Continuum Modeling for Fluid Phase-Separation

PHYS 230 Final Project

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Scientific background: What is Phase-Separation?

- Phase separation is the creation of two distinct phases from one homogeneous mixture

- Most common example is oil and water, even when mixed they will remain phase-separate

- Two components could also be two polymers, or two glassy components

Scientific Motivation

- Can we use continuum modeling techniques to model phase-separation, to see the overall changes to the system without tracking specific particles?
- Phase separation regulates cellular processes and one of the principles behind cellular organization
- Applications in materials science and engineering
- Continuum modelling allows us to see the effects of isolated parameters in a system
- Modifying parameters is straightforward

Scientific Motivation

Previous Approaches:

- Multiparticle collision dynamics (MCD)

Our Goals:

- Implementing a continuum model to view the system over time
- Implement a fluid flow as a forcing term to see how it affects the system
- Write a script to measure droplet size

Cahn-Hillard Equation:

Describes the process of phase separation, where two components of a binary fluid separate completely.

If c is the concentration of the fluid, and $c = \pm 1$ indicates the two different fluid domains after phase-separation:

$$\frac{\partial c}{\partial t} = D\nabla^2\left(c^3 - c - \gamma\nabla^2 c\right)$$

where D is the diffusion coefficient, and $\sqrt{\gamma}$ is the length of the transition regions between the domains. The chemical potential is $\mu = c^3 - c - \gamma\nabla^2 c$.

Consider a normalized density field $\vec{u}$ described by the free energy density

$$f = \left(\frac{k}{2}\right)\left[|\nabla u|^2 + \frac{1}{2}\delta^{-2}\left(u^2 - 1\right)\right]$$

This is an energy of the Landau-Ginzburg type with the second term being a "double well" with minima $u = 1$ representing one phase "oil" and $u = -1$ is "water." Here k represents the surface tension, the energy cost of having an interface between the two phases, and δ is thickness of interface.

The dynamics is given by a density conservation equation where the RHS is the divergence of a density current derived from the free energy:

$$\frac{\partial u}{\partial t} = \frac{-1}{\tau}\nabla^2\left[k\nabla^2 u + \frac{k}{\delta^2}u\left(1 - u^2\right)\right] \text{ where } \nabla^2 \text{ is the 2D Laplacian}$$

$$\Longrightarrow \frac{\partial u}{\partial t} = \frac{k}{\delta^2\tau}\nabla^2\left[\left(u^3 - u\right) - \delta^2\nabla^2 u\right]$$

$\dfrac{k}{\delta^2\tau}$ is the diffusive coefficient

δ is the length of transition regions between the domains

Different Modeling Approaches

- Explicit versus Implicit methods
- Forward Euler
- Runge-Kutta 4
- Stability concerns

Discretization

- Discretize the biharmonic operator using a 4-point laplacian linear operator applied twice, with periodic boundary conditions

- Element-wise vector multiplication for the nonlinear term

- Forward-Euler explicit scheme in time

Discretization

Scheme / Pseudo-code:

$$\frac{\partial u}{\partial t} = \frac{-k}{\tau}\nabla^2\left[\nabla^2 u + \frac{1}{\delta^2}u\left(1-u^2\right)\right]$$

$$\frac{u_{ij}^{n+1} - u_{ij}^{n}}{dt} = \frac{-1}{\tau}\nabla^2\left[k\left(\frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}}{h^2}\right) + \frac{k}{\delta^2}u_{ij}\left(1-u_{ij}^2\right)\right]^n$$

$$\Longrightarrow \frac{u_{ij}^{n+1} - u_{ij}^{n}}{dt} = \frac{-k}{\tau}\nabla^2\left(\frac{1}{h^2}\left[\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}\right)\right] + \left[\frac{1}{\delta^2}u_{ij}\left(1-u_{ij}^2\right)\right]\right)^n$$

$$\Longrightarrow u_{ij}^{n+1} = u_{ij}^{n} + \left(\frac{-k \cdot dt}{\tau}\right)\nabla^2\left(-\frac{1}{h^2}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}\right] + \left[\frac{1}{\delta^2}u_{ij}\left(1-u_{ij}^2\right)\right]\right)^n$$

Initialization and Parameters

k = surface tension

τ = density over time

δ^2 = length of interface

h = space step

Nx = number of spacial gridpoints

Nt = number of timesteps

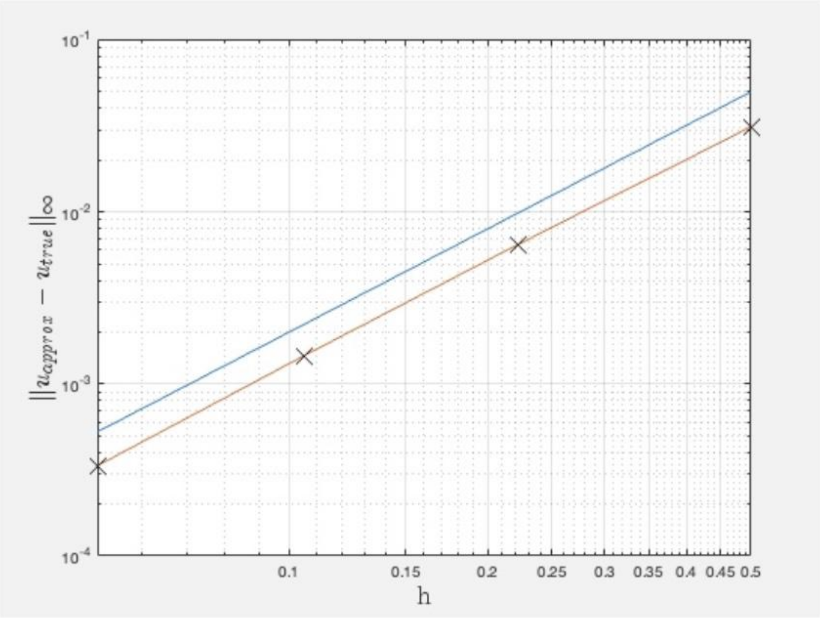
dt = timestep

Initial condition: Randomly sampled values between -1 and 1, with a bias towards -1 (water)

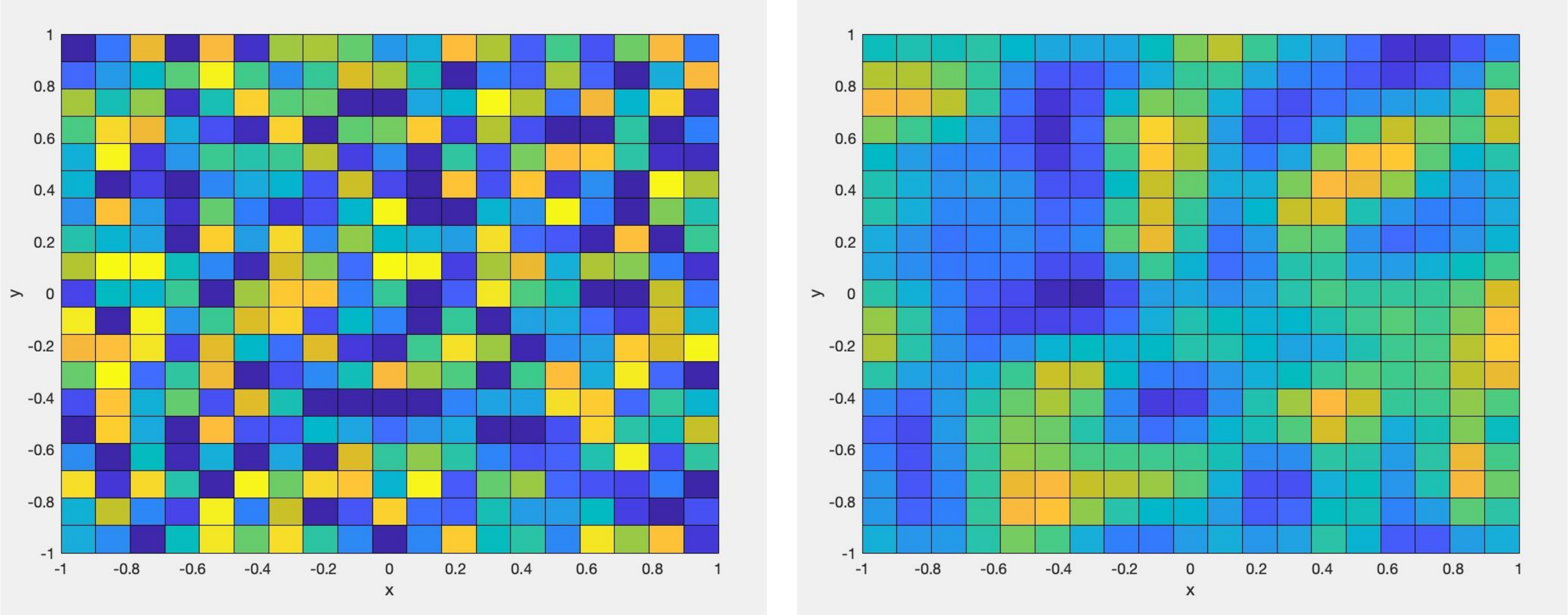
Testing Linear Operator - O(h^2) Convergence

We solve the heat equation $u_t = u_{xx}$ with periodic boundary conditions on $[-1,1]\times[-1,1]$, and can verify the expected second order convergence comparing to the true solution

$$u(x,y) = e^{-2\pi^2 t}\sin(\pi x)\sin(\pi y).$$

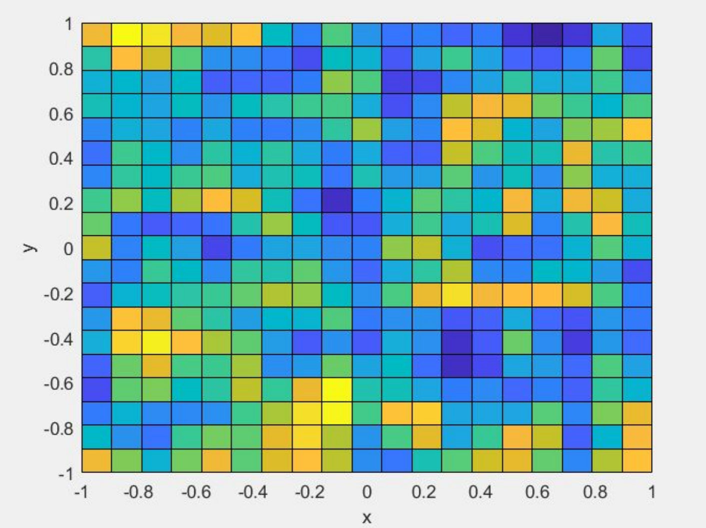


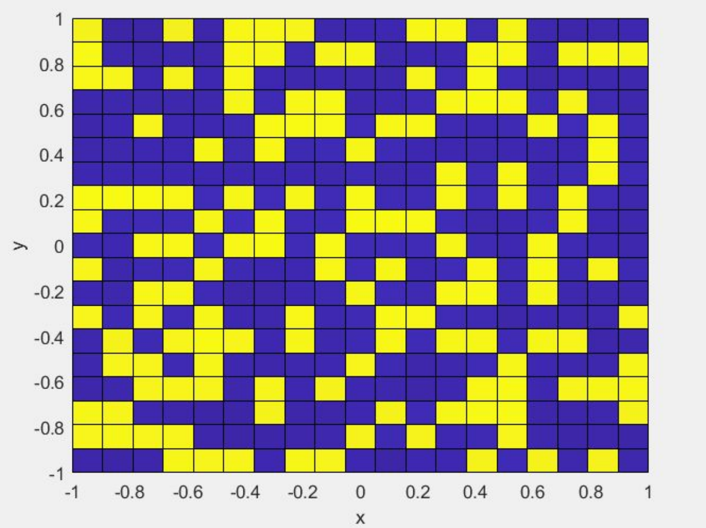
Plotted Density Field



$$k \;= 0.02,\;\; \tau = 1,\;\; \delta^2 = 1.05$$

Surface Plots

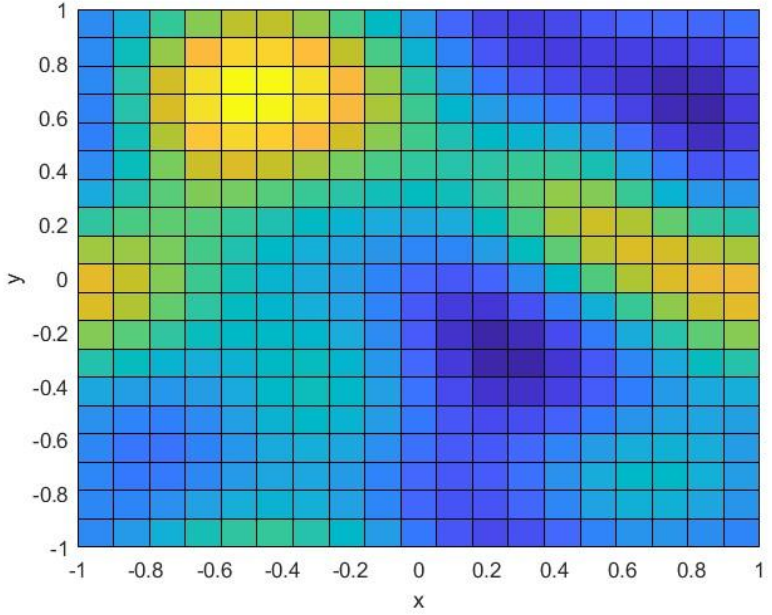




Parameters:
$\kappa = 0.02 \quad \tau = 1$
$\delta = 1 \quad Nt = 1{,}500$

Parameters:
$\kappa = 0.02 \quad \tau = 1$
$\delta = 0.1 \quad Nt = 1{,}500$

Increasing Number of Timesteps



κ = 0.02 τ = 1
δ = 100 Nt = 15,000

- Modifying parameters, we can see the effects on the final surface plot

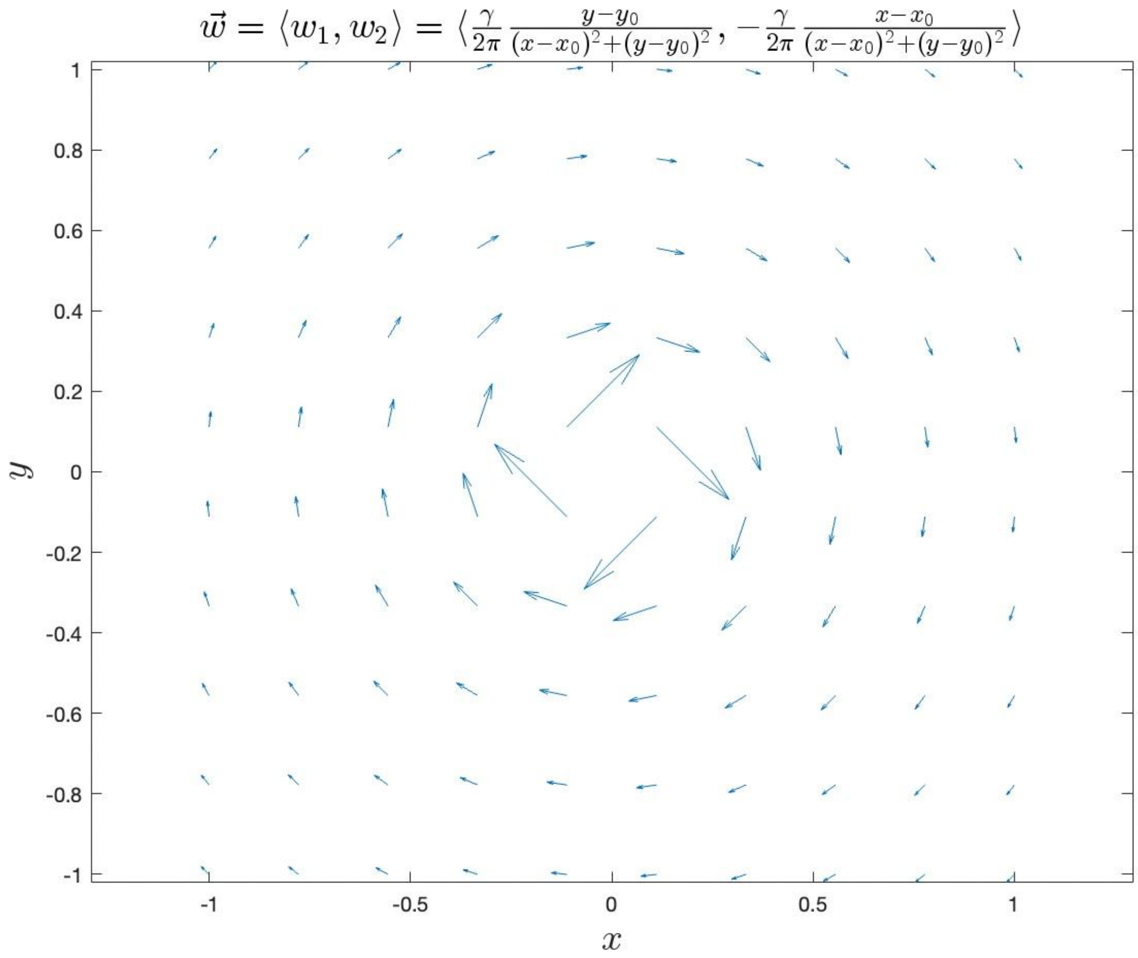
- We can also adjust for mesh refinement given a enough time

Adding Fluid Flow to our Model

Velocity Field for a Vortex:

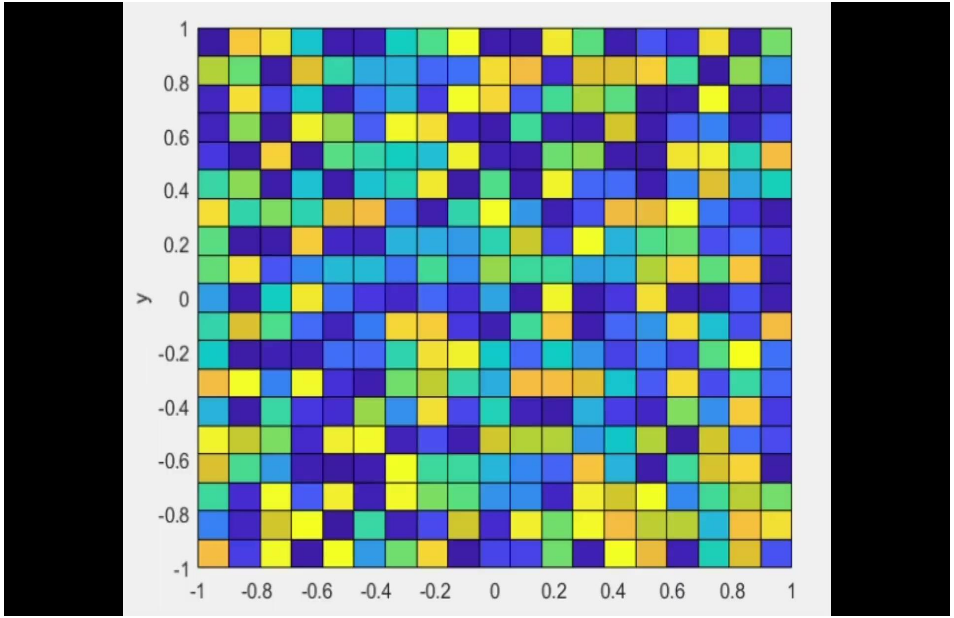
$$\vec{w} = \langle w_1, w_2 \rangle = \langle \frac{\gamma}{2\pi} \frac{y - y_0}{(x - x_0)^2 + (y - y_0)^2}, -\frac{\gamma}{2\pi} \frac{x - x_0}{(x - x_0)^2 + (y - y_0)^2} \rangle$$

```
% Calculate partial derivatives of u and v analytically
% Calculate advection terms

  adv_u = u_step .* dw1_dx(:) + v_step .* dw2_dy(:);
  adv_v = u_step .* dw1_dx(:) + v_step .* dw2_dy(:);

  u_new = u_step + (k*dt/(delta^2 * tau*h^4)) * A * ((u_step.^3-
            u_step) - (delta^2)*A*u_step + adv_u);
  v_new = v_step + (k*dt/(delta^2 * tau*h^4)) * A * ((v_step.^3-
            v_step) - (delta^2)*A*v_step + adv_v);
```

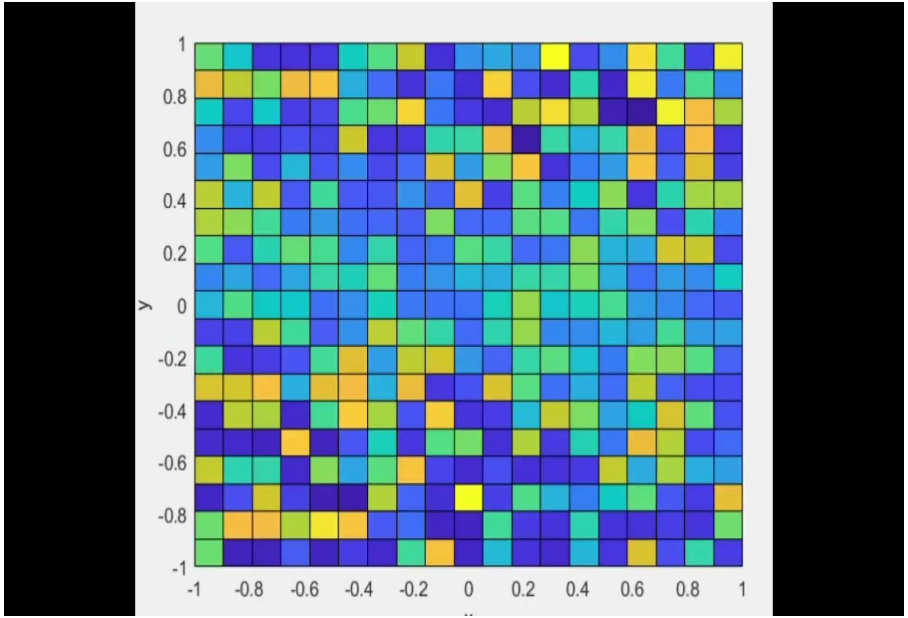

$\vec{w} = \langle w_1, w_2 \rangle = \langle \frac{\gamma}{2\pi} \frac{y-y_0}{(x-x_0)^2+(y-y_0)^2}, -\frac{\gamma}{2\pi} \frac{x-x_0}{(x-x_0)^2+(y-y_0)^2} \rangle$
y
x
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1
-0.5
0
0.5
1

Code evolution and comparison

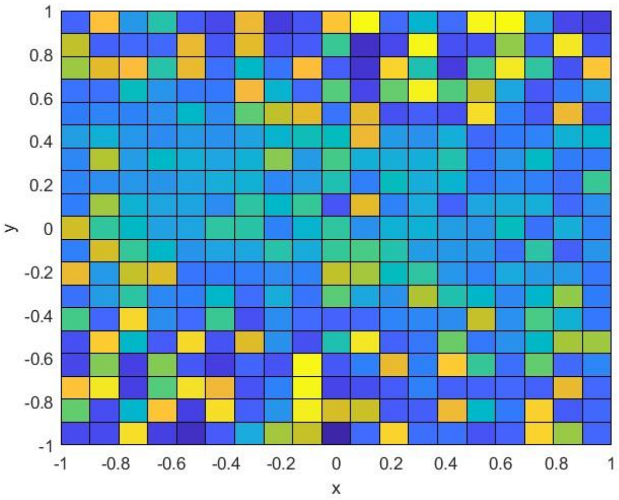
Without vortex:



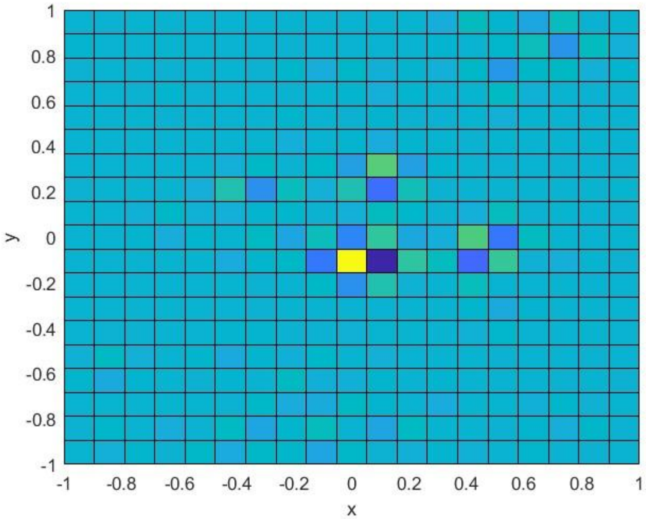
With vortex:



Instabilities and the CFL Condition

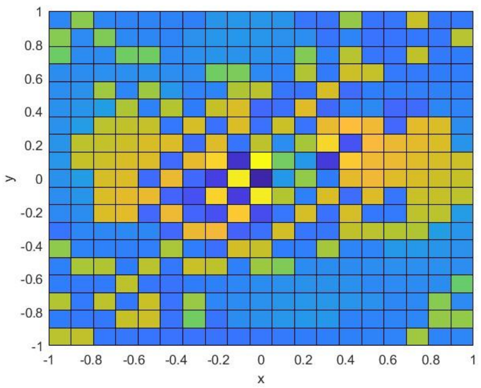


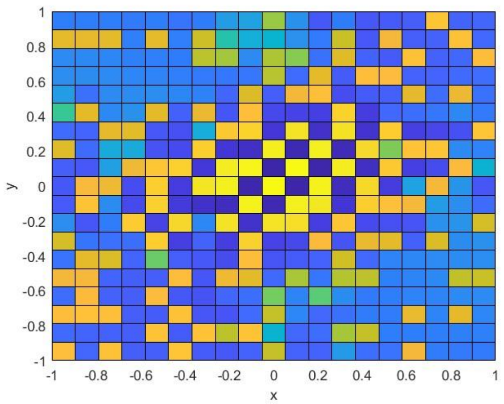
k = 0.2 $\tau = 1$
δ = 0.1 Nt = 1,500

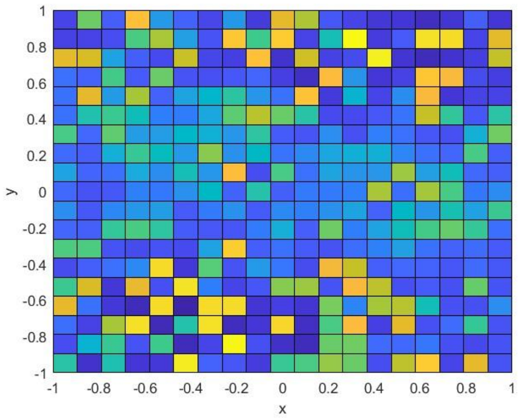


k = 2.0 $\tau = 1$
δ = 0.1 Nt = 1,500

Parameters - Density Over Time (τ)





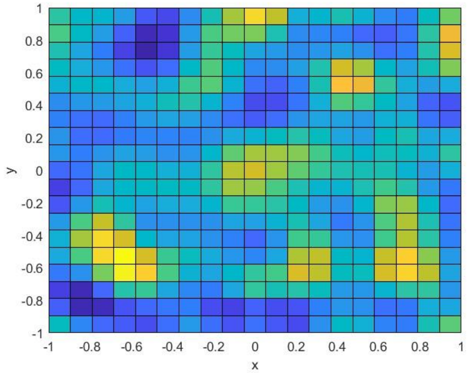


k = 0.02 τ = 0.4
δ = 0.1 Nt = 1,500

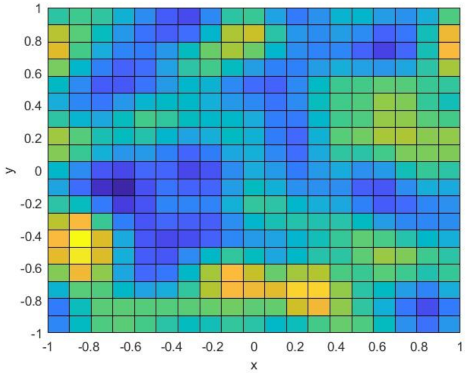
k = 0.02 τ = 10
δ = 0.1 Nt = 1,500

k = 0.02 τ = 100
δ = 0.1 Nt = 1,500

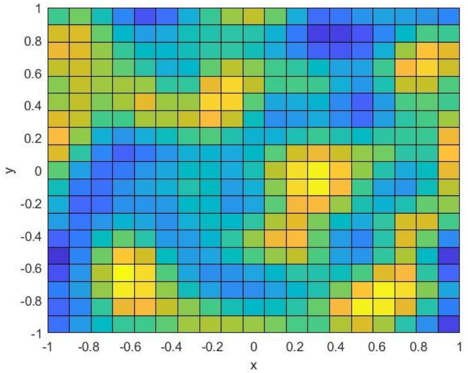
Parameters - Interface Length (δ)



k = 0.02 τ = 1
δ = 1 Nt = 1,500

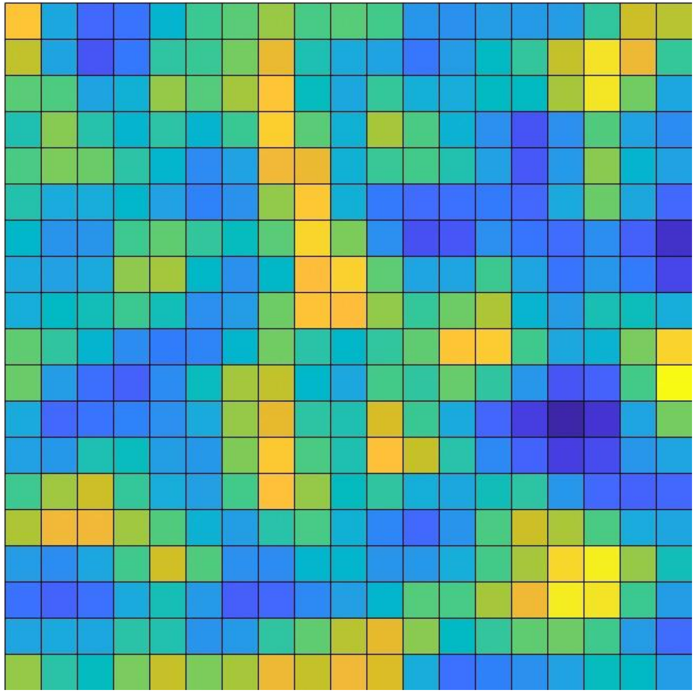


k = 0.02 τ = 1
δ = 10 Nt = 1,500



k = 0.02 τ = 1
δ = 100 Nt = 1,500

Future Plan - Droplet Size Analysis



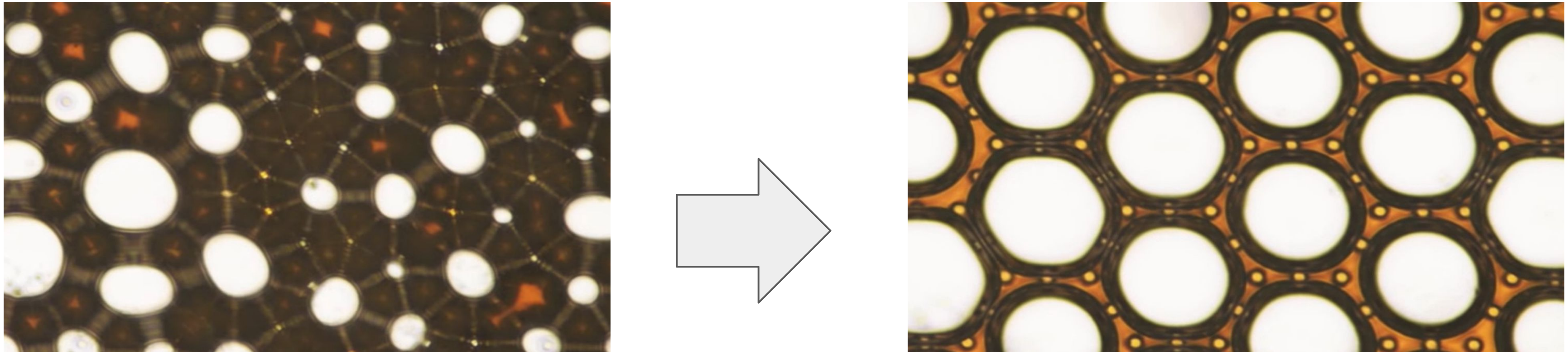
```python
# TEST SCRIPT
image_path = "/Users/jackpham/Downloads/scrnshot1.jpg"
yellow_blobs = find_yellow_circles(image_path)
average_area_pixels = calculate_average_area(yellow_blobs)

# conversion factor is 0.264583333333719 mm per 1 pixel
conversion_factor = 0.264583333333719

average_area_mm = average_area_pixels * (conversion_factor ** 2)
print("Average area of yellow circles:", average_area_mm, "mm^2")
```

✓ 0.0s

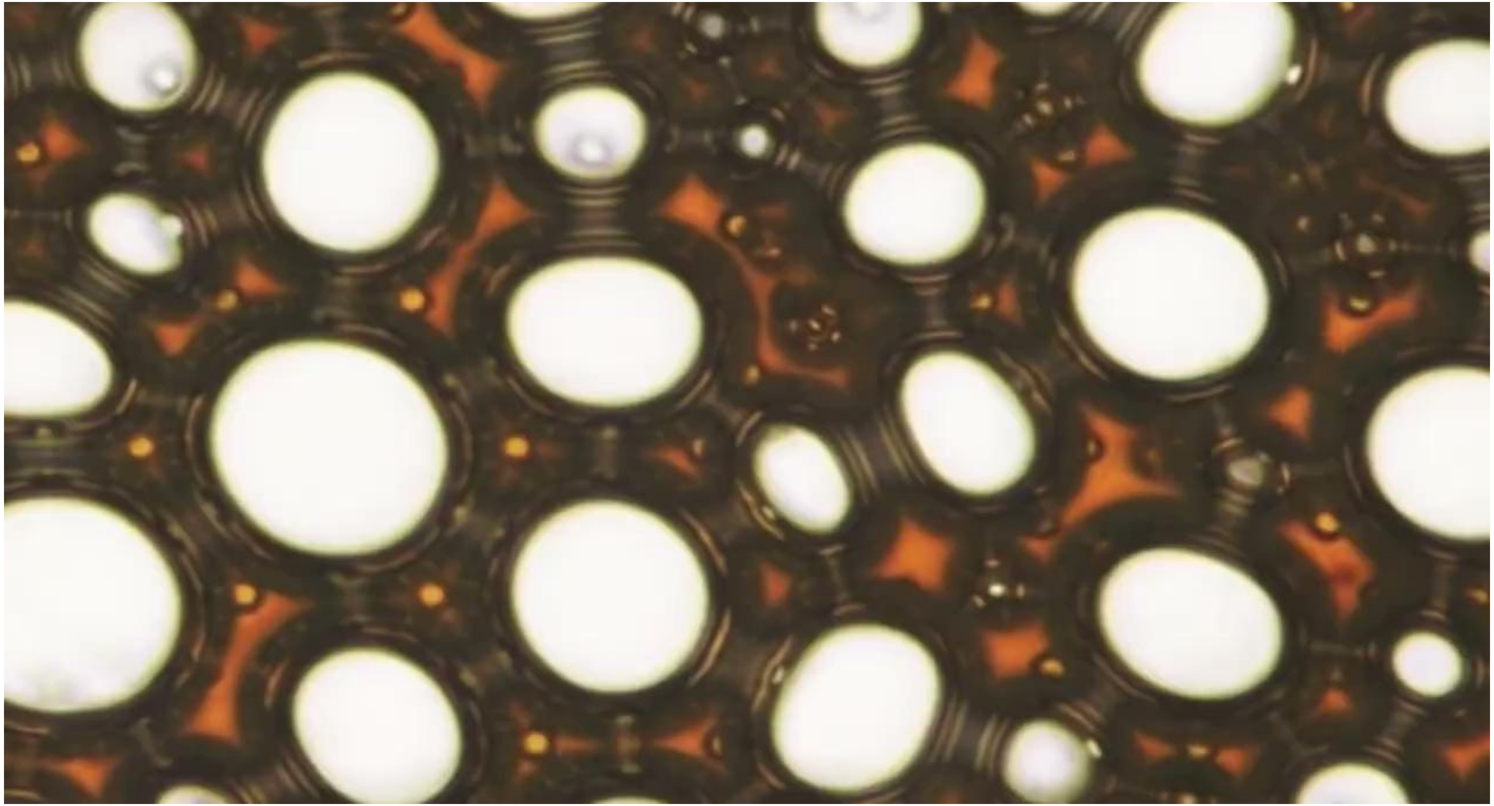
```
Average area of yellow circles: 111.50203641923643 mm^2
```

Ostwald Ripening Phenomenon

- Larger particles are more energetically favored than smaller particles.
- Involves change of inhomogeneous structure over time.
- Small solutions first dissolve and then redeposit into larger solution particles.
- Molecules on the surface of a particle are energetically less stable than ones on the interior.



Ostwald Ripening Phenomenon



Possible Future Improvements

- Spectral methods
- Can we track how fast droplets aggregate?
- More efficient way to run many experiments at once?

References

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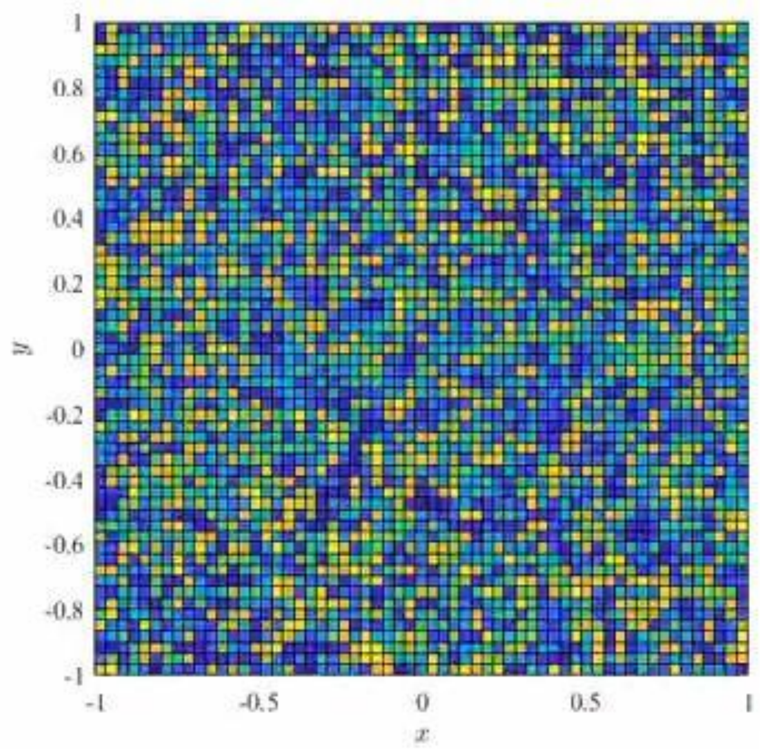
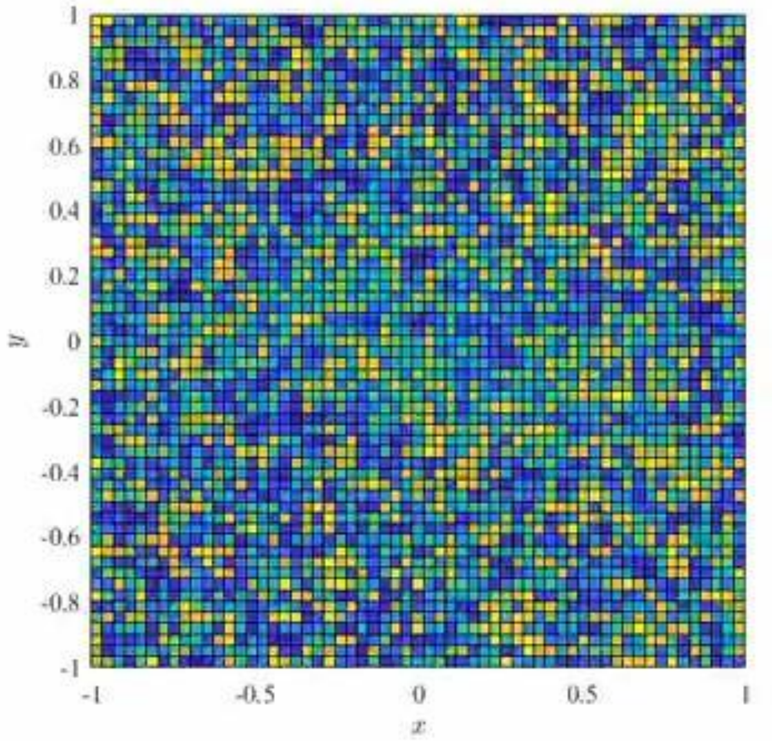
Post presentation Simulations



Parameters:
k = 0.02 τ = 1
δ = 0.65 Nt = 3000

Post presentation Simulations



Parameters:
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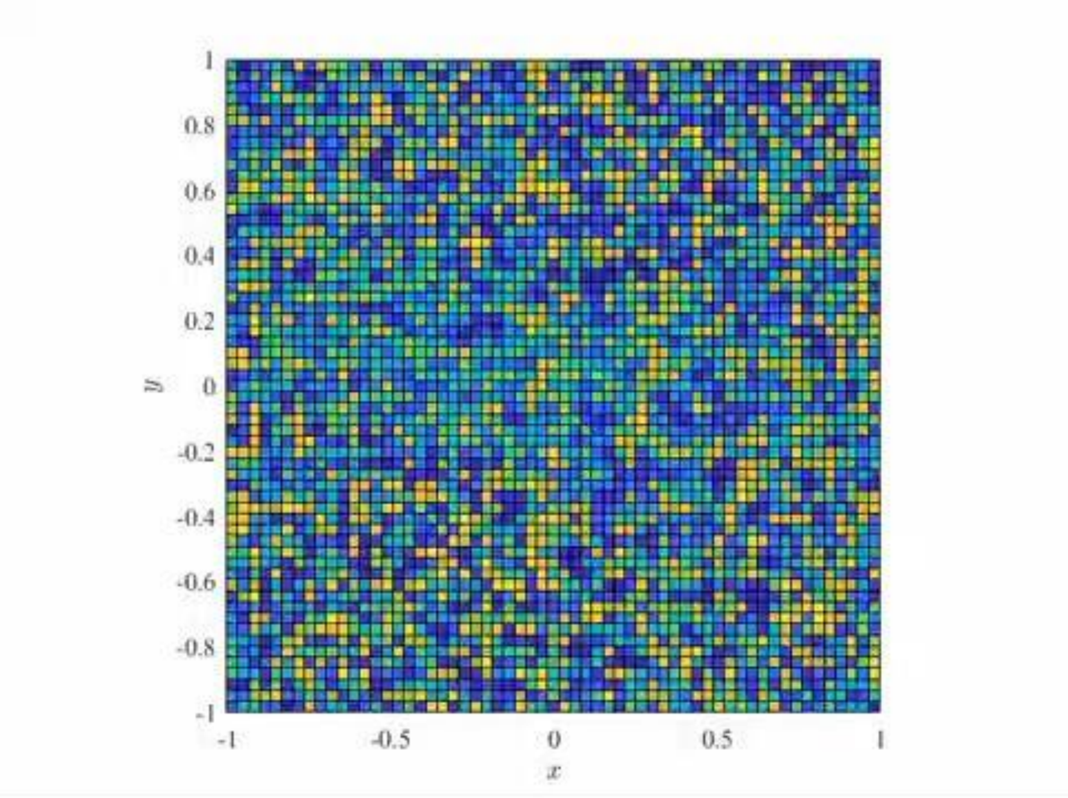
δ = 0.65 Nt = 6000

Post presentation Simulations



Parameters:
$k = 0.02 \quad \tau = 1$
$\delta = 0.65 \quad Nt = 12000$