

Soft Matter

Particle Actuation by Rotating Magnetic Fields in Microchannels: A Numerical Study

Journal:	Soft Matter
Manuscript ID	SM-ART-01-2021-000127.R1
Article Type:	Paper
Date Submitted by the Author:	04-May-2021
Complete List of Authors:	Ham, Seokgyun; Virginia Tech, Mechanical Engineering Fang, Wen-Zhen; National University of Singapore, Mechanical Engineering Qiao, Rui; Virginia Polytechnic Institute and State University, Mechanical Engineering

SCHOLARONE[™] Manuscripts

13

14

15

16

17

18

Soft Matter

1	Particle Actuation by Rotating Magnetic Fields in Microchannels:
2	A Numerical Study
3	Seokgyun Ham ¹ , Wen-Zhen Fang ² , and Rui Qiao *1
4	$^{1}\mathrm{Department}$ of Mechanical Engineering, Virginia Tech, Blacksburg, VA 24061, USA
5	² Department of Mechanical Engineering, National University of Singapore, 117575, Singapore
6	May 7, 2021
7	Abstract
8	Magnetic particles confined in microchannels can be actuated to perform translation motion
9	using a rotating magnetic field, but their actuation in such a situation is not yet well understood.
10	Here, the actuation of a ferromagnetic particle confined in square microchannels is studied using
11	immersed-boundary lattice Boltzmann simulations. In wide channels, when a sphere is away
12	from channel corners, it experiences a modest hydrodynamic actuation force parallel to the

channel walls. This force decreases as the sphere is shifted toward the bottom wall but the

opposite trend is found when the channel is narrow. When the sphere is positioned midway

between the top and bottom channel walls, the actuation force decreases as the channel width

decreases and can reverse its direction. These phenomena are elucidated by studying the flow

and pressure fields in the channel-particle system and by analyzing the viscous and pressure

components of the hydrodynamic force acting on different parts of the sphere.

^{*}To whom correspondence should be addressed, email: ruiqiao@vt.edu.

1 1 Introduction

Manipulating microscale objects in a liquid environment is challenging. One of the reasons is 2 that the motion of small objects is often governed by Stokes flows. A key characteristic of Stokes 3 flows is that reciprocal movement of a "swimmer" in these flows cannot lead to a net displacement 4 due to the time-reversibility in them, which is known as Purcell's scallop theorem.¹ Many tech-5 niques have been developed to manipulate microscopic objects in liquids, e.g., dielectrophoresis, 6 diffusiophoresis, magnetophoresis, and so on.^{2,3} Magnetism-based methods are popular because 7 they are typically bio-compatible, e.g., magnetic fields can penetrate most media without adverse 8 effects.⁴⁻⁶ Magnetism-based particle manipulation methods can be broadly divided into two cateq gories: driving particles using a net magnetic force and driving particles using a magnetic torque. 10 For particles with a characteristic dimension r, the net magnetophoresis force they experience often 11 scales as r^{3} , $r^{7,8}$ and the induced translation speed scales with r^{2} .⁹ Therefore, actuation based on net 12 magnetic force typically requires very strong magnetic fields when the particle is small. Actuation 13 based on magnetic torques, on the other hand, has more favorable scaling laws (e.g., the translation 14 speed can scale with r)¹⁰ and can provide large translation speed with weak or moderate magnetic 15 fields. As such, torque-based magnetic actuation has attracted much attention in recent years. 16

To actuate microparticles using a magnetic torque, it is essential to break the time-reversal 17 symmetry inherent in Stokes flow. Such a symmetry can be broken by using asymmetric geometry 18 such as an artificial flagella or introducing a substrate.^{11–16} Particles exhibiting magnetic torque-19 induced translation motion near substrates are often called surface walkers, and they are being 20 studied intensively by many research groups.^{10,17–22} Many interesting phenomena related to surface 21 walkers have been discovered.^{5,23–29} For example, when magnetic particles rotate above a solid wall, 22 a chain of rotating particles travel faster than an individual particle rotating near the same wall;¹⁹ 23 hydrodynamic interaction between rotating particles can leads to particle clustering;³⁰ particle 24 clustering can emerge spontaneously due to fingering instability in a swarm of particles;^{31,32} rolling 25 particles can exhibit flocking behavior at some frequencies of the applied magnetic field;³³ clusters of 26 magnetic particles can be disassembled into shorter chains near uneven substrates using three-axis 27 dynamic magnetic fields.²⁰ 28

Many potential applications of surface walkers require them to be actuated in confined spaces. ^{34,35} Therefore, it is worthwhile to study the dynamics of magnetic surface walkers under confined conditions. Research in this direction begins to receive attention only most recently, but some interesting

phenomena have already been reported. For instance, the reversible response of superparamagnetic particles confined in a microchannel has been analyzed. It was found that the particle assembly is reconfigurable and the shape of the particle assembly depends strongly on the channel-particle size ratio.³⁶ The rheology of a sphere particle suspension confined between two plates under an external uniform magnetic field was studied. It is discovered that the magnetic torque applied to the sphere is transmitted to the fluid via viscous force, and consequently, the induced shear stress drives a unidirectional flow of the suspension.³⁷

Understanding the actuation of magnetic surface walkers, or more generally, dynamics of mag-8 netic particles in fluids, using experiments alone is challenging. Computational modeling is a 9 powerful tool to complement experimental investigations. In the literature, many different meth-10 ods, including Stokesian dynamics,³⁸ dissipative particle dynamics,³⁹ finite element method,^{40,41} 11 smoothed particle hydrodynamics,^{42,43} and lattice Boltzmann method (LBM),^{44,45} have been de-12 veloped to investigate the dynamics of magnetic particles suspended in liquids. Using LBM, we 13 recently studied the dynamics of surface walkers confined between two infinite walls.⁴⁶ It was found 14 that the degree of confinement and the nature of the confining walls (slip vs no-slip) not only affect 15 the speed of a sphere actuated by a rotating field, but also its direction. For example, for a sphere 16 positioned at a fixed height above a lower no-slip wall, as the no-slip upper wall is brought closer 17 to the lower wall, the translation of the sphere first slows down, then reverses direction, and finally 18 reaches zero when the sphere is exactly in the middle way between the two walls. 19

While existing studies provided useful insights into the effects of confinement on the actuation 20 of magnetic surface walkers by rotating fields, the confinement considered so far is usually afforded 21 by two parallel walls that are normal to the rotating axis of surface walkers. In practice, a surface 22 walker may be confined in more complex environment such as inside a channel with a finite aspect 23 ratio. Understanding the actuation of surface walkers in such environment is useful for harnessing 24 them for applications such as drug delivery through capillaries.⁴⁷ However, research on this is 25 scarce at present. In particular, how the confinement by walls normal to the sphere's axis of 26 rotation changes the fluid flow and actuation force has not been studied and is poorly understood. 27 In this work, we investigate the actuation of a spherical surface walker confined in a square-shaped 28 microchannel. The flow field and actuation force acting on the sphere in the channel length direction 29 are computed numerically by varying the position of the sphere inside the channel and the dimension 30 of the microchannel. The variation of the net actuation force is elucidated by examining its various 31 components and the flow fields inside the microchannel. 32

¹ 2 Models and Methods

² 2.1 Physical and mathematical models

As shown in Fig. 1, the simulation system consists of a ferromagnetic sphere and a water-filled 3 square channel, in which the sphere is immersed. The sphere has a radius of r. The channel 4 has a width of W and a length of L. The sphere is positioned at a distance a and b from the 5 bottom wall and the purple-shaded side wall, respectively. The bottom channel wall is in the xy-6 plane and the side channel wall is in the xz- plane. Under the action of an external magnetic field 7 B, the sphere rotates around the z-axis in the clockwise direction. If the sphere is free, it may 8 move in all three directions, which changes its confinement by the channel walls (i.e., a and b) and 9 complicates the study of how confinement affects its actuation. To circumvent this problem, as is 10 widely practiced,^{48–50} the sphere is allowed to rotate but its center is fixed. The rotation-induced 11 hydrodynamic force acting on the sphere in the x-direction, F_x , is measured as the actuation force. 12



Figure 1: A three-dimensional view (a) and side view (b) of the system used to study the actuation of a magnetic sphere in a square channel. The sphere surface is divided into S_1, S_2, S_3 , and S_4 . In (b), only the channel walls closest to the sphere are shown. The origin of the coordinate system is set on the sphere's center.

¹³ Without losing generality, the sphere's radius is set to $12\mu m$. Its magnetic moment is m =¹⁴ $1.45 \times 10^{-10} \text{A} \cdot \text{m}^2$. A magnetic field $B = B \cos(2\pi f_B t) \mathbf{i} - B \sin(2\pi f_B t) \mathbf{j}$ is applied, where B is the ¹⁵ strength of the magnetic field and f_B is the rotational frequency. B and f_B are set to 3 mT and 20 ¹⁶ Hz, respectively. With the above parameters, the sphere rotates synchronously with the magnetic ¹⁷ field in all of our simulations. The rotational Reynolds number $Re_{\omega} = 2\pi\rho f_B r^2/\mu = 4.52 \times 10^{-3} \ll$ ¹⁸ 1.

We note that the sphere also experiences forces in the y- and z-directions. These forces can 1 change the position of a free particle across the channel, but they are much weaker. Specifically, 2 $F_x \sim \pi \mu \omega r^2$.^{48,50,51} Forces in the y- and z-directions (F_y and F_z), unlike F_x , originate from 3 inertia effects and scale as $F_{y,z} \sim \pi \rho \omega^2 r^4$, ^{46,50} i.e., $F_{y,z}/F_x \sim Re_\omega$. Because $Re_\omega = \ll 1$, inertia 4 effects are negligible and F_y and F_z are very small. In addition, other forces (e.g., Brownian forces) 5 in those directions may be more important in understanding how a particle is driven away from 6 walls. For these reasons, we will not elaborate on F_y and F_z . Because a free particle can depart 7 from its initial position relative to channel walls due to non-zero $F_{y,z}$, we study the implications of 8 such departure by examining how F_x varies with a and b in Fig. 1. 9

Three series of systems are studied to probe the effects of confinement on actuation by channel 10 walls (see Table 1). In all systems, the sphere is positioned at a distance b = 1.5r from the purple-11 shaded side wall. This distance is chosen so that particle actuation can be effectively studied using 12 direct numerical simulations. For surface walkers, the actuation force decreases rapidly as b/r13 increases. Hence, a small b/r is preferred. However, if b/r is too small, resolving the flow between 14 the sphere and wall necessitates an extremely fine grid and high computational cost. With b = 1.5r, 15 our tests showed that a strong actuation force is generated and the force can be computed accurately 16 using a reasonably fine grid (see below). The channel length is selected to 60r to minimize the 17 finite size effects.⁴⁶ In the first series of systems, the channel is wide (W = 6.5-30r) and the sphere 18 is fixed at various distances above the bottom wall to study the actuation near walls of a wide 19 channel. In the second series of systems, the sphere is positioned midway between top and bottom 20 walls while the channel width is varied to study the actuation with symmetric top/bottom walls. 21 In the third series of systems, the channel is narrow (W = 3.5 - 6r) and the sphere is fixed at 1.2-3r 22 above the bottom wall to study the actuation near walls of a narrow channel. 23

Series	a	b	W	L
1	1.2r to $W/2$	1.5r	6.5 to $30r$	60r
2	W/2	1.5r	3 to 30r	60r
3	1.2r to $W/2$	1.5r	3.5 to $6r$	60r

 Table 1: A summary of the simulations performed in this study.

²⁴ The fluid motion is governed by the Navier-Stokes (NS) equations:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \boldsymbol{u}) = 0 \tag{1}$$

$$\frac{\partial \rho}{\partial t} + \nabla (\rho \boldsymbol{u} \boldsymbol{u}) = -\nabla p + \nabla [\mu (\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T] + \boldsymbol{F}$$
(2)

¹ where ρ is the fluid density, \boldsymbol{u} is the velocity, p is the pressure, μ is the viscosity, and \boldsymbol{F} is the body ² force. The no-slip boundary condition is imposed on channel walls and the sphere's surface. The ³ periodic boundary condition is imposed in the x-direction. The sphere's rotation is governed by

$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \int_s (\boldsymbol{X}_s - \boldsymbol{X}_p) \times (\boldsymbol{\sigma} \cdot \boldsymbol{n}) ds + \boldsymbol{m} \times \boldsymbol{B}$$
(3)

where I_p is the sphere's moment of inertia, ω_p is the sphere's angular velocity, σ is the fluid stress tensor, n is the unit normal vector of the sphere's surface, X_s and X_p denote the sphere's center and position on the sphere's surface, respectively. Equation 3 is solved together with Eq. 1 and 2 to compute a sphere's rotation. For the rotating magnetic field considered in this work, our simulation shows that the sphere rotates synchronously with the applied magnetic field.

9 2.2 Numerical methods and code validation

The mathematical models described in the previous section are solved by combining the LBM and the immersed boundary method (IBM).^{52,53} These methods and their implementation have been described in details in our recent publication.⁴⁶ Here we highlight the salient features of these methods and present key implementation details.

The NS equations are solved using LBM. In LBM, evolution equations of the density distribution function, which can recover to the NS equations via the Chapman-Enskog expansion, are solved on a Eulerian lattice to obtain the fluid's density and velocity fields. The basic operations in LBM are the collision step and the streaming step. In the collision step, the distribution function components on each lattice is computed. In the streaming step, the post-collision distributed functions are spread to neighbor lattices by following designated microscopic velocity vectors. Because collision and streaming are local operations, LBM is highly efficient and easily parallelized.

The interactions between fluids and the solid sphere are handled using a fixed-grid method IBM.⁵³ Briefly, each solid boundary is represented using a set of Lagrangian forcing points and the flow field is solved on the Eulerian lattice, which covers both inside and outside of the solid boundary. The velocity of Lagrangian points on the solid boundary is interpolated from adjacent Eulerian lattice points through a discrete delta function. Meanwhile, the force density evaluated on Lagrangian points is spread to nearby Eulerian lattice points through the same discrete delta Page 7 of 27

Soft Matter

function. These treatments enforce the no-slip condition on the solid boundary and allow the effects
of solid boundary on fluid flow to be modeled.

When implementing LBM, we adopt the three-dimensional 19-velocity (D3Q19) multi-relationtime scheme to solve the evolution equations ^{54–56}

$$g_{\alpha}(\boldsymbol{x} + \boldsymbol{e}_{\alpha}\delta t, t + \delta t) - g_{\alpha}(\boldsymbol{x}, t) = -(\boldsymbol{M}^{-1}\boldsymbol{\Lambda}\boldsymbol{M})_{\alpha\beta}[g_{\beta} - g_{\beta}^{eq}] + \delta tF_{\alpha}, \alpha = 0 \cdots 18$$
(4)

where g is the density distribution function, e_{α} is the discrete velocity along the α direction, and Λ 5 is the collision matrix. The free relaxation parameter related to the kinematic viscosity is set to 1.25 6 while others are set to 1. The hydrodynamic force acting on fluids due to fluid-sphere interactions is 7 treated using the techniques developed by Guo et al⁵⁷ and Kang et al.⁵³ The no-slip wall boundary 8 condition is enforced using the halfway bounce-back scheme.⁵⁶ A uniform lattice spacing of r/6 is 9 used to solve the Eq. 4. For the systems listed in Table 1, the total number of grid points ranges 10 from 160,000 to 12,000,000, and there are at least two lattice points in the gap between the sphere 11 and the wall (corresponding to a/r = 1.2). Grid-dependence is tested by comparing actuation force 12 in representative cases with that obtained using a finer grid of r/10, with a deviation less than 2%. 13 When implementing IBM, the sphere's surface is discretized into 536 Lagrangian nodes according 14 to the method proposed by Feng et al,⁵² leading to the spacing between neighbor Lagrangian nodes 15 approximately equal to that between the Eulerian lattices.^{52,56} The range of kernel function (Dirac 16 delta distribution) to deal with the fluid-solid interaction function is twice the lattice spacing. 17

A code implementing the above methods has been developed and validated extensively for 18 actuation of spherical surface walkers.⁴⁶ First, the rotation of a magnetic sphere driven by a rotating 19 field in a unbounded fluid was simulated. The evolution of the sphere's rotation speed as a function 20 of the field frequency, including the transition from the synchronous regime to the asynchronous 21 regime, was accurately captured. Next, the hydrodynamic forces experienced by a sphere enclosed 22 between two no-slip walls separated by 30r were studied systematically. When the domain size 23 reaches 60r in the longitude direction and 30r in the transverse direction, the computed drag 24 acting on a sphere translating near the lower wall agrees well with the analytical prediction for 25 spheres moving parallel to a semi-infinite wall.⁴⁸ The hydrodynamic forces acting on a center-fixed 26 sphere rotating at a height of 1.5r above the lower wall computed by the code converges within 27 $\sim 5\%$ of the analytical predictions by Goldman and colleagues. 48,50 28

¹ 3 Results and Discussion

Here we study the hydrodynamic actuation force experienced by a magnetic sphere inside a 2 square channel under the actuation of a rotating magnetic field. As mentioned in Section 2.1, we 3 let the sphere rotate around the z-axis in the clockwise direction but fix its center. We measure 4 the hydrodynamic force on the sphere in the x-direction. Figure 2 summarizes the actuation force 5 F_x , for the various a and W listed in Table 1. We observe that, in a very wide channel (e.g., 6 W = 30r), when the sphere is away from the corner (e.g., a = 15r), F_x is positive as shown in 7 prior works, 46,50 but becomes negative as the sphere is shifted toward the bottom wall (i.e., as r/a8 increases). In addition, as a sphere is shifted toward the bottom wall, F_x decreases if the channel 9 is wide but increases when the channel is narrow (W < 6r). These phenomena are examined in 10 details in Sections 3.1 and 3.3, respectively. When the sphere is positioned midway between the 11 top and bottom channel walls, F_x decreases as the channel width decreases and becomes strongly 12 negative when the sphere becomes highly confined by the channel, and sharply recovers to zero 13 when the symmetry is reached at W = 3r and a = 1.5r. This series of study is discussed in Section 14 3.2.15



Figure 2: The evolution of the x-direction hydrodynamic actuation force on a rotating sphere as a function of channel width W and the sphere's distance from the bottom channel wall a. The blue, red, and black lines correspond to the Series 1, 3, and 2 simulations in Table 1.

¹ 3.1 Sphere actuation near walls of a wide channel

For the system shown in Fig. 1, the situation with $W \gg r$ and $a \gg r$ (i.e., when a sphere is positioned close to a semi-infinite vertical wall), has been studied in the literature.^{10,46} Here, we set the sphere at a distance b = 1.5r from the purple-shaded vertical wall and position the bottom wall at a distance a beneath the sphere. To understand how the sphere's actuation is affected by the corner formed by the bottom and side walls of a wide channel, we focus our discussion on a representative set of simulations where W is set to 30r and a is varied from 15r to 1.2r.

We first examine the flow and pressure fields in two sample cases with r/a = 1/15 and 1/1.5. 8 Figure 3 show sample streamlines in the channel. At r/a = 1/15, when there is little confinement by 9 the bottom wall, the rotating sphere induces a global flow in the channel in the positive x-direction 10 (see Fig. 3a). Fluids are drawn toward the vertical wall on one side of the sphere and ejected 11 away from the wall on the other side of the sphere (marked by red arrows). This global flow is 12 accompanied by two recirculations, one primarily in the horizontal plane (marked by a black arrow) 13 and one primarily in the vertical plane (marked by a blue arrow). Because the global flow is in the 14 positive x-direction, hereafter, upstream of the sphere refers to the space in which x < 0 while 15 downstream refers to the space in which x > 0. 16



Figure 3: Sample streamlines in two channel-particle systems with r/a = 1/15 (a) and r/a = 1/1.5 (b). W = 30r and b/r = 1.5 in both systems.

At r/a = 1/1.5, when there is significant confinement by the bottom wall, Fig. 3b shows that the basic features of the flow field remain similar, e.g., a global flow in the positive x-direction and recirculations still exist. Nevertheless, the additional confinement by the bottom wall leads

to important differences from those shown in Fig. 3a. First, the bending of streamlines toward 1 and away from the vertical wall becomes somewhat stronger. Practically, because there are often 2 many particles in a channel, this effect makes it easier to entrain other particles toward a rotating 3 particle located near a channel corner (note that the trajectory of entrained particles may differ 4 from the streamlines showed here if the particle density in the channel is not low). This can be 5 useful because the motion of an entrained, passive particle (e.g., a biological cell), once close enough 6 to the rotating particle, can be controlled indirectly by manipulating the rotating sphere (e.g., push 7 and pull of cells by a magnetic particle rotating near a semi-infinite wall have been demonstrated 8 in recent experiments).¹⁷ Second, in the horizontal plane, the recirculation zone moves closer to 9 the sphere, which tends to increase the velocity gradient near the sphere's surface that faces away 10 from the vertical wall. As we shall see later, this contributes to the reversal of the hydrodynamic 11 actuation force on the sphere as r/a increases from 1/15 to 1/1.5. 12

Figure 4 shows the pressure field in the horizontal (z = 0) and vertical (y = 0) planes passing 13 through the sphere's center for r/a = 1/15 and 1/1.5. As shown in Fig. 4a, at r/a = 1/15, 14 where the confinement by the bottom wall is negligible, the confinement of a rotating sphere by 15 the vertical wall induces a heterogeneous pressure field in the channel. Specifically, the rotating 16 sphere draws fluids on one of its sides toward the wall to rise the pressure there (region A in Fig. 17 4a's inset) but reduces the pressure on its other side (region B in Fig. 4a's inset). This, along with 18 the recirculation of fluids near the sphere, cause the fluid pressure to rise on one side of the sphere 19 and to decrease on the other side. Examination of the pressure fields in the z = 0 and y = 0 planes 20 (see Fig. 4a and 4c) reveals that the recirculation-induced pressure heterogeneity exists in a region 21 up to many r from the sphere, which is consistent with the global flow shown in Fig. 3a. On the 22 sphere's surface facing the vertical wall $(S_3 \text{ and } S_4)$, this kind of pressure heterogeneity creates a 23 net force pushing the sphere in the negative x-direction.^{46,50} 24

The global flow generated by the rotating sphere and its interactions with the *center-fixed* sphere, however, create a opposite pressure force on the sphere. Specifically, the pressure on the sphere's upstream surfaces is enhanced by the global flow, while the opposite occurs on the sphere's downstream surfaces. As shown in the inset of Fig. 4a, on the sphere's surface facing the vertical wall, this pressure imbalance by the global flow is weaker compared to the recirculation-induced pressure imbalance; however, on the sphere's surface facing away from the vertical wall, this pressure imbalance dominates and creates a net pressure force in the positive x-direction.

When the rotating sphere is positioned close to the bottom wall with r/a = 1/1.5, Fig. 4b



Figure 4: Pressure field and streamlines in channel-particle systems with different r/a but same b/r = 1.5. (a, b): flow in the z = 0 plane. (c, d): flow in the y = 0 plane. $\bar{p} = (p - p_{ref})/\mu\omega$.

and 4d show that the pressure field in the system is qualitatively similar to that at r/a = 1/15. 1 However, because of the stronger confinement by the horizontal wall, the pressure heterogeneity 2 due to recirculation flow is enhanced and thus the pressure imbalance on the sphere's surface facing 3 the vertical wall is enhanced (see Fig. 4b's inset). Meanwhile, the global flow around the sphere 4 is weakened and thus the pressure imbalance on sphere's surface due to the interactions between 5 the global flow and the center-fixed sphere is weakened. As a result, although this kind of pressure 6 imbalance remains important on the sphere's surface facing away from the vertical wall, the region 7 of surface where it dominates over the recirculation-induced pressure imbalance becomes smaller 8 (see Fig. 4b's inset). As we shall see later, this change contributes to the reversal of hydrodynamic 9 force on the sphere as r/a increases from 1/15 to 1/1.5. 10

Having studied the flow induced by a rotating sphere, we now evaluate the hydrodynamic force experienced by the sphere. Because the sphere rotates around the z-axis, the most significant hydrodynamic force acting on sphere is in the x-direction. Figure 5a shows the total hydrodynamic force F_x . We observe that, as r/a increases, F_x decreases and reverses sign at r/a > 1/3. In other words, as the confinement by the bottom wall increases, the actuation force decreases and ultimately reverses its direction.

To understand the origins of the observed evolution of F_x as a function of r/a, we first compute the components of F_x due to the pressure and viscous forces acting on the sphere's surface $(F_{x,p})$



Figure 5: The hydrodynamic force acting on a rotating sphere positioned near walls of a channel with W = 30r. (a) The net force in the *x*-direction and its pressure and viscous components, (b-c) The *x*-direction pressure (b) and viscous (c) forces acting on surface S_1 to S_4 labeled in the inset of panel (b) (see Fig. 1a for a 3D view).

and $F_{x,v}$). As shown in Fig. 5a, at r/a = 1/15, when the sphere is essentially confined only by 1 a semi-infinite vertical wall, $F_{x,p}$ is negative due to the large pressure difference across the sphere 2 induced by the flow recirculation. As elucidated earlier,⁴⁶ the net viscous force on the sphere is in 3 the positive x-direction and stronger than the pressure force. As r/a increases, both $F_{x,p}$ and $F_{x,v}$ 4 decreases. Eventually, at large enough r/a (i.e., the sphere is positioned close to the bottom wall), 5 pressure forces dominate the viscous forces, which differs qualitatively from the situation when the 6 sphere is close to a semi-infinite vertical wall and leads to the reversal of F_x . To gain insight into 7 the evolution of these pressure and viscous forces, we next decompose each force into that acting 8 on the sphere's four surfaces labeled in Fig. 1b $(S_1, ..., S_4)$. Hereafter, the pressure and viscous 9 force on piece i of the sphere's surface are denoted as $F_{x,p}^i$ and $F_{x,v}^i$, respectively. 10

Figure 5b shows the variation of $F_{x,p}^{1...4}$ as r/a increases (note that, throughout this work, r/bis fixed at 1/1.5). While each force becomes more negative with increasing r/a, the decrease of $F_{x,p}^2$ and $F_{x,p}^3$ are far greater than that of $F_{x,p}^1$ and $F_{x,p}^4$. This is expected because the flow near

surfaces facing toward the bottom wall $(S_2 \text{ and } S_3)$ is affected more significantly than that near 1 surface facing away from the bottom wall (S₁ and S₄). The more negative $F_{x,p}^3$ at larger r/a2 is caused by the enhanced pressure buildup on the downstream of the sphere and the pressure 3 depression on the upstream (cf. regions B and A in Fig. 4a and 4b), which is in turn caused 4 by the increased confinement by the bottom wall as explained above. The decrease and eventual 5 reversal of $F_{x,p}^2$ as r/a increases is expected. Specifically, as the confinement by the bottom wall 6 increases, recirculation-induced pressure difference along the sphere in the streamwise direction 7 (which produces a negative pressure force) is enhanced while global flow-induced pressure difference 8 in the same direction (which produces a positive pressure force) is reduced as discussed above. To 9 see this more clearly, we study the pressure field in the z = -0.4r plane when r/a = 1/15 and 10 r/a = 1/1.5. Figure 6 shows that, as r/a increases from 1/15 to 1/1.5, the pressure gradient along 11 the surface facing toward the vertical wall increases, while that along the surface facing away from 12 the vertical wall reverse direction, which is in line with the fact that $F_{x,p}^3$ becomes more negative 13 while $F_{x,p}^2$ changes from positive to negative. 14



Figure 6: Pressure field and streamlines in the z = -0.4r plane when r/a = 1/15 (a) and r/a = 1/1.5 (b).

Having analyzed the evolution of the pressure force $F_{x,p}$ acting on the sphere as r/a increases, 15 we now analyze the evolution of the viscous force $F_{x,v}$. Figure 5c shows that, similar to the pressure 16 forces, as r/a increases, only the viscous forces on the two surfaces facing the bottom wall (S_2 and 17 S_3) change markedly. Because the sphere rotates in the clockwise direction, the viscous shear on 18 S_2 and S_3 $(F_{x,v}^2)$ and $F_{x,v}^3$ are in the negative and positive x-directions, respectively. As r/a19 increases, the strength of $F_{x,v}^2$ increases monotonically. This increase is caused by the enhanced 20 velocity gradient $\nabla_r u_x$ (r denotes the sphere's radial direction) in region near surface S_2 , which 21 can be inferred from Fig. 3 as discussed earlier and is a result of the reduced distance between 22 S_2 and the no-slip bottom wall. The enhanced $\nabla_r u_x$ can also be more clearly shown in Fig. 7, in 23 which u_x along a ray OA passing through surface S_2 is shown at different r/a. 24



Figure 7: The variation of the x-component fluid velocity along rays OA and OB when the sphere is positioned at different height above the bottom wall. Both rays originate from the sphere's center and reside in the x = 0 plane. Rays OA (OB) passes through surface S_2 (S_3) and forms an angle of $3\pi/4$ ($5\pi/4$) with the positive z-axis.

The variation of $F_{x,v}^3$ with r/a however, is more complicated. As r/a increases from 1/15 to 1 $\sim 1/2$, $F_{x,v}^3$ decreases slightly; as r/a increases further, $F_{x,v}^3$ increases markedly. The initial, slight 2 decrease of $F_{x,v}^3$ as the bottom wall moves toward to the sphere is mostly caused by the increase of 3 the induced pressure gradient in the x-direction in the region between the sphere and the vertical 4 wall. Specifically, although reducing the distance between the bottom wall and the sphere tends to 5 increase $\nabla_r u_x$ near surface S_3 just like that near surface S_2 , the increased pressure gradient tends 6 to increase the fluid velocity in the region between surface S_3 and the vertical wall, thus reducing 7 $\nabla_r u_x$ near surface S_3 . The latter is supported by the velocity profile along ray OB passing through 8 surface S_3 as shown in Fig. 7. As the bottom wall moves very close to the sphere (i.e., $r/a > \sim 1/2$), 9 the enhancement of $\nabla_r u_x$ due to the proximity of the no-slip bottom wall to surface S_3 dominates 10 the reduction of $\nabla_r u_x$ due to the enhanced pressure gradient, and $F^3_{x,v}$ increases markedly. 11

Overall, as r/a increases, the increase of the positive $F_{x,v}^3$ is weaker compared to the increase of the negative $F_{x,v}^2$, leading to a decrease of $F_{x,v}$. The weakening of the positive $F_{x,v}$ and strengthening of the negative $F_{x,p}$ with the increase of r/a eventually allows the pressure force to dominate the viscous force and makes the overall actuation force negative as shown in Fig. 5.

¹⁶ 3.2 Sphere actuation in channels with symmetric top and bottom walls

¹⁷ We now fix the sphere at a distance a = W/2 from the bottom wall and vary W from 30r to ¹⁸ 3r to study the effects of confinement by four walls on the actuation of the sphere (see Series 2 in ¹⁹ Table 1 for details). In all studies, b is fixed at 1.5r. The channel has a square cross-section, and

- ¹ the system geometry is symmetric in the z-direction. As in Section 3.1, we compute the flow in
- ² the system and measure the hydrodynamic force on the sphere in the x-direction.



Figure 8: Flow in a channel-particle system with a = W/2, b = 1.5r, and W = 3.5r. (a) Sample streamlines. The sphere rotates around the z-axis in the clockwise direction. (b-c) Pressure field and streamlines in the z = 0 plane (b) and y = 0 plane (c) passing through the sphere's center (c). $\bar{p} = (p - p_{ref})/\mu\omega$.

We first study the flow field in a representative system where a = W/2 and W = 3.5r. Figure 8 a shows the streamlines near the sphere. Similar to the situation shown in Fig. 3, a global flow in the *x*-direction is induced (marked by red arrows). However, because of the proximity of the two vertical walls, the fluids drawn from the sphere's one side are ejected onto the wall on the sphere's other side. The recirculation of fluids around the sphere's surface (marked by an orange arrow) induces two predominately horizontal recirculation bubbles near the vertical wall that is further away from the sphere (marked by two black arrows).

Figure 8b and 8c show the pressure field in the horizontal (z = 0) and vertical (y = 0) planes passing through the sphere's center. Because of the small W, both vertical walls affect the fluid flow. Such a flow rises the pressure in region A and lowers it in region B near the vertical wall that is closer to the sphere. At the same time, the flow rises the pressure in region A' and lowers it in region B' near the other vertical wall that is slightly further away from the sphere. Overall, the pressure imbalance between regions A and B is higher than that between regions A' and B'. Such kind of pressure imbalance occurs very close to the vertical walls – as shown in Fig. 8c, it is hardly

noticeable in the y = 0 plane (i.e., 1.75r from the vertical walls). In addition to the above highly localized pressure heterogeneity, a pressure difference accompanying the global flow shown in Fig. 8 is developed along the channel: the pressure upstream of the sphere is lower and the pressure downstream of the sphere is higher. As discussed in Section 3.1, this pressure distribution creates a net force pushing the sphere in negative x-direction.

Figure 9a shows the variation of the hydrodynamic force acting on the sphere in the x-direction 6 (F_x) as a function of r/W. As r/W increases, F_x decreases slightly, becomes negative at r/W =7 1/3.75, then increases sharply and eventually reaches zero at r/W = 1/3. $F_x = 0$ at r/W = 1/3 is 8 expected, because at this ratio, all four channel walls are distributed symmetrically with respect to 9 the sphere. To understand the variation of F_x , we again decompose F_x into a pressure component 10 $F_{x,p}$ and a viscous component $F_{x,v}$. Figure 9a shows that the variations of $F_{x,p}$ and $F_{x,v}$ with r/W11 are both similar to that of F_x , thus indicating that the changes of these forces contribute similarly 12 to that of F_x . To understand these forces, we next decompose each pressure/viscous force into 13 that acting on the sphere's four surfaces delineated in Fig. 1b and analyze these forces (note that, 14 because the top and bottom walls are symmetric with respect to the sphere, the force acting on 15 $S_1(S_3)$ is the same as that acting on $S_2(S_4)$). Figure 9b shows the variation of $F_{x,p}^{1\dots 4}$ as a function 16 of r/W. As r/W increases from 1/30 to 1/10, $F_{x,p}^1$ to $F_{x,p}^4$ all decreases slightly; as r/W increases 17 further, all four components decrease significantly; at $r/W > \sim 1/3.5$, all four components increase 18 sharply as r/W increases. 19

The change of $F_{x,p}$ shown in Fig. 9a is a result of the modified pressure imbalance on the 20 sphere's four surfaces as r/W increases. When r/W increases, the three non-shaded walls in Fig. 21 1a all move closer to the sphere. For $r/W \ll 1/3.5$, such an enhanced confinement has a similar 22 effect on $F_{x,p}^i$ $(i = 1 \cdots 4)$ with the enhanced confinement of a sphere by the bottom wall (see Section 23 3.1 and Fig. 5b). Specifically, an increase of the confinement of the sphere by these walls enhances 24 the recirculation-induced pressure imbalance near the sphere's surface facing the shaded vertical 25 wall, which makes the negative $F_{x,p}^{3,4}$ more negative (see Fig. 9b), reduces $F_{x,p}^{1,2}$ and eventually 26 makes it negative. Because the confinement by three walls is stronger than by one bottom wall of 27 a channel corner, the variation of $F_{x,p}^i$ is stronger in the present case. For example, $F_{x,p}^2$ becomes 28 negative at $r/a \sim 1/2.5$ in Fig. 5b while $F_{x,p}^2$ becomes negative at $r/W \sim 1/9$ (i.e., $r/a \sim 1/4.5$) 29 in Fig. 9b. As r/W increases to ~ 1/3.5, the non-shaded vertical wall in Fig. 1a approaches the 30 sphere to a distance comparable to that of the purple-shaded vertical wall. Therefore, the pressure 31 imbalance across the space between by the sphere and the non-shaded vertical wall (cf. pressure 32



Figure 9: The hydrodynamic forces acting on a rotating sphere in square channels with different W (a = W/2 and b = 1.5r). (a) The net force in the x-direction and its pressure and viscous components, (b-c) The x-direction pressure (b) and viscous (c) forces acting on surface S_1 to S_4 labeled in the inset of panel (b) (see Fig. 1a for a 3D view).

¹ imbalance between regions A' and B' in Fig. 8b) becomes more positive. Further increasing r/W² enhances this pressure imbalance and eventually makes $F_{x,p}^{1,2}$ positive as shown in Fig. 9b.

Figure 9c shows the variation of $F_{x,v}^{1...4}$ as a function of r/W. As r/W increases from 1/30 to 3 1/3, $F_{x,v}^{3,4}$ decreases first and the increases sharply as r/W grows larger than 1/3.5. Meanwhile, 4 $F_{x,v}^{1,2}$ generally becomes more negative as r/W increases but increases minutely at r/W > 1/3.5. 5 These trends are similar to those shown in Fig. 5c. As in Section 3.1, they can be attributed 6 to the evolution of the velocity gradient near the sphere with the confinement by channel walls, 7 which depends on the sphere's proximity to the no-slip walls and is also regulated by the pressure 8 gradient along the gaps between the sphere and its adjacent walls. At r/W = 1/3, when the two 9 vertical walls are distributed symmetrically with respect to the sphere, $F_{x,v}^{1,2}$ and $F_{x,v}^{3,4}$ become equal 10 as expected. 11

17

¹ 3.3 Sphere actuation near walls of a narrow channel

In the previous section, we studied the actuation of a sphere in narrow channels by keeping the distance of the sphere to the top and bottom channel walls the same (i.e., a = W/2). Here, we relax this symmetric restriction by varying a and W independently (see Series 3 in Table 1). As before, b is fixed at 1.5r and the sphere rotates around the x-axis in the clockwise direction.



Figure 10: Flow in a channel-particle system with a = 1.2r, b = 1.5r, and W = 3.5r. (a) Sample 3D streamlines. The sphere rotates around the z-axis in the clockwise direction. (b-c) Pressure field and streamlines in the z = 0 plane (b) and y = 0 plane (c) passing through the sphere's center. $\bar{p} = (p - p_{ref})/\mu\omega$.

We first investigate the flow field in a representative case with a = 1.2r and W = 3.5r. Figure 6 10a shows sample streamlines near the sphere. Like the flow field of Series 2 shown in Fig. 8, a 7 global flow is induced in the x-direction (marked by red arrows), the fluids drawn from the sphere's 8 one side are ejected onto the wall on the sphere's other side, and the recirculation of fluids around 9 the sphere's surface (marked by an orange arrow) induces two horizontal recirculation bubbles 10 (marked by two black arrows). However, unlike that shown in Fig. 8a, because the sphere is closer 11 to the bottom wall than the top wall, a vertical recirculation (marked by a blue arrow) is created. 12 Further, a recirculation around the sphere's surface (marked by an orange arrow) is formed near 13 the bottom wall. Because of this recirculation, compared to those shown in 8c, the streamlines near 14 the top wall are shifted toward the bottom wall as they approach the sphere (see Fig. 10c). 15

Figure 10b and 10c show the pressure field in the horizontal (z = 0) and vertical (y = 0)

planes passing through the sphere's center. The pressure field is similar to that in Series 2 with the 1 same W (see Fig. 8b and c) in that two kinds of pressure heterogeneities exist. First, a pressure 2 imbalance arises due to the interactions between the recirculating fluids around the sphere and the 3 vertical walls. This pressure imbalance is localized near the vertical walls (e.g., in regions marked 4 by A, B, A', and B' in Fig. 10b) and is hardly noticeable at a distance $\sim r$ away from the vertical 5 walls. Second, as shown in Fig. 10c, a pressure difference caused by the global flow is created 6 along the channel so that the pressure upstream of the sphere is lower while the opposite occurs 7 in downstream. As mentioned earlier, this pressure distribution generates a net force pushing the 8 sphere in the negative x-direction. 9



Figure 11: The hydrodynamic forces acting on a rotating sphere in square channels with different r/a (W = 3.5r and b = 1.5r). (a) The net force in the x-direction and its pressure and viscous components, (b-c) The x-direction pressure (b) and viscous (c) forces acting on surface S_1 to S_4 labeled in the inset of panel (b) (see Fig. 1a for a 3D view).

Figure 11a shows the evolution of the hydrodynamic force and its components due to pressure and viscous forces as a function of r/a when W is fixed at 3.5r. As r/a increases from 1/1.75 to 1/1.2, F_x , $F_{x,p}$, and $F_{x,v}$ all increase. The trend of these forces is opposite to that in the Series 1 study (where W = 30r) but is similar to that shown in the Series 2 study over the same range of

¹ r/a (i.e., in the range of 1/3.5 < r/W < 1/2.4 in Series 2 study). These differences highlight the ² importance of confinement by narrow channels on particle actuation. To understand the origins of ³ the observed evolution of the hydrodynamic force as a function of r/a, we again decompose each ⁴ force into that acting on the sphere's four surfaces labeled in Fig. 1b (S_1, \ldots, S_4) .

Figure 11b shows that, as r/a increases, $F_{x,p}^{1,2,4}$ become less negative but $F_{x,p}^3$ changes little. 5 These changes originate from the different responses of pressure in different regions near the sphere 6 as it is shifted toward the bottom wall. As r/a increases, the sphere is confined more by the bottom 7 channel wall while less confined by the top channel wall. The pressure field in the gap between 8 the purple-shaded vertical wall and surface S_3 changes little, which is supported by the comparison 9 of pressure fields in the z = -0.6r plane for r/a = 1/1.75 and 1/1.2 (see Fig. 12a and b). As 10 such, $F_{x,p}^3$ changes little. On the other hand, as r/a increases, the local pressure imbalance between 11 regions A' and B' becomes stronger (see Fig. 12a and b) and thus $F_{x,p}^2$ becomes less negative. A 12 similar trend is found for the pressure imbalance along the gap between surface S_1 and its adjacent 13 wall (see region A' and B' in Fig. 12c and d, where the pressure fields in the z = 0.6r plane are 14 compared). Thus $F_{x,p}^1$ also becomes less negative as r/a increases. A comparison of the pressure 15 along the gap between surface S_4 and the purple-shaded wall shows that, as r/a increases, the 16 pressure imbalance along the gap (e.g., between region A and B in Fig. 12c and d) decreases and 17 hence $F_{x,p}^4$ becomes less negative. 18

Figure 11c shows the variation of $F_{x,v}^{1\cdots 4}$ as r/a increases from 1/1.75 to 1/1.2. Similar to those 19 shown in Section 3.1, as r/a increases, $F_{x,v}^2$ becomes more negative and $F_{x,v}^3$ becomes more positive. 20 These behaviors and their origins are similar to those discussed in Section 3.1. Specifically, because 21 the sphere is already very close to the no-slip bottom wall (r/a > 1/2), shifting the sphere closer 22 to the no-slip bottom wall enhances the radial gradient of the x-velocity $(\nabla_r u_x)$ and thus the 23 magnitude of the viscous shear stress and $F_{x,v}^2$ and $F_{x,v}^3$. On the other hand, as r/a increases, $F_{x,v}^1$ 24 and $F_{x,v}^4$ show little change. This is because, for the r/a considered here, $\nabla_r u_x$ near and on the 25 sphere surface is affected primarily by the no-slip non-shaded vertical wall rather than by the top 26 wall (note that the sphere rotates around the z-axis). Since the distance between the sphere and 27 the vertical wall is fixed as r/a increases, $F_{x,v}^1$ and $F_{x,v}^4$ show little variation. 28



Figure 12: (a-b) Pressure field and streamlines in the z = -0.6r plane when r/a = 1/1.75 (a) and 1/1.2 (b). (c-d) Pressure field and streamlines in the z = 0.6r plane when r/a = 1/1.75 (c) and 1/1.2 (d). W = 3.5r and b = 1.5r in all cases. $\bar{p} = (p - p_{ref})/\mu\omega$.

1 4 CONCLUSIONS

In summary, the actuation of magnetic spheres confined inside square channels by a rotating magnetic field is studied using immersed-boundary lattice Boltzmann simulations. The sphere is positioned at a fixed distance from one of the vertical channel walls and rotates around the z-axis with a small rotational Reynolds number. The hydrodynamic actuation force acting on the sphere in the x-direction, F_x , is computed as a function of the channel width and the sphere's distance to the bottom channel wall.

Our simulations show that, in very wide channels, when a sphere is away from top and bottom 8 walls, F_x is positive. F_x decreases and eventually reverses its direction as the sphere is shifted toward 9 the channel corner. The opposite trend is discovered in channels that are sufficiently narrow. When 10 the sphere is positioned midway between top and bottom walls, F_x decreases to become negative 11 as the channel width decreases but then recovers to zero when all four channel walls are symmetric 12 with respect to the sphere. These different trends are traced to the modulation of the flow in 13 the channel, which features both recirculation near the sphere and a more global flow across the 14 entire channel, by the confinement of channel walls. Such modulation is more complicated than 15 that encountered when a rotating sphere is confined between two parallel walls.⁴⁶ In particular, the 16 pressure heterogeneity near the sphere induced by fluid recirculation and global flow is modified 17

greatly as the confinement by the four channel walls changes. The resulting pressure force can dominate the viscous force on the sphere and control the direction of F_x . The observed variations of F_x and their underlying mechanisms highlight the rich behavior of magnetic actuation inside microchannels and can be important for the application of magnetic actuation in microfluidic environment.

6 ACKNOWLEDGMENTS

The authors thank the ARC at Virginia Tech for generous allocation of computing time. R.Q.
acknowledges support by the NSF under grant number 1808307.

⁹ References

- 10 (1) Purcell, E. M. Life at low Reynolds number. American Journal of Physics 1977, 45, 3–11.
- (2) Yang, F.; Qian, S.; Zhao, Y.; Qiao, R. Self-diffusiophoresis of Janus catalytic micromotors in
 confined geometries. *Langmuir* 2016, *32*, 5580–5592.
- (3) Ma, F.; Yang, X.; Zhao, H.; Wu, N. Inducing propulsion of colloidal dimers by breaking the
 symmetry in electrohydrodynamic flow. *Physical review letters* 2015, 115, 208302.
- (4) Qian, S.; Bau, H. H. Magneto-hydrodynamics based microfluidics. Mechanics research com munications 2009, 36, 10–21.
- (5) Driscoll, M.; Delmotte, B. Leveraging collective effects in externally driven colloidal suspensions: Experiments and simulations. *Current Opinion in Colloid & Interface Science* 2019, 40, 42–57.
- (6) Yang, Z.; Zhang, L. Magnetic Actuation Systems for Miniature Robots: A Review. Advanced
 Intelligent Systems 2000082.
- (7) Lim, B.; Vavassori, P.; Sooryakumar, R.; Kim, C. Nano/micro-scale magnetophoretic devices
 for biomedical applications. *Journal of Physics D: Applied Physics* 2016, *50*, 033002.
- (8) Barbillon, G.; Bosseboeuf, A.; Chun, K.; Ferrigno, R.; Français, O. Engineering of Micro/Nano
 Biosystems; Springer, 2020.

22

1	(9) Kirby, B. J. Micro-and Nanoscale Fluid Mechanics: Transport in Microfluidic Devices; Cam-
2	bridge university press, 2010.

(10) Sing, C. E.; Schmid, L.; Schneider, M. F.; Franke, T.; Alexander-Katz, A. Controlled surface induced flows from the motion of self-assembled colloidal walkers. *Proceedings of the National Academy of Sciences* 2010, 107, 535–540.

6 (11) Tottori, S.; Zhang, L.; Qiu, F.; Krawczyk, K. K.; Franco-Obregón, A.; Nelson, B. J. Mag7 netic helical micromachines: fabrication, controlled swimming, and cargo transport. *Advanced*8 *Materials* 2012, 24, 811–816.

(12) Khalil, I. S.; Tabak, A. F.; Hamed, Y.; Mitwally, M. E.; Tawakol, M.; Klingner, A.; Sitti, M.
 Swimming back and forth using planar flagellar propulsion at low Reynolds numbers. *Advanced Science* 2018, *5*, 1700461.

(13) Yu, J.; Jin, D.; Chan, K.-F.; Wang, Q.; Yuan, K.; Zhang, L. Active generation and magnetic
 actuation of microrobotic swarms in bio-fluids. *Nature Communications* 2019, 10, 1–12.

(14) Rogowski, L. W.; Oxner, M.; Tang, J.; Kim, M. J. Heterogeneously flagellated microswimmer
 behavior in viscous fluids. *Biomicrofluidics* 2020, 14, 024112.

(15) Khalil, I. S.; Magdanz, V.; Simmchen, J.; Klingner, A.; Misra, S. Resemblance between motile
 and magnetically actuated sperm cells. *Applied Physics Letters* 2020, *116*, 063702.

- (16) El Alaoui-Faris, Y.; Pomet, J.-B.; Régnier, S.; Giraldi, L. Optimal actuation of flagellar magnetic microswimmers. *Physical Review E* 2020, 101, 042604.
- (17) Zhu, L.; Huang, W.; Yang, F.; Yin, L.; Liang, S.; Zhao, W.; Mao, L.; Yu, X.; Qiao, R.;
 Zhao, Y. Manipulation of Single Cells Using a Ferromagnetic Nanorod Cluster Actuated by
 Weak AC Magnetic Fields. Advanced Biosystems 2019, 3, 1800246.

(18) Tierno, P.; Golestanian, R.; Pagonabarraga, I.; Sagués, F. Controlled swimming in confined
 fluids of magnetically actuated colloidal rotors. *Physical Review Letters* 2008, 101, 218304.

(19) Martinez-Pedrero, F.; Ortiz-Ambriz, A.; Pagonabarraga, I.; Tierno, P. Colloidal microworms
 propelling via a cooperative hydrodynamic conveyor belt. *Physical Review Letters* 2015, 115, 138301.

23

1 2	(20)	Wang, Q.; Yu, J.; Yuan, K.; Yang, L.; Jin, D.; Zhang, L. Disassembly and spreading of magnetic nanoparticle clusters on uneven surfaces. <i>Applied Materials Today</i> 2020 , <i>18</i> , 100489.
3 4	(21)	Sprinkle, B.; van der Wee, E. B.; Luo, Y.; Driscoll, M. M.; Donev, A. Driven dynamics in dense suspensions of microrollers. <i>Soft Matter</i> 2020 ,
5 6	(22)	Helgesen, G. Magnetic propulsion of microspheres at liquid-glass interfaces. <i>Journal of Applied Physics</i> 2018 , <i>123</i> , 064902.
7 8	(23)	Zhang, S.; Wang, Y.; Onck, P.; den Toonder, J. A concise review of microfluidic particle manipulation methods. <i>Microfluidics and Nanofluidics</i> 2020 , <i>24</i> , 1–20.
9 10	(24)	Martínez-Pedrero, F.; Tierno, P. Advances in colloidal manipulation and transport via hydro- dynamic interactions. <i>Journal of Colloid and Interface Science</i> 2018 , <i>519</i> , 296–311.
11 12	(25)	Erb, R. M.; Martin, J. J.; Soheilian, R.; Pan, C.; Barber, J. R. Actuating soft matter with magnetic torque. <i>Advanced Functional Materials</i> 2016 , <i>26</i> , 3859–3880.
13 14	(26)	Elgeti, J.; Winkler, R. G.; Gompper, G. Physics of microswimmers—single particle motion and collective behavior: a review. <i>Reports on Progress in Physics</i> 2015 , <i>78</i> , 056601.
15 16 17	(27)	Van Reenen, A.; de Jong, A. M.; den Toonder, J. M.; Prins, M. W. Integrated lab-on-chip biosensing systems based on magnetic particle actuation–a comprehensive review. <i>Lab on a Chip</i> 2014 , <i>14</i> , 1966–1986.
18 19	(28)	Tierno, P. Recent advances in anisotropic magnetic colloids: realization, assembly and appli- cations. <i>Physical Chemistry Chemical Physics</i> 2014 , <i>16</i> , 23515–23528.
20 21 22	(29)	Rikken, R. S.; Nolte, R. J.; Maan, J. C.; van Hest, J. C.; Wilson, D. A.; Christianen, P. C. Manipulation of micro-and nanostructure motion with magnetic fields. <i>Soft Matter</i> 2014 , <i>10</i> , 1295–1308.
23 24 25	(30)	Martinez-Pedrero, F.; Navarro-Argemí, E.; Ortiz-Ambriz, A.; Pagonabarraga, I.; Tierno, P. Emergent hydrodynamic bound states between magnetically powered micropropellers. <i>Science advances</i> 2018 , <i>4</i> , eaap9379.
26	(31)	Driscoll, M.; Delmotte, B.; Youssef, M.; Sacanna, S.; Donev, A.; Chaikin, P. Unstable fronts

and motile structures formed by microrollers. *Nature Physics* **2017**, *13*, 375–379.

1	(32) Delmotte, B.; Driscoll, M.; Chaikin, P.; Donev, A. Hydrodynamic shocks in microroller su	ıs-
2	pensions. Physical Review Fluids 2017, 2, 092301.	

5 (34) Xiao, Z.; Wei, M.; Wang, W. A review of micromotors in confinements: Pores, channels,
6 grooves, steps, interfaces, chains, and swimming in the bulk. ACS applied materials & inter7 faces 2018, 11, 6667–6684.

8 (35) Singh, A.; Li, J.; Jiang, X.; Hernández-Ortiz, J. P.; Jaeger, H. M.; de Pablo, J. J. Shape
9 induced segregation and anomalous particle transport under spherical confinement. *Physics*10 of Fluids 2020, 32, 053307.

(36) Liu, P.; De Folter, J. W.; Petukhov, A. V.; Philipse, A. P. Reconfigurable assembly of superparamagnetic colloids confined in thermo-reversible microtubes. *Soft Matter* 2015, *11*, 6201–6211.

(37) Alonso-Matilla, R.; Saintillan, D. Microfluidic flow actuation using magnetoactive suspensions.
 EPL (Europhysics Letters) 2018, 121, 24002.

(38) Sherman, Z. M.; Pallone, J. L.; Erb, R. M.; Swan, J. W. Enhanced diffusion and magnetic tophoresis of paramagnetic colloidal particles in rotating magnetic fields. *Soft matter* 2019, 15, 6677–6689.

(39) Satoh, A.; Chantrell, R. W. Application of the dissipative particle dynamics method to mag netic colloidal dispersions. *Molecular Physics* 2006, 104, 3287–3302.

(40) Kang, T. G.; Hulsen, M. A.; Anderson, P. D.; den Toonder, J. M.; Meijer, H. E. Chaotic
mixing induced by a magnetic chain in a rotating magnetic field. *Physical Review E* 2007,
76, 066303.

(41) Kang, T. G.; Hulsen, M. A.; den Toonder, J. M.; Anderson, P. D.; Meijer, H. E. A direct
 simulation method for flows with suspended paramagnetic particles. *Journal of Computational Physics* 2008, 227, 4441–4458.

27 (42) Lagger, H. G.; Breinlinger, T.; Korvink, J. G.; Moseler, M.; Di Renzo, A.; Di Maio, F.;

 ^{3 (33)} Kaiser, A.; Snezhko, A.; Aranson, I. S. Flocking ferromagnetic colloids. *Science Advances* 4 2017, 3, e1601469.

Bierwisch, C. Influence of hydrodynamic drag model on shear stress in the simulation of 1 magnetorheological fluids. Journal of Non-Newtonian Fluid Mechanics 2015, 218, 16–26. 2 (43) Rossi, E.; Ruiz-Lopez, J. A.; Vazquez-Quesada, A.; Ellero, M. Dynamics and rheology of a 3 super-paramagnetic chain suspension under the combined effect of a shear flow and a rotating 4 magnetic field. Soft Matter 2021, 5 (44) Krishnamurthy, S.; Yadav, A.; Phelan, P.; Calhoun, R.; Vuppu, A.; Garcia, A.; Hayes, M. 6 Dynamics of rotating paramagnetic particle chains simulated by particle dynamics, Stokesian 7 dynamics and lattice Boltzmann methods. *Microfluidics and Nanofluidics* 2008, 5, 33–41. 8 (45) Han, K.; Feng, Y.; Owen, D. Modelling of magnetorheological fluids with combined lattice 9 Boltzmann and discrete element approach. Communications in Computational Physics 2010, 10 7, 1095. 11 (46) Fang, W.-Z.; Ham, S.; Qiao, R.; Tao, W.-Q. Magnetic Actuation of Surface Walkers: The 12 Effects of Confinement and Inertia. Langmuir 2020, 13 (47) Cheng, R.; Huang, W.; Huang, L.; Yang, B.; Mao, L.; Jin, K.; ZhuGe, Q.; Zhao, Y. Ac-14 celeration of tissue plasminogen activator-mediated thrombolysis by magnetically powered 15 nanomotors. ACS Nano 2014, 8, 7746-7754. 16 (48) Goldman, A. J.; Cox, R. G.; Brenner, H. Slow viscous motion of a sphere parallel to a plane 17 wall—I Motion through a quiescent fluid. Chemical Engineering Science 1967, 22, 637–651. 18 (49) Zeng, L.; Balachandar, S.; Fischer, P. Wall-induced forces on a rigid sphere at finite Reynolds 19 number; 2004. 20 (50) Liu, Q.; Prosperetti, A. Wall effects on a rotating sphere. Journal of Fluid Mechanics 2010, 21 657, 1. 22 (51) Fang, C.; Sun, S.; Qiao, R. Structure, thermodynamics, and dynamics of thin brine films in 23 oil-brine-rock systems. Langmuir 2019, 35, 10341-10353. 24 (52) Feng, Z.-G.; Michaelides, E. E. Robust treatment of no-slip boundary condition and velocity 25 updating for the lattice-Boltzmann simulation of particulate flows. Computers & Fluids 2009, 26

27 *38*, 370–381.

26

Soft Matter

1	(53)	Kang, S. K.; Hassan, Y. A. A comparative study of direct-forcing immersed boundary-lattice
2		Boltzmann methods for stationary complex boundaries. International Journal for Numerical
3		Methods in Fluids 2011 , 66, 1132–1158.
4	(54)	Zhang, D.; Papadikis, K.; Gu, S. Three-dimensional multi-relaxation time lattice-Boltzmann
5		model for the drop impact on a dry surface at large density ratio. International Journal of
6		Multiphase Flow 2014 , 64, 11–18.
7	(55)	$\label{eq:constraint} d'Humieres, D. \ Multiple-relaxation-time \ lattice \ Boltzmann \ models \ in \ three \ dimensions. \ Philo-interval \$
8		sophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and
9		Engineering Sciences 2002 , 360, 437–451.
10	(56)	Krüger, T.; Kusumaatmaja, H.; Kuzmin, A.; Shardt, O.; Silva, G.; Viggen, E. M. The lattice
11		Boltzmann method. Springer International Publishing 2017, 10, 4–15.

(57) Guo, Z.; Zheng, C.; Shi, B. Discrete lattice effects on the forcing term in the lattice Boltzmann 12 method. Physical Review E 2002, 65, 046308. 13