Supporting Information

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SI Methods and Materials

Numerical Simulation. We used a numerical model to solve the 3D incompressible Navier–Stokes equations in the reference frame of a particle moving in a rectangular channel (1). For these simulations, whereas the position of particle is fixed, the dynamics of the system are updated to achieve force- and torque-free conditions for the particle (i.e., the steady-state behavior). More precisely, a sphere, of diameter a, is stationary in a $w \times h$ rectangular channel, with sidewalls moving backward at the presumptive sphere velocity u_p. The flow at the position of the sphere was determined for one isolated particle by specifying a volumetric flow rate q, through setting inlet or outlet boundary conditions to fully developed laminar inflow or outflow in software (no periodic boundary conditions). Scripts run by COMSOL Multiphysics are used to solve the Navier–Stokes equations and update conditions to achieve steady state. Rotation is modeled by modifying the slip velocity at the surface of the sphere according to its rigid rotation. In addition to these boundary conditions, fluid density ρ and viscosity μ, were set to values of water, or ρ was set to zero for the Stokes flow case. Beginning with the initial condition of a stationary sphere (i.e., particle and walls at rest), we determined forces and torques by integrating force per area (F'') and torque density ($r \times F''$) across the particle surface in software. We then iteratively updated the wall velocity (u_p) and particle rotation until the sphere was force-free in the axial (x) direction and experienced zero net torque in all directions, to the limit in numerical precision. The streamlines in the frame of reference of a translating particle that is rotating at steady state could then be obtained.

Using this method, first, we conducted simulations for particle positions 1 μm apart along the short axis of the channel to determine the inertial focusing position. Varying the sphere position yielded the steady state lateral force for a particle held to a particular y-position in the channel cross section at ($z = 0$). Based on interpolating the position where the lateral force curve crossed zero we found the focusing position of the particle. Placing a particle at this position we solved the Navier-Stokes equations to obtain the flow fields in the microchannel for several conditions (reported in Fig. 3).

Image Analysis. Particle motion was captured with a high-speed camera (Phantom V7.3) at up to 100,000 frame/s rate. To study the interaction between particles, it was necessary to follow the particle motion as long as possible. Therefore we used a low magnification objective lens to achieve a large field of view, while sacrificing resolution. The ×2 magnification objective lens allowed an 8.8 mm wide field of view with our optical setup. With a typical flow rate of ∼80 μL/ min in a 25 μm × 90 μm channel, it takes ∼14 ms for particles to move across the whole field of view. Movies were taken at ∼5 mm downstream from inlet, at which point the particles are mostly at the same y-position but not fully focused yet (possibly at different z-positions). Captured movie frames are combined to build a 3D stack (*x*-*y*-*t*) with Image J (Fig. S1). Then the 3D stack was resliced in the *x*-*t* plane. With the choice of y equal to the focusing position, we get a particle trajectory in *x*-*t* plane. Graphs showing particle dynamics, as in Fig. 2 and 5, are achieved by skewing the *x*-*t* image horizontally, which is equivalent to a coordinate transformation of $x' = x - vt$ ($v = \frac{\Delta x}{\Delta t} = \tan\theta$, where θ is the skewed angle).

1. Di Carlo D, Edd JF, Humphry KJ, Stone HA, Toner M (2009) Particle segregation and dynamics in confined flows. *Phys Rev Lett* 102:094503.

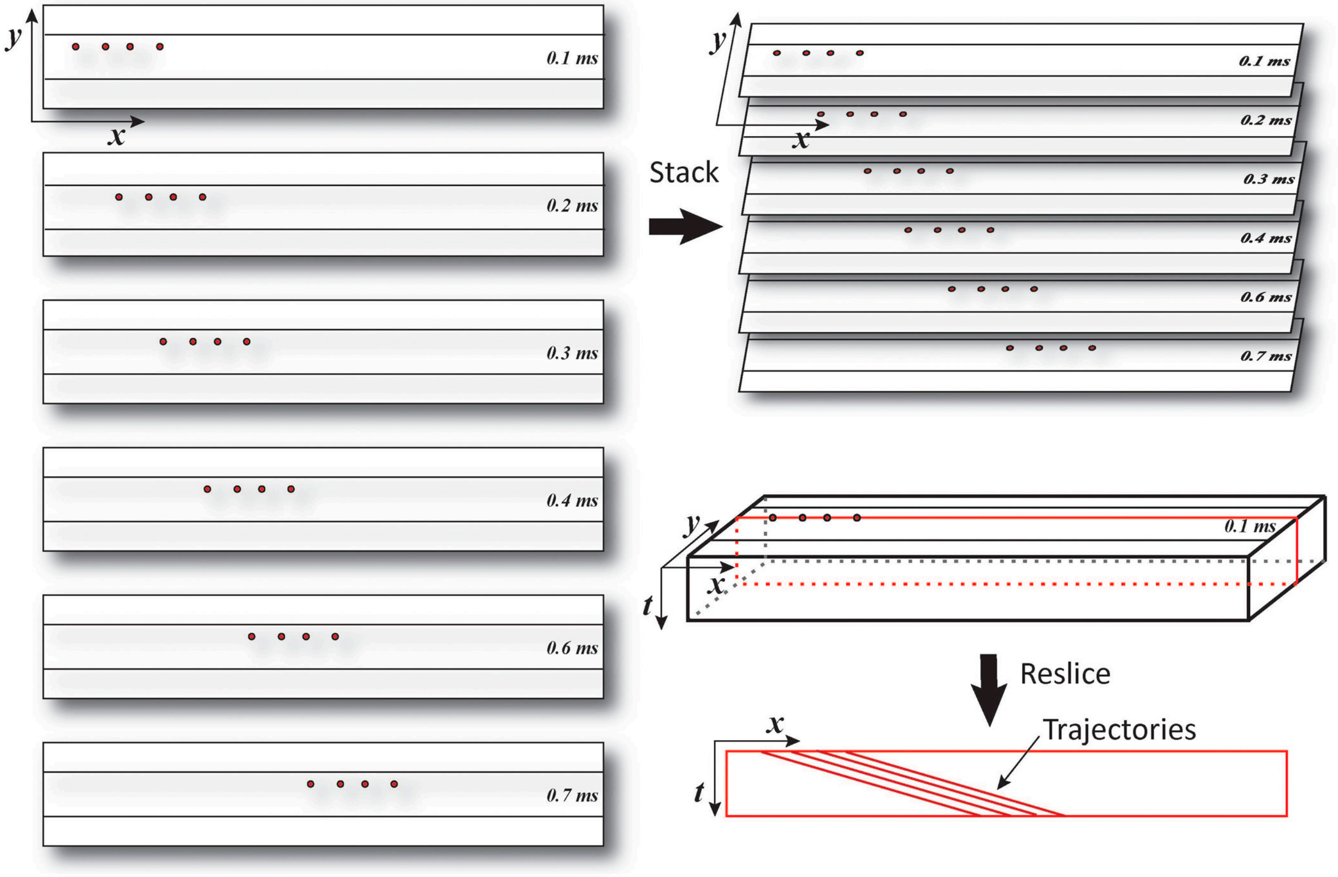


Fig. S1. *x-t* graph conversion. High-speed movie frames are stacked to build a 3D stack (*x-y-t*) and resliced through another plane (*x-t*). The plane contains particle trajectory is chosen for further analysis.

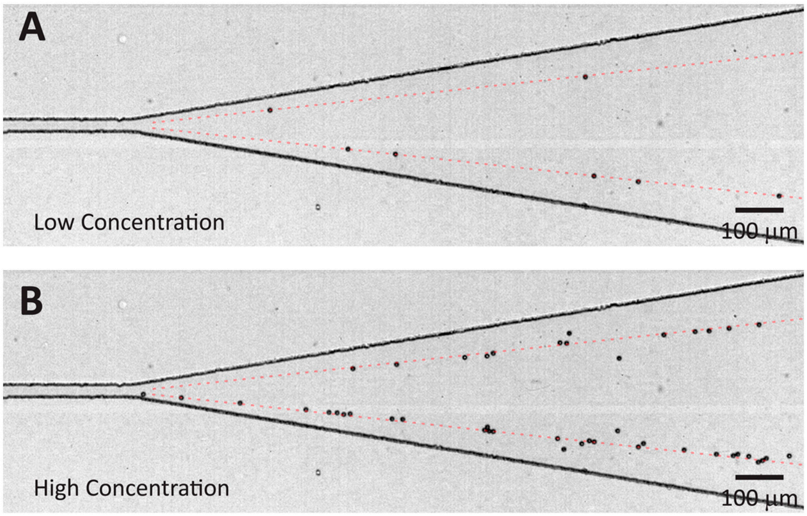


Fig. S2. Defocusing at expanding channels. (*A*) At low concentration in expanding channels, inertially focused particles follow the same streamlines. (*B*) At high concentration, particles migrate across the streamlines due to particle–particle interactions resulting in defocusing.

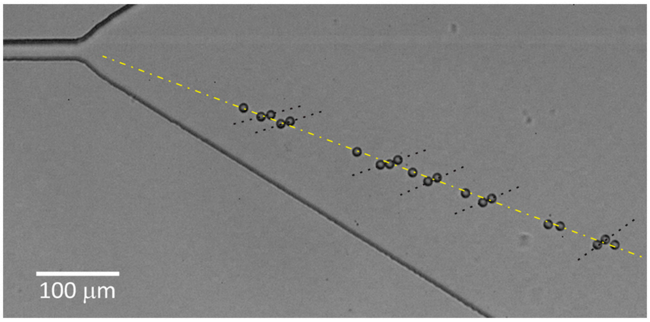
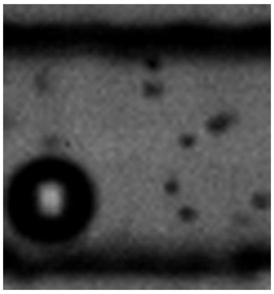
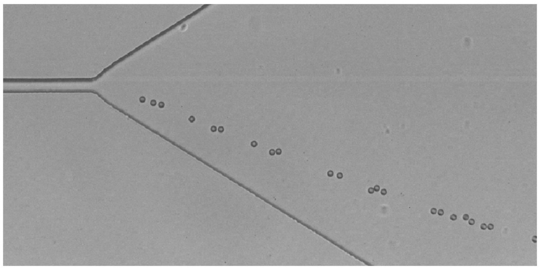


Fig. S3. Ordering induced by expansion flow. Particles develop a unique pattern at the expanding channel due to deterministic defocusing for an appropriate particle concentration.

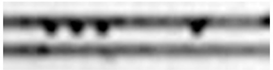
Movie S1. Dynamic self-assembly of a particle pair. Particle pair motion in a translating reference of frame shows settling to a preferred interparticle spacing after oscillations. Channel dimension: 25 μm wide, 90 μm high. Particle size: 9.9 μm. Re = 13. The movie is ~800 times slowed from real time (total ~15 ms).
Movie S1 (MOV)



Movie S2. Reversing flow. The 1 μm tracer particles change direction near the 10 μm particle indicating the reversing flow. The video is assembled in a translating reference frame. Channel dimension: 25 μm wide, 90 μm high. Re = 0.36. The movie is ~300 times slowed from real time (total ~23 ms).
Movie S2 (MOV)



Movie S3. Particle ordering at an expanding channel. Particles form unique deterministic patterns at the expanding channel with an appropriate particle concentration. Particle size: 9.9 μm. The movie is ~1300 times slowed from real time (total ~9 ms).
Movie S3 (MOV)



Movie S4. Elongation of a particle train. The dynamic self-assembly process of a single particle joining a particle train shows wave-like momentum transfer. The video is assembled in a translating reference frame. Channel dimension: 25 μm wide, 90 μm high. Particle size: 9.9 μm. Re = 26. The movie is ~2000 times slowed from real time (total ~13 ms).
Movie S4 (MOV)

Movie S5. Tuning of particle spacing with an expansion-contraction channel. The interparticle spacing of the particle pair changes along the channel; first, decreasing at the expansion then slowly increasing, and finally increasing further at the contraction. Channel dimension: 25 μm wide at narrow region and 45 μm at wide region, 85 μm high. Particle size: 9.9 μm. Re = 16 at the narrow region. The movie is ∼600 times slowed from real time (total ∼16 ms).
Movie S5 (MOV)