Spatio-Temporal Pattern Formation in the Gray-Scott Model

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Reaction-Diffusion Systems

Reaction-diffusion systems are mathematical models that explain how the concentration of one or more substances change under the influence of:

- Local reactions between chemical species, and
- Diffusion of reactants over space.

Simple reaction-diffusion systems are known to display an amazing diversity of spatiotemporal patterns.

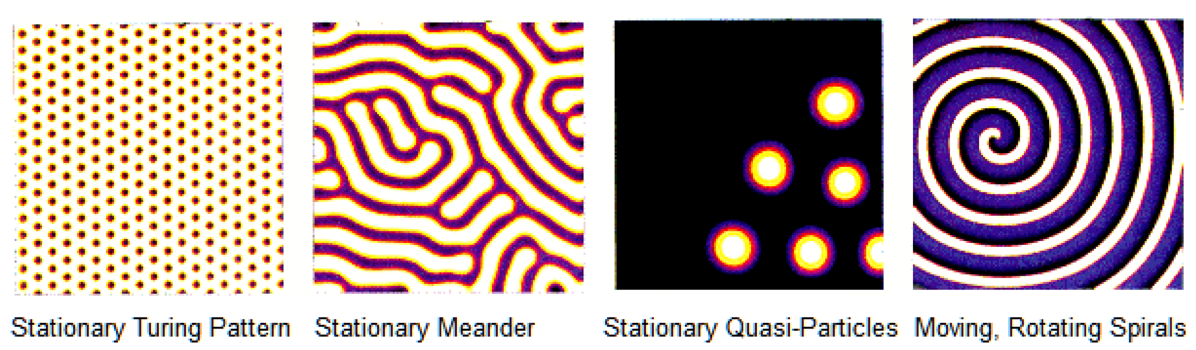

Figure 1: Example Turing patterns (adapted from [1]).

The Gray-Scott Model

The Gray-Scott model describes an autocatalytic reacting system involving chemical reactants U and V [2][3]. The governing equations are:

$$\frac{\partial U}{\partial t} = \underbrace{D_U \nabla^2 U}_{Diffusion} - \underbrace{UV^2 + F(1-U)}_{Reaction} \qquad (1)$$

$$\frac{\partial V}{\partial t} = \underbrace{D_V \nabla^2 V}_{Diffusion} + \underbrace{UV^2 - (F+k)V}_{Reaction} \qquad (2)$$

where U and V are concentrations, D_U and D_V are diffusion coefficients, and F and k are order parameters.

Simulation Method

- Grid: 256×256 (2D) / $128 \times 128 \times 128$ (3D).
- Integrator: explicit forward Euler's method.
- Laplacian solver: 5-point (2D) / 7-point (3D). [4]
- Boundaries: periodic boundary conditions.
- Initialization: $(U, V) = (0.5, 0.25) \pm 1\%$ in the 20×20 mesh point area located symmetrically about the center of the grid, $(1, 0)$ everywhere else.

Simulation Results

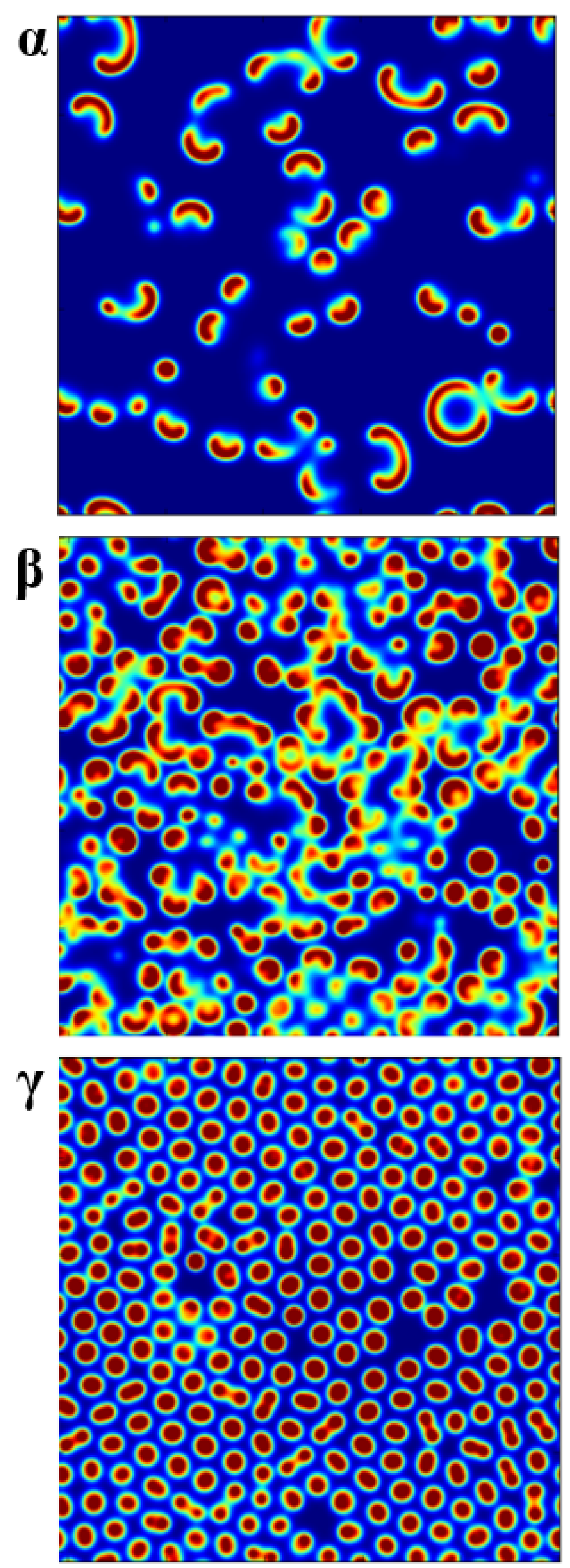

Figure 2: Simulation results of steady-state oscillating patterns from the Gray-Scott model after 200,000 steps. High values of V are shown in red. Order parameters (k, F) for patterns α, β, and γ are $(0.043, 0.006)$, $(0.050, 0.016)$, and $(0.056, 0.020)$, respectively.

Research Goals

1. Characterize the spatio-temporal behaviour of patterns emerging from the Gray-Scott model.
2. Extend the Gray-Scott model into three dimensions.

Time-Domain Fourier Analysis

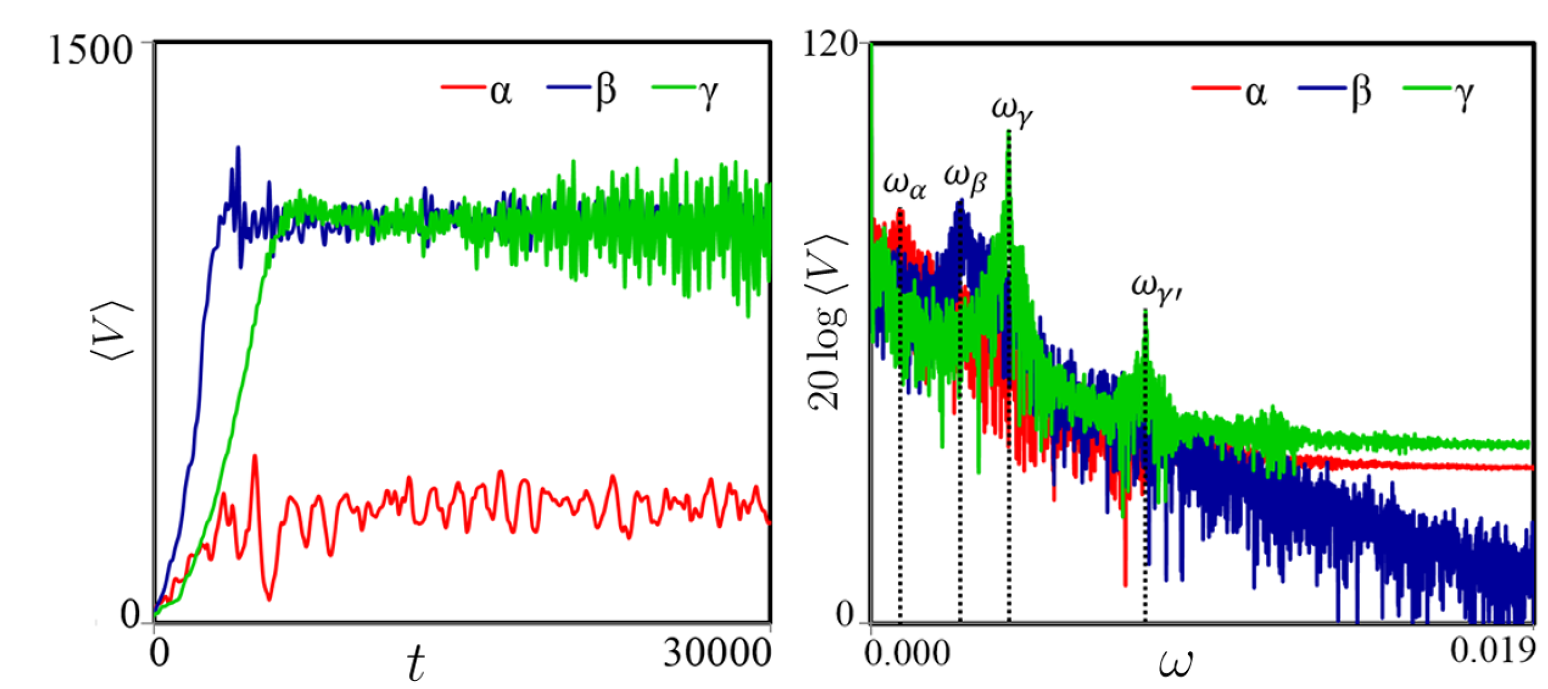

Figure 3: Left: Time evolution of the spatial average concentration of V (denoted as $\langle V \rangle$). Right: Power spectrum of $\langle V \rangle$. ω_α, ω_β, ω_γ are resonant frequencies for patterns α, β, and γ, respectively. $\omega_{\gamma'}$ denotes a second order resonance mode.

Phase Diagrams

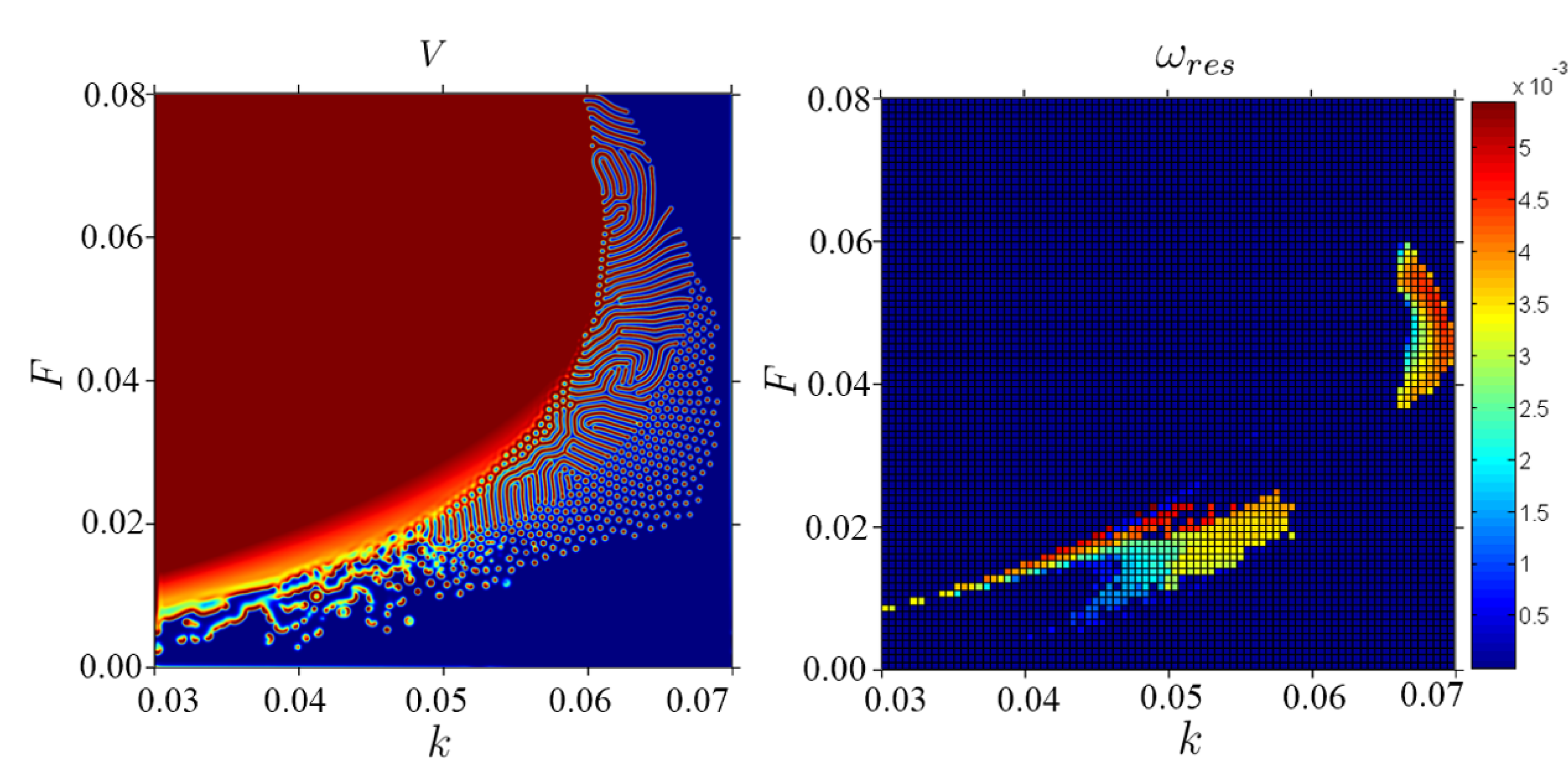

Figure 4: Left: Phase diagram of the Gray-Scott model, illustrating the variety of final patterns produced by the system. Right: Fundamental resonant frequencies of patterns as a function of (k, F)-coordinates. Each point corresponds to a separate simulation from a set of 6,400 simulations (one simulation for each element on an 80×80 (k, F) grid).

Three-Dimensionalization

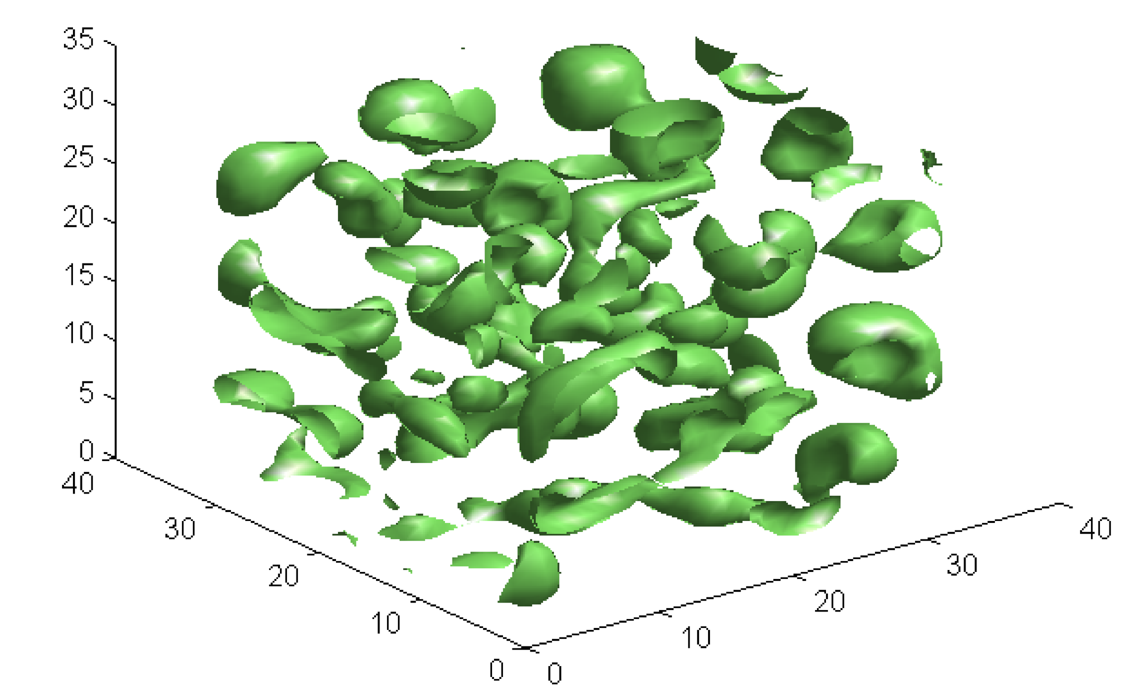

Figure 5: Example simulation result from the 3D Gray-Scott model. Here, $(k, F) = (0.056, 0.02)$. The isosurface plot shows $V = 0.23$.

Conclusions and Outlook

Fourier analysis was used to extract characteristic time scales of patterns arising from the Gray-Scott model. This technique can be extended to find characteristic length scales. The 3D Gray-Scott model can also be characterized in a similar way. The next steps in this project are to:

- Extend spatio-temporal characterization to the 3D Gray-Scott model; and
- Couple elastic equations into the model.

References

[1] [URL: http://www.uni-muenster.de/Physik.AP/Purwins/RD/index-en.html], Accessed May 19, 2013.

[2] Gray P, Scott S.K, Chemical Engineering Science **39**(6):1087-97 (1984)

[3] Pearson J.E., Science **261**, 189-192 (1993).

[4] Patra M, Karttunen M, Numerical Methods for Partial Differential Equations, **2**(4), 936-953 (2005)

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