The crucial role of adhesion in the transmigration of active droplets through interstitial orifices
Supplementary information

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SUPPLEMENTARY NOTE 1: SUPPRESSION OF TRANSMIGRATION IN THE PRESENCE OF ADHESION

As discussed in the main text, the transmigration through sufficiently narrow constrictions is generally inhibited if a constant and uniform value of γ is set between droplet and pillars. In Fig.2 of the main text we have shown that the process can actually occur if the adhesion coefficient at the entry of the pore, γ_L, is larger than the one the exit, γ_R, provided that $\gamma_L \geq \gamma_{c,L}$ and $\gamma_R \leq \gamma_{c,R}$.

In Supplementary Movie SM1 we show an active droplet moving within a microchannel where $\lambda \simeq 0.5$, $\gamma_L = 5 \times 10^{-2}$ and $\gamma_R = 3 \times 10^{-2}$. Note that, with this value of λ, $\gamma_L > \gamma_{c,L} \simeq 2 \times 10^{-2}$ and $\gamma_R > \gamma_{c,R} \simeq 2 \times 10^{-2}$, thus the transmigration is expected to be suppressed. At the entry of the pore the dynamics is overall akin to that discussed in Fig.2 of the main text for $\lambda \simeq 0.5$. Indeed, portions of the interface, approximately located on opposite sides with respect to the longitudinal midline of the microchannel, adhere to pillars enabling the droplet to squeeze in. However, once a large part (more than half) of the droplet has passed the center of the pore, the motion stops and the droplet gets stuck in a peanulike configuration. This occurs because the droplet propulsion is not sufficient to overcome the excess of adhesion (controlled by γ_R) which, increasing the connectivity between interface and pillars, ultimately prevents the transmigration.

In Supplementary Movie SM2 we show the case in which $\lambda \simeq 0.2$, $\gamma_L = 1.5 \times 10^{-2}$ and $\gamma_R = 10^{-2}$. Here $\gamma_L < \gamma_{c,L} \simeq 2 \times 10^{-2}$ while $\gamma_R < \gamma_{c,R} \simeq 1.5 \times 10^{-2}$, hence once again the crossing should be inhibited. Indeed, once the droplet hits the pore, the low adhesion forces at the entry (controlled by γ_L) do not guarantee enough and prolonged contact between interface and pillars, thus basically impeding the droplet to snake in. The rearrangement of the liquid crystal orientation due to the internal fluid flow drives the droplet downwards and then backwards, causing its detachment from the pore.

As mentioned in the main text we note that, the values of the adhesion coefficients depends upon other thermodynamic parameters, such as elasticity of the liquid crystal and interfacial tension, speed of the droplet, viscosity, diffusion constant, repulsion as well as initial position, whose modification would require an adjustment of γ_L and γ_R.

SUPPLEMENTARY NOTE 2: NUMERICAL ASPECTS

In this section we provide further details about the computational model and the simulation parameters.

The equation of the order parameter ϕ_1 (Equation 2 of the main text), the one of the polarization $\mathbf{P}$ (Equation 3 of the main text) and the Navier-Stokes equations (Equation 4 and 5 of the main text) are integrated by using a hybrid lattice Boltzmann (LB) method [1], where the first two are solved via a finite-difference predictor-corrector scheme and the latter through a standard LB approach.

Simulations are run on rectangular boxes, where the vertical direction is kept constant at $L_z = 170$ while the horizontal one L_y ranges between 400 and 700 lattice sites. We set periodic boundary conditions along the y-axis and two flat walls along the z-axis, placed at $z = 0$ and $z = L_z$. Within the microchannel we place a droplet containing an active gel, whose concentration is described by the scalar field $\phi_1(\mathbf{r}, t)$, kept approximately equal to 2 inside and 0 everywhere else, and whose orientation is captured by the polar field $\mathbf{P}(\mathbf{r}, t)$, initially uniform and parallel to the y direction within the drop ($\mathbf{P}(\mathbf{r}, 0) = \mathbf{P}_y(\mathbf{r}, 0)$, with $|\mathbf{P}_y| = 1$) and zero outside. At the walls of the channel we impose no-slip conditions for the velocity field, i.e. $v|_{z=0,L_z} = 0$, and no wetting for ϕ_1, i.e. $\phi_1|_{z=0,L_z} = 0$ throughout the simulation. No specific anchoring conditions (such as perpendicular or parallel) are imposed at the walls for the polar field $\mathbf{P}$.

Following the design proposed in Ref.[2], the constriction is represented by two semi-circular pillars placed symmetrically at distance h and attached at opposite walls (see Fig.2 of the main text). Their solid structure is modeled through two auxiliary *static* phase fields $\phi_2(\mathbf{r})$ and $\phi_3(\mathbf{r})$, positive within each pillar and zero outside. In addition, the velocity field is set to zero inside throughout the simulation. Finally, to ensure that their interface remains perpendicular to the flat walls, we impose neutral wetting condition for both phase fields. Al-

though a more accurate modeling of the constriction is possible (using, for example, a full lattice Boltzmann approach [1, 3]), this one combines a good numerical stability with a relatively easy implementation of mesoscale interactions (such as repulsion and adhesion controlled by proper free energy terms, see Eq.1 of the main text) between the active droplet and the pore.

Thermodynamic parameters have been chosen as follows: $a = 0.04$, $k = 0.06$, $\alpha = 0.1$, $\kappa = 0.04$, $M = 0.1$, $\xi = 1.1$, $\Gamma = 1$, $\eta \simeq 1.67$, $\epsilon_{ij,i<j} = \epsilon = 0.1$. The first two values, a and k, control the surface tension σ of the active droplet, given by $\sigma = \sqrt{8ak/9} \simeq 0.045$, while the latter means that an equal repulsion is set between droplet and pillars. Lattice spacing and integration timestep are kept fixed to $\Delta x = 1$ and $\Delta t = 1$. The contractile activity ζ has been varied between -10^{-4} and -10^{-3}. Keeping fixed the thermodynamic parameters defined above, the optimal values of ζ ensuring a balance between interfacial deformations and splay distortions (guaranteeing a rectilinear motion) range roughly between -5×10^{-4} and -10^{-3}. Finally, the constant γ_{ij} in Eq.1 of the main text gauges the strength of the adhesion forces. We impose an equal value of adhesion coefficient between drop and each pillars, i.e. $\gamma_{12} = \gamma_{13}$, while other entries are set to zero. Since a constant value of γ throughout the pore generally does not yield a complete crossing, we set two different values γ_L and γ_R of adhesiveness on the half left of the pore (entry) and on the half right (exit) respectively, with $\gamma_L > \gamma_R$, to ensure a transmigration along the positive direction of the y-axis. In our simulations they approximately vary between 10^{-3} and 5×10^{-2}, while optimal values generally depend on the previous thermodynamic parameters as well as on the ratio $\lambda = h/D$, where D is the diameter of the droplet. As discussed in the main text, λ ranges from 0.2 to 0.8.

SUPPLEMENTARY NOTE 3: MAPPING TO PHYSICAL UNITS

Here we provide an approximate mapping between simulation parameters and real physical units. Our runs are performed on a rectangular mesh of size varying from $L_y = 500 \div 700$ (length of the channel) to $L_z = 170$ (height of the channel), with lattice spacing $\Delta x = 1$ and integration time step $\Delta t = 1$. A droplet of radius $R = 45$ lattice sites is placed within the microchannel, sufficiently far away from the constriction. Following previous works on self-propelled active fluid droplets [4, 5], we fix the length, time and force scales to the following values: $L = 1\mu$m, the time scale $T = 10$ms and the force scale $F = 100$nN (in simulation units these scales are all equal to one). Hence, our simulation would approximately correspond to a microfluidic channel of length ranging from 0.5 to 1mm in which an active droplet of diameter $D \simeq 90\mu$m has an effective shear viscosity $\eta_{eff} \simeq 1.5$kPa·s and an effective elastic constant $\kappa \simeq 0.04$nN, moving with speed $1 \div 10\ \mu m/s$ in a Newtonian fluid, such as water. Also, one would have a rotational viscosity $\Gamma \simeq 1$kPa·s and a diffusion coefficient $D = Ma \simeq 0.4\ \mu$m^2/s. Finally, the drop speed in simulation units varies between $v \simeq 10^{-4}$ and $v \simeq 10^{-3}$, values that keep the Reynolds number lower than 0.1 and ensure that inertial effects can be neglected. In addition, the capillary number ranges approximately between 0.1 and 0.001, thus droplet rupture remains an unlikely event.

SUPPLEMENTARY REFERENCES

[1] L. N. Carenza, G. Gonnella, A. Lamura, G. Negro, A. Tiribocchi, Lattice Boltzmann Methods and Active Fluids, Eur. Phys. Journ. E **42**, 81 (2019).

[2] P. M. Davidson, J. Sliz, P. Isermann, C. Denais, J. Lammerding, Design of a microfluidic device to quantify dynamic intra-nuclear deformation during cell migration through confining environments, Integrative Biology **7**, 1534-1546 (2015).

[3] T. Krüger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva, E.M. Viggen, *The Lattice Boltzmann Method: Principles and Practice*, Springer International Publishing, (2016).

[4] E. Tjhung, D. Marenduzzo, M. E. Cates, Spontaneous symmetry breaking in active droplets provides a generic route to motility, Proc. Nat. Acad. Sci. USA **109**, 12381 (2012).

[5] E. Tjhung, A. Tiribocchi, D. Marenduzzo, M. E. Cates, A minimal physical model captures the shapes of crawling cells, Nature. Commun **6**, 5420 (2015).