Instabilities in thin nematic liquid crystal films

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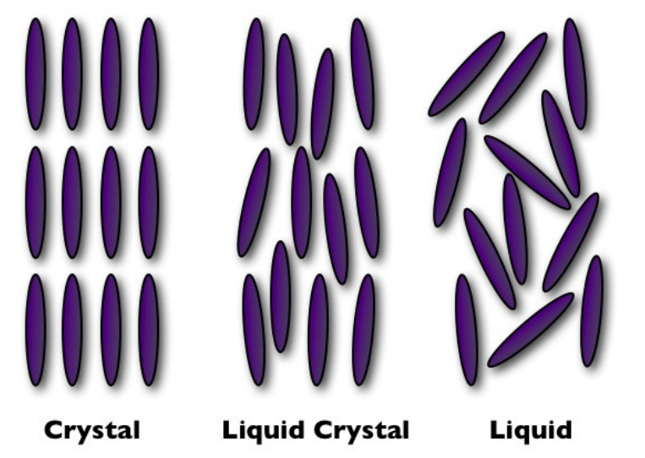
Abstract

The breakup of nematic liquid crystals (NLCs) films with thicknesses less than a micrometer is studied. Paying particular attention to the interplay between the bulk elasticity and the anchoring (boundary) conditions at the substrate and free surface, a fourth order nonlinear partial differential equation (PDE) is derived for the free surface height within the framework of the long wave approximation. Numerical simulations of a perturbed flat film show that, depending on the initial average thickness of the film, satellite droplets may form and persist on time scales much longer than dewetting.

Model derivation

Nematic liquid crystals (NLCs) are fluid like substances typically composed of rod like molecules with a dipole moment. The molecular interactions induce an elastic response under deformation, making NLCs behave as a state of matter intermediate between a fluid and a solid, having some short-range order to their molecular structure but no positional order.



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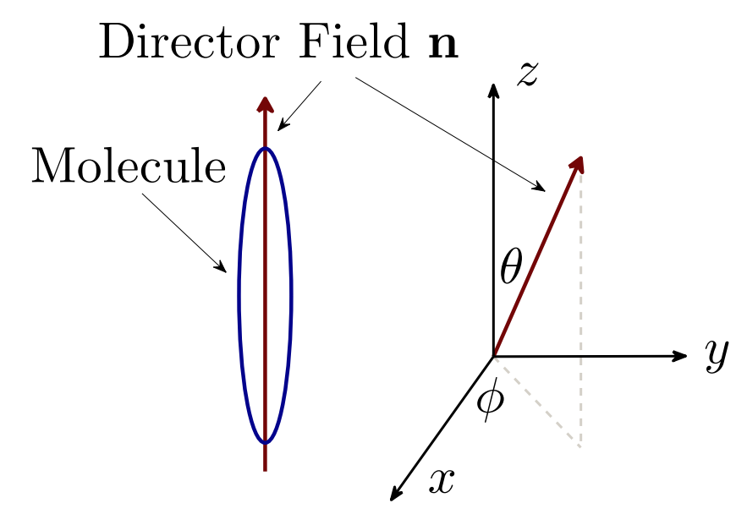
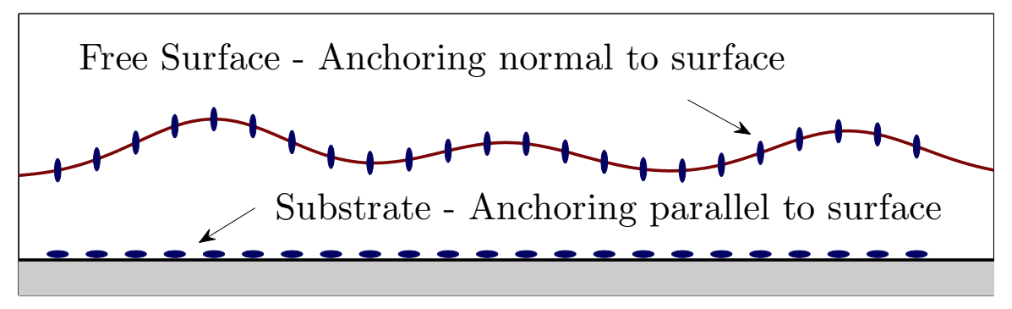
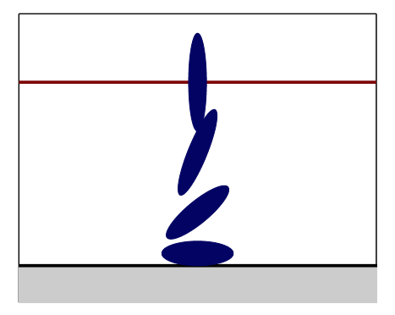


The dynamics of a NLC may be described by its velocity field $\boldsymbol{v} = (u, v, w)$ and the director field $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ representing the averaged orientation of the anisotropic axis in the liquid crystal.

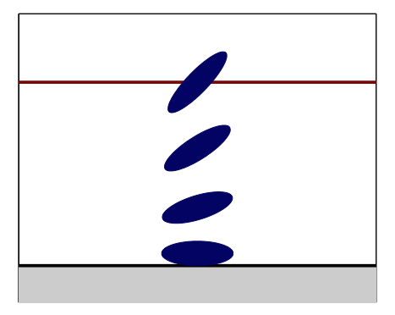
Weak Anchoring: The boundary condition on the director field at an interface is commonly called the anchoring condition. For thick films anchoring is typically homeotropic (perpendicular) at the free surface and planar on the substrate.



However, for very thin films, the antagonistic anchoring conditions impose a high energy penalty in the bulk of the film, therefore molecules prefer to be planar (or nearly so) on the free surface. Therefore a weak anchoring model is introduced that relaxes the homeotropic anchoring condition on the free surface for thinner films.



Strong Anchoring



Weak Anchoring

Governing Equation: The free surface height, h of a very thin films of NLC can be modeled by the fourth order nonlinear PDE,

$$h_t + \nabla\cdot\left[\mathcal{C}h^3\tilde{\nabla}\nabla^2 h + \Pi_S{}'(h)\tilde{\nabla}h\right] = 0\,, \quad \Pi_S(h) = \mathcal{K}\left[\left(\frac{b}{h}\right)^3 - \left(\frac{b}{h}\right)^2\right] + \frac{\mathcal{N}}{2}\left(\frac{m(h)}{h}\right)^2,$$

$$\tilde{\nabla} = \left[\lambda I + \nu\begin{pmatrix}\cos 2\phi & \sin 2\phi, \\ \sin 2\phi & -\cos 2\phi\end{pmatrix}\right]\nabla\,, \qquad m(h) = \frac{1}{2}\left[1 + \tanh\left(\frac{h-2b}{0.05}\right)\right]\frac{h^2}{h^2+\beta^2}$$

$\delta = H/L$ is the aspect ratio, $H = 100$ nm, $L = 10$ μm;

$\beta = 1$ is the lengthscale on which surface anchoring energy becomes comparable to bulk elastic energy;

$\mathcal{C} = \delta^3\gamma/\mu U = 0.87$ is the inverse capillary number, a ratio of capillary to viscous forces;

$\mathcal{N} = \pi^2 K/4\mu U L = 1.67$, a ratio of elastic to viscous forces;

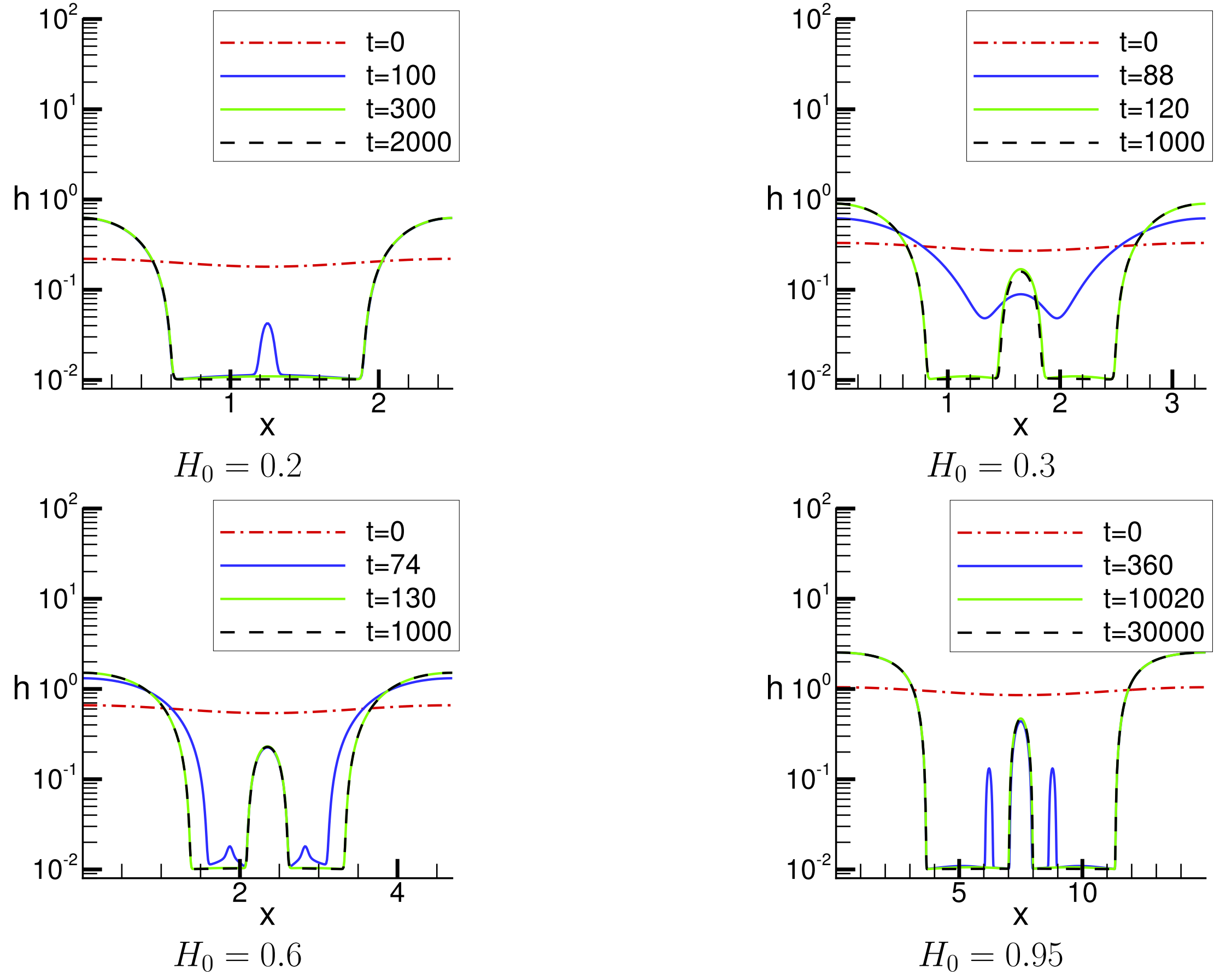
$\mathcal{K} = \delta^2 AL/\mu U = 36$ is a ratio of van der Waals forces to viscous forces; and

$\lambda = 1, \nu = 0$ are scaled anisotropic viscosities (ignored for now).

Physical parameters are chosen to match experimental values for 4-Cyano-4'-pentylbiphenyl.

Metastability and Satellite Drops

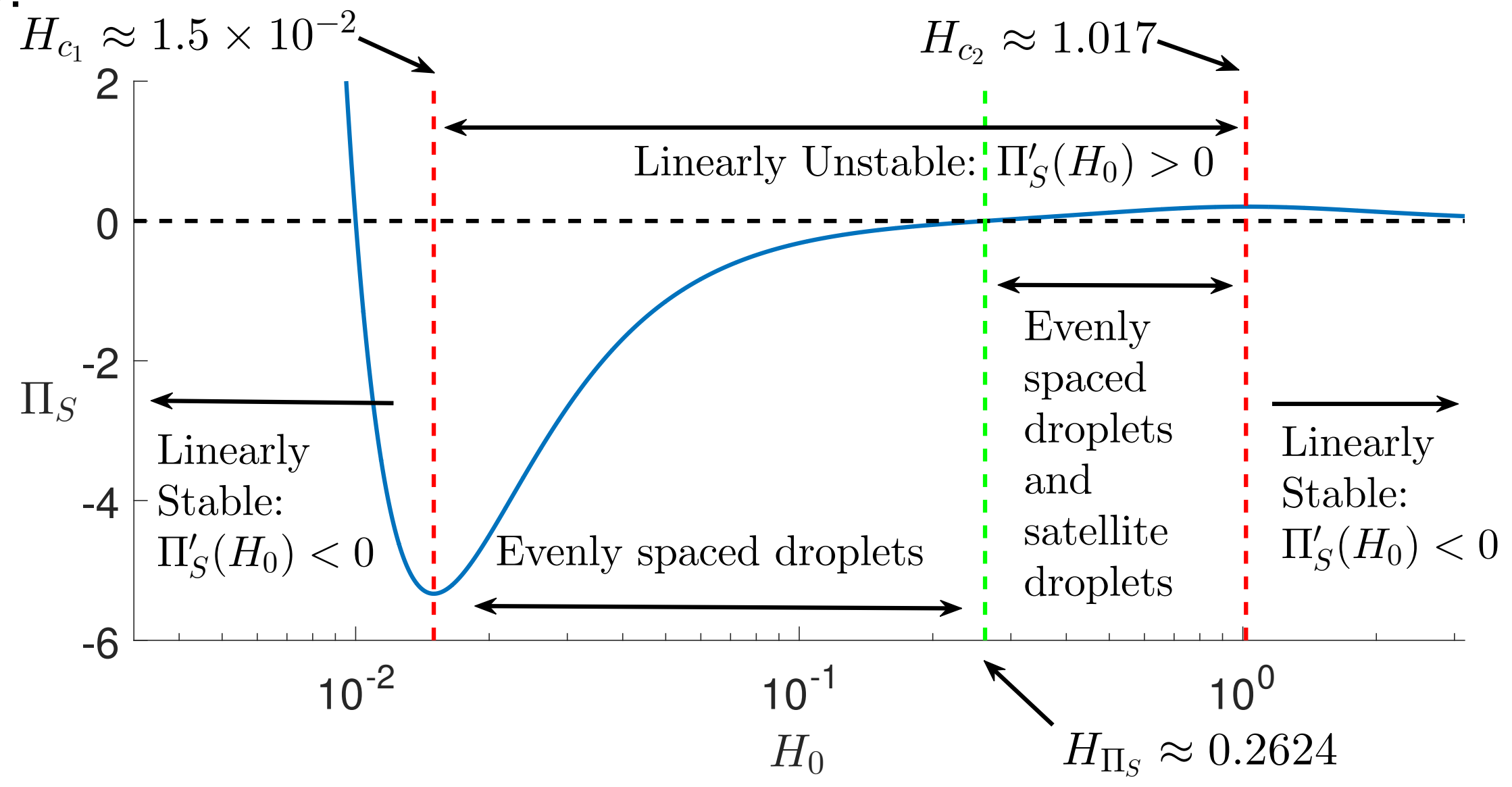
We are interested in the stability of a flat film of NLC, in particular its dependence on the initial film thickness, H_0. Below are 2D simulations for four different values of H_0 in the unstable regime. In each case the domain length is equal to the wavelength of maximum growth (linear stability analysis).



$H_0 = 0.2$ $H_0 = 0.3$

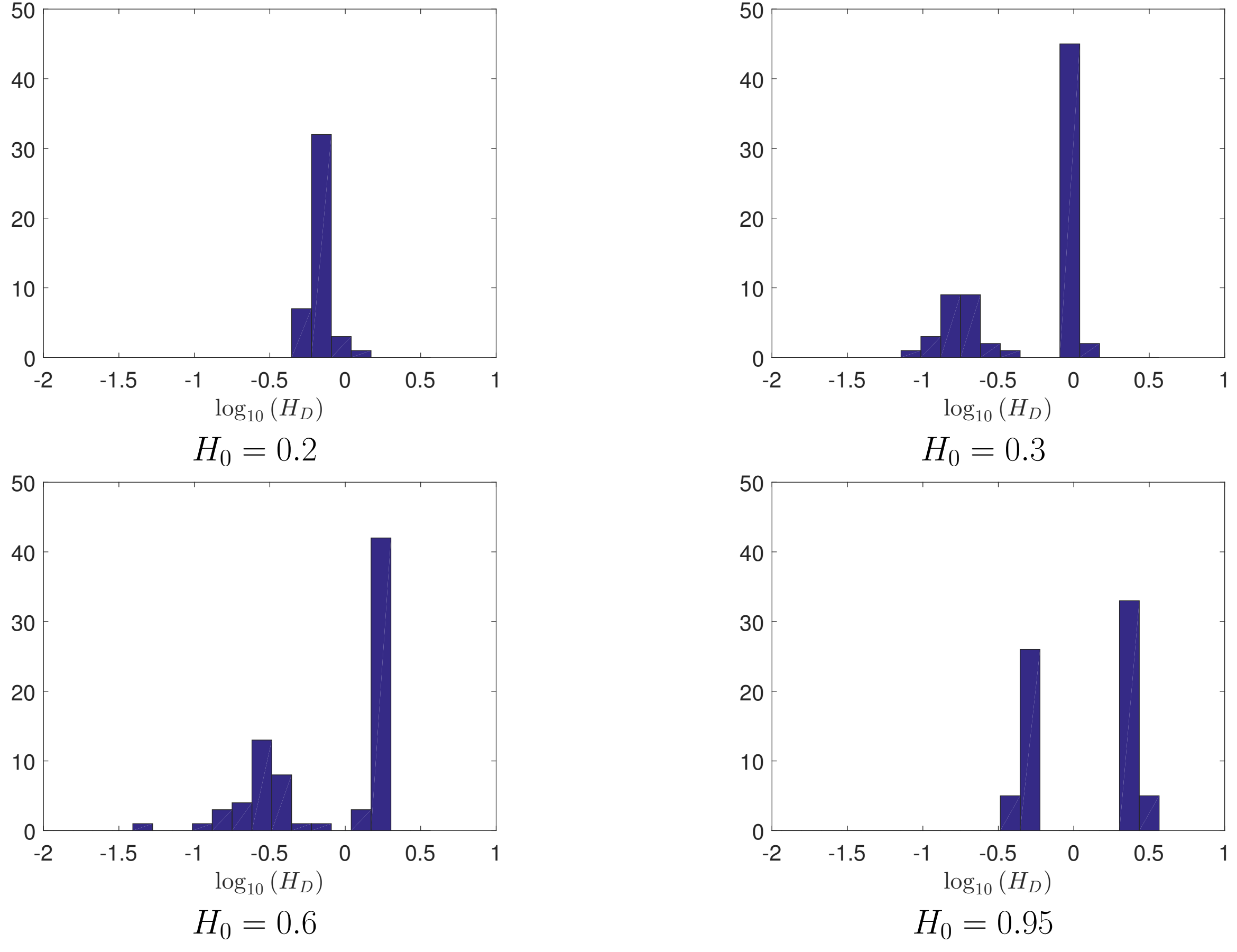
$H_0 = 0.6$ $H_0 = 0.95$

For thicker films satellite droplets exist on a a longer timescale (green curve to black curve) than dewetting (red curve to blue curve) The final dewetting pattern depends strongly on the disjoining pressure associated with the initial film thickness, as summarized below:



The region between the red vertical lines is the linearly unstable regime and the center vertical green line denotes the zero of the structural disjoining pressure, $\Pi_S(H_0)$.

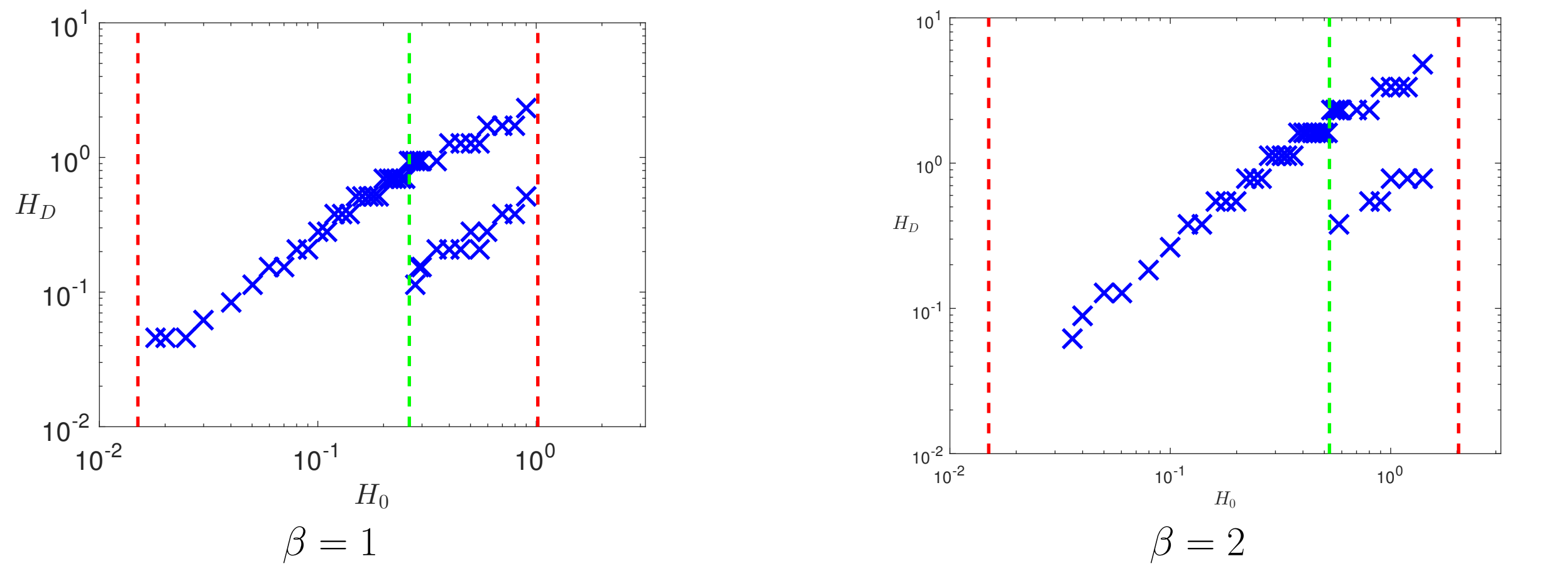
To further probe the dependence on $\Pi_S(H_0)$, simulations are carried out for a randomly perturbed film on a domain of length 50× wavelength of maximum growth. The height of droplets is extracted from simulations and plotted as histograms below:



$H_0 = 0.2$ $H_0 = 0.3$

$H_0 = 0.6$ $H_0 = 0.95$

The histograms reveal a multimodal drop height distribution. Below we extend the histogram data to a much wider range of H_0 values, plotting for each H_0 the modal droplet height(s). Statistics for simulations with $\beta = 2$ (doubles the value of the zero of the disjoining pressure) are also plotted.

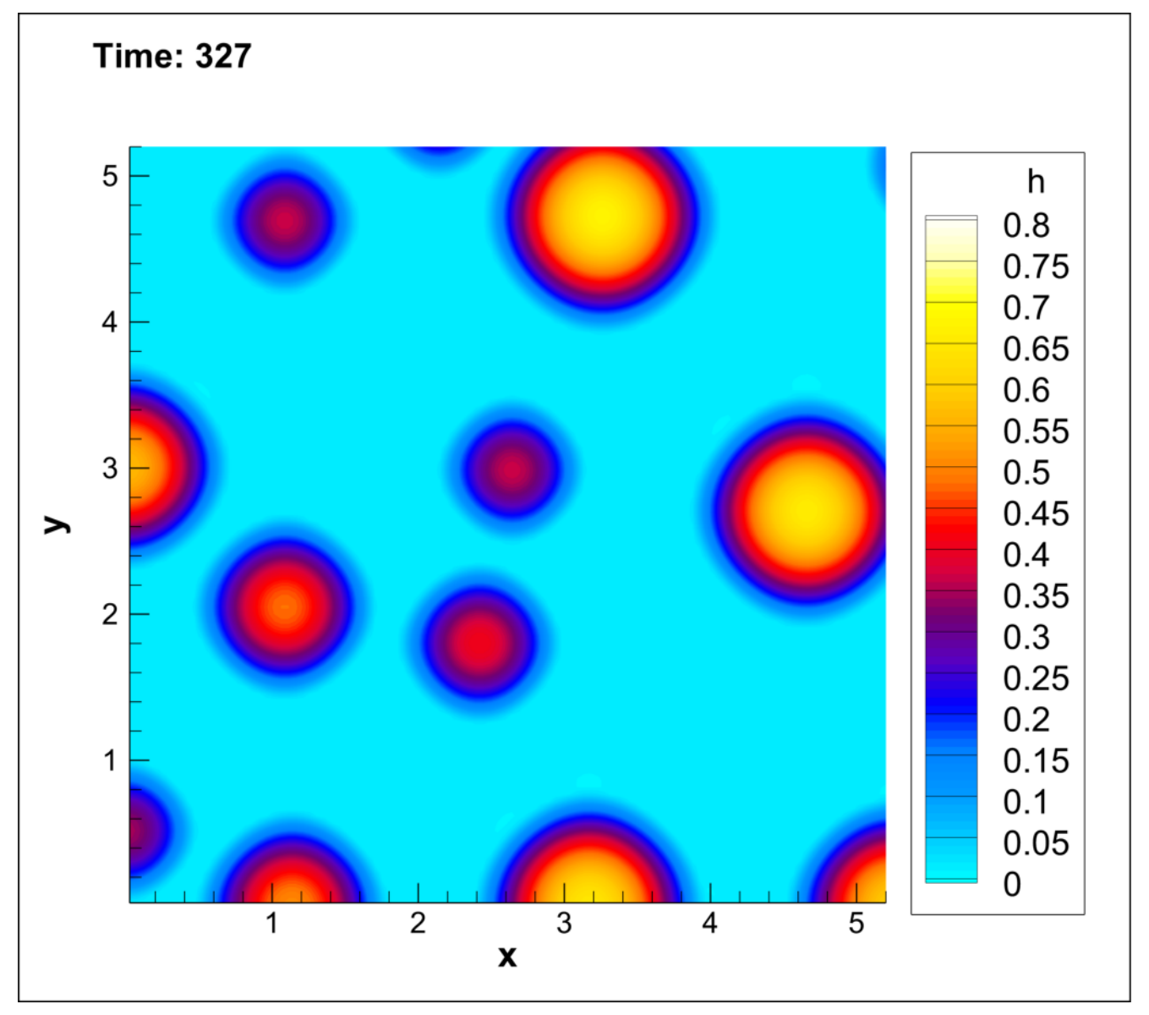


$\beta = 1$ $\beta = 2$

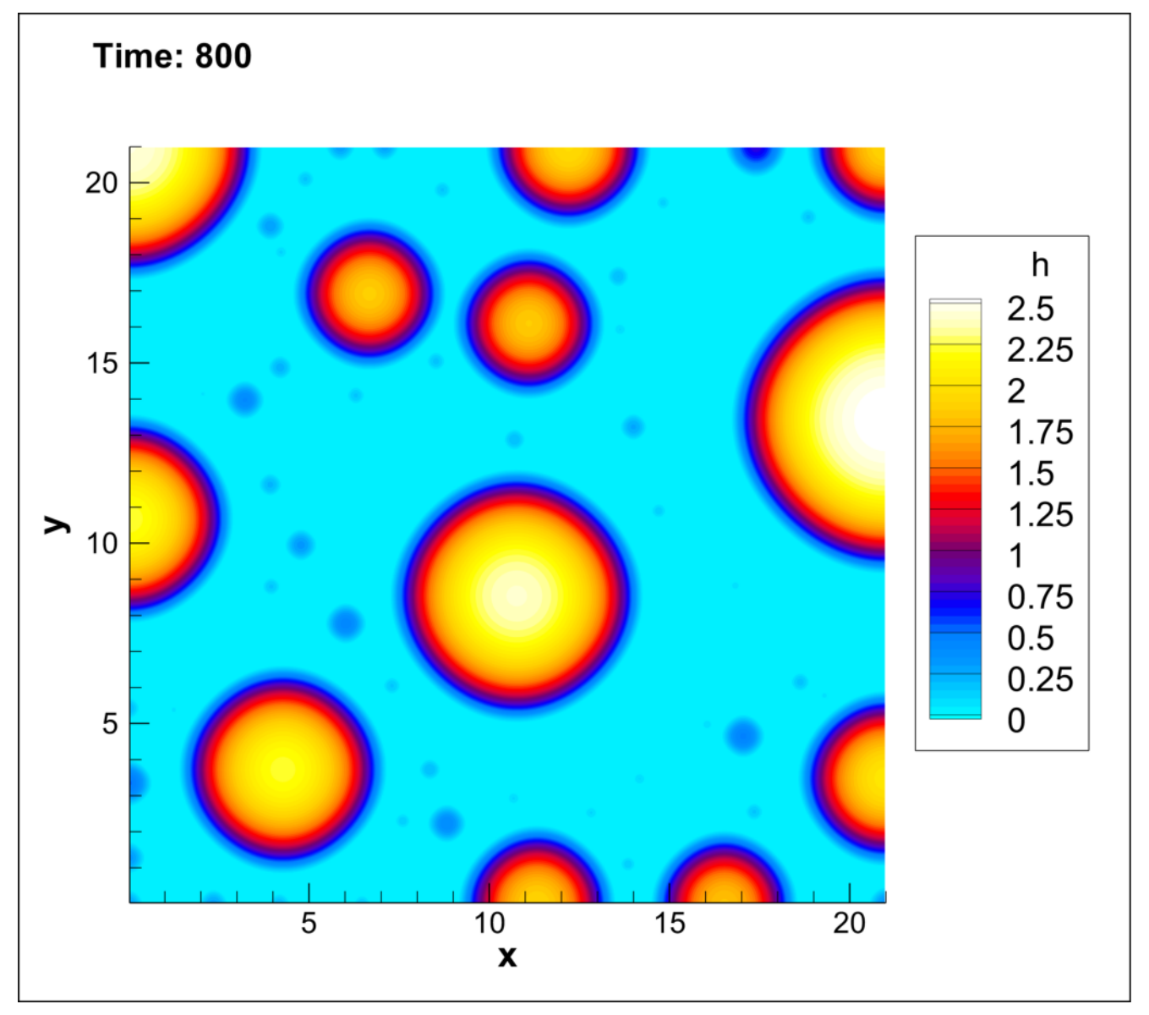
These results suggest that the formation of satellite droplets existing on a timescale longer than detwetting depends strongly on the sign of the disjoining pressure at the initial film thickness.

3D Flow Simulations

We now present preliminary simulation results for 3D flow. These confirm our expectations from the 2D results: for negative structural disjoining, $H_0 = 0.1$, no satellite drops form; however for a thicker film, $H_0 = 0.5$, smaller satellite drops form and exists on a longer timescale than detwetting.



$H_0 = 0.1$



$H_0 = 0.5$

Conclusion

The inclusion of the interplay between the bulk elastic energy and surface anchoring energy lead to interesting novel results describing stability of thin films. In particular, our simulations suggest that there is a correlation between the structural disjoining pressure and the formation of satellite drops.

References

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