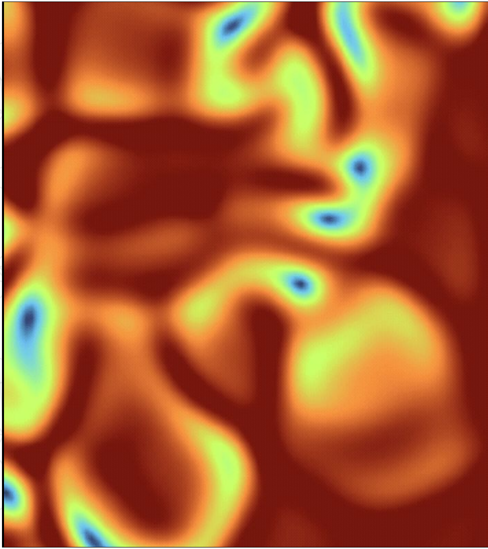
FEM & Pattern Formation Group

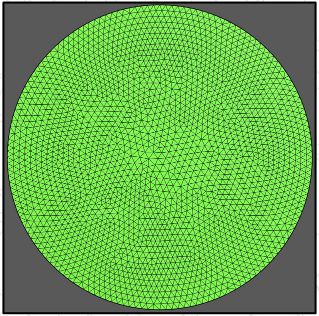
Lead by Alice Quillen, Additional Lectures by Nathan Skerrett

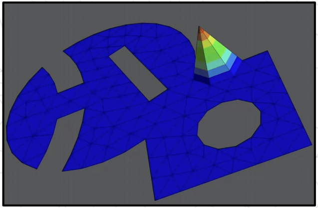
Students: Laura Quiñonez, Abobakar Sediq Miakhel, Benjamin Gutowski, and Edward Caine



The Finite Element Model (FEM)

- PDEs are very hard to solve, and even harder to solve on irregular domains!
- Numerically, we can discretize any domain into a mesh of simpler pieces.
- Next, define a vector space with a basis over the mesh you've created.
- Approximate your solution with this basis!
- A finer mesh means a better approximation.
- Store the solution in in this basis as a vector and evolve it with an operator dependent on the PDE.





Example: The Heat Equation with FEM

- First, we invoke a weak formulation of the PDE by multiplying both sides of it by a "test function" v and then integrating over the domain.
- Next, we rewrite the Laplacian term (integration by parts) and introduce the numerical implicit Eulerian scheme, after choosing a dt and mesh.
- The n index represents timestep number, and the basis on this mesh incorporates our boundary conditions.
- We define the mass matrix M and bilinear form L as linear operators in our finite element space, and are able to compute the next timestep!

$$\partial_t u = \nabla^2 u,\ u_x|_{\partial D=0}$$

$$\int \partial_t uv\, dx + \int \nabla u \nabla v dx = 0 \qquad \forall v$$

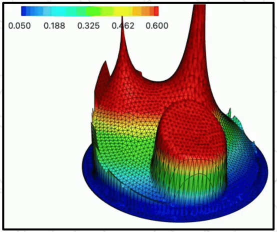
$$\int \frac{(u^{n+1} - u^n)}{dt} v\, dx + \int \nabla u^{n+1} \nabla v dx = 0$$

$$Mu := \int uvdx \text{ and } Lu := \int \nabla u \nabla v dx$$

$$Mu^{n+1} - Mu^n + dtLu^{n+1} = 0$$

$$(M + dtL)(u^{n+1} - u^n) + dtLu^n = 0$$

$$u^{n+1} - u^n = (M + dtL)^{-1}(-dtLu^n)$$



Pattern Formation and the Reaction-Diffusion Equation

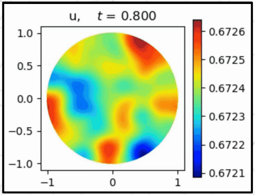
- Chemical concentration populations u and v are reacting on a domain. The D terms represent diffusivity, and the R terms represent interactions.

$$\partial_t u = D_u \nabla^2 u + R_u(u,v)$$
$$\partial_t v = D_v \nabla^2 v + R_v(u,v)$$

- The Brusselator Model assumes a specific set of 2 non-linear reactions R between u and v, including feed terms F and kill terms K for u.

$$\partial_t u = D_u \nabla^2 u + F_u - R_1 u + R_2 u^2 v - K_u u$$
$$\partial_t v = D_v \nabla^2 v + R_1 u - R_2 u^2 v$$

- A pattern is any noticeably distinct behavior of the system, such as waves, dots, or constant value. The system will often converge to them, but a pattern can also be oscillatory or unstable.



- Reaction-diffusion equations are very good at forming patterns! (Turing instability)

Brusselator

The **Brusselator** is a model for a **chemical oscillator** it describes how two chemical species interact and diffuse in space. The concentrations X(t) and Y(t) change continuously over time in a repetitive, wave-like manner, showing periodic increases and decreases.

It describes the interaction between two chemical species usually denoted X and Y, that participate in a hypothetical reaction scheme

$$A \to X$$

$$2X + Y \to 3X$$

$$B + X \to Y + D$$

$$X \to E$$

A and B are constant feed chemicals. D and E are waste products. The step: 2 $X + Y \to$ 3X , 2X+Y→3X makes X replicate itself.

Reaction terms

$$\frac{\partial X}{\partial t} = A - (B+1)X + X^2Y + D_X\nabla^2 X$$

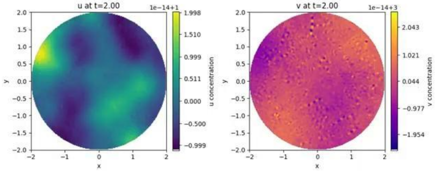
$$\frac{\partial Y}{\partial t} = BX - X^2Y + D_Y\nabla^2 Y$$

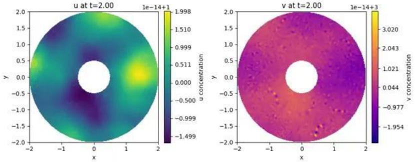
Numerical method

$$\left(I - \frac{\Delta t}{2} D_X \nabla^2\right) X^{n+1} = \left(I + \frac{\Delta t}{2} D_X \nabla^2\right) X^n + \Delta t \cdot R_X\left(X^n, Y^n\right)$$

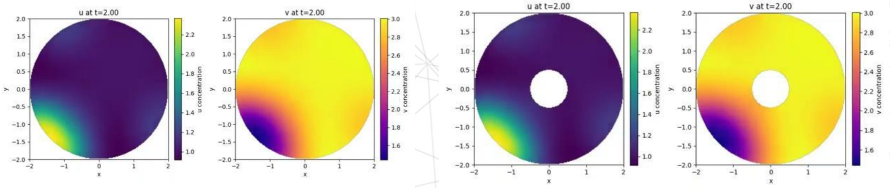
$$\left(I - \frac{\Delta t}{2} D_Y \nabla^2\right) Y^{n+1} = \left(I + \frac{\Delta t}{2} D_Y \nabla^2\right) Y^n + \Delta t \cdot R_Y\left(X^n, Y^n\right)$$

X= 1, Y= 3


u at t=2.00
1e−14+1
u concentration
v at t=2.00
1e−14+3
v concentration
x
y


u at t=2.00
1e−14+1
u concentration
v at t=2.00
1e−14+3
v concentration
x
y

X= 1, Y= B/A + 0.1 * exp(-20 * ((x-1.5)**2 + y**2)), x, y are positions.



Gray Scott Model

$$f_u(u,v) = -uv^2 + \alpha(1-u)$$
$$f_v(u,v) = uv^2 - (\alpha+\beta)v$$

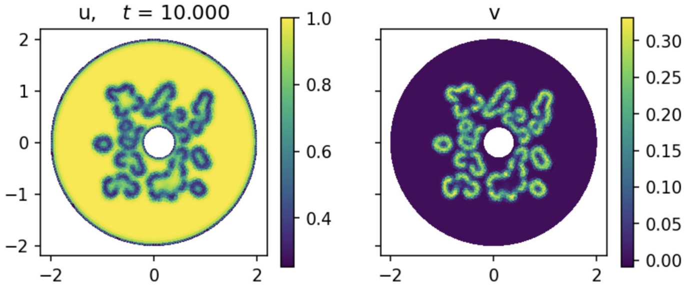
$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + f_u(u,v)$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + f_v(u,v).$$

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

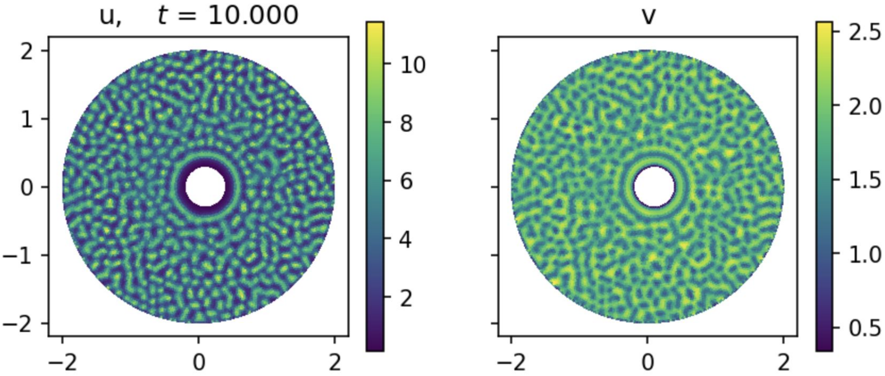
Gray Scott Model

With the following parameters:

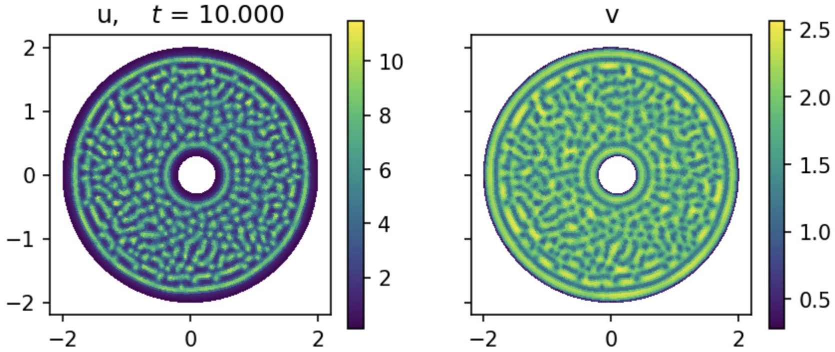
$$D_u = 3.0 * 10^{-5}$$
$$D_v = D_u/2$$
$$\alpha = 0.035;$$
$$\beta = 0.06$$



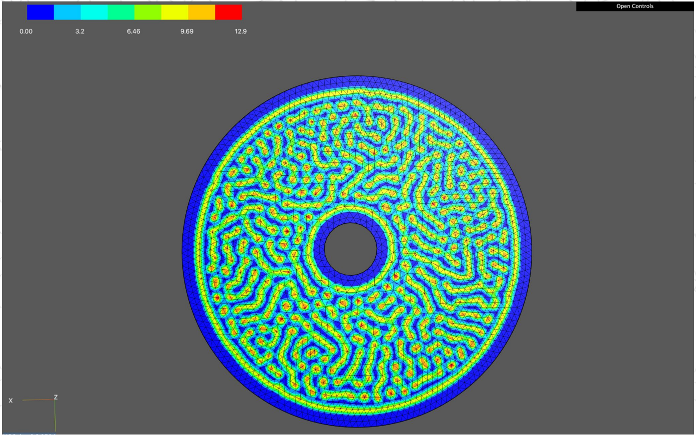
Brusselator: Inner circle with Dirichlet Boundary condition. Order = 1.



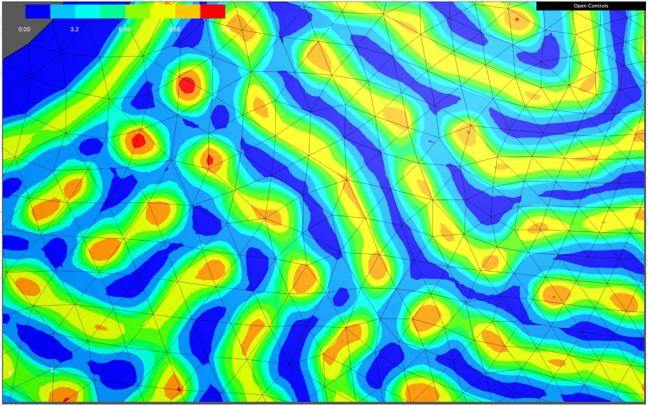
Brusselator: Inner and Outer circles with Dirichlet Boundary Condition. Order = 1.



Brusselator: Inner and Outer circles with Dirichlet Boundary Condition. Order = 2.



Brusselator: Inner and Outer circles with Dirichlet Boundary Condition. Order = 2.



Finite Difference for Wave Chimeras in Reaction Diffusion

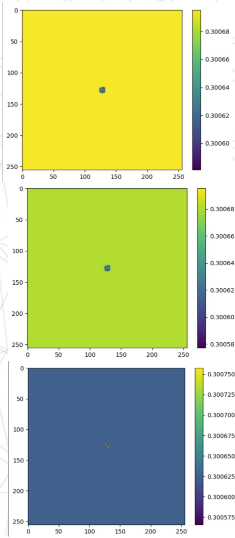
- Oscillator-environment coupled reaction-diffusion (OECRD) model
  - Model random perturbations in center
  - Expected to get get spirals or concentric waves around center
    - Grid spacing too large
    - Laplacian package
    - Initial Conditions
- Finite Difference Method
  - Simpler elements (cartesian grid)
  - These finite differences are substituted for derivatives in the original equation
    - Transforming PDE into a collection of algebraic equations

$$\frac{\partial u}{\partial t} = f(u, v) - K(w - u) \quad (1)$$

$$\frac{\partial v}{\partial t} = g(u, v) \quad (2)$$

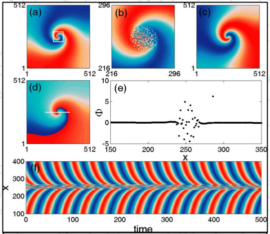
$$\frac{\partial w}{\partial t} = \epsilon(u - w) + \nabla^2 w \quad (3)$$

Li, B.-W., Xiao, J., Li, T.-C., Panfilov, A. V., & Dierckx, H. (2024). Self-organized target wave chimeras in reaction-diffusion media. Physical Review Letters, 133(20). https://doi.org/10.1103/PhysRevLett.133.207203

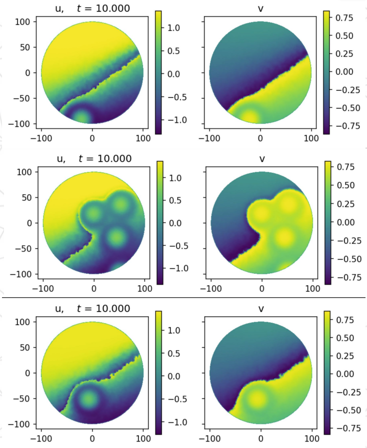


Finite Element for Wave Chimeras In reaction Diffusion

- Bubbles come from initial conditions
  - Random, gaussian bumps
  - Local Oscillator out of phase with surroundings
- Sharp line indicates discontinuity
  - Phase discontinuity



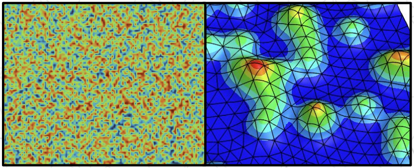
Li, Bing-Wei & Dierckx, Hans. (2015). Spiral wave chimeras in locally coupled oscillator systems. Physical Review E. 93. 10.1103/PhysRevE.93.020202.

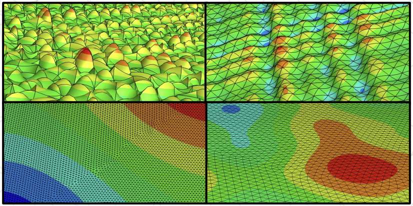


Initial Conditions and the Complex Ginzburg-Landau Eq.

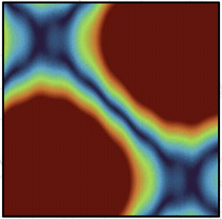
$$\partial_t u = (1 + i\alpha)\nabla^2 u + u - (1 + i\beta)u|u|^2$$

- Existing research often does not describe what initial conditions are needed to obtain particular patterns.
- Common initial conditions (IC) vary between fine noise and ones seeding
- Studying how changing these IC affects pattern formation can allow targeted choice of IC to produce specific patterns
- In the α=1, $\beta \in$[-5,5] regime, I investigated how varying IC noise grain affected pattern formation.



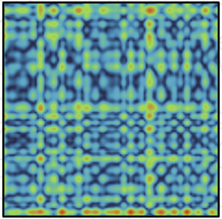


Pattern Formation in the Complex Ginzburg-Landau Eq.

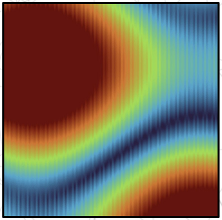


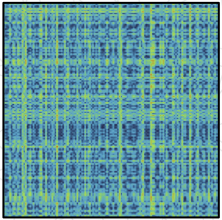
⬅ "Worms With Defects"

➡ "Defects"

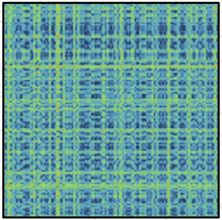


➡ "Defects"



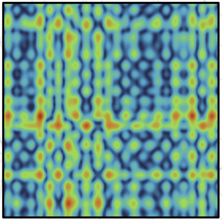


⬅ "Cells With Defects"



⬅ "Shiny Cells"

➡ "Dancing Worms"



Pattern Formation in the Complex Ginzburg-Landau Eq.

- IC noise was formed by adding 20 sin terms with wavelengths sampled from the uniform range $[\lambda_{min}, \lambda_{max}]$, with random phase offsets.
- The noise grain was characterized by λ_{min}. Neumann BC and a square 100x100 grid were used, with dx=0.5 and dt=0.04.
- I observed patterns being largely independent of noise grain in the $-5 \lesssim \beta \lesssim -0.5$ and $\beta=5$ regimes, but strong dependence in the $0.5 \lesssim \beta \lesssim 4$ regime.

$$\partial_t u = (1+i\alpha)\nabla^2 u + u - (1+i\beta)u|u|^2$$