A Finite Element Approach to Reaction-Diffusion Systems

Gavin Engelstad

Fall 2024

Math 494: Partial Differential Equations

Big Idea

I want to solve reaction-diffusion PDEs using the finite element method

Reaction-Diffusion Equations

Model the concentration of compounds over time that are simultaneously reacting with each other and diffusing away from itself

$$\partial_t u = \underbrace{\Gamma \nabla^2 u}_{\text{Diffusion}} + \underbrace{R(u)}_{\text{Reaction}}$$

Where:

u	Vector function of concentrations
Γ	Diagonal matrix of diffusion coefficients
R	Reaction function

Method

The Weak Form

The reaction-diffusion equation for one compound:

$$\partial_t u_n = \gamma_n \nabla^2 u_n + r_n \left(\{u_m\}_{m=1}^N\right)$$

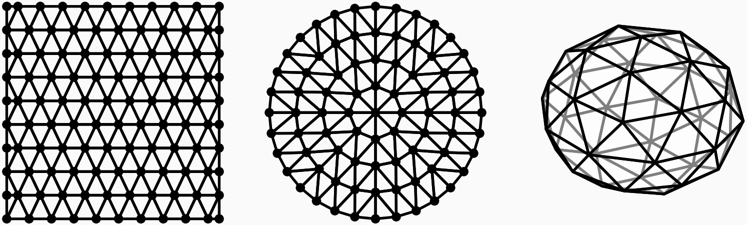
Multiplying by v and integrating gets the weak form:

$$\int_\Omega v \partial_t u_n dA = -\gamma_n \int_\Omega \nabla v \cdot \nabla u_n dA + \int_\Omega v r_n \left(\{u_m\}_{m=1}^N\right) dA$$

I approximate the weak form of the PDE

Triangulation

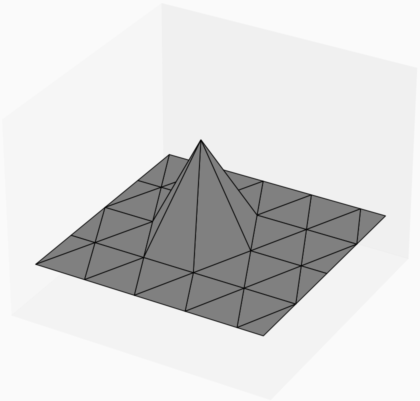
I approximate $\boldsymbol{u}$ at the vertices of a triangulation of Ω



Spacial Discretization (1/2)

Define a function ψ_i at each vertex v_i that's linear on each triangle and

$$\psi_i(v_i) = 1$$
$$\psi_i(v_j) = 0$$



Spacial Discretization (2/2)

Define

$$\hat{u}_n(t,x,y) = \sum_i \psi_i(x,y) u_{n,i}(t) \approx u_n(t,x,y)$$

$$\hat{r}_n(t,x,y) = \sum_i \psi_i(x,y) r_n\left(\{u_{m,i}(t)\}_{m=1}^N\right) \approx r_n\left(\{u_m(t,x,y)\}_{m=1}^N\right)$$

Discretized weak form is

$$\sum_j \partial_t u_{n,j} d_{i,j} = -\gamma_n \sum_j u_{n,j} s_{i,j} + \sum_j r_n\left(\{u_{m,j}\}_{m=1}^N\right) d_{i,j}$$

where

$$d_{i,j} = \int_\Omega \psi_i \psi_j dA \quad \text{and} \quad s_{i,j} = \int_\Omega \nabla\psi_i \cdot \nabla\psi_j dA$$

Temporal Discretization

I combine an explicit (forwards) and implicit (backwards) Euler method

$$\sum_j \frac{u_{n,j}(t+\Delta t) - u_{n,j}(t)}{\Delta t} d_{i,j} = \underbrace{-\gamma_n \sum_j u_{n,j}(t+\Delta t) s_{i,j}}_{\text{Implicit}} + \underbrace{\sum_j r_n \left(\{u_{m,j}(t)\}_{m=1}^{N} \right) d_{i,j}}_{\text{Explicit}}$$

Linear System

Altogether, I solve for $u_n^{t+\Delta t}$ using the linear system

$$(D + \Delta t \gamma_n S) u_n^{t+\Delta t} = D\left(u_n^t + \Delta t r_n\left(\{u_m^t\}_{m=1}^N\right)\right)$$

Where

u_n^t	The vector of u values at the vertices at time t
D	"Damping Matrix" of $d_{i,j}$ values
S	"Stiffness Matrix" of $s_{i,j}$ values

Solutions

The Equation

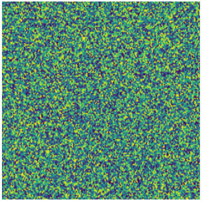
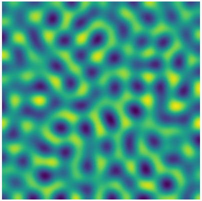
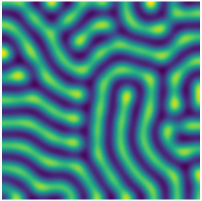
As an example reaction-diffusion equation, I use

$$\frac{\partial u}{\partial t} = \gamma_u \nabla^2 u + k_1 \left(v - \frac{uv}{1 + v^2} \right)$$
$$\frac{\partial v}{\partial t} = \gamma_v \nabla^2 v + k_2 - v - \frac{4uv}{1 + v^2}$$

with $\gamma_u = 1$, $\gamma_v = 0.02$, $k_1 = 9$, $k_2 = 11$

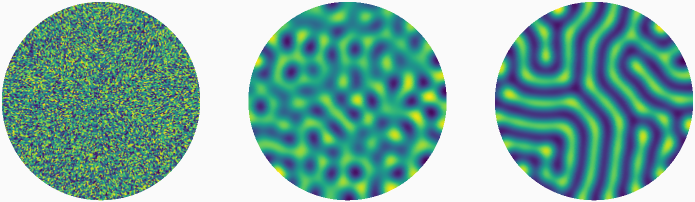
Solution (Square)

$t = 0$ $t = 10$ $t = 100$

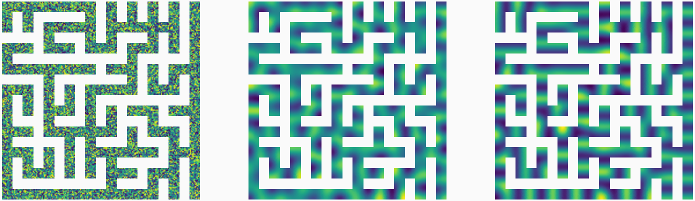
Solution (Circle)

$t = 0$ $t = 10$ $t = 100$



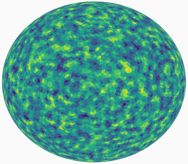
Solution (Maze)

$t = 0$ $t = 10$ $t = 100$

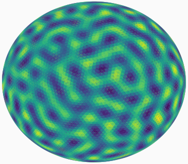


Solution (Sphere)

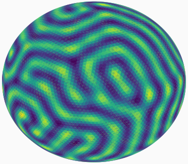
$t = 0$



$t = 10$

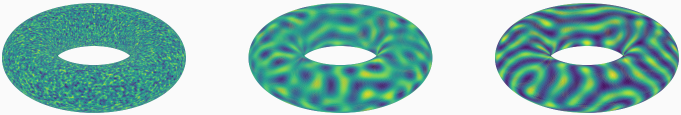


$t = 100$



Solution (Torus)

$t = 0$ $\quad$ $t = 10$ $\quad$ $t = 100$



Conclusion

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I used a finite element approach to numerically solve reaction-diffusion PDEs

Potential next steps:

- More accurate solutions
    - Spectral element method
    - Account for curvature
- More realistic solutions
    - The effects of tissue growth
    - Realistic reaction functions

Questions?