Dewetting in Thin Liquid Films: Using Sparse Optimization to Learn Evolution Equations

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Abstract
An investigation using machine learning to determine the evolution equation of soft matter from experimental data. The LASSO shrinkage method performs variable selection to determine dominant features of the system.

1. Motivation

- Refine theories describing soft matter evolution such as the dewetting of thin liquid films
- Simplest description may have physics unaccounted for, so we want to determine the PDE from experimental data
- Develop with statistical methods allowing AI to learn unknown equations from scattering data

2. Theory

Dewetting of thin films occurs when a liquid retracts itself from the substrate and forms droplets.

$$h_t = -\frac{1}{3\mu}\nabla\cdot\left(h^3\nabla\left(\gamma\nabla^2 h - \Pi(h)\right)\right)$$

The addition of *disjoining pressure* $\Pi(h)$ accounts for intermolecular forces usually negligible in thick films[1].

Unstable surface → Preferred low energy state → Self-assembly

3. Machine Learning Method

Following Schaeffer's method[2] we start with a PDE of terms relevant to the system, here the Navier-Stokes equations. Coefficients are separated into vector $\boldsymbol{\alpha}$:

$$h_t = \begin{bmatrix} | & | & | & | & | & & | \\ \Delta h & \Delta h^2 & \Delta h_x & \Delta {h_x}^2 & \Delta h_{xx} & \cdots & \Delta^3 h \\ | & | & | & | & | & & | \end{bmatrix}\cdot\boldsymbol{\alpha}$$

The feature selection algorithm used is known as the least absolute shrinkage and selection operator, *LASSO.*

- The system is linear in $\boldsymbol{\alpha}$, solved using the L^1 norm
- Penalizes nonzero terms, promoting sparsity until only coefficients of the dominant features remain[2]

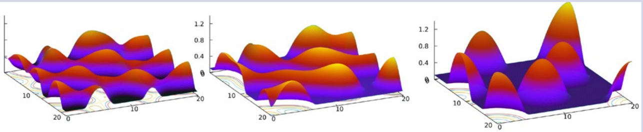

Figure 1. The stages of dewetting in a thin film. Small disturbances of a nearly-uniform layer evolve over time into droplets[3].

4. Results and Discussion

Numerical simulations accurately modelled the system's dynamics, as shown in Figure 2.

The algorithm has shown in previous work to identify Δh, Δh^3, and $\Delta^2 h$ as the dominant features[2]. Ongoing analysis of the film data is expected to support these findings.

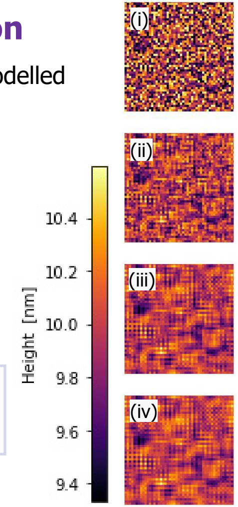

Figure 2. Time dependence of the film height on a 50x50 lattice at (i) 0, (ii) 72 000, (iii) 216 000, and (iv) 288 000 s.

5. Further Work

We continue this project in applying the above methodology to experimental scattering data

- Observe differing dewetting morphologies
- Applications from solar cells to nanoscale sensors[4]

References
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