Long wave dynamics in heterogeneous environments

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5 July 2023

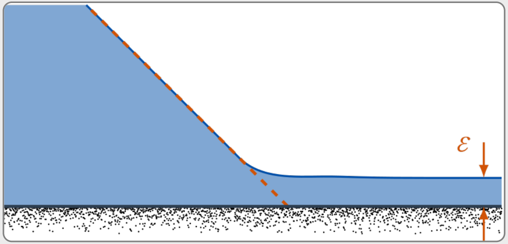
Outline

- Precursor film models (PFM)
- PFM with environmental heterogeneities
- Implementing the PFM solver in Basilisk
- Numerical applications
  - Strong scaling plots
  - Validations cases
  - Examples under heterogeneous effects
- Electrowetting

Precursor film model

Based on the long-wave approximation. PFMs avoid the contact line singularity by introducing an utlra-thin film ahead of the moving contact line.

Ideally the precursor film $\varepsilon \ll 1$. The smaller, the stiffer the equation becomes.



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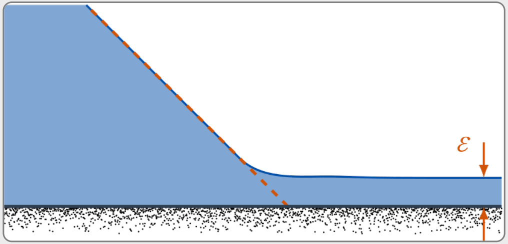


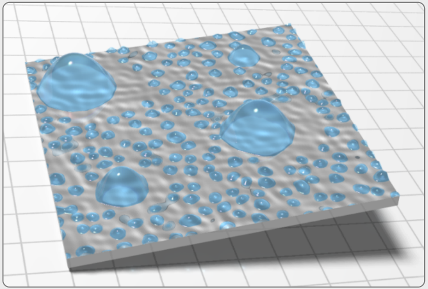
Main assumptions: Thin flow, negligible inertia, small contact angles.

Advantages compared to DNS: Computational cost (dimension reduction), single equation, valid in small contact angles, easier to include additional effects.

Types of environmental heterogeneities

How are droplet dynamics affected by the presence of:

1. Topographical defects
2. Substrate chemical heterogeneities
3. Body-forces
4. Thermal effects
5. Electric fields*



Case of multiple droplets moving on an inclined, chemically heterogeneous substrate. AMR. $67K < nc < 220K$

Aim: Development of a PFM solver that incorporates these heterogeneities and can deal with isolated and multiple droplets.

The governing equation for the film height is written as $h(\mathbf{x}, t)$

$$\partial_t h + \nabla \cdot \mathbf{F}\left(h, \nabla h, \Delta h\right) \qquad = 0$$

with

$$\mathbf{F} = h^3 \left[\nabla \underbrace{\Delta(h \qquad)}_{\text{curvature}} - \nabla \underbrace{\Pi(h \quad)}_{\text{disjoining}} \qquad \right]$$

Heterogeneity augmented PFM

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- Substrate Chemical Heterogeneity
- Body Forces (gravity and/or external forces)

Heterogeneity augmented PFM

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$$\partial_t h + \nabla \cdot \mathbf{F}\,(h, \nabla h, \Delta h) + S\,(h, \nabla h, \Delta h) = 0$$

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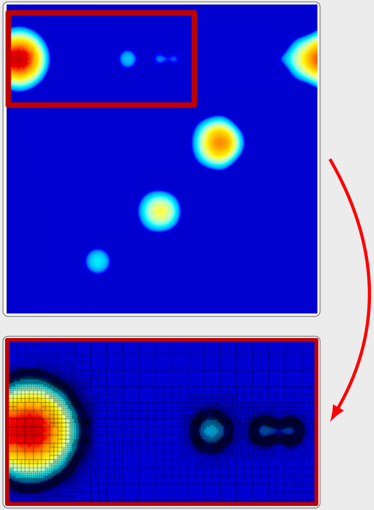
$$S = J = \frac{\mathcal{E} - \delta(\Delta(h+s) - \nabla\Pi(h, x) - w_1 \nabla(h+s))}{\mathcal{K} + h + s}$$

- Substrate Roughness
- Substrate Chemical Heterogeneity
- Body Forces (gravity and/or external forces)
- Thermal Effects (evaporation/condensation)

Numerical implementation - Discretization

Implicit discretization to ease PDE stiffness
Different heterogeneity combinations call for modularity



Discretization

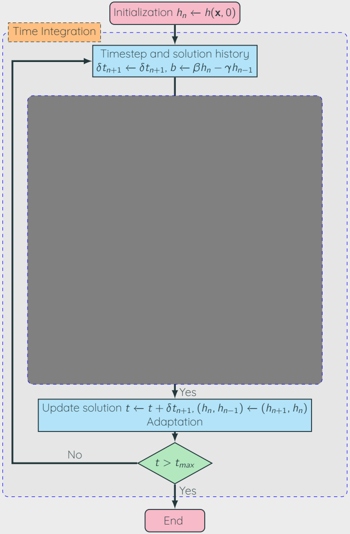
- 2^{nd} order time discretization with variable time-stepping (a-BDF2)
- Newton linearization
- 2^{nd} order space discretization
- Geometric multigrid method

Precursor film solver framework

Implicit time discretization

$$\mathcal{R}(h_{n+1}, \hat{h}_{n+1})\delta t_{n+1} + \alpha h_{n+1} = \beta h_n - \gamma h_{n-1},$$

δt_{n+1} defined based on number of MG cycles



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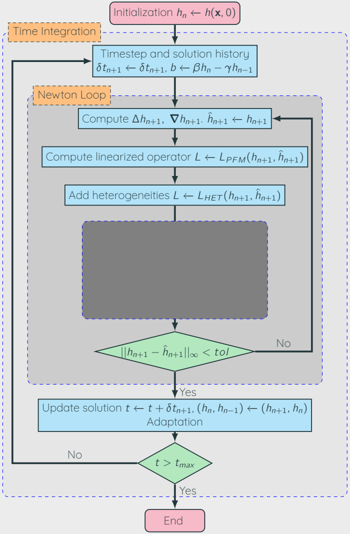
Linearization

Find linearized operator (L) for MG.

$\partial_t h = -\nabla \cdot \mathbf{F} \approx -\nabla \cdot \mathbf{F} - \nabla \cdot (\partial_h \mathbf{F}\, \delta h)\,, \; \delta h = h - \hat{h}$

Newton iterations until $h_{n+1} \approx \hat{h}_{n+1}$



Precursor film solver solution process

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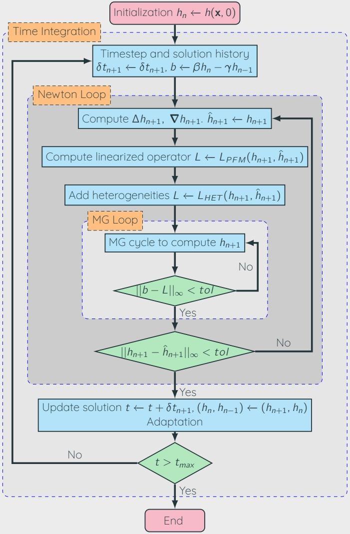
Basilisk details

FDs for residual and relaxation functions

```
static double residual_thin( ... ) { ... }
static void relax_thin( ... ) { ... }
```

Conditional compilation for heterogeneities

```
#if ROUGH
 addRoughnessContributions( ... );
#endif
```

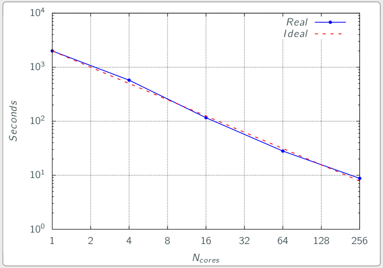


Scalability

Strong scaling plots obtained from simulations of a single droplet (1000 timesteps) on the HPC VEGA using AMD EPYC Rome 7H12 @ 2.6 GHz CPUs.

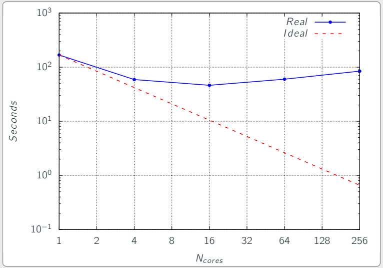
Uniform mesh - ***multigrid.h***

$N = 262K \ (L = 9)$



Adaptive mesh - ***quadtree.h***

$16K < N < 22K \ (4 < L < 9)$



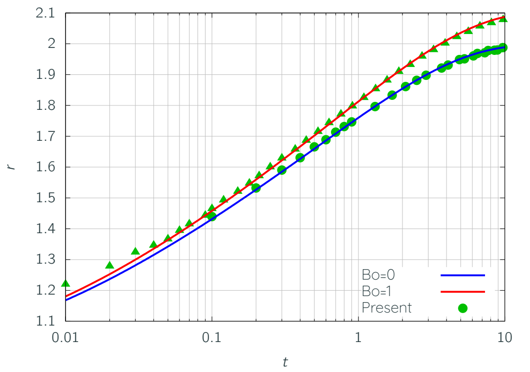
Adaptive mesh refinement ➔ significant communication overhead.

Increasing adaptation intervals or avoiding it for small cell count changes can help.

Solver validation - Comparison with ODE models[1]

Comparison of sessile droplet radius expansion rate with $(Bo = 1)$ and without $(Bo = 0)$ gravity effects.

$r(t = 0) = 1,\ h_{max}(t = 0) = 4,\ V = 2\pi,\ L0 = 5,\ L = 9,\ \varepsilon = 3 \times 10^{-3}$



[1]Bikerman J., (1950), J. Colloid Sci., 5, 349–359.

Solver validation - Comparison with ODE models

Comparison of droplet contact lines at different simulation times to validate substrate chemical heterogeneity effects between Basilisk and ODE.

Contours refer to the Hamaker coefficient with values; $1 < \mathcal{H}(x) < 10 = 1$ (white to black).

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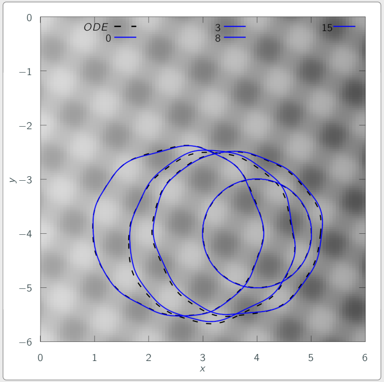
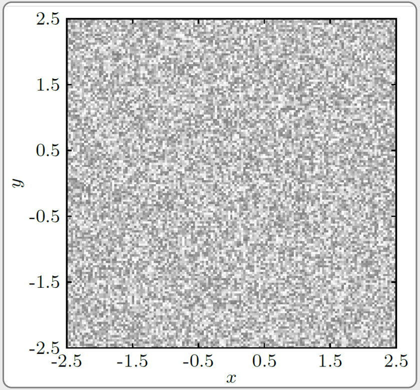


Simulation Examples - Multiple droplets

Case of multiple droplets moving on an inclined, chemically heterogeneous substrate.

Small droplets either get absorbed by the much larger ones or coalesce with other small droplets.

Contours refer to $0.08 < h < 0.8$ values. Low h values are excluded for clarity.



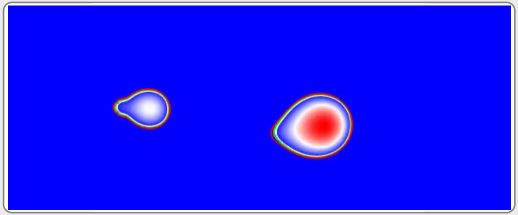
Simulation examples - Dropwise condensation

Simulations aiming to qualitatively capture the drop-wise condensation on an inclined substrate.

The area of low Hamaker coefficient, i.e. high hydrophilicity act as droplet inception point

As the droplet increases in size, it de-pinns from the inception point and starts to move downstream.

Hamaker coefficient profile. Blue: 0.1; Red: 1.0

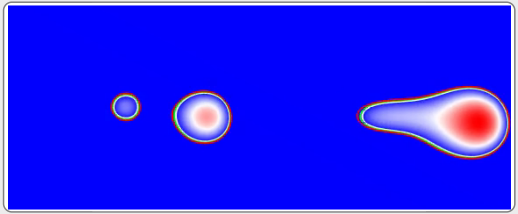


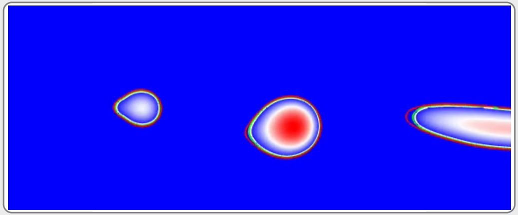
Simulation examples - Dropwise condensation

Since the droplet is larger, it is able to condensate on its own increasing in volume and accelerating downstream.

After a critical mass is reached, the corner becomes unstable and ejects a drop.[a]

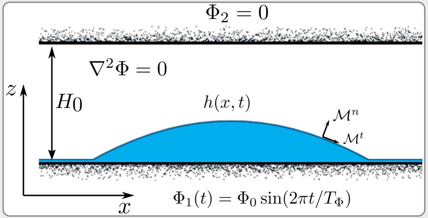
The droplets grow until reaching the boundaries. Here $h_{max} \approx 0.4$.





[a] Podgorski T et al., (2001), Phys. Rev. Lett., 87, 036102.

Electrowetting - Droplet dynamics under electric fields



In the **thin film limit**, $\nabla^2\Phi = \partial_{zz}\Phi_i$ leading to closed-form $\Phi_i(z)$ expressions[a],

$$\Phi_1(z) = \Phi_1(t) - z\frac{\Phi_1(t) - (\beta - h)Q}{h(1-\epsilon) + \epsilon\beta}$$

$$\Phi_2(z) = (\beta - z)\frac{\epsilon\Phi_1(t) + hQ}{h(1-\epsilon) + \epsilon\beta}$$

[a] Kainikkara M, et al., (2021), npj Microgravity, 7,1-47.

Assuming **negligible inertia** and the **leaky dielectric model**[b]

$$\partial_t h + \nabla \cdot \mathbf{F}^e(h,Q) = 0$$

$$\partial_t Q + \nabla \cdot \left(\frac{Q}{2h}\mathbf{F}^e(h,Q)\right) = \Psi_c\left(\partial_z\Phi_2 - \sigma\partial_z\Phi_1\right)_{z=h}$$

$$\mathbf{F}^e(h,Q) = \mathbf{F}(h) \underbrace{- \frac{3h^2}{2}E\mathcal{M}^t - h^3 E\mathcal{M}^n}_{\text{Maxwell Stresses}}$$

where Q the interfacial free charge density.

Coupled system of equations of Q and h is solved by modifying the existing thin film Multigrid solver.

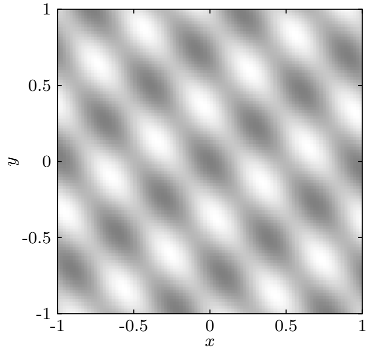
[b] Melcher JR, Taylor GI, (1969), Annu. Rev. Fluid Mech., 1,111–46

Electrowetting with thermal effects

Evaporating droplet on a chemically heterogeneous substrate under the effect of an electric field.

The presence of a time-varying electric field ($\Phi_0 = 12, T_\Phi = 5s$) causes the Maxwell stresses to vary in time, leading to a vibrating droplet.

Simultaneously, the droplet decreases in size due to it evaporating.



Concluding remarks/Challenges

Remarks

- Optimal scaling with uniform meshes. Adaptation could be better with some fine-tuning
- Good agreement with ODE data
- Effect of precursor film on condensing case

Challenges/ Future Work

- Pseudo-3D formulations for diffusion-limited evaporation
- Extension to non-rigid substrates

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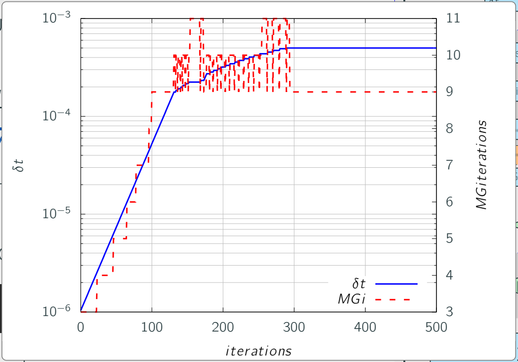

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