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Supplementary Information: Feedback control of inertial microfluidics using axial control forces

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S1 The lattice Boltzmann method

Here we explain details of our lattice Boltzmann simulations and start with explaining the collision and streaming step.

In the collision step the fluid particles at each lattice point exchange momentum by a local collision rule. Here we employ the common Bhatnagar-Gross-Krook collision model, where the velocity distribution function relaxes towards a local equilibrium distribution f_i^{eq} with a single relaxation time τ. This results in the post-collision distribution

$$f_i^\star(\vec{x},t) = f_i(\vec{x}) + \frac{1}{\tau}\left[f_i^{\mathrm{eq}}(\vec{x},t) - f_i(\vec{x},t)\right]. \tag{S1}$$

For the local thermal equilibrium distribution we use an expansion of the local Maxwell-Boltzmann distribution up to second order in the mean velocity $\vec{u}$, which results in

$$f_i^{\mathrm{eq}} = w_i\rho\left(1 + \frac{\vec{c}_i\cdot\vec{u}}{c_s^2} + \frac{(\vec{c}_i\cdot\vec{u})^2}{2c_s^4} - \frac{|\vec{u}|^2}{2c_s^2}\right). \tag{S2}$$

The weights w_i ensure that all moments of the equilibrium distribution up to the third order are correctly reproduced including the number density ρ (zeroth order) and the mean velocity $\vec{u}$ at lattice point $\vec{x}$ (first order). $c_s = \sqrt{k_BT/m}$ is the speed of sound[1]. Note that the collision step locally conserves mass and momentum.

After collision the fluid particles move to adjacent lattice positions according to their velocities and the new distribution functions at time $t + \Delta t$ become

$$f_i(\vec{x} + \Delta t\vec{c}_i, t + \Delta t) = f_i^\star(\vec{x},t). \tag{S3}$$

Here we use the D3Q19 scheme[1], where the velocities connect each lattice point to its nearest and next-nearest neighbors. To simplify the following discussion,

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in the remainder of this section we set $\Delta x = 1$ and $\Delta t = 1$ and rescale all quantities accordingly.

Note that on length and time scales much larger than Δx and Δt, respectively, one can derive the Navier-Stokes equation by a Chapman-Enskog expansion using the formulated streaming and collision steps[1]. The internal pressure follows an ideal gas law with $p = c_s^2\rho$, where $c_s = 1/\sqrt{3}$ is the speed of sound, and the kinematic viscosity is given by $\nu = c_s^2(\tau - 1/2)$.

To implement the no-slip boundary condition on the channel walls, we employ the regularized boundary condition introduced by Latt and Chopard[2]. It treats boundary nodes just like fluid nodes but modifies the distribution function before the collision such that the correct velocity is imposed. The method uses the bounce-back rule for the nonequilibrium distribution introduced by Zou and He[3].

S2 Inamuro Immersed Boundary method

We model the colloidal particle by the Inamuro Immersed Boundary (IB) method[4] with "five iterations". In this section we review the details of the implementation.

The colloid surface is approximated by a triangular mesh with vertices i at positions $\vec{x}_i^m$. To obtain the mesh, we start from a an icosahedron and successively refine it by splitting each triangle into four until the edge length is smaller than the lattice spacing. The positions of the resulting vertices continuously vary in space and hence do not necessarily coincide with the lattice sites. For clarity we will denote here the lattice sites by $\vec{x}_j$. We couple mesh vertices and lattice sites to each other using a smoothed delta function $\delta_h(\vec{x})$. We follow Peskin[5] and employ $\delta_h(\vec{x}) = \phi(x)\phi(x)\phi(z)$ with

$$\phi(x) = \begin{cases} \frac{1}{8}\left(3 - 2|x| + \sqrt{1 + 4|x| - 4x^2}\right) & 0 \le |x| \le 1 \\ \frac{1}{8}\left(5 - 2|x| - \sqrt{7 + 12|x| - 4x^2}\right) & 1 \le |x| \le 2 \\ 0 & 2 \le |x| \end{cases} \tag{S4}$$

and the same form for $\phi(y)$ and $\phi(z)$. In the IB method one determines the fluid velocity $\vec{u}_i^m$ at mesh point i by interpolating the fluid velocity from the lattice sites with the help of the smoothed delta function,

$$\vec{u}_i^m = \sum_j \delta_h(\vec{x}_i^m - \vec{x}_j)\vec{u}_j. \tag{S5}$$

To enforce the no-slip boundary condition at the colloid surface, we introduce the penalty force $\vec{f}_i^m = \vec{u}_i^m - \vec{v}_i^s$ as the difference between the fluid velocity and the surface velocity $\vec{v}_i^s = \vec{v} + \vec{\omega} \times (\vec{x}_i^m - \vec{r})$ of the colloid at the position $\vec{x}_i^m$ of mesh vertex i. The penalty force $\vec{f}_i^m$ acts on the mesh vertex i and, to conserve momentum, its negative $-\vec{f}_i^m$ acts on the surrounding fluid. We interpolate the

penalty force on lattice site $\vec{x}_j$ from the neighboring mesh vertices,

$$\vec{f}_j = -\sum_i \delta_h(\vec{x}_i^m - \vec{x}_j)\vec{f}_i^m. \tag{S6}$$

To apply the penalty force to the fluid, we use the same method as for the body force. We calculate modified fluid velocities at the mesh points i, which do not obey the no-slip boundary condition exactly since we interpolate forces and velocities between the mesh and lattice points. To decrease the slip velocity further, we therefore refine the penalty force iteratively by repeating the procedure five times and thereby implement the no-slip boundary condition in good approximation. Note that the total penalty force experienced by the fluid and hence by the colloid is the sum over all iterations.

As just introduced, the fluid interacts with a colloid which results in a hydrodynamic coupling. We can quantify it by a force and torque acting on the colloid given by the sum of the vertex contributions just introduced,

$$\vec{F}_{\text{fluid}} = \sum_i \vec{f}_i^m \tag{S7}$$

$$\vec{T}_{\text{fluid}} = \sum_i (\vec{x}_i^m - \vec{r}) \times \vec{f}_i^m. \tag{S8}$$

The force and torque contain two contributions. The first one comes from the fluid particles outside the colloid. The second contribution resulting from fluid particles inside the colloid is unphysical. We therefore compensate this contribution using Feng's rigid body approximation[6] and denote the respective force and torque by $\vec{F}_{\text{Feng}}$, $\vec{T}_{\text{Feng}}$.

With all force contributions the equations of motion for the colloid are given by

$$\begin{aligned} \vec{r}(t+1) &= \vec{r}(t) + \vec{v}(t), \\ M\vec{v}(t+1) &= M\vec{v}(t) + \vec{F}_{\text{fluid}} + \vec{F}_{\text{Feng}} + \vec{F}_{\text{ctl}}, \\ I\vec{\omega}(t+1) &= I\vec{\omega}(t) + \vec{T}_{\text{fluid}} + \vec{T}_{\text{Feng}}, \end{aligned} \tag{S9}$$

where M and I are the respective mass and moment of inertia of the colloid and $\vec{F}_{\text{ctl}}$ is the axial control force which we will introduce in Sects. 4 and 5 of the main text.

References

[1] B. Dünweg and A. J. Ladd, *Advances in Polymer Science*, Springer Berlin Heidelberg, 2008, pp. 1–78.

[2] J. Latt, B. Chopard, O. Malaspinas, M. Deville and A. Michler, *Phys. Rev. E*, 2008, **77**, 056703.

[3] Q. Zou and X. He, *Phys. Fluids*, 1997, **9**, 1591.

[4] T. Inamuro, *Fluid Dyn. Res.*, 2012, **44**, 024001.

[5] C. S. Peskin, *Acta numerica*, 2002, **11**, 479–517.

[6] Z.-G. Feng and E. E. Michaelides, *Comput. Fluids*, 2009, **38**, 370–381.