

Finite Element Method Applied to Gray-Scott Reaction-Diffusion Problem. Using FEniCs Software

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Abstract
The Gray-Scott problem is among the reaction –diffusion systems showing patterns that stand out by showing self-replicating patterns (spots). This pattern formulation is a suitable interplay between diffusion and reaction. Here we show in details the spot multiplication process of the Gray-Scott reaction-diffusion problem using finite element method, where the finite element mesh is generated using an external and a free three dimensional finite element mesh generator called Gmsh. And Numerical experiment is performed using a free software package called FEniCs.
Keywords: Finite Element Methods, Gray-Scott, self-replication, FEniCs, Gmsh

1. Introduction

The Gray-Scott model was originally introduced in Gray and Scott [1985] as an isothermal system with chemical feedback in a continuously fed, well-stirred tank reactor, where the last property implied the lack of diffusion. The complex interplay between activator and inhibitor or substrate chemical , aided by the reaction and diffusion components create most starling spatio-temporal patterns, such as spots, stripes, traveling waves, spot replication, and spatio-temporal chaos, in a nut-shell, a clear example of Turing patterns. The Turing patterns are characterized by the active role that diffusion plays in destabilizing the homogenous steady state of the system. Interesting enough, the replication characteristics are a particularity of the diffusive Gray-Scott model alone, which makes it the ideal model for the unfolding development of a proto-organism. The Turing patterns from the work of Pearson[1993] on the diffusive Gray-Scott model were confirmed experimentally by Lee et al.[1993], including the spot replication[Lee et al.1994]. Theoretically, extensive work exists in the literature on the dynamics of this model concerning the spot replication in one, two and three dimensional [Muratov and Osipov 2000]. In this part of this paper effort is made to solve the Gray-Scott reaction-diffusion using finite element method by using FEniCs software.

2. Model Formulation

The model was originally introduced in the Gray and Scott[1985] as an isothermal system with chemical feedback in a continuously fed, well-stirred tank reactor, where the last property implied the lack of diffusion. The analysis of the system revealed stationary states, sustained oscillations and even chaotic behavior. The Gray-Scott model involves two generic chemical species $U(x,t)$ and $V(x,t)$ at a given point in space which governs the following irreversible chemical reaction

$$\begin{aligned} &U + 2V \to U + 3V \\ &V \to Q \end{aligned} \tag{1}$$

The model considers the chemical reactions describing the autocatalytic growth of an activator $V(x,t)$ on the continuously fed substrate, $U(x,t)$ and the decay of the former in the inert product $P(x,t)$, subsequently removed from the system. A major development was performed by Pearson[1993] who introduced the role of space by relaxing the constraint of a well-stirred tank and studied the system in two dimensions, in the limit of small diffusion. Suppose u and v represents the concentration of the chemical species $U(x,t)$ and $V(x,t)$ respectively. Then the coupled reaction diffusion equations governing the Gray-Scott model are:

$$\begin{aligned} u_t &= D_1 \Delta u - uv^2 + \gamma(1-u) \\ v_t &= D_2 \Delta v + uv^2 - (\gamma+\kappa)v \end{aligned} \tag{2}$$

Where the parameters D_1 and D_2 are their diffusion rates of u and v respectively, κ represents the rate of conversion of V to Q (decay constant of the activator V), γ represents the rate of the process that feeds U and drain U, V and Q.

At the boundaries a homogeneous Neumann condition is imposed for both u and v. That is

$$\frac{\partial u}{\partial n}=0,\frac{\partial v}{\partial n}=0 \quad (3)$$

The initial values are

$$u(x,y,0)=1-2v(x,y,0)$$

$$v(x,y,0)=\begin{cases} v(x,y,0)=\frac{1}{4}\sin^2(4\pi x)\sin^2(4\pi y), if\, 1\le x,y\le 1.5 \\ 0, elsewhere \end{cases} \quad (4)$$

Important Given Parameters

Domain: $\Omega=(0,2)\times(0,2)$

Time Step-size: $\Delta t=0.5$

$D_1=8.0\times10^{-0.05}, D_2=4.0\times10^{-0.05}$

$\gamma=0.024$

$\kappa=0.06$

3. Variational Formulation/Weak formulation

Let us write the weak/variation formulation (2) - (4). The unknowns are u and v. The weak (or the variational) form of the problem reads: find $(u,v)\in V\times V$ satisfying the initial and the natural boundary conditions such that,

$$\begin{aligned} \int_\Omega qu_t dx &= -\int_\Omega D_1\nabla q.\nabla u dx-\int_\Omega quv^2 dx+\int_\Omega \gamma q(1-u)dx \\ \int_\Omega wv_t dx &= -\int_\Omega D_2\nabla w.\nabla v dx+\int_\Omega wuv^2 dx-\int_\Omega (\gamma+\kappa)wv dx \end{aligned} \quad (6)$$

Holds for all admissible test functions $(q,w)\in V\times V$.

4. Time Discretization

The time derivative must be dealt before able to solve this problem. Sampling the semi-discrete equation at some reference time, say k , and applying the Backward Euler method for the coupled semi-discrete weak form of the equations () and ():

$$\begin{aligned} \int_\Omega \frac{u^k-u^{k-1}}{\Delta t}q dx &= -\int_\Omega D_1\nabla q.\nabla u^k dx-\int_\Omega qu^k(v^k)^2 dx+\int_\Omega \gamma q(1-u^k)dx \\ \int_\Omega \frac{v^k-v^{k-1}}{\Delta t}w dx &= -\int_\Omega D_2\nabla w.\nabla v^k dx+\int_\Omega wu^k(v^k)^2 dx-\int_\Omega (\gamma+\kappa)wv^k dx \end{aligned} \quad (7)$$

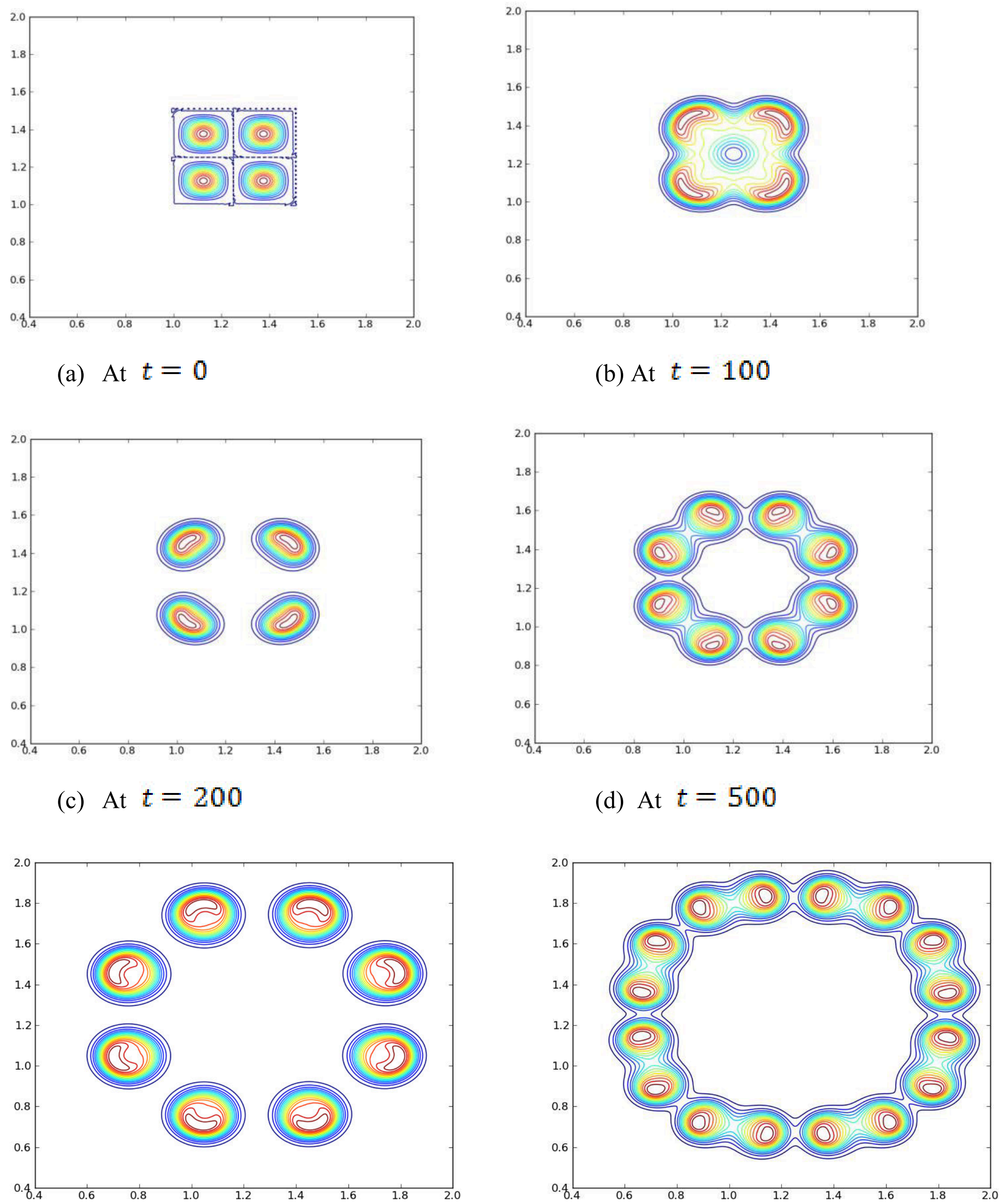
Where $\Delta t=t_{n+1}-t_n$.

5. Numerical Simulation

For the numerically study of the partial differential equations we used a system of size $R\times R$, with $R=0.5$ discretized through $x\to(x_0,x_1,x_2,...,x_N)$ and $y\to(y_0,y_1,y_2,...,y_N)$, with $N=n_x=n_y=64$.

The task is now: given u^{k-1} and v^{k-1} solve the equations to find u^k and v^k. The implementation for this problem is included in the appendix part. The figure () shows the time evolution of the v component by contour lines in the $(x,y)-$plane at various times; for clarity the solutions are only displayed for $0.5\le x,y\le 2$.

With the parameters and initial values given above the solution of the Gray-Scott model gives repeated replication of the initial spots.



(a) At $t = 0$

(b) At $t = 100$

(c) At $t = 200$

(d) At $t = 500$

(e) At $t = 1000$

(f) At $t = 1500$

Figure 1: Illustrative the spot-multiplication process. The complex interplay between activator and inhibitor or substrate chemical, aided by the reaction and diffusion components creates spot-replication.

6. Conclusion

The Gray-Scott problem is among the reaction –diffusion systems showing patterns that stand out by showing self-replicating patterns (spots). This pattern formulation is a suitable interplay between diffusion and reaction. The complex interplay between activator and inhibitor or substrate chemical aided by the reaction and diffusion components creates spot-replication. The replication characteristic is a particularity of the diffusive Gray-Scott model alone, which makes it the ideal model for the unfolding development of a proto-organism. In this case, cell-like localized structures grow, deform and make replica of themselves until they occupy the entire space.

Reference

1. Anders Logg, Kent-Andre Mardal, and Garth N. Wells, Automated Scientific H.P. Langtangen, A FEniCs Tutorial,Aug. 19,2010.

2. Anders Logg, Automating the Finite Element Method, Toyota Technological Institute at Chicago.
3. Anders Logg, Automating the Finite Element Method, 22 March 2006 / Accepted: 13 March 2007 Published online: 15 May 2007 © CIMNE, Barcelona, Spain 200.
4. A. Logg and G. N. Wells, Automated Finite Element Computing, accepted for publication in ACM Transactions on Mathematical Software, 2009.
5. Christophe Geuzaine and Jean-François Remacle, A three-dimensional finite element mesh generator with built-in pre- and post-processing facilities, Version 2.5.0, Oct 15 2010.
6. Doelman, T.Kaper, and P.A.Zegaling, Pattern formation in the one dimensional Gray-Scott model, Nonlinearity 10, 523-563.
7. Gmsh GUI Tutorial I, How to create a simple 2D model (from on-line source).
8. J.E.Pearson, Complex patterns in a simple system, Science 261, page 189-92
9. J.Reynolds, J.Pearson and S.Ponce-Dawson, Dynamics of Self-replicating spots in the reaction-diffusion system, phy.Rev.E 56(1)1997, 185-198.
10. K. B. Oelgaard, A. Logg and G. N. Wells SIAM J. Sci., Automated Code Generation for Discontinuous Galerkin Methods vol. 31, pp. 849-864, 2008.
11. P.Gray and S.K.Scott, Auto-catalytic reaction in the isothermal, continuous stirred tank reactor: Oscillation and instabilities in the system A+2B $\rightarrow$ 3B, B $\rightarrow$ C, Chem.Eng.Sci.39 (1984), 1087-1097.
12. T. Dupont J.Hoffman, C.Johnson, R. Kirby, M. Larson, A.Logg, and R. Scott. Chalmers, Finite Element Center, Chalmers University of Technology, SE–412 96 Goteborg, Sweden.
13. W.Hundsdorfer,J.G.Verwer,Numerical solution of Time-dependent Advection-Diffusion-Reaction Equations,Page(21 - 22).