Task 3.5: AI for wetting hydrodynamics

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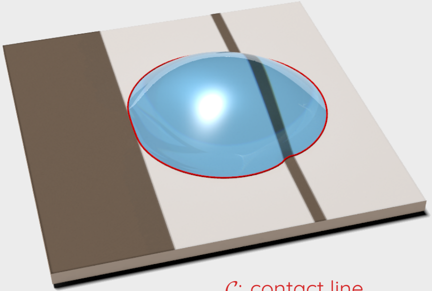
The Cyprus Institute

Raise AHM

Iceland, August 28, 2023

Task 3.5 overview

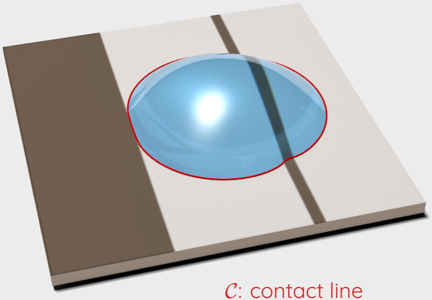
Simulation Data → Evolution of Contact Line



$\mathcal{C}$: contact line

Task 3.5 overview

Simulation Data → Evolution of Contact Line → (data-driven modelling) → Surrogate low-order models



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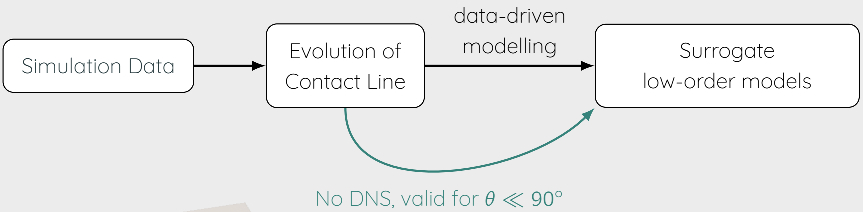

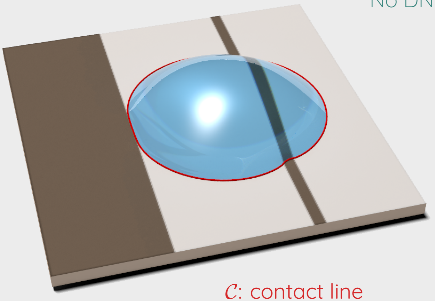

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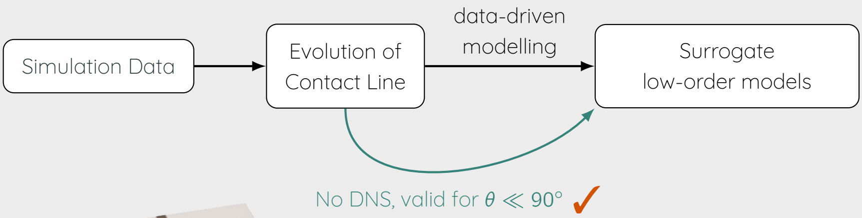

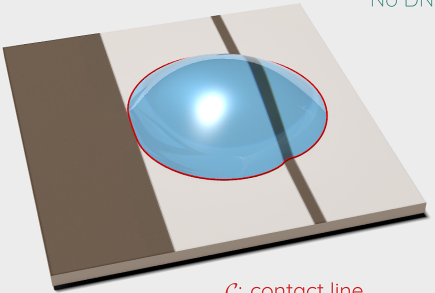

$\mathcal{C}$: contact line

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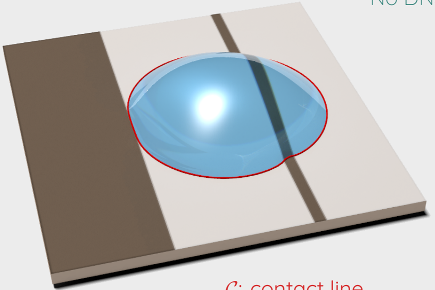
Simulation Data → Evolution of Contact Line → (data-driven modelling; CFD data ✓) → Surrogate low-order models

Evolution of Contact Line → Surrogate low-order models: No DNS, valid for $\theta \ll 90°$ ✓



$\mathcal{C}$: contact line

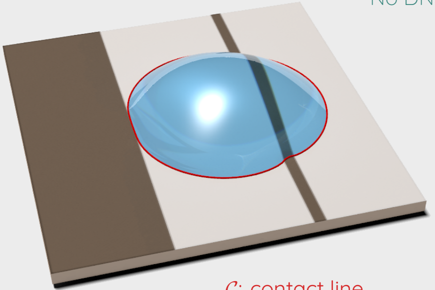
Task 3.5 overview

Simulation Data → Evolution of Contact Line

Evolution of Contact Line → Surrogate low-order models (data-driven modelling; CFD data ✓)

Evolution of Contact Line → Surrogate low-order models (No DNS, valid for $\theta \ll 90^\circ$ ✓)

Surrogate low-order models → Efficient data generation



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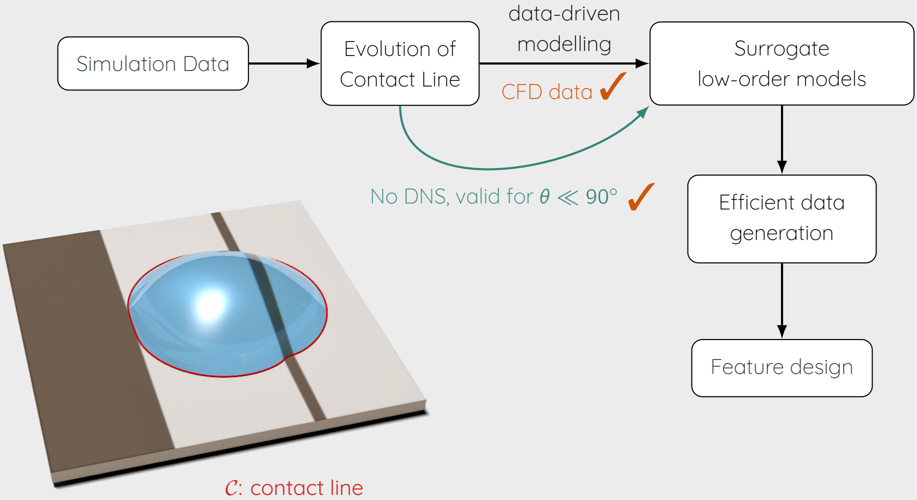

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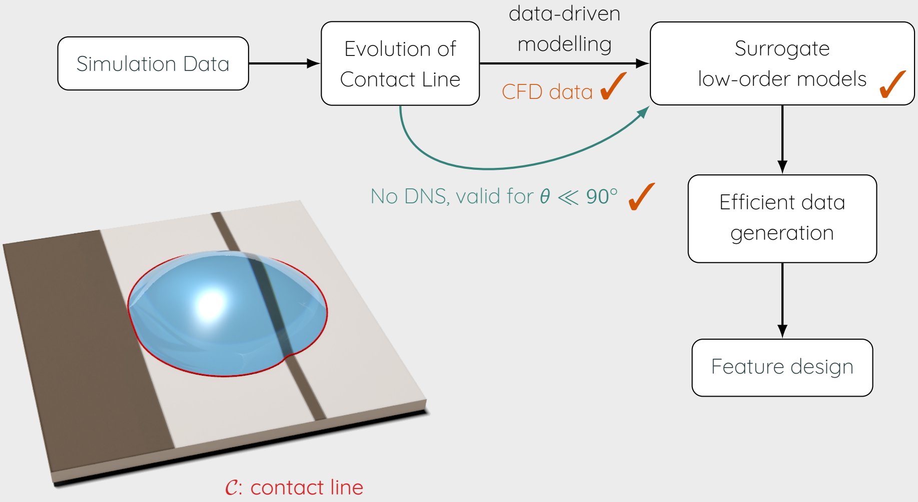

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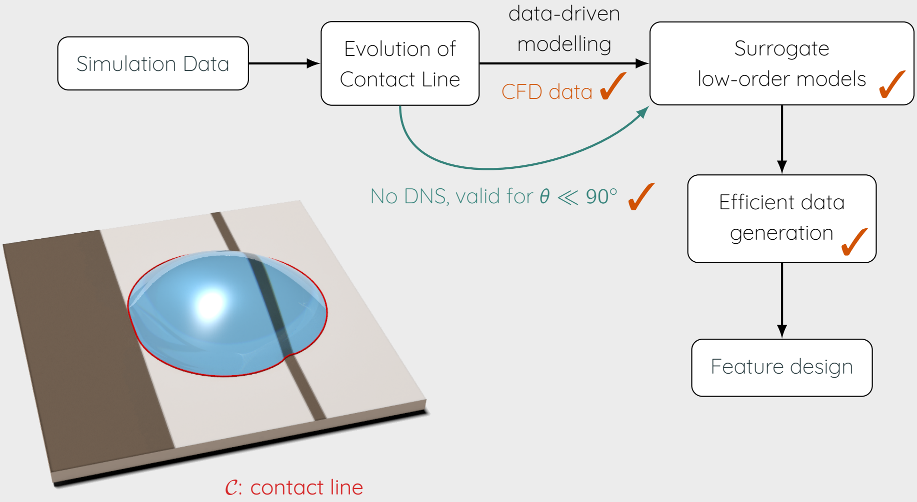

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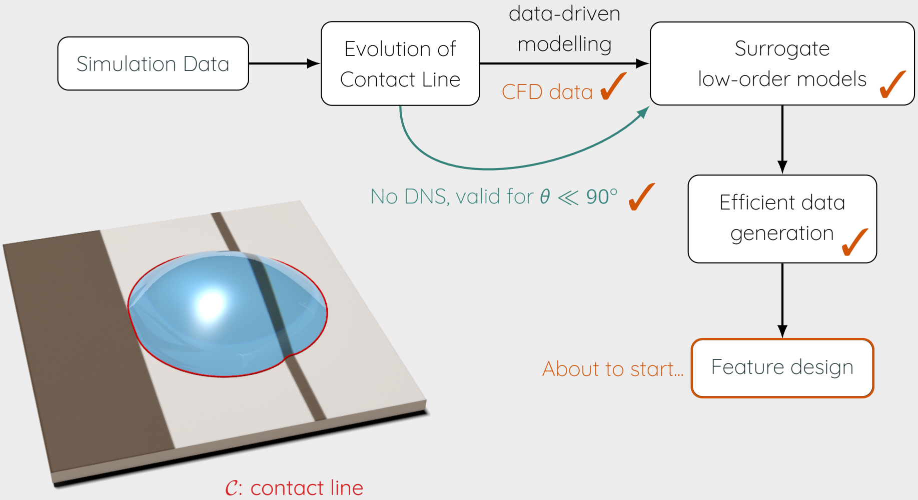
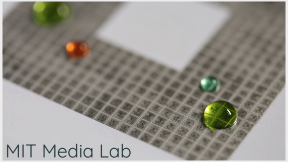
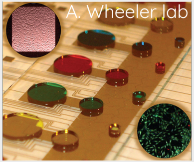
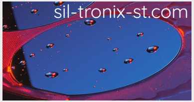


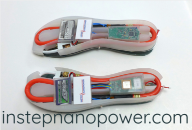
Motivation; some applications

- Industry
  - Pesticide deposition
  - Coating processes
  - Wetting agents
- Technology
  - Inkjet printing
  - Microfluidic & lab-on-a-chip devices
  - Display technologies
- Surface design
  - Surface cleaning
  - Waterproofing
  - Water harvesting
- Energy
  - Oil recovery
  - Fuel cells
  - Mechanical Energy harvesting









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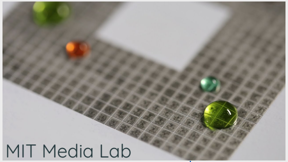

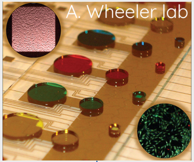

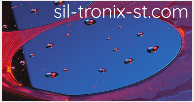

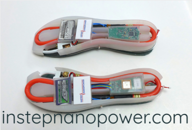

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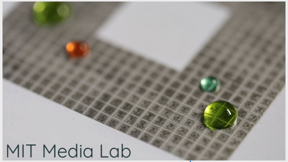

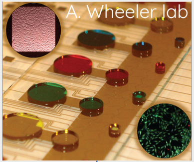

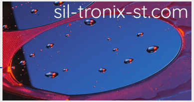

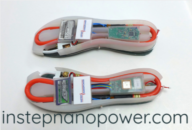

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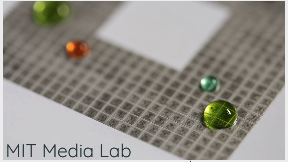

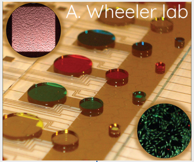

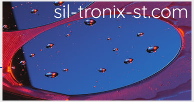

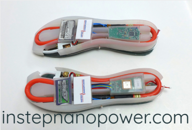

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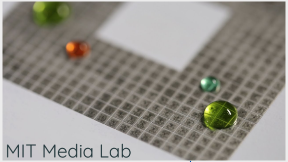

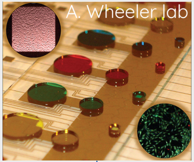

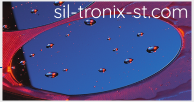

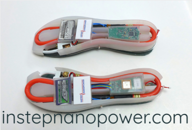

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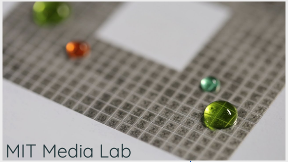

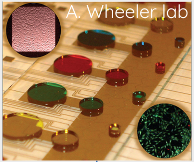

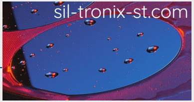

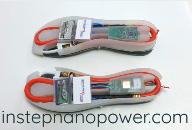

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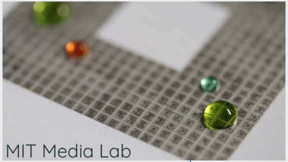
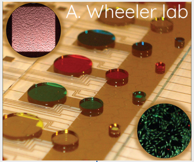
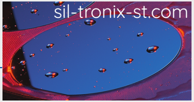




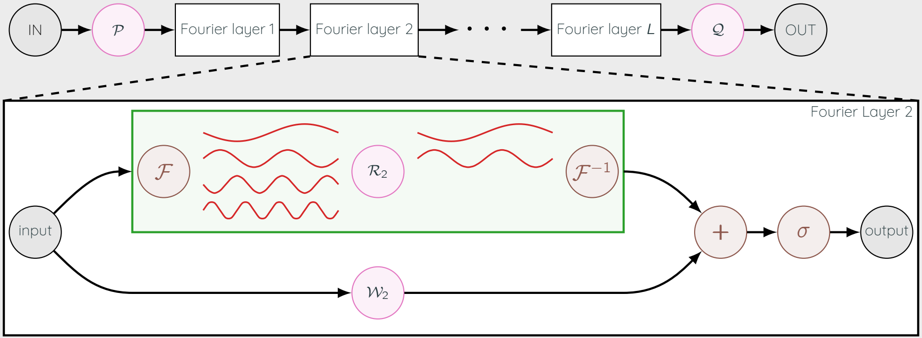


AI modelling - Fourier Neural Operator (FNO)

Learn contact line dynamics in a data-driven manner, by considering the mapping:

$$G = (\text{aux. data}) \to \{\text{Solution}\}$$

Key idea: A neural operator can approximate G through the Fourier space.



Completed work
Modelling thin-film data

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Assumptions

- strong surface tension
- negligible inertial effects
- small contact angles

Non-dimensional governing PDE

$$\partial_t h + \boldsymbol{\nabla} \cdot \left[h(h^2 + \lambda^2) \boldsymbol{\nabla} \nabla^2 h \right] = 0$$

Boundary conditions along the contact line $\mathcal{C}$ ($\boldsymbol{\nu}$ is the unit outward normal on $\mathcal{C}$)

Thickness vanishes: $h|_{\mathcal{C}} = 0$

Contact angle: $|\boldsymbol{\nabla} h|_{\mathcal{C}} = -h_\nu = \vartheta_*$

Kinematic BC: $\left(\partial_t \boldsymbol{c} - \lambda^2 \boldsymbol{\nabla} \nabla^2 h \big|_{\mathcal{C}} \right) \cdot \boldsymbol{\nu} = 0$

Contact line $\boldsymbol{c}(t_i)$ is discretised with 128 points and time t_i is discretised uniformly.

Auto-regressive approach

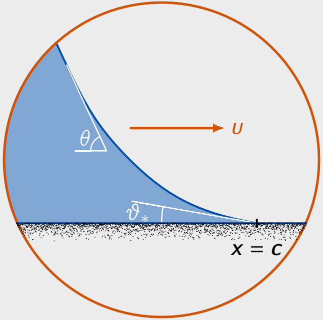
Input: $\{\boldsymbol{c}(t_1), \boldsymbol{c}(t_2), \ldots, \boldsymbol{c}(t_{10}), \vartheta_*(t_1), \vartheta_*(t_2), \ldots, \vartheta_*(t_{10})\}$

Output: $\boldsymbol{c}(t_{11})$, i.e. subsequent solution

AI-assisted, hybrid approach

Droplet velocity normal to the contact line, u_ν,

$$u_\nu = \bar{u}_\nu + G\left(\boldsymbol{c}, \bar{u}_\nu\right) \quad \text{with} \quad \bar{u}_\nu = \frac{\theta^3 - \vartheta_*^3}{3\,|\ln\lambda|}$$



Input: $\{\boldsymbol{c}(t_i), \bar{u}_\nu(t_i)\}$

Output: $G(\boldsymbol{c}, \bar{u}_\nu)$

Contact line $\boldsymbol{c}(t_i)$ is discretised with 128 points and time t_i is discretised uniformly.

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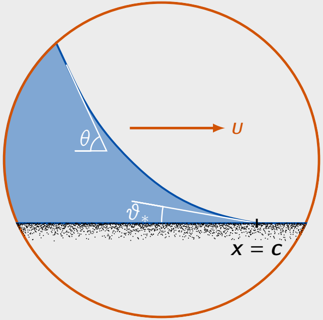
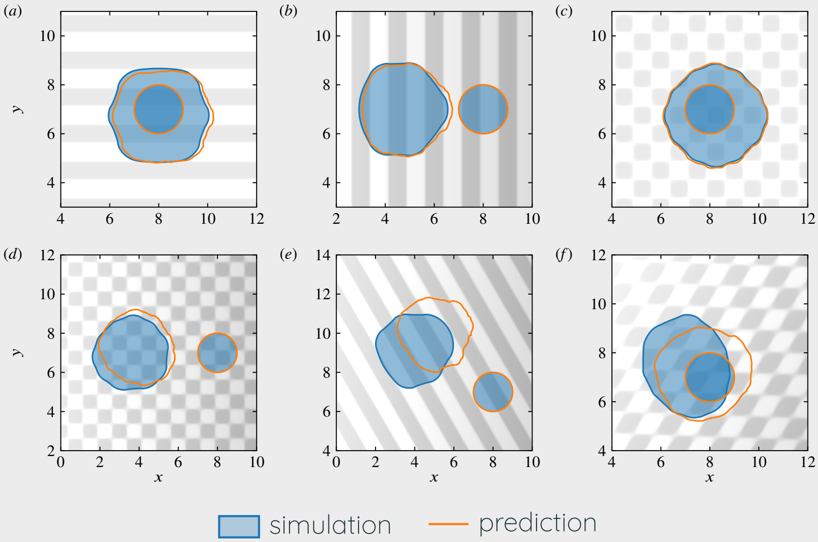
Input: $\{\boldsymbol{c}(t_i), \bar{u}_\nu(t_i)\}$

Output: $G(\boldsymbol{c}, \bar{u}_\nu)$

data-driven, implicit in t



Auto-regressive approach - Tests



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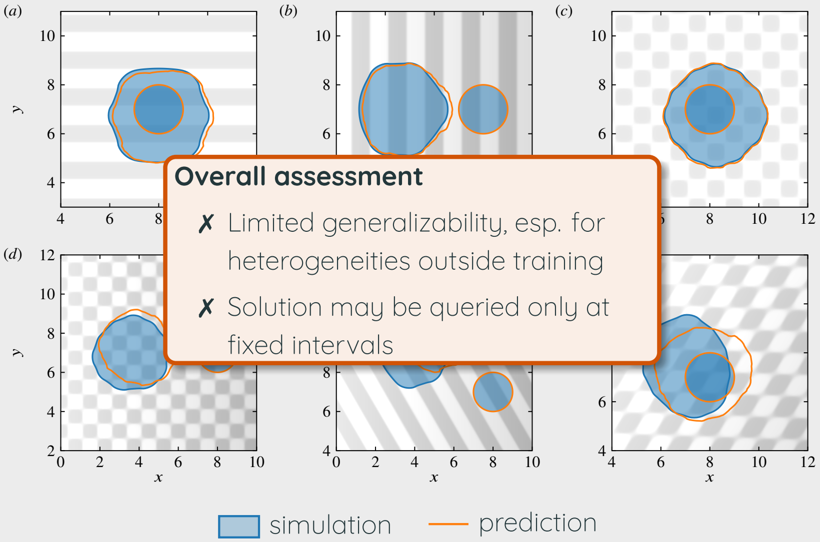
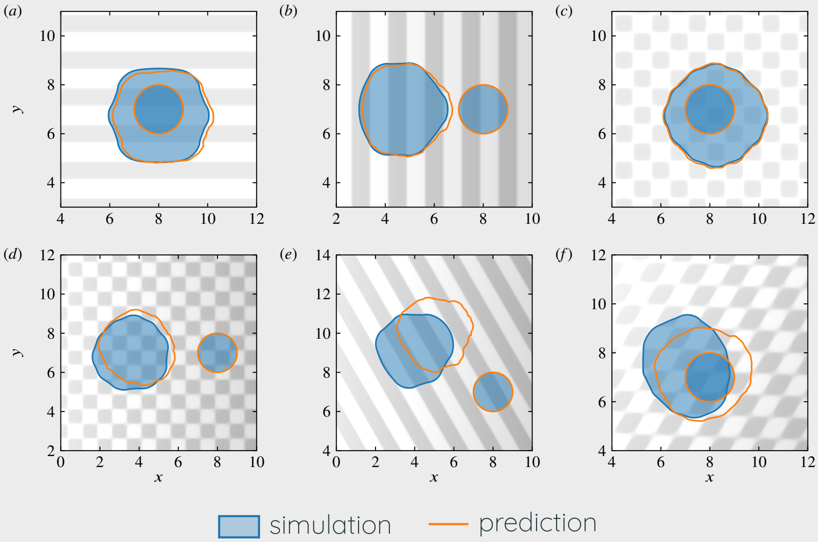


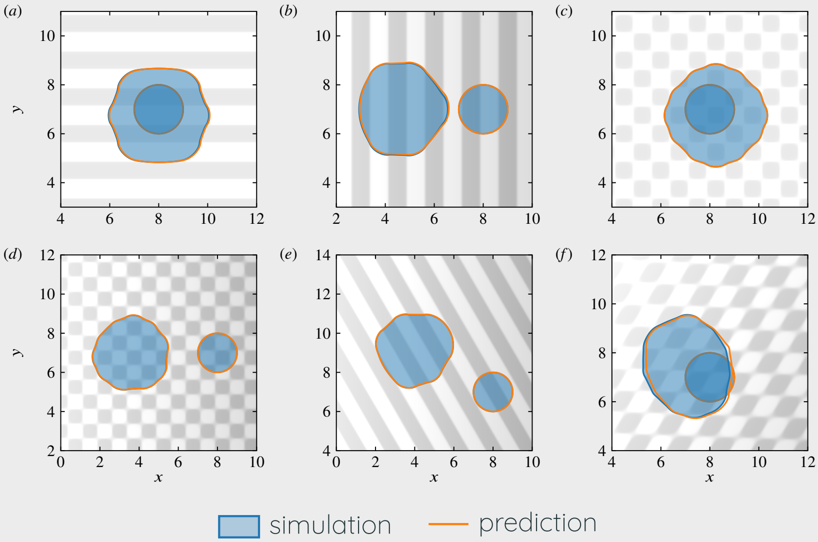
Overall assessment

- ✗ Limited generalizability, esp. for heterogeneities outside training
- ✗ Solution may be queried only at fixed intervals

Auto-regressive approach - Tests



AI-assisted approach - Tests



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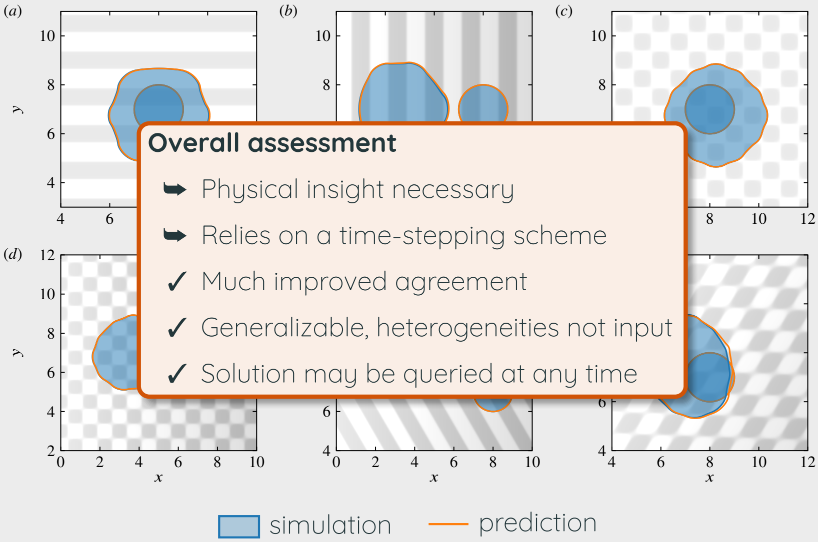
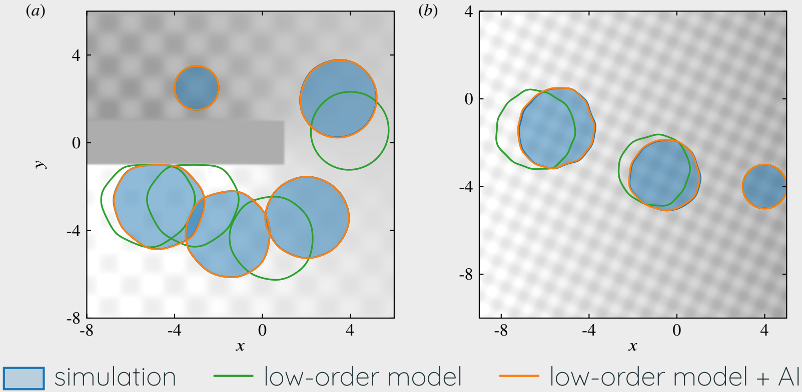


Overall assessment

- ➥ Physical insight necessary
- ➥ Relies on a time-stepping scheme
- ✓ Much improved agreement
- ✓ Generalizable, heterogeneities not input
- ✓ Solution may be queried at any time

AI-assisted approach - Out of distribution



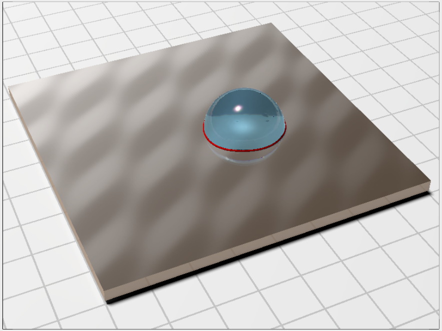
Under review in **Data-centric Engineering** (Cambridge University Press)

Reviewer: “This paper is absolutely excellent. It is well-written and convincing. It should be accepted.”

On-going work
Modelling CFD data

Code: Basilisk

- random heterogeneities, from a 7-parameter functional form
- 10–50 dimensionless times, snapshot saved every 0.1 time units
- adaptive mesh refinement, local grid size between $1/2^5 - 1/2^8$



Dataset:

- 300 DNS cases
- 80,000 contact line snapshots

Cox (J. Fluid Mech. 1986)

Analysis near the contact line reveals

$$u_\nu^{COX} = \frac{\sigma}{\mu}\left(\frac{F(\vartheta_*) - F(\theta)}{\ln\left(\frac{\lambda}{r_0}\right) + \frac{Q_o}{f(\theta)} - \frac{Q_i}{f(\vartheta_*)}}\right)$$

- λ, slip length, scales with Δx
- σ surface tension; μ viscosity
- Q_o and Q_i are unspecified
- F and f are known

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Obtaining θ assuming quasi-static dynamics

Given $\boldsymbol{c}$, obtain θ from the slope of the solution to the Young–Laplace eqn

$$-\sigma\nabla\cdot\hat{\boldsymbol{n}} = \Delta p, \quad \hat{\boldsymbol{n}} \text{ the surface unit normal}$$

Δp is constant specified by the volume constraint.

➥ Using the open source code, **Surface Evolver** (SE). Repeated calls to SE during training/testing through a dedicated Python interface.

Analysis near the contact line reveals

$$u_{\nu}^{COX} = \frac{\sigma}{\mu}\left(\frac{F(\vartheta_*) - F(\theta)}{\ln\left(\frac{\lambda}{r_0}\right) + \frac{Q_o}{f(\theta)} - \frac{Q_i}{f(\vartheta_*)}}\right)$$

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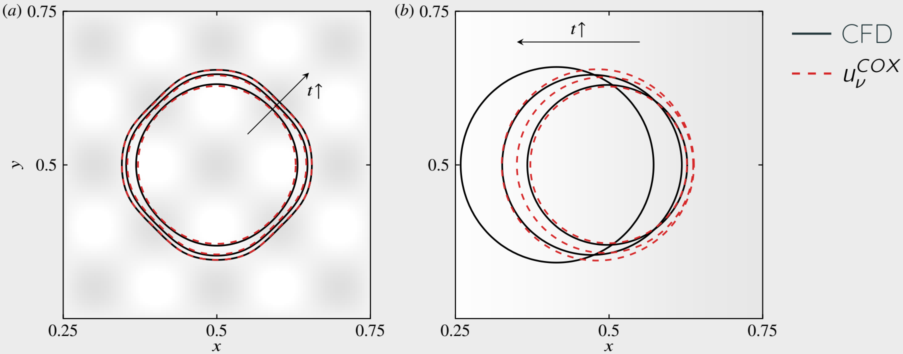

Reduced-order model

Cox (J. Fluid Mech. 1986)

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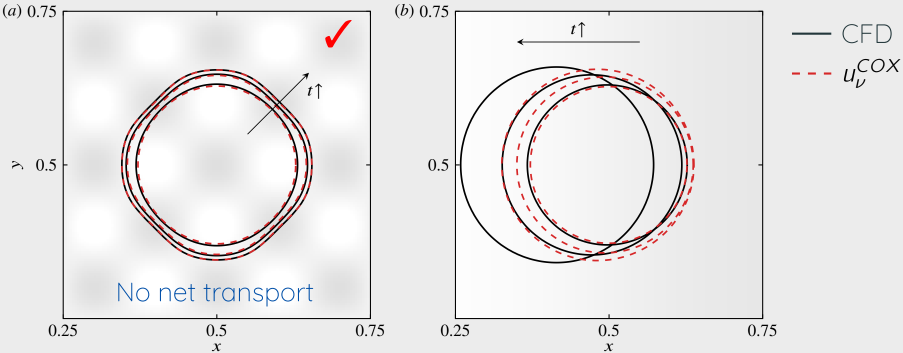
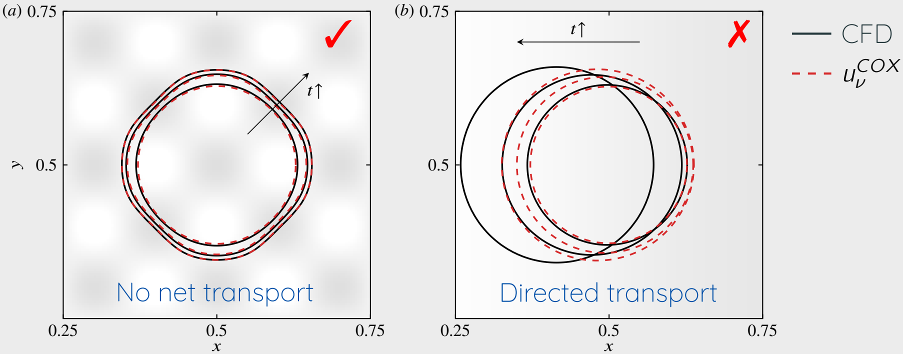


Cox (J. Fluid Mech. 1986)

Analysis near the contact line reveals

$$u_\nu^{COX} = \frac{\sigma}{\mu}\left(\frac{F(\vartheta_*) - F(\theta)}{\ln\left(\frac{\lambda}{r_0}\right) + \frac{Q_o}{f(\theta)} - \frac{Q_i}{f(\vartheta_*)}}\right)$$

- λ, slip length, scales with Δx
- σ surface tension; μ viscosity
- Q_o and Q_i are unspecified
- F and f are known



Cox (J. Fluid Mech. 1986)

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Analysis near the contact line reveals

$$u_\nu^{COX} = \frac{\sigma}{\mu}\left(\frac{F(\vartheta \ldots}{\ln\left(\frac{\lambda}{r_0}\right) - \ldots}\right.$$

- λ, slip length, scales with Δx

Cox's model underestimates net transport

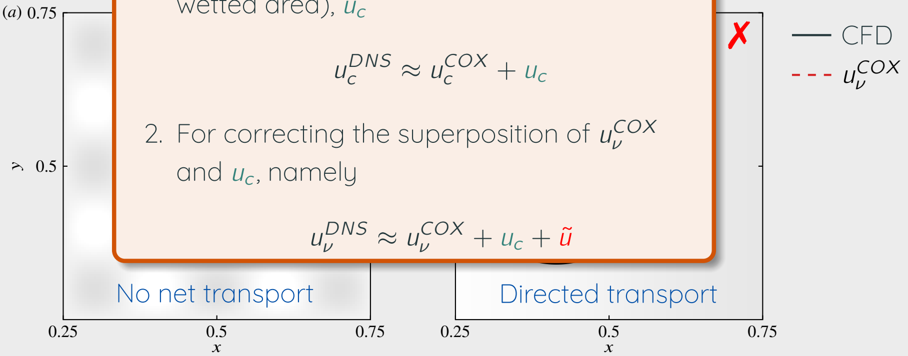
Approach: train two models

1. For net transport (speed of the centroid of wetted area), u_c

$$u_c^{DNS} \approx u_c^{COX} + u_c$$

2. For correcting the superposition of u_ν^{COX} and u_c, namely

$$u_\nu^{DNS} \approx u_\nu^{COX} + u_c + \tilde{u}$$



AI model for correcting net transport motion

Net transport captured by first harmonic; contact line evolves such that contact line has no first harmonic

Input: snapshots of first harmonics of θ and ϑ_*

Output: snapshots of first harmonics of $u_\nu^{DNS} - u_\nu^{COX} = u_c^{DNS} - u_c^{COX} \rightarrow u_c$

AI model for correcting net transport motion

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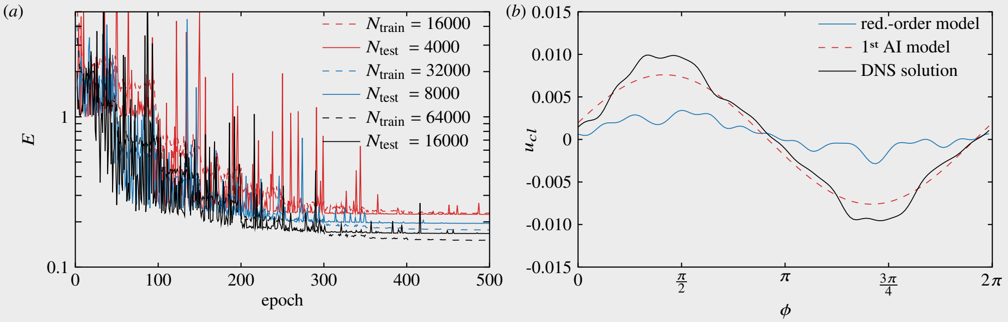

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Input: snapshots of $\{\boldsymbol{c},\ u_\nu^{COX} + u_c\}$

Output: snapshots of $u_\nu^{DNS} - (u_\nu^{COX} + u_c) \rightarrow \tilde{u}$

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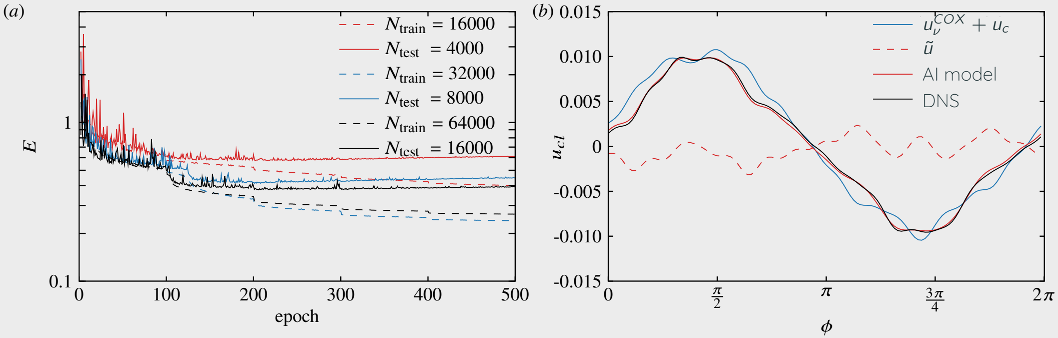
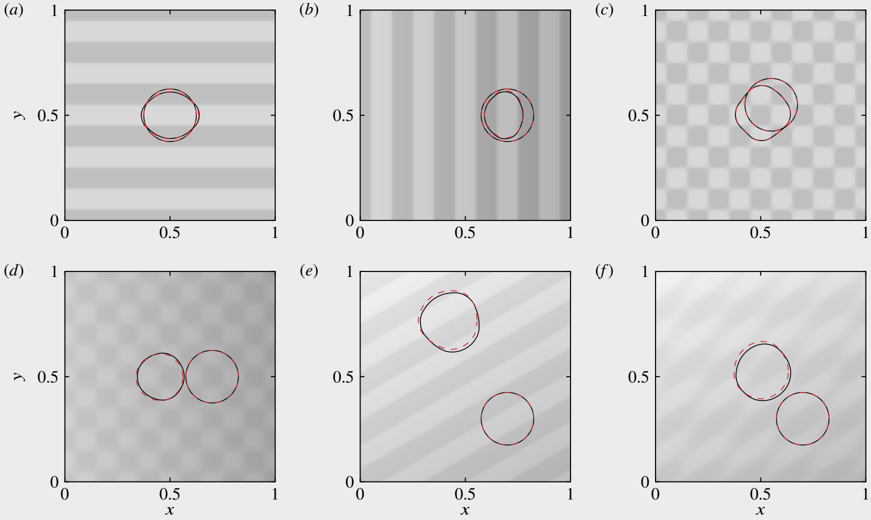
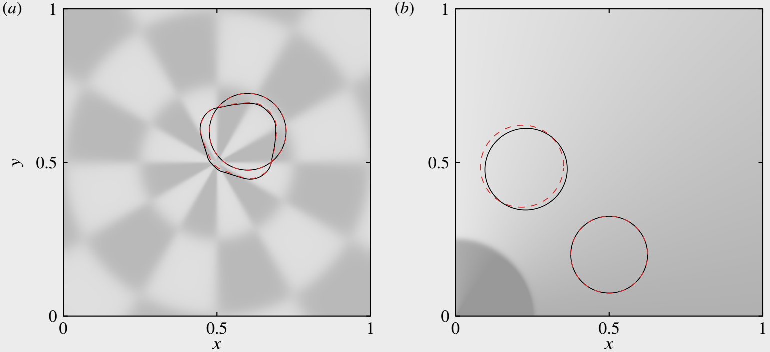
Output: snapshots of $u_\nu^{DNS} - (u_\nu^{COX} + u_c) \rightarrow \tilde{u}$



AI-assisted approach for CFD - Tests



AI-assisted approach for CFD - Out of distribution



Paper in preparation, to be submitted in the coming weeks.

Future tasks

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Employ similar workflow:

$$u_\nu = u_\nu^{COX} + u_c + \tilde{u}$$

- u_ν^{COX} - function of (θ, ϑ_*, r).
- u_c - for net transport as a function of the first harmonics of (θ, ϑ_*) and the gravity vector.
- $\tilde{u}$ - for higher-order corrections as a function of $(\boldsymbol{c}, u_\nu^{COX} + u_c)$.

- Currently post-processing data from 100 extra DNS for inclined surfaces.
- Further analytical understanding may be necessary.

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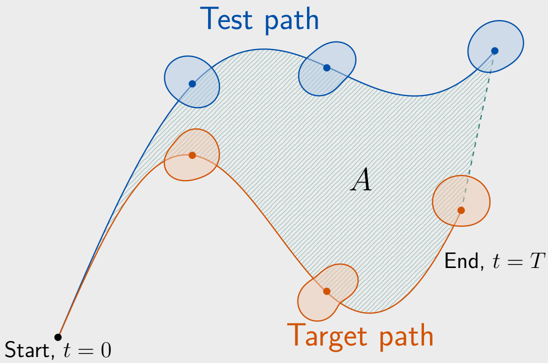
Given a target droplet path, what heterogenity profile ϑ_* can induce it?



General het. profile given by:

$$\vartheta_* = \sum_{m,n} a_{m,n} \exp^{ik_m x + ik_n y},$$

$a_{m,n}$ ‘design’ variables

Optimisation procedure to obtain:

$$a^*_{m,n} = \text{argmin } J$$

where J is a cost function that depends on A and some metric that penalizes non-circular contact lines

Successes enabled by RAISE

Successes enabled by RAISE

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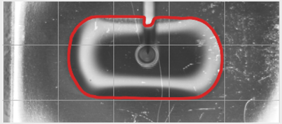
- **Research funding**: three successful proposals involving AI for wetting projects
  2 EU-funded MSCA ITNs; 1 CY-Funded Excellence Hubs project as PI
- **Computing time grants**: three successful proposals for computing time.
  1 under EuroHPC JU*; 2 on the national machine
  *to be featured in EuroHPC JU's "success stories" webpage
- **Industrial collaboration** with a tribology R&D company in Austria



  Surface texturing effectively guides lubricant flow
  CFD simulations infeasible (micron-scale texturing to centi-metre scale drops)
  Develop reduced-order surrogates to inform texture design

drive. enable. innovate.

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The CoE RAISE project have received funding from
the European Union's Horizon 2020 –
Research and Innovation Framework Programme
H2020-INFRAEDI-2019-1 under grant agreement no. 951733

Extra slides

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Two-phase Stokes

$$\vec{\nabla} \cdot \vec{u} = 0,$$

$$\rho \frac{\partial \vec{u}}{\partial t} = -\vec{\nabla} p + \vec{\nabla} \cdot \left[\mu \left(\vec{\nabla} \vec{u} + \vec{\nabla} \vec{u}^T\right)\right] + \sigma \kappa \delta_\Gamma \vec{n} + \hat{\rho} \vec{g},$$

$$\frac{\partial C}{\partial t} + \vec{\nabla} \cdot (\vec{u} C) = 0, \text{ where } C(\vec{x}, t) = \begin{cases} 1 & \text{if } \vec{x} \in \text{liquid}, \\ 0 & \text{if } \vec{x} \in \text{gas}. \end{cases}$$

Physical properties ξ calculation: $\xi(\vec{x}, t) = \xi_1 C(\vec{x}, t) + \xi_2 (1 - C(\vec{x}, t)).$

Boundary conditions: impose local contact angle (chemical heterogeneity) on surface.