of a particle after a collision in a square lattice of finite-sized obstacles.**
  - **Incorporates finite obstacle size/hydrodynamics**
  - **Converges to +/- r in the infinitesimal obstacle limit**
  - **Could this Risbud-Drazer parameter be the key to extending this theory to finite sized obstacles?**

Acknowledgements

Kirby Research Group

E. Bowins
R. George
M. Harnett
A. Jayaraman
A. Kang
B. J. Kirby, Ph.D.
A. Paranjape
J. Radzio
A. Rodriguez-Gonzalez
A. Sanchez
P. Sehgal
K. Wellmerling

External Collaborators

J. Gleghorn

Funding:

Alfred P. Sloan Foundation
Graduate Scholarships
Program

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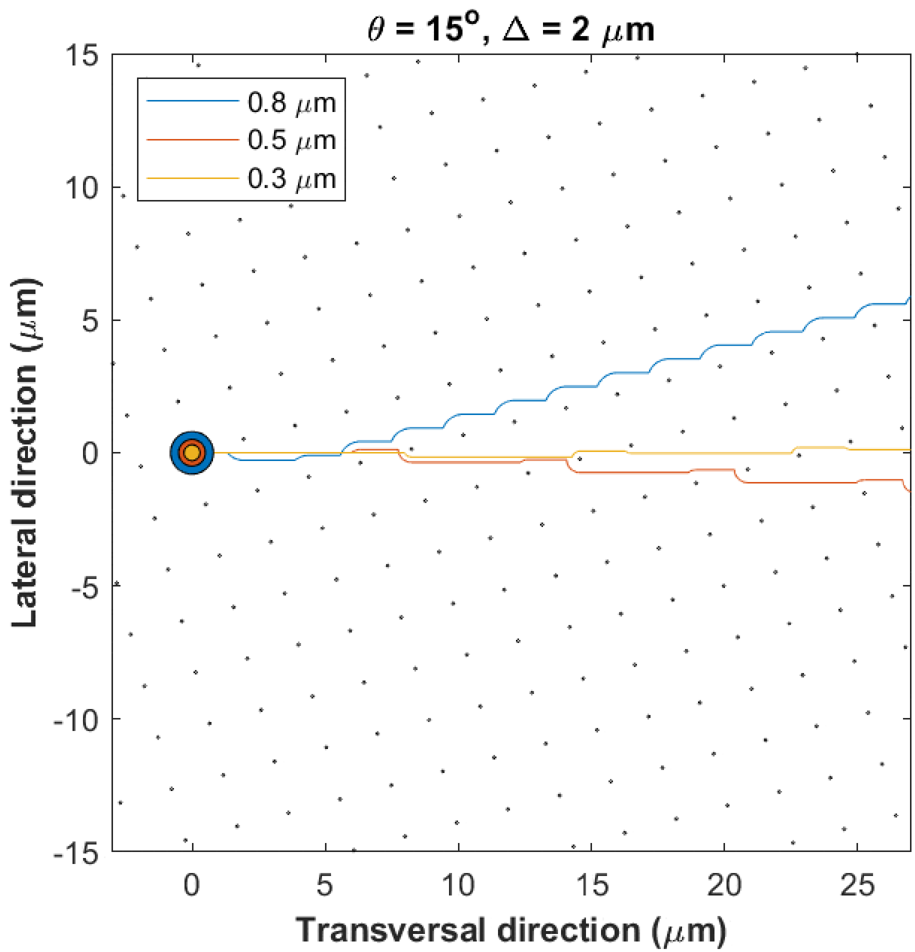
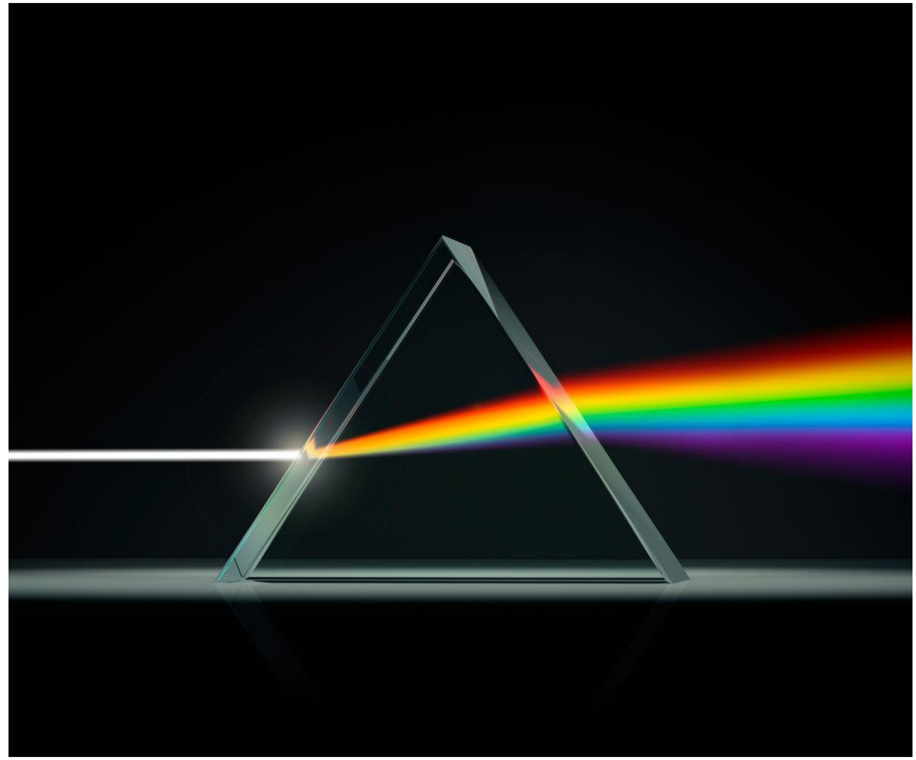


Chaining Obstacle Lattices Lets Us Generate Versatile Particle Sorting Microdevices

- **We can chain obstacle lattices with different parameters to obtain displacement behaviors unavailable in single lattices.**

- **Total lateral displacement and collision number are additive.**



Total lateral displacement

$$d = \sum_{i=1}^{N} d_i = \sum_{i=1}^{N} \ell_i \Upsilon_i$$

Lateral displacement per length

Total no. of collisions

$$c = \sum_{i=1}^{N} c_i = \sum_{i=1}^{N} \ell_i \omega_i$$

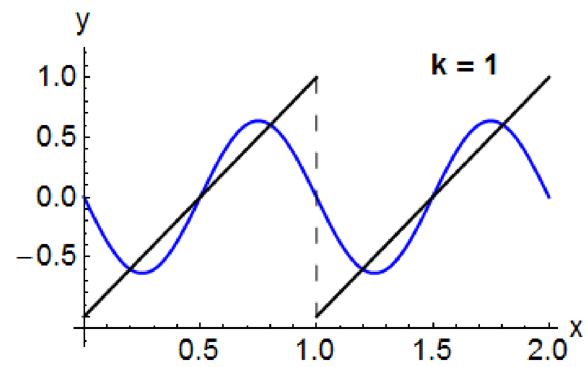
Spatial collision frequency

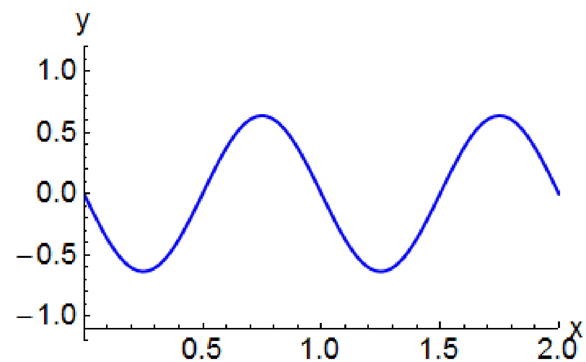
Lattice length (streamwise)

Our method of approximating target functions is very similar to Fourier series approximation

$$d(r) = \sum_{i=1}^{n} \ell_i \Upsilon_i$$

$$f(x) = \sum_{k=0}^{\infty} \left(a_k \cos \frac{k\pi x}{L} + b_k \sin \frac{k\pi x}{L} \right)$$





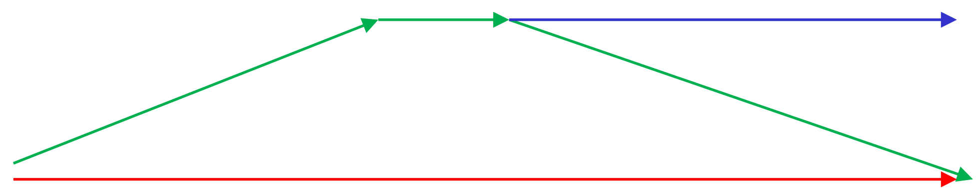
Same mathematical structure, but Υ_i are not orthonormal!

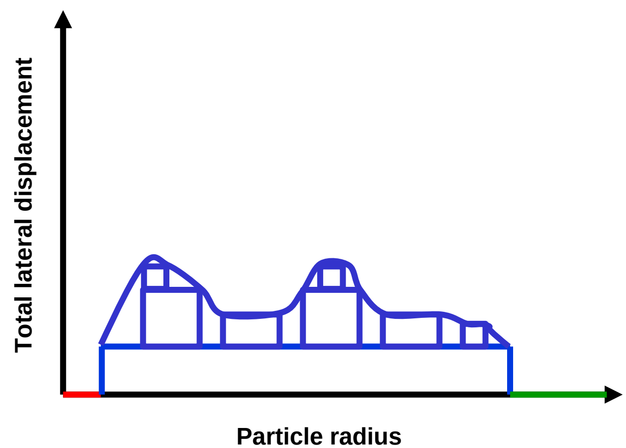
How do we know this kind of approximation process can always work?

We've shown that we can approximate any given lateral displacement function of size with chained lattices

- We *can* approximate any lateral displacement function of particle size using a sequence of specific pairs of rotated square lattices.

- The type of approximation we use is convergent with respect to many common error metrics, like least squares and least absolute deviation for both continuous and discrete functions.





We have developed a systematic inverse design algorithm for microfluidic lattice chains

- For a chain of n lattices, we find the individual lattice parameters that best approximate some target function.
  - Lattice parameters $\ell_i, \vec{a}_i, \vec{b}_i \rightarrow \ell_i, \Delta_i, \theta_i$

- We approximate by sequentially increasing lattice number.
  - Lattice complexity reduced as much as possible.
  - Accuracy thresholds can be established.
  - Convergence guaranteed.

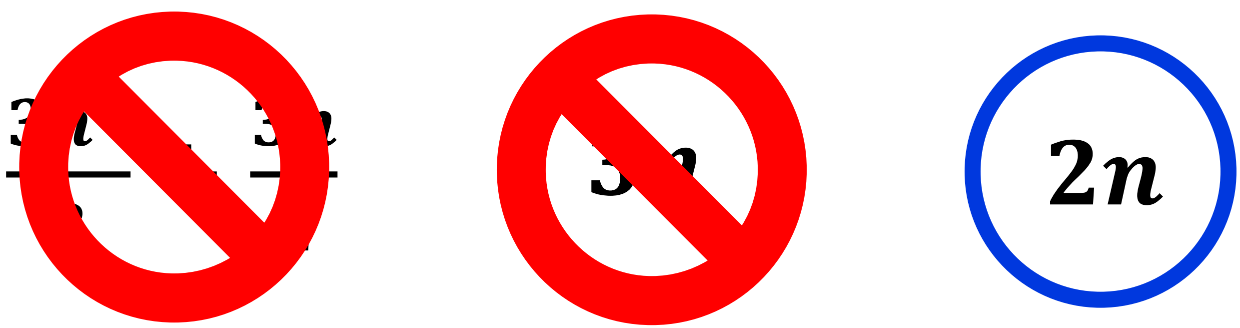
Optimization algorithm dimension:

$$\frac{3n^2}{2} + \frac{3n}{2}$$

n	Dimensions
1	3
2	9
3	18
4	30

We have significantly improved dimensionality constraints by applying mathematical tools

- **Least-squares solving reduces dimensionality drastically.**
  - **Hilbert projection theorem ensures sequential solutions are still global solutions.**
  - **Since lateral displacement is linear in lattice lengths, closed-form solutions for lengths exist given the other two parameters.**



- **To ensure unique solutions, we maximize the inner product of the target function with the lateral displacement per length function when lattice length is zero.**

To validate our designs, we utilize three different techniques and three different design metrics

Metrics

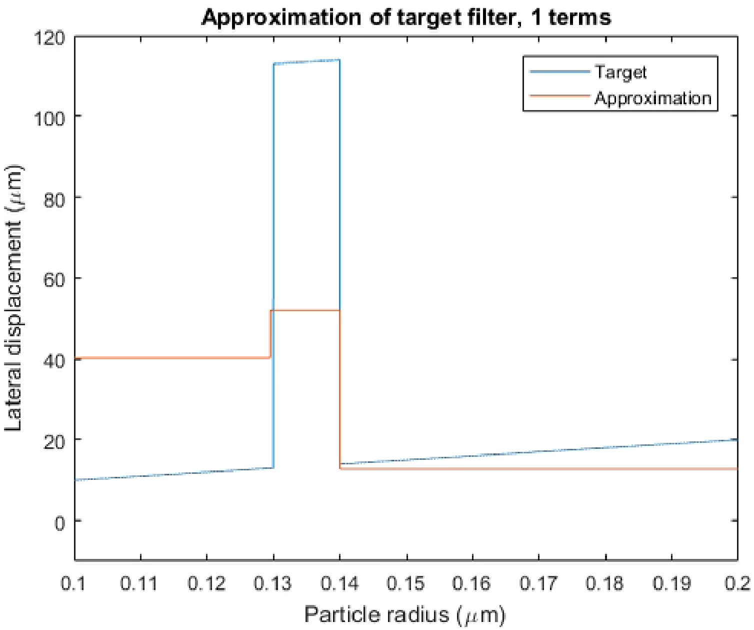
- **Device complexity (# of lattices)**
  - **High complexity leads to amplification of edge effect/lock-in errors between lattices**
- **Total device length**
  - **Large device lengths cause lateral pressure gradients to develop, harming the DLD effect**
- **Mean square error to target**
  - **Large error diminishes intended device performance**

Techniques

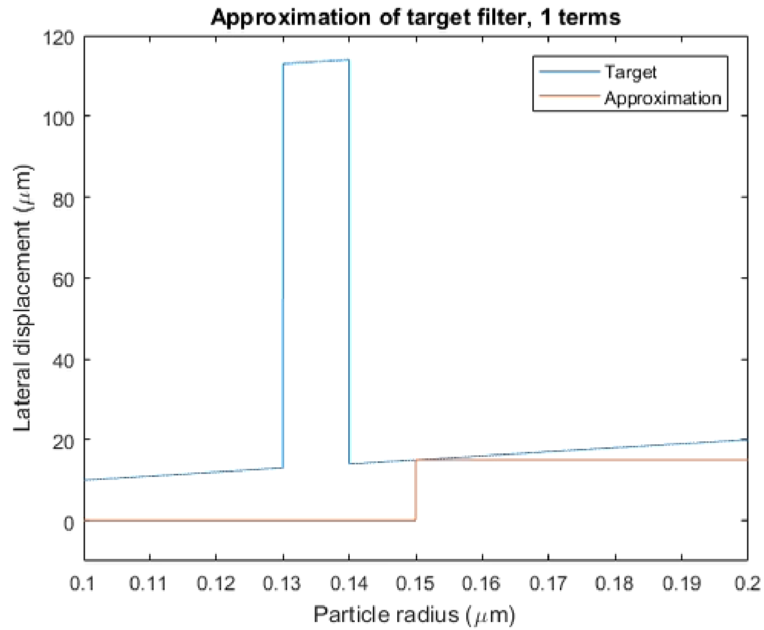
- **Direct L2**
  - **Directly finds the lattice parameters that minimize the cost function with no extra constraints.**
- **θ-restricted L2**
  - **As above, but fixing the angle such that LD function are step functions.**
- **Riemann**
  - **Doesn't use optimization, fits the target with step functions. Consistent with current design strategies.**

Optimization improves error convergence considerably for nearly every target function

Direct L2 method



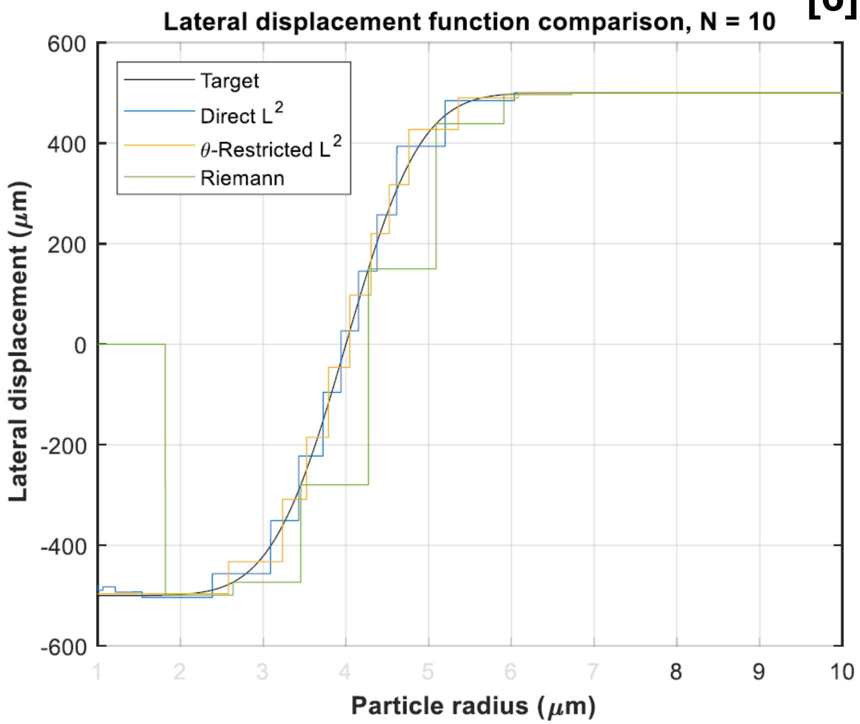
Riemann method



Our algorithms are considerably better at constructing "prismatic" microdevices than the unoptimized approach

$$n = 10$$

[6]



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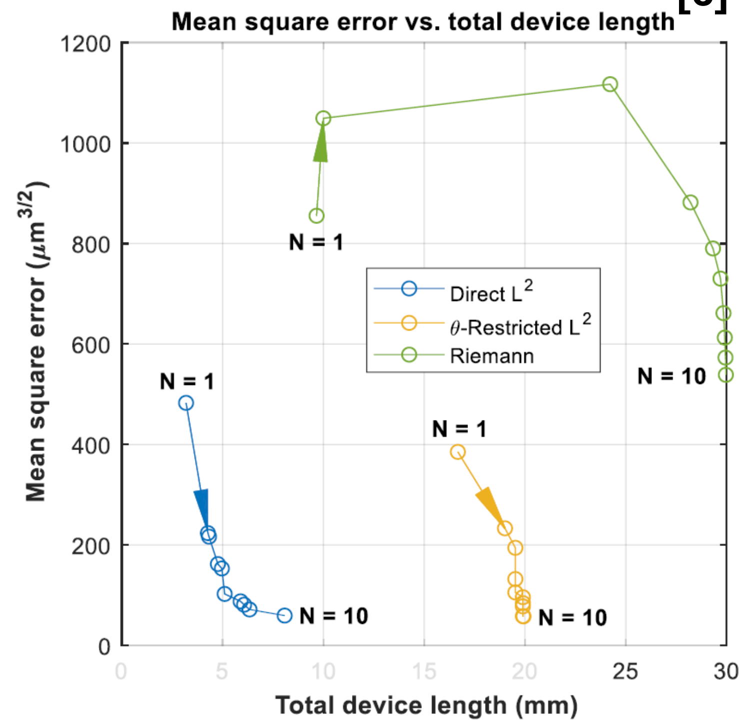
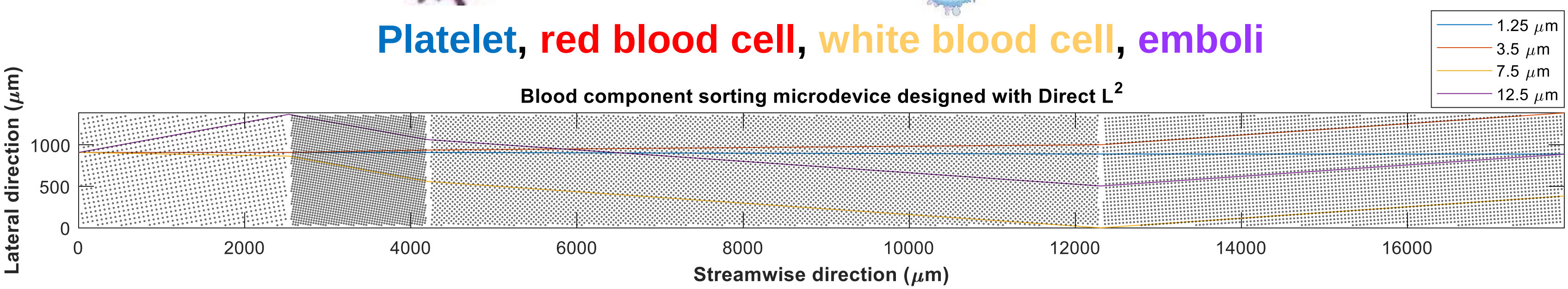


We can use novel knowledge about these colloidal dynamics to construct devices that sort arbitrary polydisperse suspensions

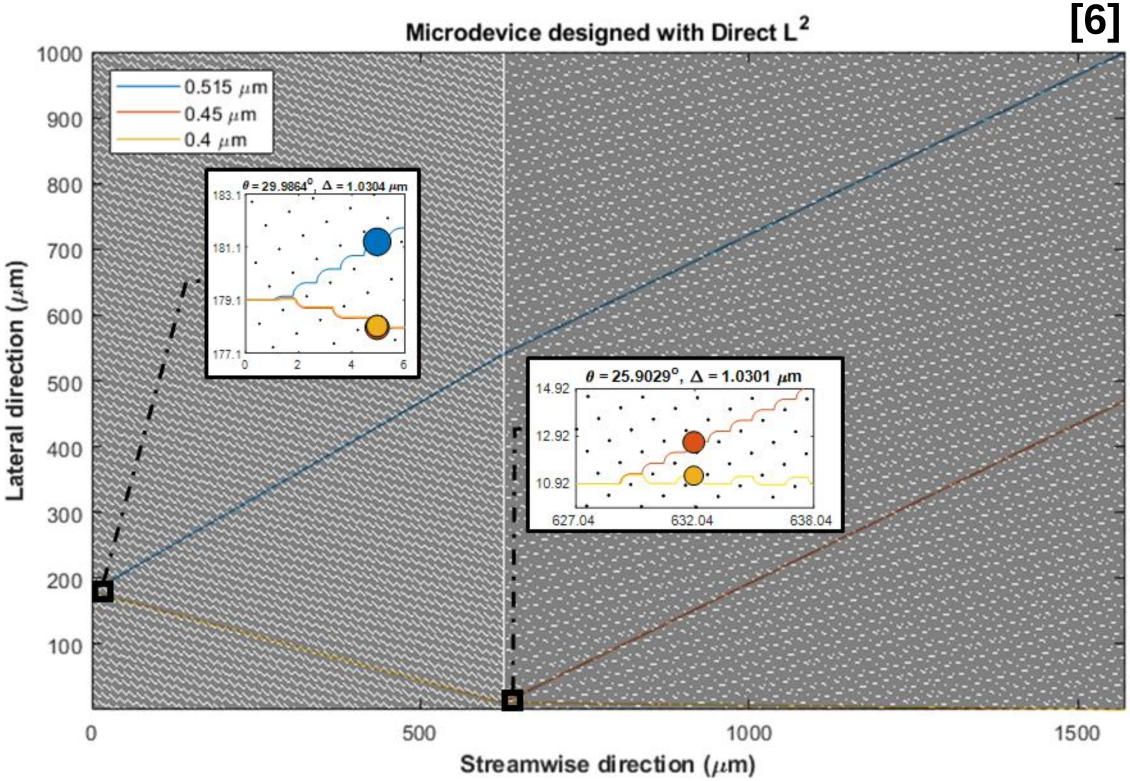
[6]

Platelet, red blood cell, white blood cell, emboli

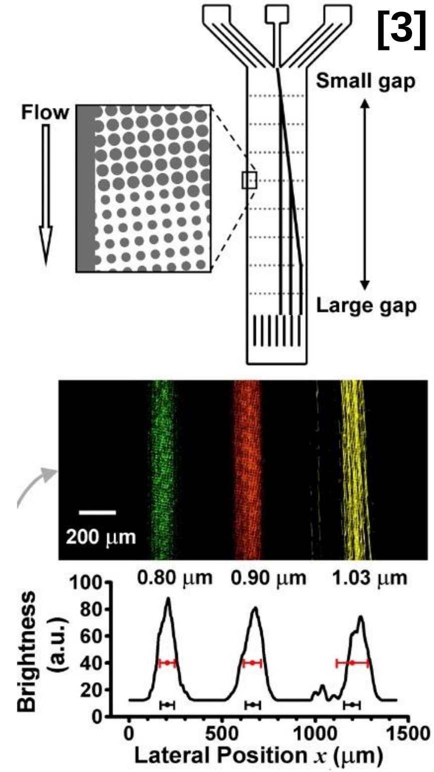


Our device designs vastly outperform those reported in literature, in theory

[6]



[3]



	Huang et al. (2004)	Rodriguez-Gonzalez et al. (2020)
Number of lattices	8	2
Total device length	14 mm	1.57 mm

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