NYS Task 2

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1 Introduction

$$A + 2B \rightarrow 3B$$

Species A (u): substrate/prey particles
Species B (v): autocatalyst/predator particles

Writing the update equation per cell *(i, j)* based on material balance and reaction terms with time step Δt

$$A_{i,j}^{\text{new}} = A_{i,j} + \Delta t \cdot \left(d_A \cdot \Delta A_{i,j} + f \cdot (1 - A_{i,j}) - r \cdot A_{i,j} \cdot B_{i,j}^2\right)$$
$$B_{i,j}^{\text{new}} = B_{i,j} + \Delta t \cdot \left(d_B \cdot \Delta B_{i,j} - k \cdot B_{i,j} + r \cdot A_{i,j} \cdot B_{i,j}^2\right)$$

where the Laplacian operator ∇^2 is approximated using the 5-point stencil:

$$\nabla^2 A_{i,j}^n \approx A_{i+1,j}^n + A_{i-1,j}^n + A_{i,j+1}^n + A_{i,j-1}^n - 4A_{i,j}^n$$

We can write the same equation such that A and B are entire 2D arrays (grids), and all operations are applied element-wise:

$$A_{\text{new}} = A + \Delta t \cdot \left(d_A \cdot \Delta A + f(1 - A) - r \cdot A \cdot B^2\right)$$
$$B_{\text{new}} = B + \Delta t \cdot \left(d_B \cdot \Delta B - k \cdot B + r \cdot A \cdot B^2\right)$$

Converting this discretized equation into PDEs, we have the following:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u \ - uv^2 + F(1 - u)$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v \ + uv^2 - (F + k)v$$

2 Non-Dimensionalization of the Gray-Scott Model

The Gray-Scott reaction-diffusion system describes the interaction of two chemical species $u(x, y, t)$ and $v(x, y, t)$, governed by the equations:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1 - u), \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (F + k)v. \tag{2}$$

2.1 Scaling and Dimensionless Variables

To simplify the system and identify the dominant parameters, we introduce the following dimensionless variables:

$$\tilde{x} = \frac{x}{L}, \quad \tilde{y} = \frac{y}{L}, \quad \tilde{t} = \frac{t}{T}, \quad \tilde{u} = \frac{u}{U_0}, \quad \tilde{v} = \frac{v}{V_0},$$

where L, T, U_0, and V_0 are characteristic length, time, and concentration scales.

2.2 Choice of Scaling Parameters

To simplify the equations and reduce the number of parameters, we choose the following dimensionless scaling:

- $U_0 = 1$, $V_0 = \sqrt{\frac{F}{k}}$: normalize the concentrations of species u and v.
- $T = \frac{1}{F}$: scale the characteristic time based on the feed rate F.
- $L = \sqrt{\frac{D_u}{F}}$: scale the characteristic length based on the diffusion coefficient D_u and the feed rate F.

Differential operators transform as:

$$\nabla^2 = \frac{1}{L^2} \nabla^2_{\tilde{x}}, \quad \frac{\partial}{\partial t} = \frac{1}{T} \frac{\partial}{\partial \tilde{t}}.$$

2.3 Substituting into the Equations

Substituting into equation (1):

$$\begin{aligned}
\frac{1}{T} \frac{\partial \tilde{u}}{\partial \tilde{t}} &= D_u \cdot \frac{1}{L^2} \nabla^2_{\tilde{x}} \tilde{u} - \tilde{u}\tilde{v}^2 \frac{F}{k} + F(1 - \tilde{u}) \\
\Rightarrow \frac{\partial \tilde{u}}{\partial \tilde{t}} &= \frac{D_u T}{L^2} \nabla^2_{\tilde{x}} \tilde{u} - T\tilde{u}\tilde{v}^2 \frac{F}{k} + TF(1 - \tilde{u}) \\
&= \nabla^2_{\tilde{x}} \tilde{u} - \frac{1}{k} \tilde{u}\tilde{v}^2 + \frac{L^2}{D_u} F(1 - \tilde{u}).
\end{aligned}$$

Choosing $T = \frac{L^2}{D_u}$ simplifies the diffusion term. Define the dimensionless feed rate:

$$\tilde{F} = \frac{L^2}{D_u} F.$$

Similarly, for equation (2):

$$\begin{aligned}
\frac{1}{T}\frac{\partial \tilde{v}}{\partial \tilde{t}} &= D_v \cdot \frac{1}{L^2}\nabla^2_{\tilde{x}}\tilde{v} + \tilde{u}\tilde{v}^2\sqrt{\frac{F}{k}} - (F+k)\tilde{v} \\
\Rightarrow \frac{\partial \tilde{v}}{\partial \tilde{t}} &= \frac{D_v T}{L^2}\nabla^2_{\tilde{x}}\tilde{v} + T\tilde{u}\tilde{v}^2\sqrt{\frac{F}{k}} - T(F+k)\tilde{v} \\
&= \frac{D_v}{D_u}\nabla^2_{\tilde{x}}\tilde{v} + \frac{L^2}{D_u}\tilde{u}\tilde{v}^2\sqrt{\frac{F}{k}} - \frac{L^2}{D_u}(F+k)\tilde{v}.
\end{aligned}$$

Define the dimensionless parameters:

$$D = \frac{D_v}{D_u}, \quad \tilde{\kappa} = \frac{L^2}{D_u}(F+k) = k/F.$$

2.4 Final Dimensionless Equations

Dropping the tildes for clarity, we arrive at the dimensionless Gray-Scott system:

$$\frac{\partial u}{\partial t} = \nabla^2 u - \psi_1 u v^2 + (1-u), \tag{3}$$

$$\frac{\partial v}{\partial t} = D\nabla^2 v + \psi_2 u v^2 - (\kappa+1)v. \tag{4}$$

These equations are simpler, highlight the key governing parameters D,ψ_1,ψ_2, F, and k, and are more suitable for numerical simulation and analysis of pattern formation.

3 Mathematical Solution Using Finite Differences

To solve the dimensionless Gray-Scott equations on a square grid, we apply the finite difference method.

3.1 Spatial Discretization

We approximate the Laplacian operator ∇^2 using the standard five-point stencil:

$$\nabla^2 u_{i,j} \approx \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{(\Delta x)^2}$$

The same approximation applies for $v_{i,j}$.

3.2 Time Integration

We use the Forward Euler method to advance the solution in time. Let $u_{i,j}^n$ and $v_{i,j}^n$ denote the values of u and v at grid point (i, j) and time step n. Then:

$$u_{i,j}^{n+1} = u_{i,j}^n + \Delta t \left[D_u \nabla^2 u_{i,j}^n - u_{i,j}^n (v_{i,j}^n)^2 + F(1 - u_{i,j}^n) \right]$$

$$v_{i,j}^{n+1} = v_{i,j}^n + \Delta t \left[D_v \nabla^2 v_{i,j}^n + u_{i,j}^n (v_{i,j}^n)^2 - (F + k) v_{i,j}^n \right]$$

Here, Δt is the time step size and Δx is the spatial step size.

4 Boundary Conditions for the Finite Difference Gray-Scott Model

To solve the Gray-Scott reaction-diffusion equations on a square grid using finite differences, we must define appropriate boundary conditions (BCs). Below, we describe the mathematical formulation and discrete implementation of Dirichlet, Neumann, and Periodic boundary conditions.

4.1 Grid Setup and Notation

- Grid size: $N \times N$
- Grid spacing: $\Delta x = \Delta y = 1$ (for simplicity)
- Concentrations: $u_{i,j}, v_{i,j}$ at grid point (i, j)
- Index range: $i, j \in \{0, 1, \ldots, N - 1\}$

4.2 Dirichlet Boundary Conditions

Mathematical Condition: Fixed concentrations at the boundaries:

$$u(0, y, t) = u_L, \quad u(L, y, t) = u_R, \quad u(x, 0, t) = u_B, \quad u(x, L, t) = u_T$$

$$u_{0,j} = u_{\text{left}}, \quad u_{N-1,j} = u_{\text{right}}, \quad u_{i,0} = u_{\text{top}}, \quad u_{i,N-1} = u_{\text{bottom}}$$

(Similarly for v.)

Discrete Laplacian at Boundaries:
Standard five-point stencil:

$$\nabla^2 u_{i,j} \approx u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}$$

At the left boundary ($i = 0$):

$$\nabla^2 u_{0,j} = u_{1,j} + u_{\text{left}} + u_{0,j+1} + u_{0,j-1} - 4u_{0,j}$$

At the right boundary ($i = N - 1$):

$$\nabla^2 u_{N-1,j} = u_{\text{right}} + u_{N-2,j} + u_{N-1,j+1} + u_{N-1,j-1} - 4u_{N-1,j}$$

Implementation Steps:

- Initialize boundary cells with fixed values.
- Update interior cells using standard Laplacian.
- Reset boundary values after each time step.

4.3 Neumann Boundary Conditions

Mathematical Condition: Zero-flux (no material crosses boundary):

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = 0, \quad \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0$$

Discrete Implementation Using Ghost Cells:

- At $i = 0$: the ghost cell$u_{-1,j} = u_{1,j}$
- At $i = N - 1$: the ghost cell$u_{N,j} = u_{N-2,j}$

Laplacian at the Left Boundary ($i = 0$):

$$\nabla^2 u_{0,j} = 2u_{1,j} + u_{0,j+1} + u_{0,j-1} - 4u_{0,j}$$

Laplacian at the Right Boundary ($i = N - 1$):

$$\nabla^2 u_{N-1,j} = 2u_{N-2,j} + u_{N-1,j+1} + u_{N-1,j-1} - 4u_{N-1,j}$$

Implementation Steps:

- Use ghost cell values for boundary approximation.
- Update interior cells as normal.
- Enforce ghost cell values before or after each time step.

4.4 Periodic Boundary Conditions

Mathematical Condition: Grid wraps around (toroidal topology):

$$u(0, y, t) = u(L, y, t), \quad u(x, 0, t) = u(x, L, t)$$

$$u_{0,j} = u_{N,j}, \quad u_{i,0} = u_{i,N}$$

Laplacian at the Left Boundary ($i = 0$):

$$\nabla^2 u_{0,j} = u_{1,j} + u_{N-1,j} + u_{0,j+1} + u_{0,j-1} - 4u_{0,j}$$

Laplacian at the Right Boundary ($i = N - 1$):

$$\nabla^2 u_{N-1,j} = u_{0,j} + u_{N-2,j} + u_{N-1,j+1} + u_{N-1,j-1} - 4u_{N-1,j}$$