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Simulation of pattern formation in a Volume-Filling Chemotaxis Model using Mimetic Differences

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Abstract

In this paper, the Chemotaxis driven pattern for a reaction-diffusion-chemotaxis with volume-filling effect is modeled in two dimensions using mimetic differences with operators from the MOLE library [**?**]. The coupled diffusion-chemotaxis system is discretized using Gradient, Divergence, and Laplace operators. Appropriate interpolation was applied to move cells to its appropriate place and apply the operators, then semi-implicit scheme is applied to the stiff diffusion term. Afterwards, addscalarBC2D is used to enforce the system with periodic boundary condition obtaining a pattern formation for both cells diffusion (U) and their chemical concentration (V) that align with the equations behavior.

Introduction

Chemotaxis is the movement of biological cells in response to chemical signals which is a mechanism that drives many processes, including bacterial movement towards nutrients, embryonic development, immune cell response, and tumor invasion. Similar to Turing pattern mechanism, mathematical models of chemotaxis provide an understanding of how local interactions between cells and chemical fields give rise to large-scale spatial patterns.

One of the most widely studied model is Keller-Segel, in which a cell density evolves under the combined effects of diffusion and directed movement along gradients of a chemoattractant [1]. This model however, produces numerical difficulty of finite-time blow-up, which is not a physical behavior

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where cell density becomes unbounded. To address this limitation, volume-filling models have been introduced, incorporating density-dependent diffusion and chemotactic sensitivity to account for crowding effects and finite cell size [2].

In this work, we use the two-dimensional diffusion-chemotaxis system with nonlinear (volume-filling) diffusion, density-dependent chemotactic sensitivity, and logistic growth which is obtained from [3]. The chemoattractant is produced by the cells and evolves according to a diffusion-reaction equation, creating a feedback loop in which cells both shape and respond to their chemical environment.

Mimetic differences are numerical methods used to discretize the differential operators associated to space in partial differential equations while preserving key structural properties of the continuous equations such as compatibility between gradient and divergence. This is important for chemotaxis models as it helps prevent nonphysical artifacts and numerical inconsistencies and generate pure model related pattern formation.

The system is discretized using mimetic difference operators from the MOLE library [6, 4]. Time integration is performed using a semi-implicit scheme for the cell density and an explicit scheme for the chemoattractant to account for numerical stability and computational efficiency for the chosen spatial size. Periodic boundary conditions are imposed to eliminate artificial boundary effects and to approximate a subdomain of a larger homogeneous system. This allows pattern formation to arise solely from the intrinsic dynamics of diffusion, chemotaxis, and reaction, without effects of boundary constraints.

Model

The following model is obtained from Ma and Gao [3]

$$\begin{cases} u_t = \nabla \cdot (D(1-u)^{-\alpha}\nabla u - \chi u(1-u)^{\beta}\nabla v) + \mu u(1-\frac{u}{u_c}), x, y \in \Omega \\ v_t = \Delta v - v + u, x, y \in \Omega \\ u(x,y) = v(x,y) = u_0(x,y), x, y \in \Omega, \end{cases} \tag{1}$$

where specific parameters were chosen to be applied:

$$D_0 = 0.18,\ \mu = 0.89,\ u_c = 0.2,\ \alpha = 1.0,\ \beta = 0.1,\ \chi = 10.2768, \tag{2}$$

and initial conditions :

$$u_0 = v_0 = u_c + 10^{-7} \tag{3}$$

The spatial domain and temporal domains are chosen as :

$$x, y \in \Omega, \Omega = [0, 3\pi] \times [0, 3\pi], t \in [0, 100] \tag{4}$$

and $u(x, y, t), v(x, y, t)$ satisfy periodic boundary conditions on $\partial\Omega$ as described in figure [1].

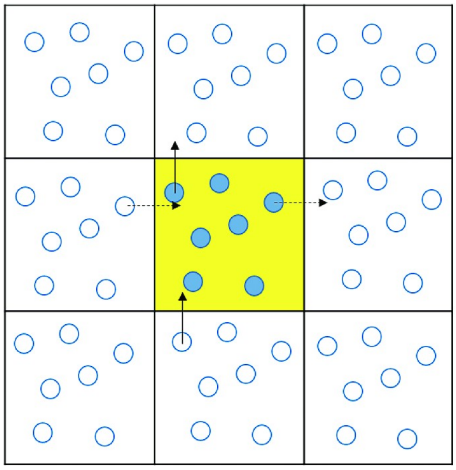

Figure 1: Two-dimensional representation of periodic boundary conditions (Reproduced from Katiyar and Jha (2018) [5]).

Mimetic Difference Discretization with Newton's time step:

Diffusion term $= A(U^n) = D_0(1-U^n)^{-\alpha}$
Chemical term $= B(U^n) = \chi U^n(1-U^n)^{\beta}$
Reaction term $= C(U^n) = \mu U^n(1-\frac{U^n}{u_c})$

$$\frac{U^{n+1}-U^n}{dt} = Div(A(U^n)Grad * U^{n+1} - B(U^n)Grad * V) + C(U^n)$$

$$(I - Div(A(U^n)Grad)U^{n+1} = U^n - dt * [B(U^n)Grad * V - C(U^n)]$$

Then the system can be solved as $LU^{n+1} = b$

$$U^{n+1} = L \backslash b$$

$$\frac{V^{n+1}-V^n}{dt} = Lap(V^n) - V^n + U^{n+1}$$
$$V^{n+1} = V + dt * (Lap(V^n) - V^n + U^{n+1})$$

Similarly, $V^{n+1} = L \backslash b$ where $L = I$, the identity matrix.

Results

Figure 2 illustrates the pattern formation with volume-filling effect with the applied mimetic operators using the MOLE library. Diffusion of cells (U) contains sharp peaks and cluster tightly, whereas the chemotaxis (V) which

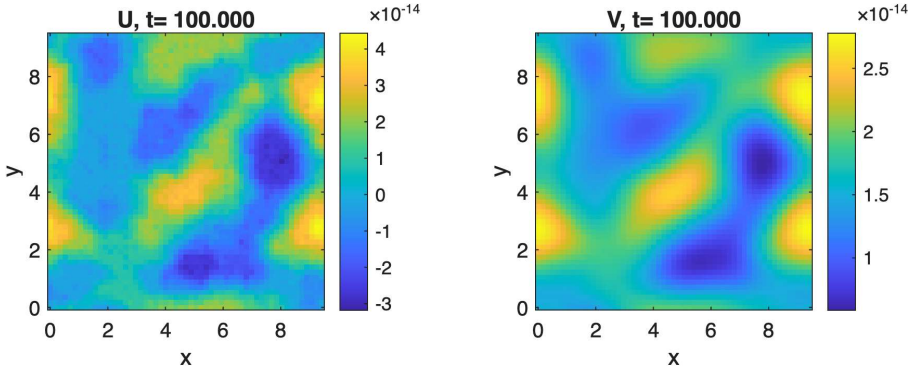

Figure 2: Diffusion, U and Chemoattractant V are displayed at 100 seconds with 55 x-grids, and 55 y-grids and 0.01 time step. The difference of solution and 0.2 is plotted to show the precise difference in colorbar. Diffusion shows sharper contrasts while Chemoattractant shows smoother and more diffused version.

provides signal field and cells' direction diffuses through space and shows where cells are. This is consistent with what is proposed in the papers referenced.

Discussion

Discretizing the system with MOLE and introducing Neumann boundary conditions of zero resulted in singular and ill conditioned matrices even in fully implicit regime. The solution was resolved with periodic boundary conditions as it is more stable numerically.

It is important to note that the choice of periodic boundary condition for pattern forming dynamics does not eliminate the physics of the system. While zero-flux (zero Neumann boundary conditions) are usually used in the papers referenced and patterns can be influenced by boundaries by showing aggregation near edges, periodic conditions isolate the intrinsic pattern-forming dynamics of the chemotaxis and eliminate boundary driven effects and thus the accumulation at the edges. Therefore, diffusion, chemotactic drive (moving up ΔV), and growth of the system is preserved.

From the given terms, only the diffusion terms is stiff and requires smaller time steps due to the denominator term possibly blowing up. Therefore, to gain more stability, it can be treated implicitly while leaving other terms explicit.

Conclusion

The reaction-diffusion-chemotaxis with volume-filling effect is modeled with mimetic differences using the MOLE library [**?**] operators and applying periodic boundary conditions. The simulation shows the cells diffusion (U) with sharp peaks showing clear density pattern, whereas the chemotaxis (V) showed smoothed pattern of the concentration of cells. These results are consistent with the proposed equations behaviors as U produces V and V guides U which means cells follow the chemical, and the chemical reflects the cells.

References

[1] T. Hillen and K. J. Painter, A User's Guide to PDE Models for Chemotaxis, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, vol. 17, no. 3, 037101, 2007.

[2] K. J. Painter and T. Hillen, Volume-Filling and Quorum-Sensing in Models for Chemosensitive Movement, *Canadian Applied Mathematics Quarterly*, vol. 10, no. 4, pp. 501–543, 2002.

[3] M. Ma, M. Gao, C. Tong, and Y. Han, Chemotaxis-Driven Pattern Formation for a Reaction-Diffusion-Chemotaxis Model with Volume-Filling Effect, *Applied Mathematics and Computation*, 2016.

[4] J Corbino and J. E. Castillo, High-Order Mimetic Difference Operators Satisfying the Extended Gauss Divergence Theorem. Journal of Computational and Applied Mathematics (364) (2020) 112326.

[5] R.S. Katiyar and P.K. Jha, Molecular simulations in drug delivery: Opportunities and challenges, WIREs Computational Molecular Science, 2018.

[6] J. Corbino, M. Dumett, and J. E. Castillo, *MOLE: Mimetic Operators Library Enhanced*, Journal of Open Source Software, vol. 9, no. 99, p. 6288, Jul. 2024, doi: 10.21105/joss.06288.