High-Fidelity CFD and Reduced-Order Modelling of Capillary Filling in Microchannels

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A multipronged strategy: 3D HPC for detailed microfluidic design + high-fidelity CFD and reduced-order modelling for transient wetting dynamics.

The story: from high-fidelity computation to efficient prediction

Aim: Efficient computational tools for microfluidic applications: **separating red blood cells** (RBCs) from plasma and **transient capillary filling** in microchannels

Topology optimisation

Blood-based microfluidic devices require detailed multiphase physics; HPC and adjoint methods make shape optimisation feasible

Transient capillary filling

High-fidelity CFD resolves the evolving liquid–gas interface; repeated simulations and microscopic slip scales are computationally demanding

Physics-based ROM

Generalised lubrication and limited CFD information retains the relevant wetting physics, enabling rapid transient predictions

1. Application: microfluidic transport and separation



Representative microfluidic device: small channels amplify interfacial, wall and multiphase effects.

- Applications: **diagnostics, plasma separation and lab-on-a-chip systems**.
- High-fidelity simulation resolves physics but is expensive.
- Combine **HPC** with physics-based **reduced models**.

2. Two complementary computational routes

3D steady blood flow

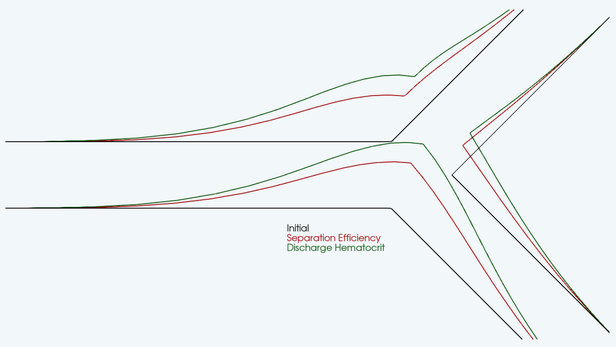
- blood transport in complex geometries
- CFD + **adjoint shape optimisation**
- maintained detailed 3D physics

2D transient wetting

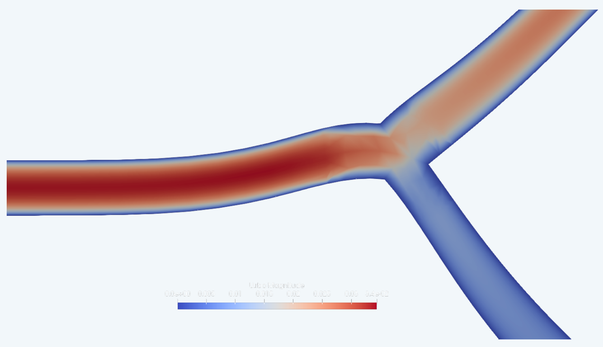
- features a moving air-liquid interface
- use CFD simulation as reference
- fast ROM to match CFD predictions

Why models for interfacial flows? Fully 3D transient moving-contact-line CFD simulations are prohibitively expensive for realistic scale separations.

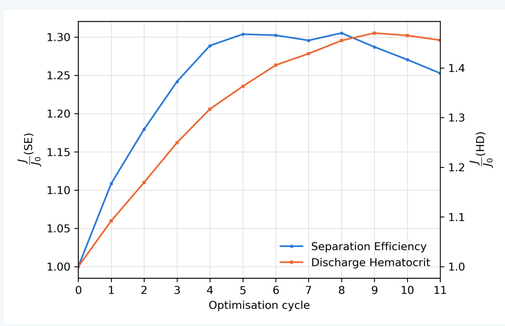
3. HPC in action: adjoint optimisation of 3D blood flow



The channel geometry evolves to promote plasma/RBC separation.



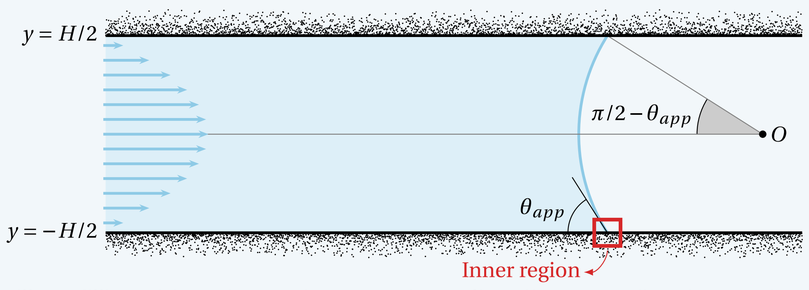
Velocity field in an optimised Y-junction. Blood is modelled as coupled RBC and plasma phases.



Adjoint-based optimisation substantially improves both separation metrics relative to the initial geometry.

- **Two-fluid OpenFOAM model** for the migration of RBCs and near-wall cell-free layer physics
- Objectives: separation efficiency and discharge-haematocrit difference.
- One grid-converged flow + adjoint solve: ∼1 day on 20 processors.
- Desirable feature: Adjoint gradient cost is essentially **independent of the number of design variables**.

4. Transient capillary filling; the need for a reduced-order model



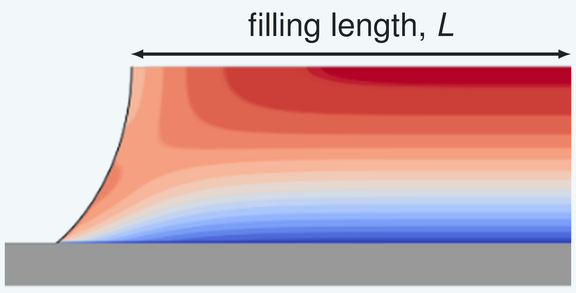
Capillary filling driven by surface tension; slip effects confined near the contact line.

- **Classical Lucas–Washburn**: misses **extra near-contact-line viscous stresses** (Poiseuille flow).
- High-fidelity CFD resolves interface dynamics but requires extreme contact-line resolution.
- Realistic slip lengths are typically too small to resolve in parameter studies.
- CFD parameter sweeps are currently infeasible regardless of available computing power

Idea: use a physics-based ROM to avoid resolving microscopic details with CFD

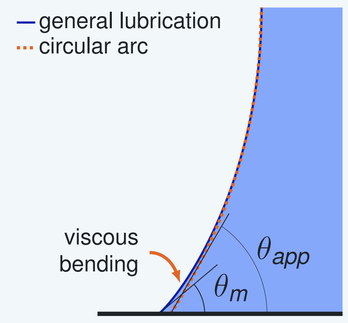
5. How the reduced-order model works

High-fidelity reference



CFD simulation for $\theta_m = 40°$

Generalised lubrication



Non-circular meniscus near the contact line; behaviour matches CFD ($\theta_m = 40°$).

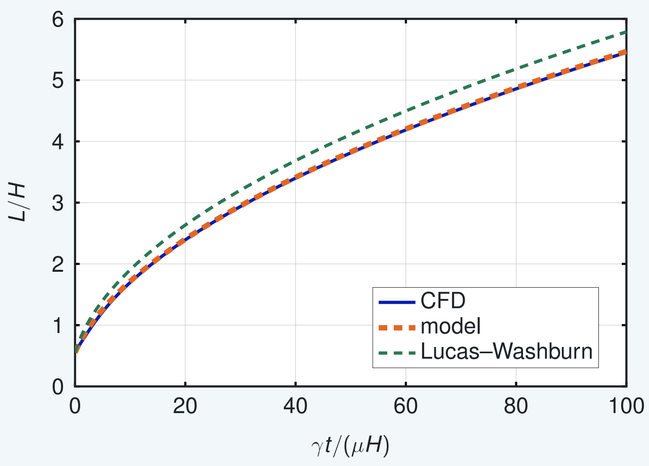
For γ surface tension, μ viscosity, λ slip length and H channel height

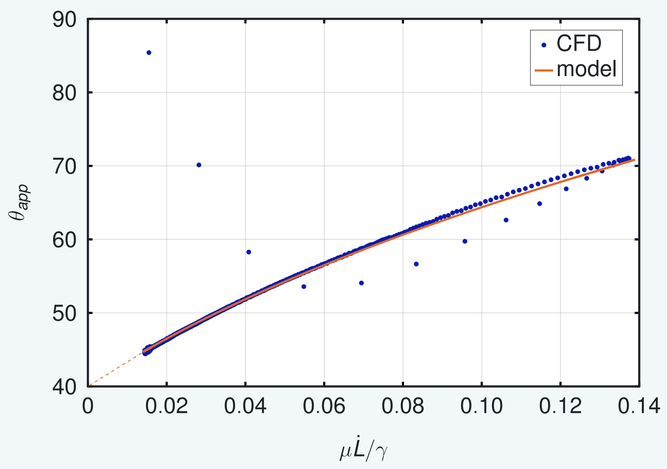
$$\frac{dL}{dt} = \frac{\gamma \cos\theta_{app}}{\mu(L-\delta)}\left(\frac{H}{6} + \lambda\right)$$

Compare with classical Lucas–Washburn ($\theta_{app} \to \theta_m$, $\delta \to 0$)

- **Step 1 – generalised lubrication:** reconstructs the meniscus and yields θ_{app}.
- **Step 2 – correcting unaccounted stresses:** Obtain δ through two routes
  - CFD calibration beyond transients requiring a short CFD run
  - analytical estimate through analysis, a rapid parameter sweep
- **Step 3 – rapid prediction:** subsequent ROM run completes under 2 mins vs days

6. Validation: meniscus position and apparent contact angle





Observations

- Without correction, classical Lucas–Washburn predicts faster speeds
- Our model exhibits excellent agreement with CFD
- The physics of the moving meniscus are captured accurately (after a transient of $\sim$ 0.5 µs)

In progress: extensions underway

- 3D geometries of arbitrary cross section
- heterogeneous channel walls

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