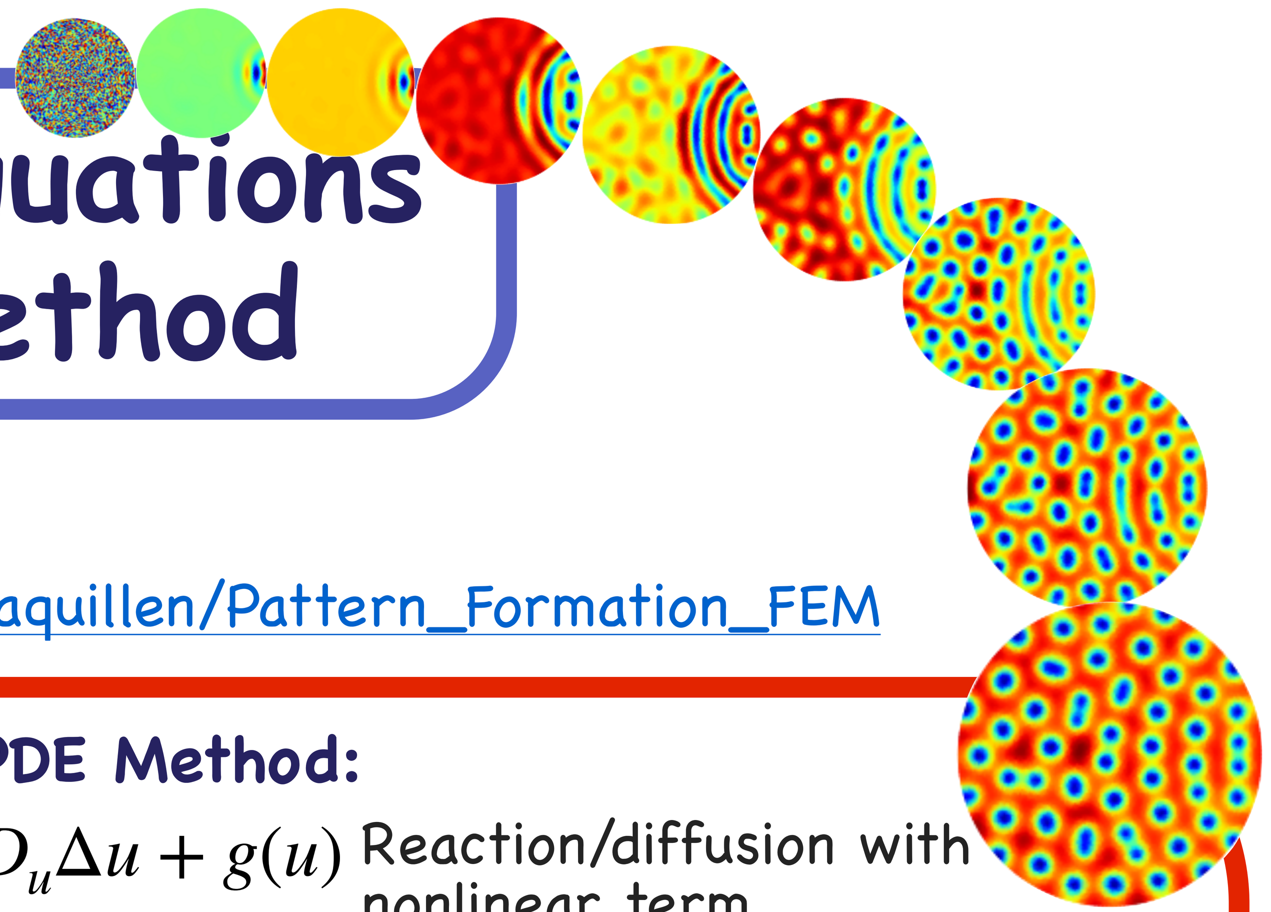
Solving Pattern Formation Partial Differential Equations on Triangular Meshes with a Finite Element Method



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code: https://github.com/aquillen/Pattern_Formation_FEM

Motivation:

Biological/Chemical/Active matter continuum systems are necessarily confined. Pattern formation models are often solved on square Cartesian grids with periodic boundary conditions. Finite element methods make it possible to study these systems on different shaped domains with different types of boundary conditions.

Abstract:

We solve pattern formation partial differential equations with a finite element method on 2D triangular meshes, in different shaped domains and with a variety of boundary conditions. We solve reaction-diffusion Brusselator and Gray-Scott systems, the complex Landau-Ginzburg model and the 4-th order Swift-Hohenberg model. The Brusselator model is more sensitive to the boundary than the Gray-Scott model, with crystallization or linear features likely to be present on the boundary after equilibrium is reached.

Implementation:

We built on https://github.com/kinnala/scikit-fem
Tom Gustafsson and GD McBain's Finite element code
In python and with minimal dependancies
Spirit of FEniCS but actually works
Galerkin method: turn the weak formulation into a discrete method using a finite set of orthogonal basis functions. The approximate solution is a linear combination of the basis functions which are defined on "elements". The problem is approximated by a linear algebra problem, with sparse matrices (sparse because interactions are local)

PDE Method:

$\partial_t u = D_u \Delta u + g(u)$ Reaction/diffusion with nonlinear term

$$\int_\Omega \partial_t u \; w \, dx = \int_\Omega D_u (\Delta u) \; w \, dx + \int_\Omega g(u) \; w \, dx$$ Weak form of PDE

Integrate by parts — w is a test function

$$\int_\Omega \partial_t u \; w \, dx = - D_u \int_\Omega \nabla u \nabla w \, dx + D_u \int_{\partial\Omega} \nabla u \; w \, ds + \int_\Omega g(u) \; w \, dx$$

linear operator — boundary term

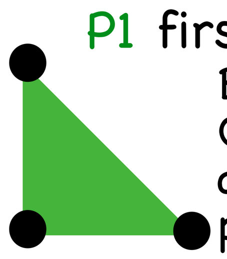
$$u^{n+1} = \left(1 - \frac{\Delta t}{2} D_u L\right)^{-1} \left(1 + \frac{\Delta t}{2} D_u L\right) u^n + \Delta t \; g(u^n)$$

Crank-Nicholson method for linear operators

Nonlinear part Added in by hand (Operator split)

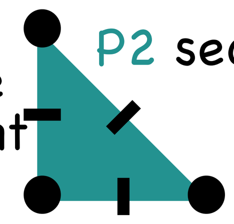
The elements:

Lagrange finite element
PDE contains Δ
Test functions in H^1



P1 first order polynomials
Basis elements {1, x, y}
Gradients can be described with polynomials in this basis

Morley element
PDE contains Δ^2 then we need a quadratic element
Test functions $\in H^2$, $\int_\Omega \sqrt{|\nabla^2 w|^2} dx$ finite



P2 second order polynomials
Basis elements {1,x,y,x^2,y^2,xy}
Normal derivatives at edge midpoints, giving continuity for derivatives across cells

Reaction diffusion equations

$$\partial_t u = D_u \Delta u + R_u(u,v)$$
$$\partial_t v = D_v \Delta v + R_v(u,v)$$

Boundary Conditions Natural Neumann $\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$

Brusselator model

$R_u = \alpha - (\beta+1)u + u^2 v$

$R_v = \beta u - u^2 v$

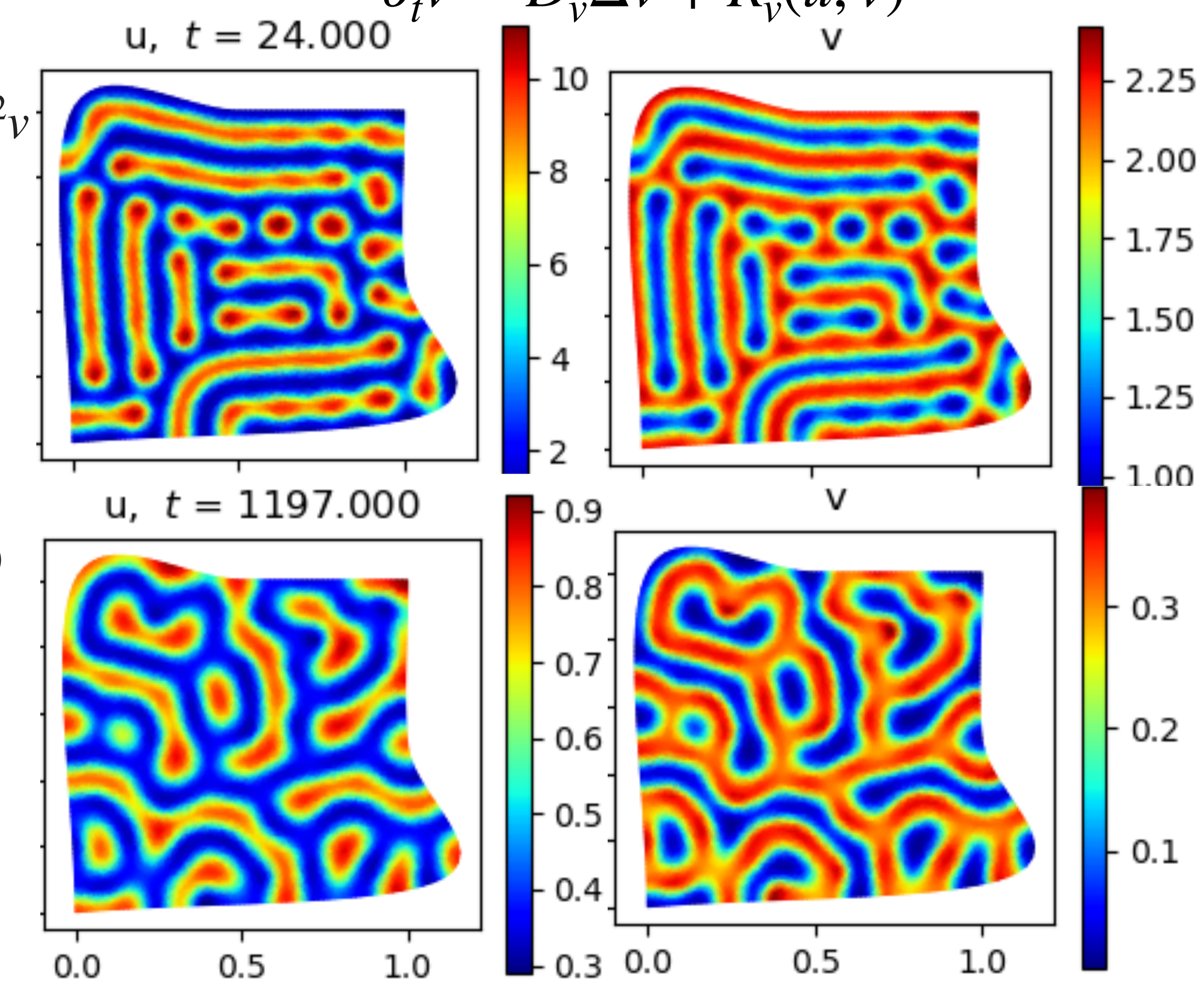
α=5, β=9, $D_u = 10^{-3}, D_v = 11 D_u$

Gray-Scott model

$R_u = -uv^2 + \alpha(1-u)$

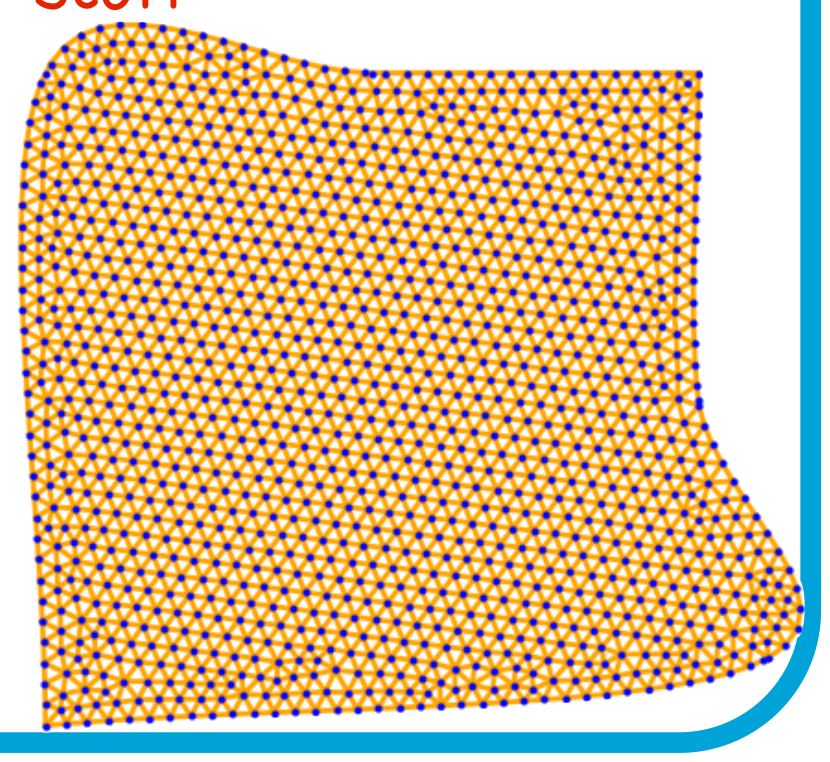
$R_v = uv^2 - (\alpha+\beta)v$

α=0.05, β=0.063, $D_u = 3 \times 10^{-5}, D_v = D_u/2$



Initial conditions:
In most cases noise

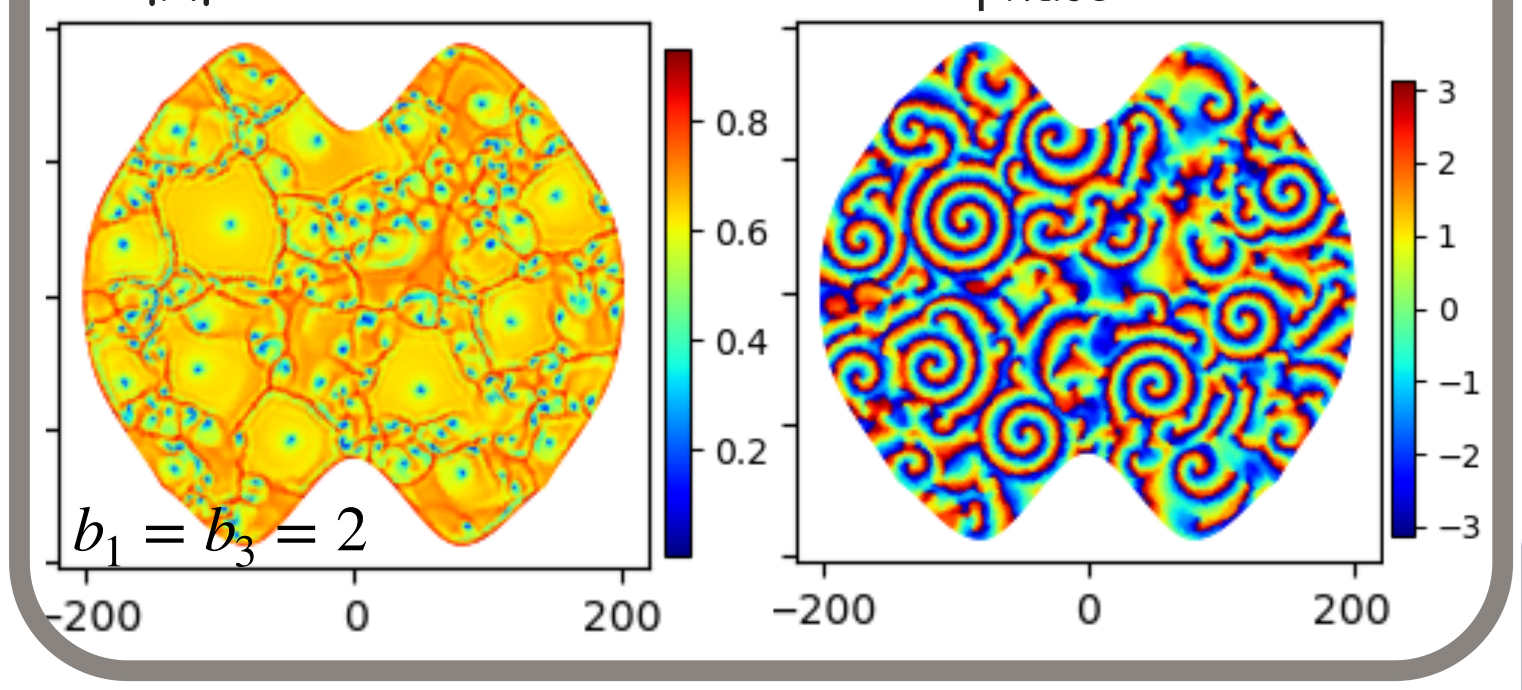
Brusselator is more sensitive to the boundary than Gray-Scott



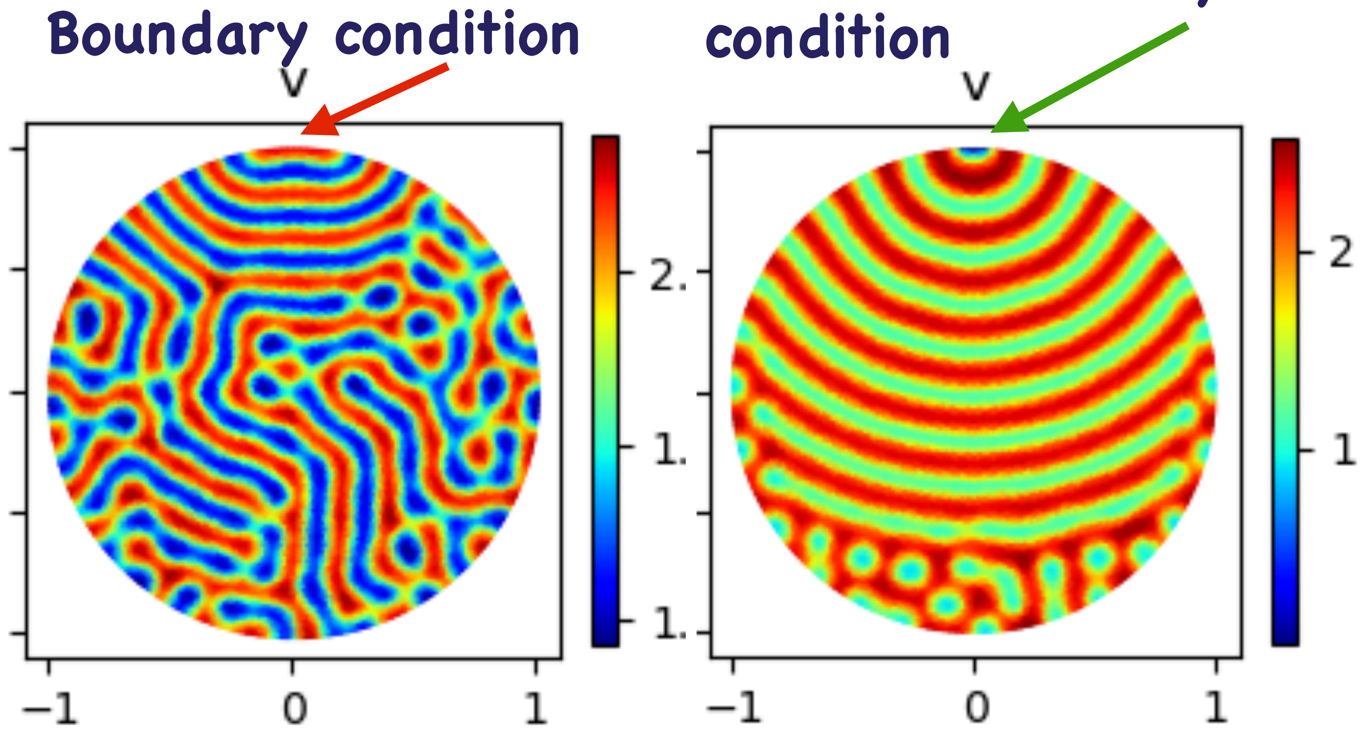
Complex Landau-Ginzburg

Natural BC

$$\partial_t A = A + (1 + ib_1)\Delta A - (b_3 - i)|A|^2 A$$



non-zero Neumann Boundary condition — Dirichlet Boundary condition



Brusselator is quite sensitive to boundary!

Discussion

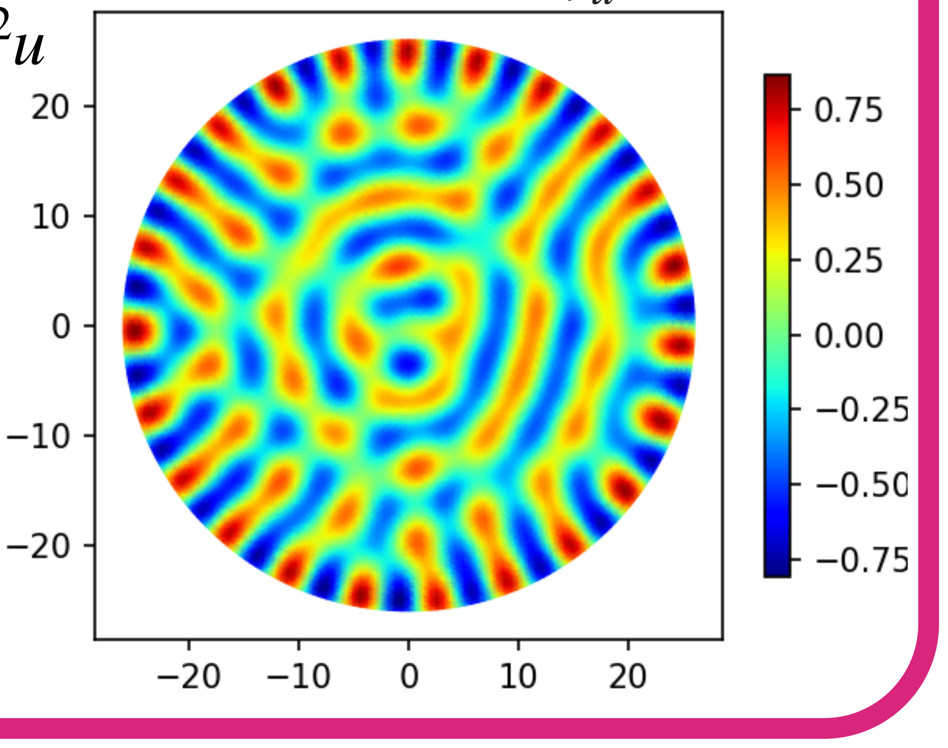
We find that we can simulate growth of patterns in 2D domains with a variety of shapes. Patterns are least affected by natural (zero Neumann) boundary conditions. We adjusted domain and element size so that the most unstable wavelength fits within the domain. We find that there is a characteristic distance over which the boundary affects the patterns which form. Boundaries can be used to control some of the behavior of pattern formation models.

Swift-Hohenberg model

$r = 0.2, \gamma_u = 0$

$$\partial_t u = ru - (1+\Delta)^2 u + \gamma_u u^2 - u^3$$

Biharmonic so we use a quadratic element.
Both first and second derivatives are zero on the boundary



References:
Seeing phenomena similar to ours: Krause, A.L et al., 2021, Isolating Patterns in Open Reaction-Diffusion Systems, Bulletin of Mathematical Biology, 2021, 83, 82

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