MS5033
Mesoscale Microstructure Modeling
Report

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Problem Statement

In this project, we simulate the growth of a solid tumor using a Cahn–Hilliard-type convection-reaction-diffusion model. The goal is to capture the evolution of tumor volume fraction, nutrient concentration, and velocity fields in a confined domain over time. This type of modeling is useful for understanding tumor development, interactions with the microenvironment, and for testing hypothetical therapies.

1 Mathematical Model

Governing equtaions are as follows:

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (M(\phi)\nabla\mu) + \bar{\rho}_S(P\sigma - A)h(\phi) - \nabla\nu\phi \tag{1}$$

Equation 1, consists of three terms:

- Diffusion term: Describes the diffusion of the tumor phase ϕ.
- Source term: Represents the growth of the tumor due to nutrient availability.
- Chemotaxis term: Represents the chemotactic response of the tumor to nutrient gradients.

$$\mu = \frac{\beta}{\epsilon}\psi(\phi) - \beta\epsilon\Delta\phi - \chi_\phi\sigma \tag{2}$$

$$\frac{\partial \sigma}{\partial t} = \nabla \cdot (n(\phi)(\chi_\sigma\nabla\sigma - \chi_\phi\nabla\phi)) - C\sigma h(\phi) \tag{3}$$

$$\nu = -K(\nabla P - \mu\nabla\phi - \chi_\phi\sigma\nabla\phi) \tag{4}$$

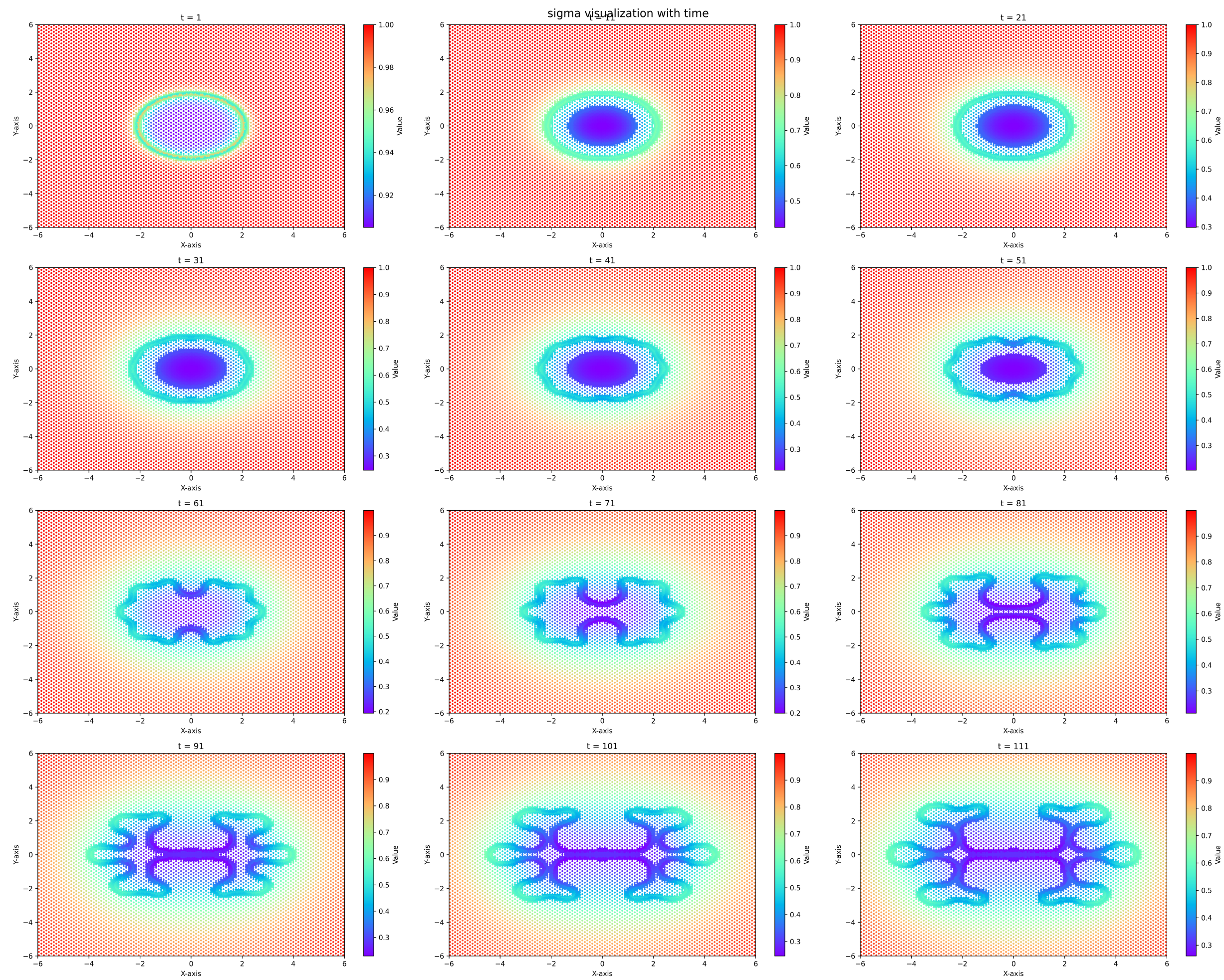

Figure 1: Scatter plot of σ with time evolution.

Results

- Here $t = 1$ signifies, 1000 timesteps, with stepsize of 0.001.
- χ is the chemotaxis parameter.
- σ denotes the unspecified chemical species that serves as nutrients for tumor.
- ϕ phase variable denotes the tumor volume fraction.

σ Evolution

Figure 1 and 2 show the evolution of σ with time for $\chi_\phi = 5$ by plotting the scatter and contour plots respectively.

Figure 3 and 4 show the evolution of σ with time for $\chi_\phi = 10$ by plotting the scatter and contour plots respectively. Here $t = 1$ signifies, 1000 timesteps, with stepsize of 0.001.

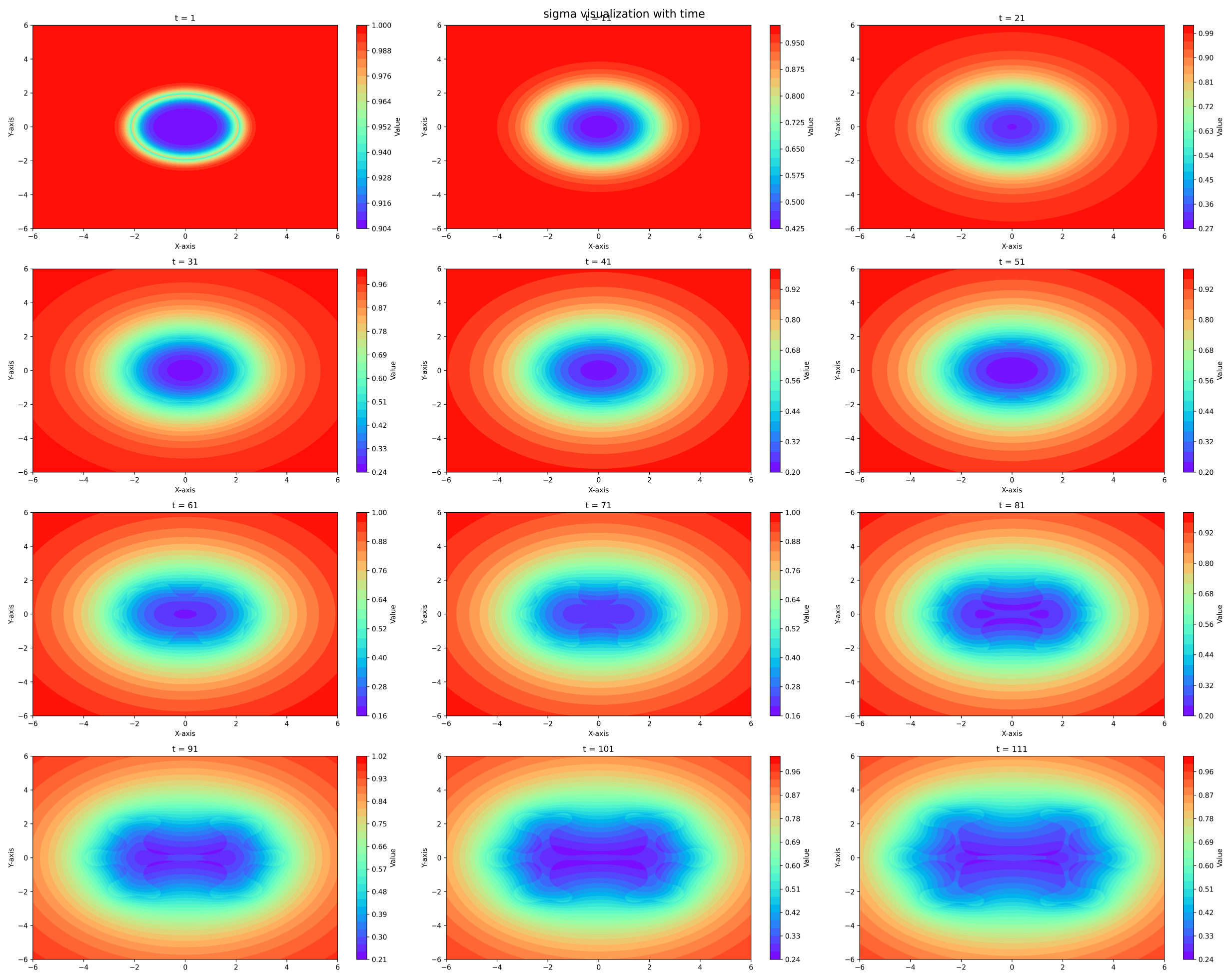

Figure 2: Contour plot of σ with time evolution.

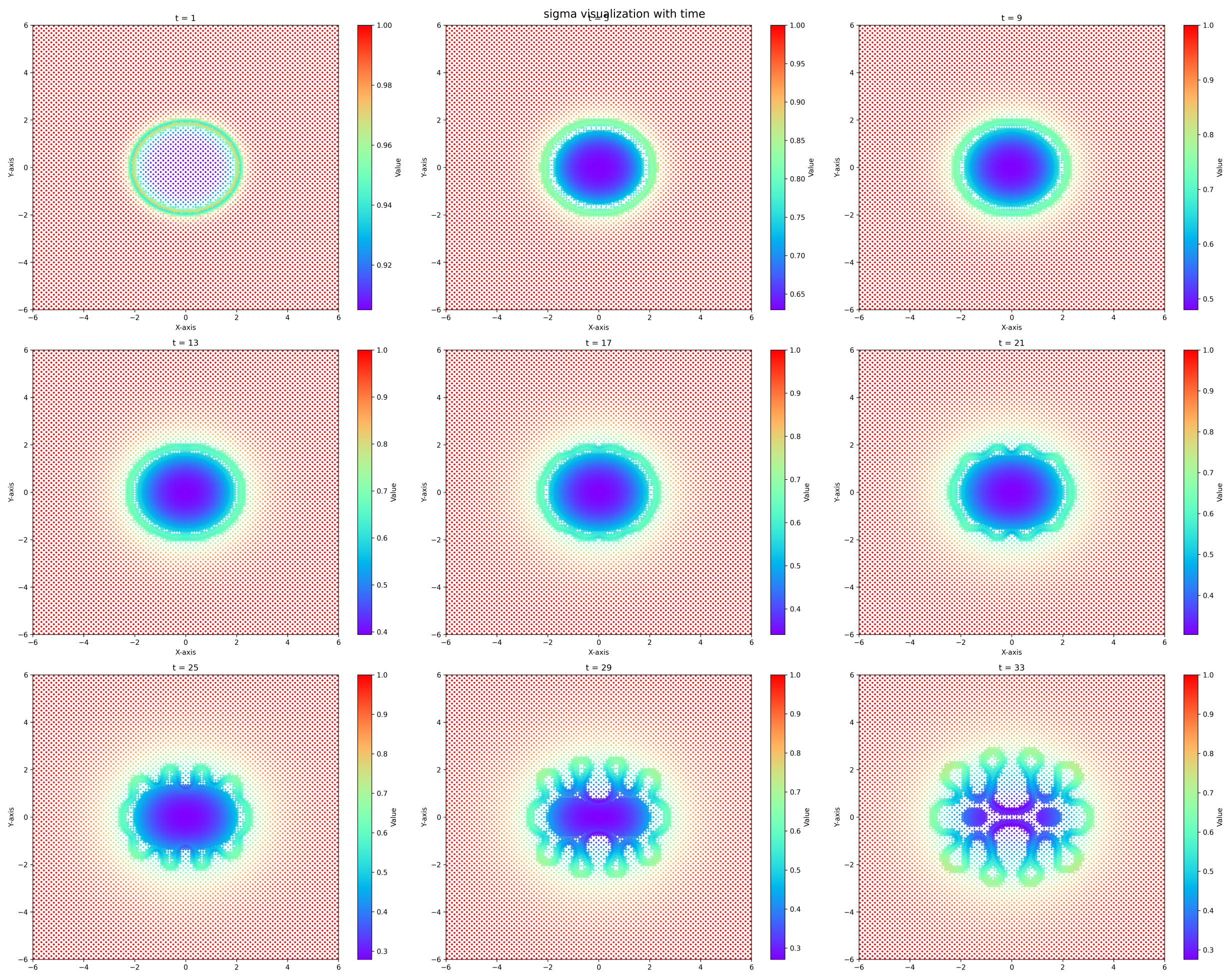

Figure 3: Scatter plot of σ with time evolution.

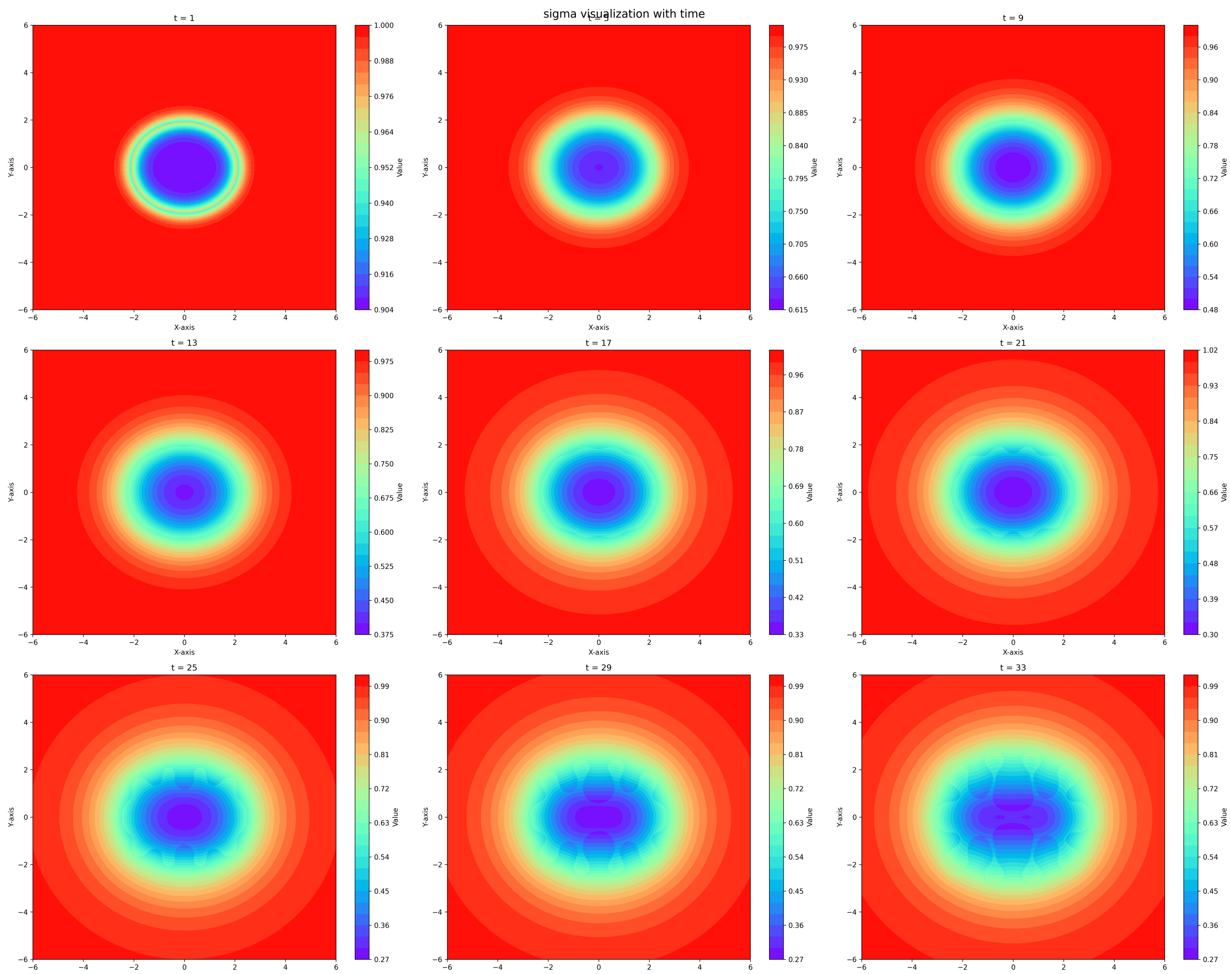

Figure 4: Contour plot of σ with time evolution.

ϕ Evolution

Explained by Yoshita Kondapalli in her report.

Observations

- For larger values of χ formation and evolution of the branches of tumor is quicker.
- More branches are formed in the case of $\chi = 10$ as compared to $\chi = 5$.
- For $\chi = 5$, $t = 111$ and for $\chi = 10$, $t = 33$ shows similar evoltion of σ.
- Results are similar to the reference results.

Time for execution of the code is around 3-5 seconds per iteration of timestep. We have ran for $t = 150$ i.e., 15000 timesteps with stepsize of 0.001 for $chi = 5$ and it took around a day to run the simulation. We have ran for $t = 50$ i.e., 5000 timesteps with stepsize of 0.001 for $chi = 10$ and it took around 12 hours to run the simulation.

Reference Results

Reference results are obtained from the paper 1.

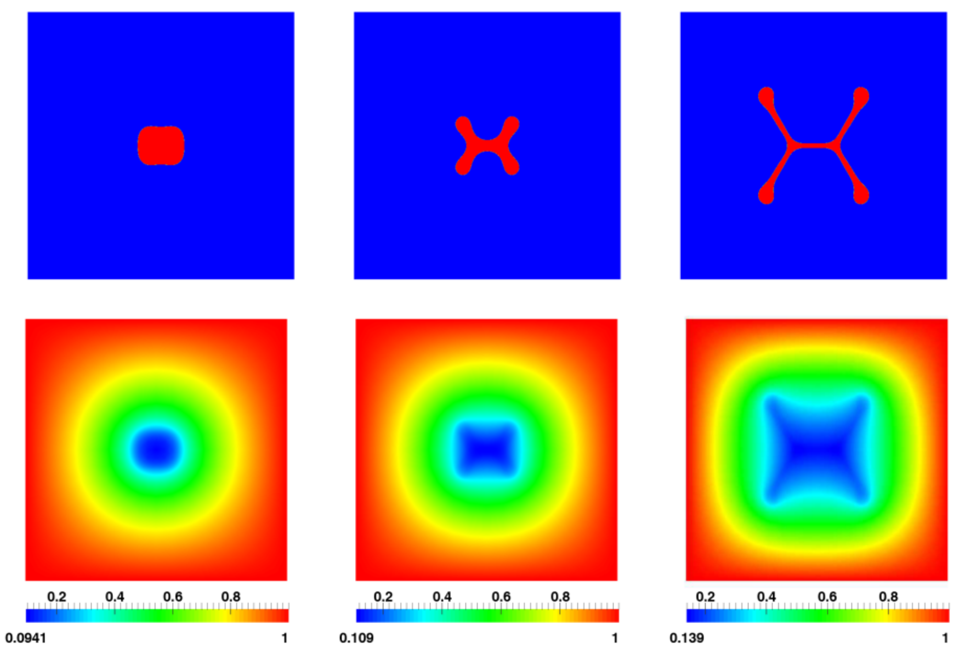

Figure 5: Reference Result: Solution with$P = 0.1, \chi_p hi = 5$, at $t = 5, 10, 20$

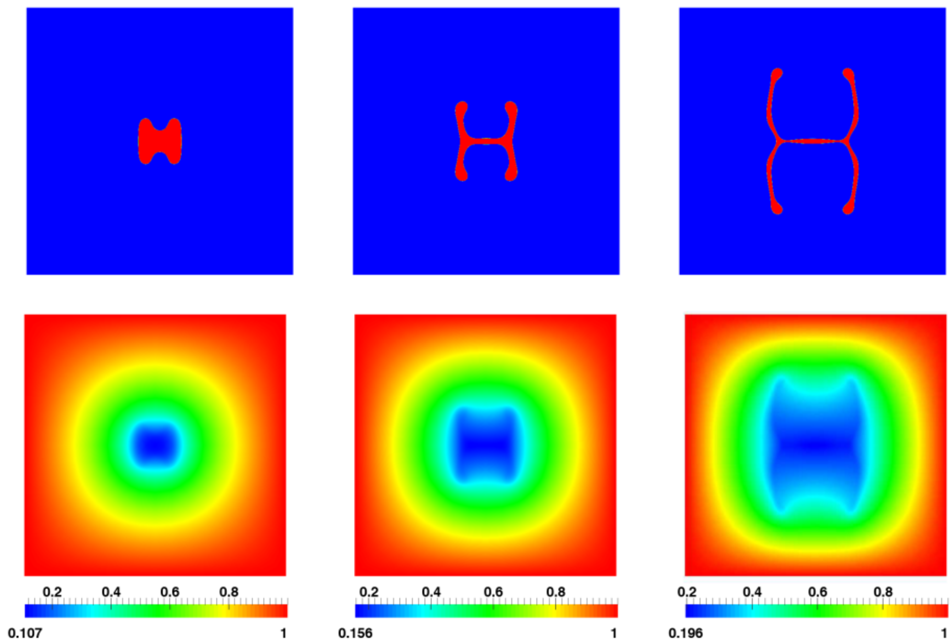

Figure 6: Reference Result: Solution with $P = 0.1, \chi_\phi = 10$, at $t = 5, 10, 20$

Reference

1. Garcke, Harald & Lam, Kei & Sitka, Emanuel & Styles, Vanessa. (2016). A Cahn–Hilliard–Darcy model for tumour growth with chemotaxis and active transport. Mathematical Models and Methods in Applied Sciences. 26. 1095-1148. 10.1142/S0218202516500263.

2. Non-linear Cahn-Hillard equation using FEM and Newton method. `https://docs.fenicsproject.org/dolfinx/main/python/demos/demo_cahn-hilliard.html`

3. Wise, S. M., Lowengrub, J. S., & Cristini, V. (2011). An adaptive multigrid algorithm for simulating solid tumor growth using mixture models. *Mathematical and Computer Modelling*, 53, 1–20.

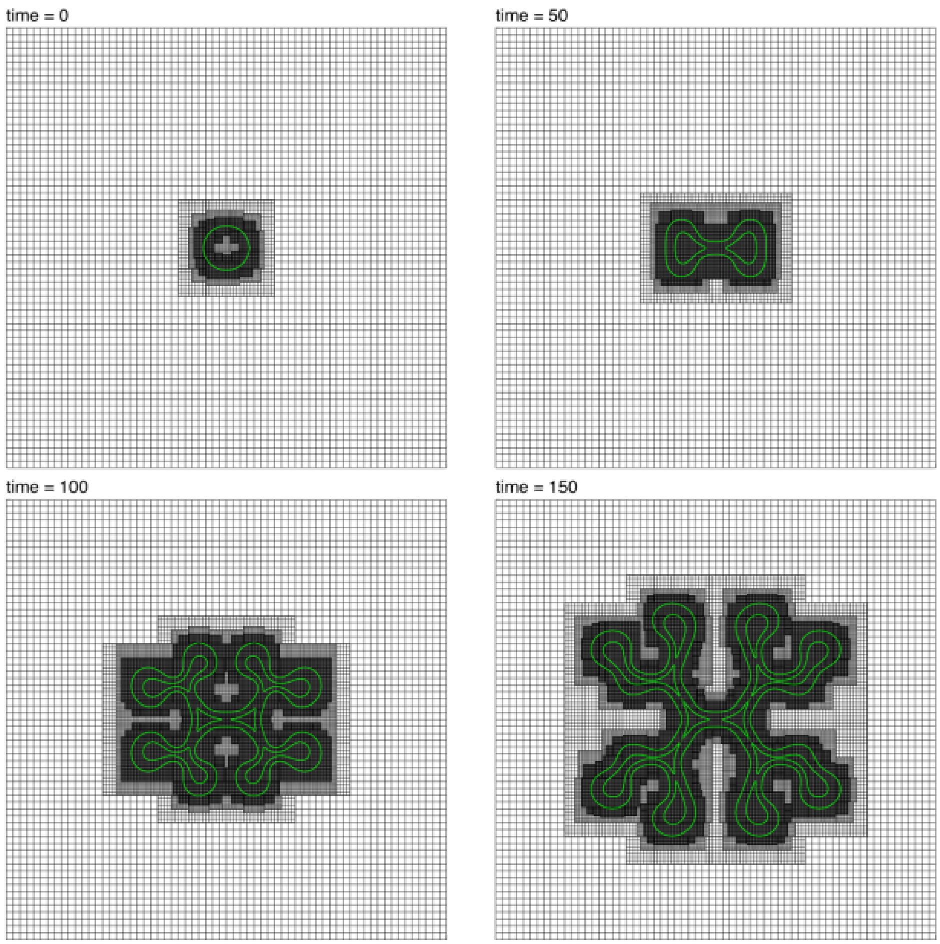

Figure 7: Reference Result: From the paper 3