

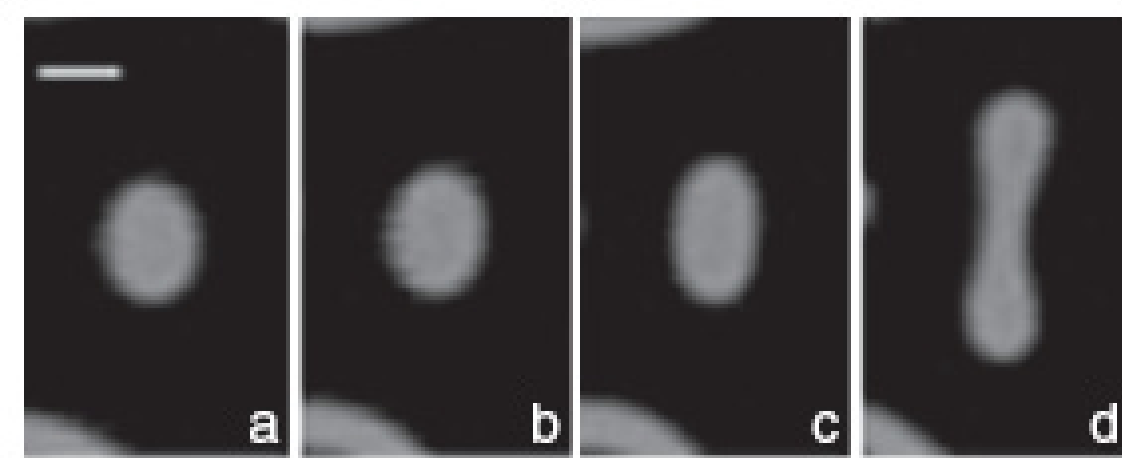
# HARVEY MUDD COLLEGE Formation of Labyrinth Patterns in Langmuir Films

George Tucker



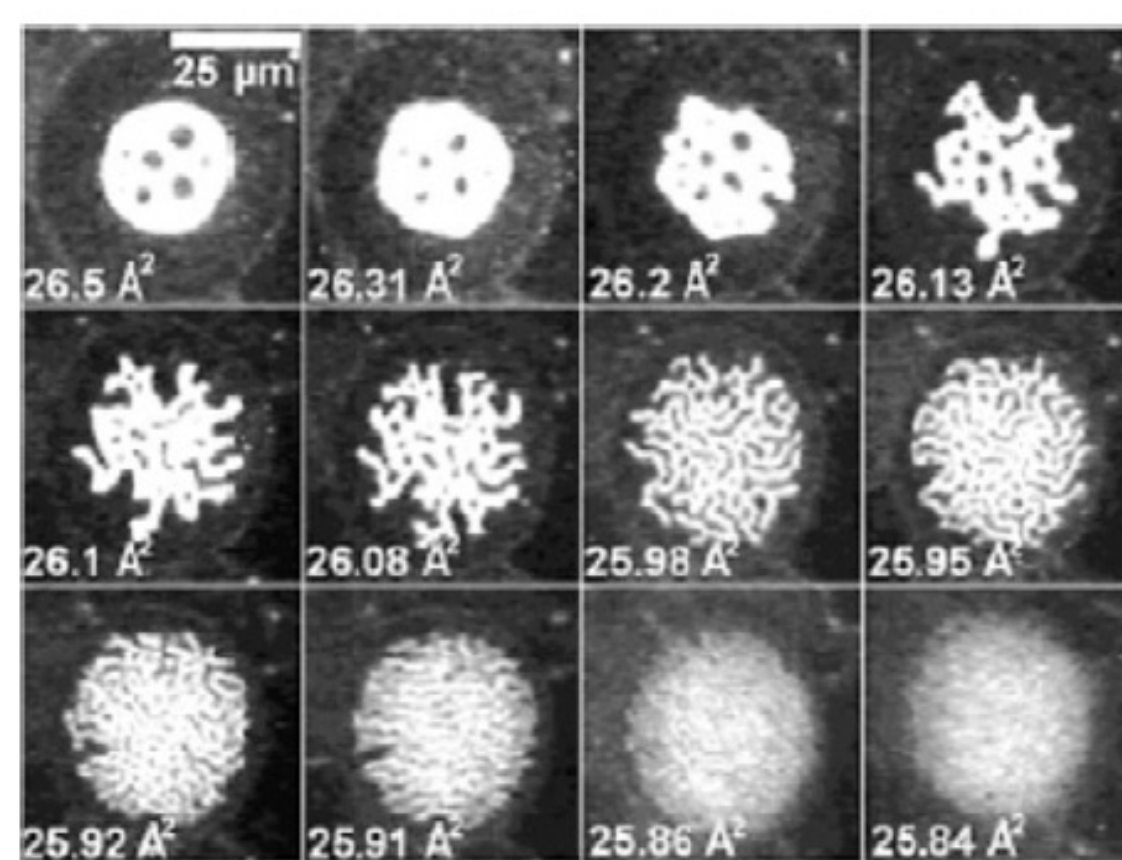
## Introduction

A Langmuir film is a molecularly thin fluid layer on the surface of a subfluid; a classic example is the lipid bi-layer that forms the external membrane of a biological cell. Langmuir layers can have multiple phases, which can evolve a variety of morphologies. When dipole-dipole forces are negligible, bounded films relax to energy-minimizing circular domains. If the molecules in a phase have a strong vertical dipole moment (often a result of hydrophilic/hydrophobic chains orienting themselves on the subfluid), exotic morphologies such as dog-bone shapes and labyrinth patterns manifest themselves. Similar morphologies are observed in numerous other physical systems, including type-1 superconductors, chemical reaction-diffusion systems, and films of ferrofluids.



**Figure 1:** A circle to dog-bone transition observed experimentally. Courtesy of Heinig et al. (1).

We investigate numerically the case where dipole-dipole interactions are strong enough to deform the domain into highly distorted patterns.

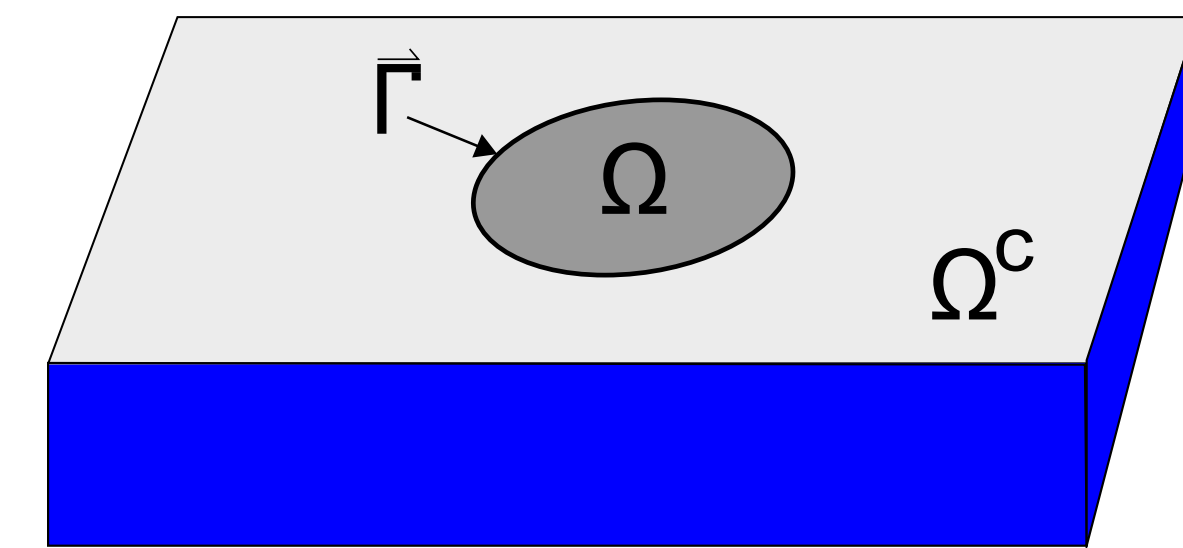


**Figure 2:** A labyrinth pattern observed experimentally. Courtesy of Heinig et al. (1).

## Model

In our model, two phases form different domains within the Langmuir film. We assume that one phase is a localized domain  $\Omega$ , that its complement  $\Omega^c$  is a second phase that extends infinitely in the horizontal plane. The domain boundary  $\partial\Omega$  is described by a po-

sition vector  $\vec{\Gamma}(s, t)$  parameterized by arc-length  $s$  and time  $t$ .



Modeling assumptions:

- Domains in the film are incompressible inviscid 2D Newtonian fluids.
- A constant line tension and the dipole-dipole interaction can be modeled as a force per unit length along the phase boundary ( $\vec{\Gamma}$ ).
- The subfluid is Stokesian.

## Equations of Motion

From the model of the fluid, we can determine the equations of motion that govern the interface:

$$\vec{\Gamma}_t = \left( \frac{\partial \Psi}{\partial s} \right) \hat{n},$$

where  $\Psi(s)$  is the stream function restricted to the boundary of the domain. The velocity stream function is computed as a boundary integral:

$$\Psi(s) = -\frac{1}{2\pi} \oint \mathcal{F}(s') [\hat{t}(s') \cdot \hat{r}(s, s')] ds',$$

where  $\mathcal{F}$  is the amplitude of the normal force per unit length at the boundary,  $\hat{t}$  is the unit tangent vector, and  $\hat{r}(s, s')$  is a unit vector pointing from  $\vec{\Gamma}(s)$  to  $\vec{\Gamma}(s')$ . For dipolar interactions, the force is given by:

$$\mathcal{F}(s) = \lambda\kappa(s) - \mu^2 \oint \frac{\hat{n}(s') \cdot \hat{r}(s, s')}{r(s, s') \sqrt{r(s, s')^2 + \Delta^2}} ds',$$

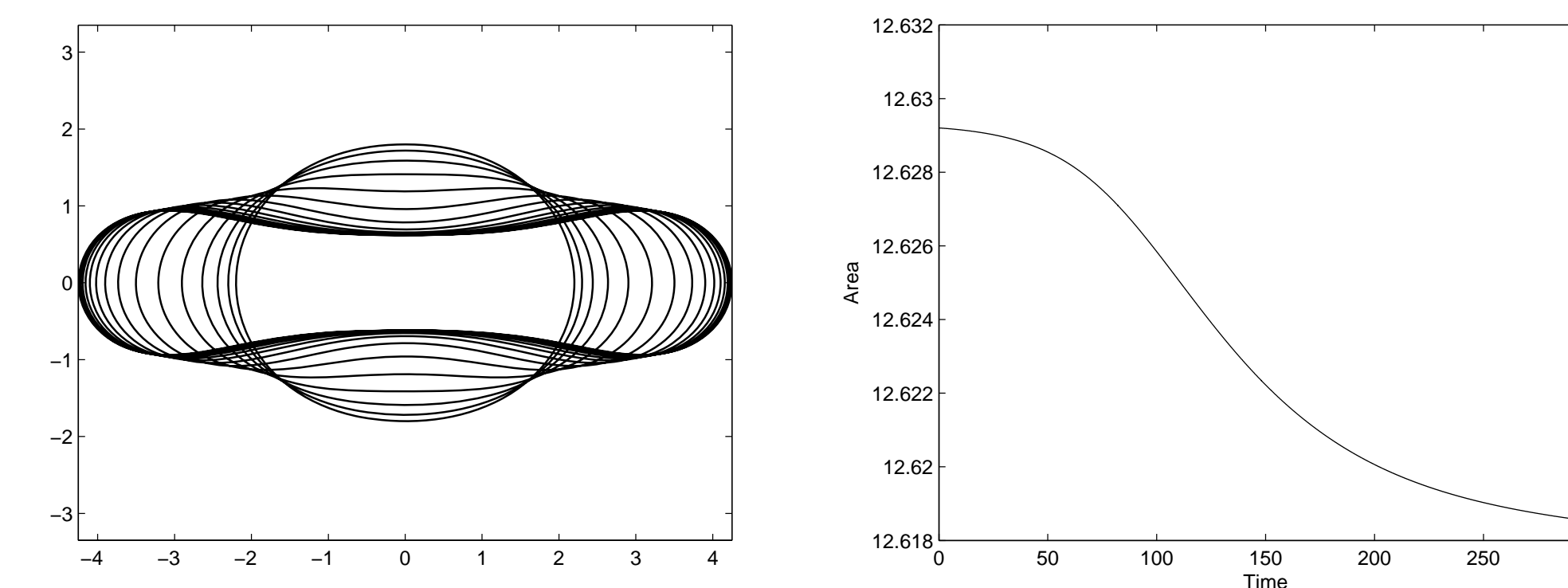
where  $\Delta$  is a small parameter that prevents the integrand from becoming singular. Its physical meaning is that of the thickness of the phase boundaries in the case of Langmuir monolayers.

## Outline of the Numerical Method

The force term includes a regularization parameter  $\Delta$  that keeps the integral from diverging. Different values of  $\Delta$  give different numerical results. Yet, the precise value of  $\Delta$  should only affect the short-range interactions (line tension forces) (2). To this end, we reformulate the integral to separate out the  $\Delta$  dependence

of the force into a term that affects the short range line tension term and a term independent of  $\Delta$ .

We store the boundary of the domain numerically as a set of discrete equally spaced points on the boundary. To evolve the domain in time, we move the points on the boundary according to the equations of motion.

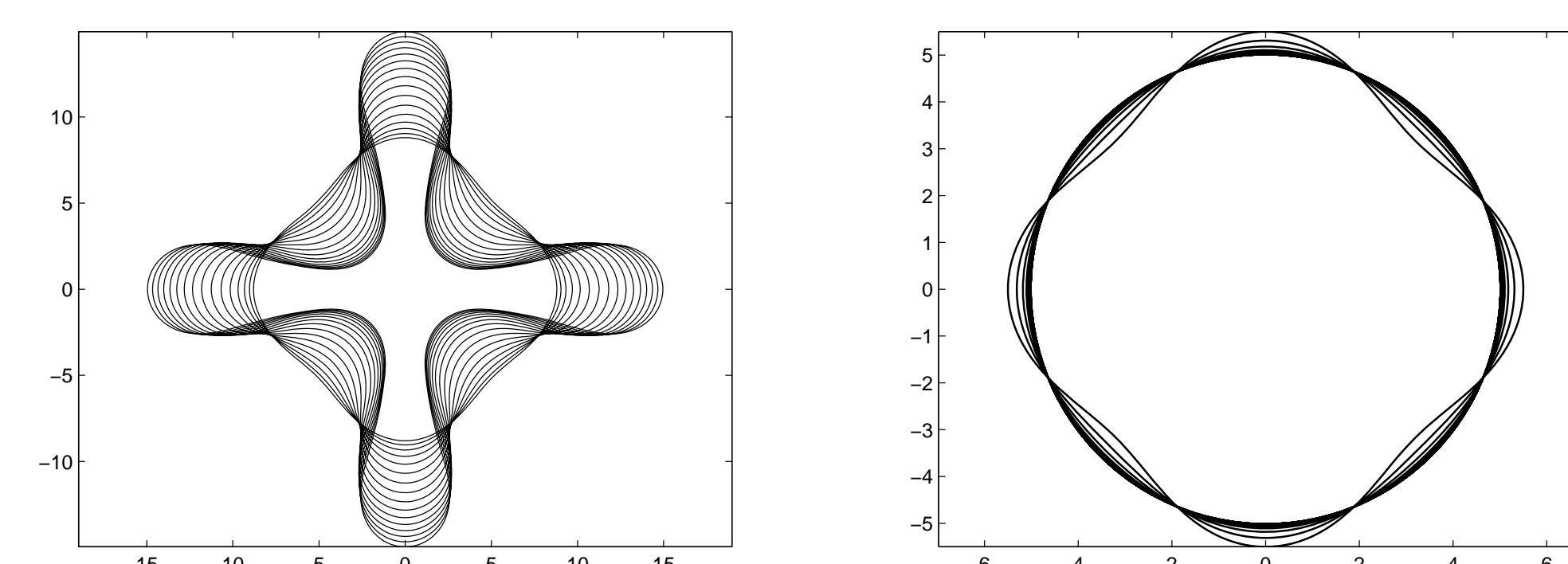


**Figure 3:** The left graph shows a numerical simulation of an elliptical domain evolving into a stable dog-bone shape domain. The curve at different times is superimposed. The right graph shows that the area loss during the simulation is minimal.

## Results

From the literature, as the radius of a circular domain increases, it becomes unstable. In Fig. 3, we have a perturbed circle (an ellipse) with a radius greater than the stability radius, and instead of relaxing back to a circle, it transitions into a dog-bone shape.

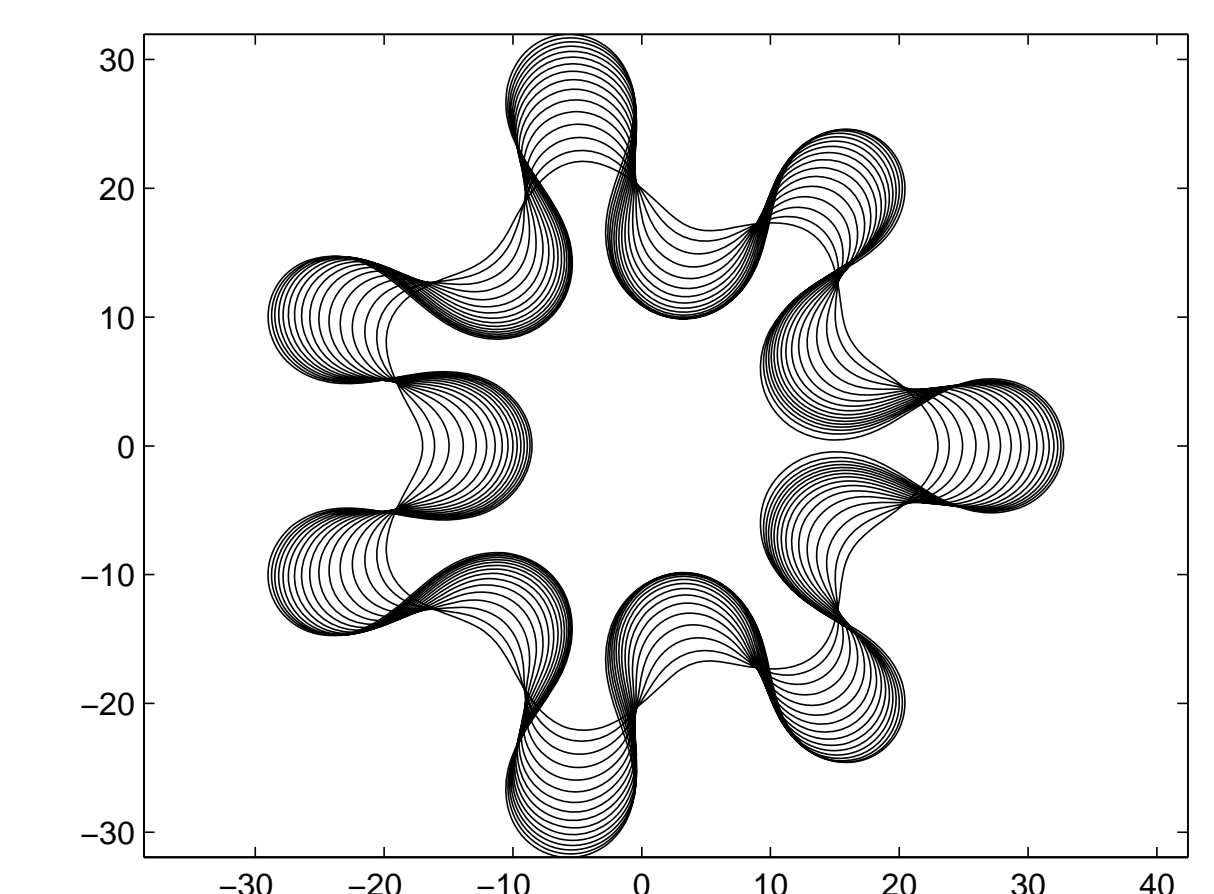
We are also able to simulate more complex patterns, such as in Fig. 5. Our simulations qualitatively agree with experimental data. Previous numerical simulations have been done, but they have experienced significant area loss (5 percent), whereas from the right panel of Fig. 3 we observe that the area loss is minimal. Our numerical method achieves higher accuracy and better stability than previous work.



**Figure 4:** A large-radius unstable domain and a smaller-radius stable domain.

## Conclusions

Our numerical method allows us to simulate Langmuir films with dipolar forces. The next step is to verify that our simulation conform with experimental data. Then we can numerically determine regions of stability for different materials that would not be possible by experiments alone.



**Figure 5:** A perturbed circle evolves into a complicated domain. The total area loss over the entire simulation was less than 0.8%.

## References

- [1] HEINIG, P., HELSETH, L. E. & FISHER, T. M. 2004 Relaxation of patterns in 2D modulated phases. *New J. of Phys.* **6**, 189.
- [2] DE KOKER, R. & H. M. MCCONNELL. 1993 Circle to Dogbone: Shapes and Shape Transitions of Lipid Monolayer Domains. *J. Phys. Chemistry* **97**, 13419-13424.

## Acknowledgments

I would like to thank my advisor, Professor Andrew Bernoff, for his invaluable guidance.

## For Further Information

<http://www.math.hmc.edu/~gtucker/thesis>