Surface wettability inverse design for programmable droplet transport and sorting

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1 Problem & design space

Wettability gradients drive droplets towards more wettable regions, with no pumps, electrodes or external fields. Patterning a substrate's chemistry could therefore *program* droplet transport and sorting passively, e.g. on low-cost lab-on-a-chip platforms.

Inverse problem. Given a target centroid path, find the heterogeneity field $\Phi(x, y)$, the local contact angle, that makes a droplet follow it. The design space is *high-dimensional*, so gradient-free search is prohibitive: we optimize Φ by gradient descent through a differentiable droplet model.

Gradients. Reverse-mode AD through the solver (JAX/diffrax) gives a *discrete adjoint* whose cost is largely independent of the number of design variables.

Surface parametrization.

$$\Phi(x,y) = b_0 + \underbrace{\frac{b_{\ell,0}}{L_x}x + \frac{b_{\ell,1}}{L_y}y}_{\text{linear}} + \underbrace{\mathrm{Re}\sum_{n,m}\mu_m B_{nm}\, e^{\mathrm{i}(k_x^{(n)}x + k_y^{(m)}y)}}_{\text{truncated Fourier}}$$

The *linear* term captures non-periodic, path-scale trends; the *Fourier* modes add the local structure curved paths need, with fewer modes and faster convergence than Fourier alone.

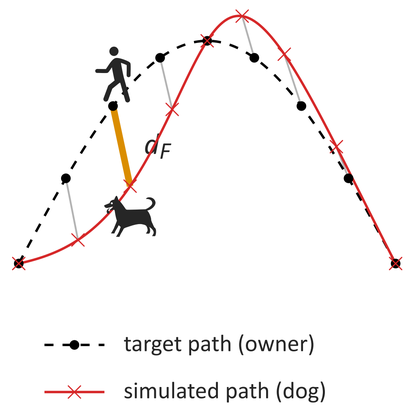
2 Method

Forward model. Lubrication theory and matched asymptotics reduce the droplet to *ODEs for the Fourier harmonics of its contact line* (Savva et al., 2019): cheap enough for thousands of forward solves inside the optimization loop. The system *stiffens* as the slip length $\lambda \to 0$; we integrate it with the implicit Kværno 5/4 scheme and adaptive steps.

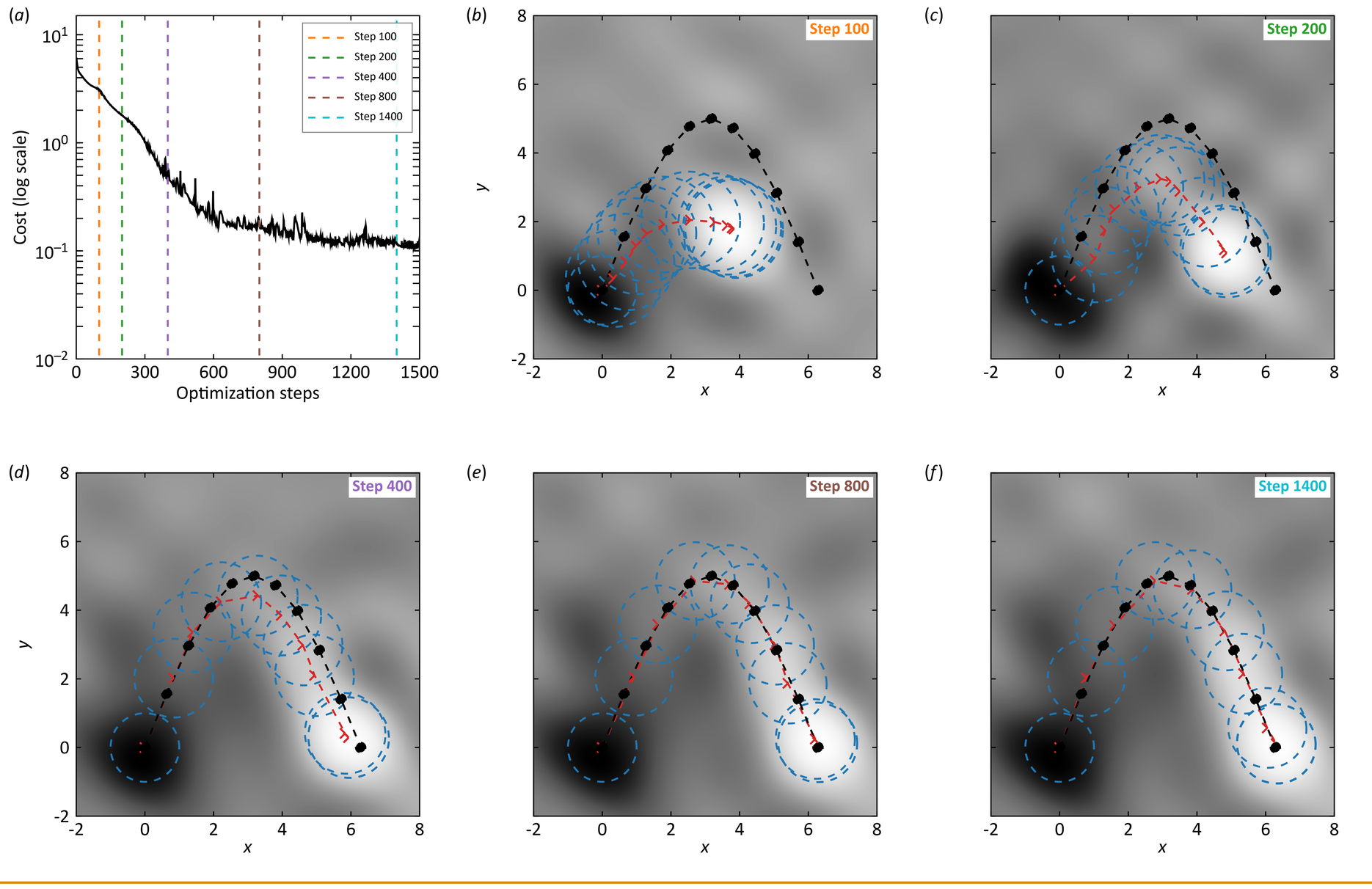
Loss function.

$$\mathcal{J} = \sqrt{d_F^2 + \beta\,\langle \sigma_r^2 \rangle_t}$$

- d_F: *Fréchet distance* between simulated and target centroid paths: the shortest leash that lets an owner and a dog walk the two paths without either going back. Sensitive to both location and ordering along the path.
- $\langle \sigma_r^2 \rangle_t$: time-averaged variance of the contact-line radius. Keeps the droplet near-circular, away from near-breakup states where the solver fails and the asymptotic model no longer holds ($\beta = 1$ or 0.1).



3 Optimization progression



The field is frozen at five optimization steps and the droplet re-simulated.

Fast phase ($\lesssim 400$ steps): the cost drops by over an order of magnitude and the path is captured *coarsely*.

Refinement (400–1400): remaining discrepancies are resolved *slowly*.

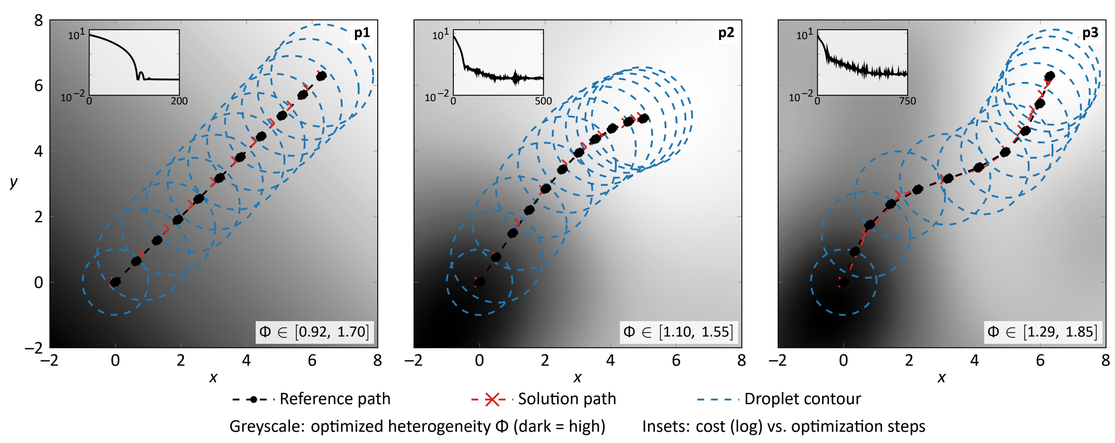
Emerging design: a hydrophobic patch at the start (dark) and a wettable basin at the end (light).

wettable (low Φ) — hydrophobic (high Φ)

greyscale normalized per panel

4 Validation: paths of increasing complexity

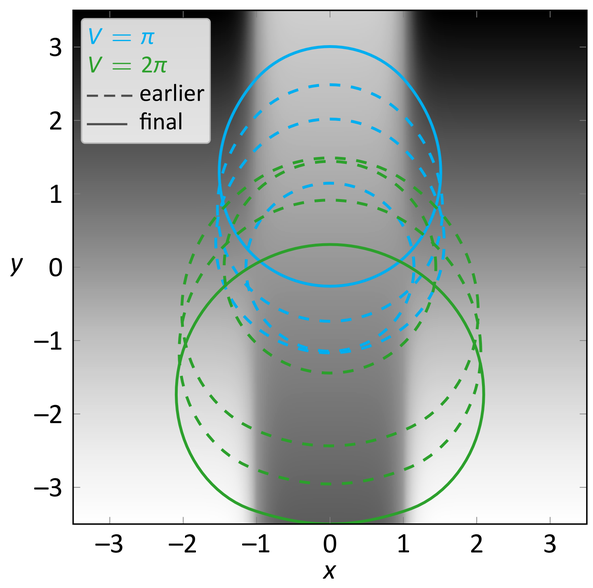
Straight line (p1), straight + turn (p2), oscillation + straight run (p3) and the sinusoidal arch (p4, in box 3) are all reproduced, with *nearly circular* contact lines throughout. Richer paths need more Fourier modes ($0 \to 13$) and more optimization steps ($200 \to 1500$).



5 Passive droplet sorting

One surface with inner and outer regions of *opposing linear wettability gradients* (smooth tanh transition). The droplet's *footprint* decides which gradient dominates: small droplets feel only the inner region, large ones also span the outer region, and the net drive reverses.

With its four parameters optimized over 100 droplets of different volume, droplets below and above $V_c = 3\pi/2$ move in opposite directions, *with no detection stage and no external fields*. Only droplets close to V_c barely move.



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