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Kristy Le* Miguel A. Dumett‡

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Abstract

We solve the Fizhugh-Nagumo reaction diffusion equations with mimetic differences using the MOLE library.

Introduction

The Fitzhugh-Nagumo reaction diffusion equations models a system of quantities that spreads through space by diffusion while also changing through nonlinear reaction terms. The problem being solved is a coupled two-variable system on the square domain [0, π] x [0, π] with periodic boundary conditions. The variables u(x, y, t) and v(x, y, t) represents the two interacting fields that both diffuse and react over time.

$$\partial_t u = D_1 \triangle u + (a-u)(u-1)u - v, (x,y) \epsilon [0,\pi] \times [0,\pi] \tag{1}$$

$$\partial_t v = D_2 \triangle v + e(bu - v), (x,y) \epsilon [0,\pi] \times [0,\pi] \tag{2}$$

$\partial_t u$ and $\partial_t v$ are time derivatives on u and v. $D_1 \triangle u$ and $D_2 \triangle v$ are the diffusion terms that spreads information across the [0, π]x[0, π] grid. The reaction terms are (a - u)(u - 1)u - v for u and e(bu - v) for v. The cubic term (a - u)(u - 1)u - v introduces nonlinear local dynamics, while e(bu - v) term couples to two variables such that each field influences the other through time.

The initial conditions are simple and symmetric as cos(x)cos(y) for both u and v. The problem has a periodic boundary condition where the opposite sides of the bounds repeats the system. Thus, the left and right edges behave as neighbors and the same is true for the bottom and top edges. So,

$$u(x,y,0) = cos(x)cos(y), (x,y) \epsilon [0,\pi] \times [0,\pi] \tag{3}$$

$$v(x,y,0) = cos(x)cos(y), (x,y) \epsilon [0,\pi] \times [0,\pi] \tag{4}$$

D_1 and D_2 represents the diffusion coefficients which are set to 10^{-4}. Because D_1 and D_2 are very small, they represent a weak diffusion. The reaction terms dominate and have relatively large parameter values a = 1, e = 3, b = 30 indicating v responds strongly to the current state of u.

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MOLE Spatial Discretization

Mimetic differences construct numerical schemes that use high-order approximate discrete analogs of vector calculus operators to be used for solving partial differential equations [3, 2]. The Mimetic Operators Library Enhanced (MOLE) is a repository that contains mimetic difference operators [1].

The Laplacian is represented by L and is the discrete 2D Laplacian produced by MOLE rather than the continuous Laplacian $\triangle$. It is built using the function Lap2D(k, m, dx, n, dy) where k is the order of accuracy, m and n are the grid intervals in the x and y directions, and dx and dy are the grid spacing. For our problem, k=2, and m and n are set to 50. Since the domain is [0, π]x[0, π], the grid spacing is set to:

$$dx = \frac{\pi}{m} = \frac{\pi}{50} \tag{5}$$

$$dx = \frac{\pi}{n} = \frac{\pi}{50} \tag{6}$$

With MOLE, the semidiscrete form of our problem is:

$$\partial_t u = D_1 L u + (a - u)(u - 1)u - v \tag{7}$$

$$\partial_t v = D_2 L v + e(bu - v) \tag{8}$$

The periodic boundaries are set when the Dirichlet and Neumann conditions passes zero boundary vectors. AddScalarBC2D is called and imposes a periodic boundary condition rather than enforcing a zero value or zero flux condition on the boundaries. With the spatial operator from MOLE, the PDE system becomes a large algebraic ODE system.

Time Integration

After spatial discretization, the remaining task is to move the discrete vectors forward from t=0 to t=T. In our problem, T is set to 10 with dt = 0.01. Therefore, the simulation runs 1,000 steps before the final approximation is drawn.

At each iteration, we discretize the time derivative with the forward Euler method. Nevertheless, the update for u is not a plain Euler step since it treats the diffusion and part of the nonlinear reaction term implicitly.

$$u_t = \frac{u^{n+1} - u^n}{dt} = D_1 L u^{n+1} + (a - u^n)(u^n - 1)u^{n+1} - v^n \tag{9}$$

The equation is restructured into a linear system $A_u u^{n+1} = u_{rhs}$ where A_u is a matrix containing the diffusion and cubic reaction terms.

$$A_u = I - dt(D_1 L + (a - u^n)(u^n - 1)) \tag{10}$$

$$u_{rhs} = u^n - dtv^n \tag{11}$$

$$(I - dt(D_1 L + (a - u^n)(u^n - 1)))u^{n+1} = u^n - dtv^n \tag{12}$$

The update for v is handled with explicit Euler. It uses the newest value of u so the two equations are advanced with a staggered coupling strategy.

$$v^{n+1} = dt(D_2 L v^n - ev^n + ebu^{n+1}) + v^n \tag{13}$$

Results

At the start of the simulation, the two fields u and v are identical since they are both initialized with the same conditions cos(x)cos(y). As the simulation progresses, the two variables no longer evolves identically. The difference in structure means the time history of u reflects both a local nonlinear response and weak diffusion, while v is strongly driven by u.

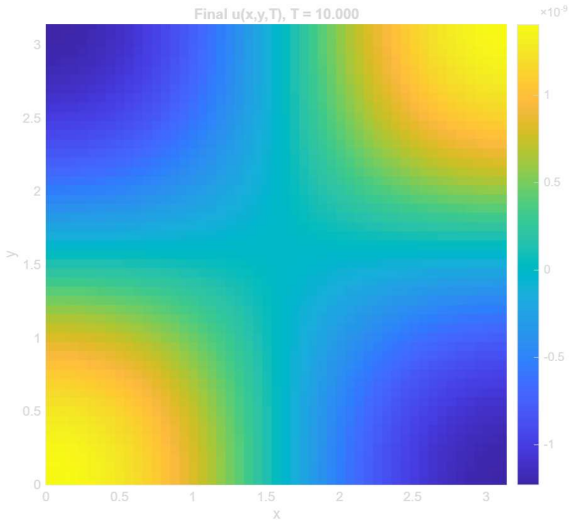

Figure 9: u(x,y,t) at T=10

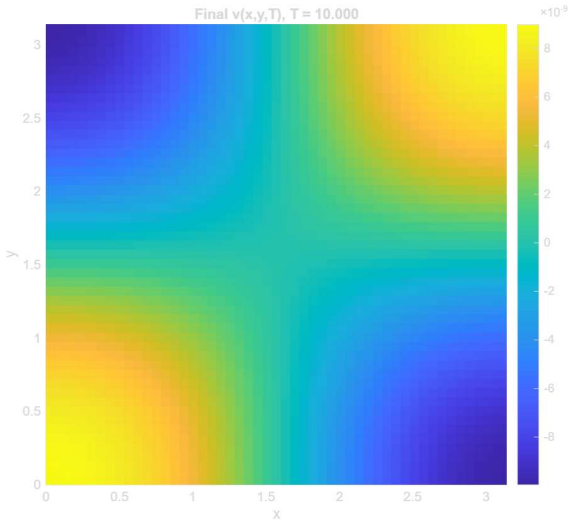

Figure 10: v(x,y,t) at T=10

Figure 11: Top 2D view of u and v at T=10

The simulation of the 2D reaction diffusion equation appears stable. It shows a short oscillatory transient, and then both fields settle towards a near-steady state close to zero. The max/min plots for both u and v started with oscillations and then decayed rapidly towards zero. The v-field has a much larger amplitude than u which is representative of the large parameters set for v with e = 3 and b = 30. The spatial-average plot shows the average of both fields oscillating briefly and then converging towards zero as well. This indicates that this problem setup does not produce persistent patterns, and diffuses out towards a zero state. The successive-step-difference plot indicates strong stability since both curves decreases over time, and the numerical solution is approaching a steady state rather than blowing up or continuing with large persistent oscillations. A clean decay of the step-to-step norms suggests that the chosen dt = 0.01 works well for the parameters set.

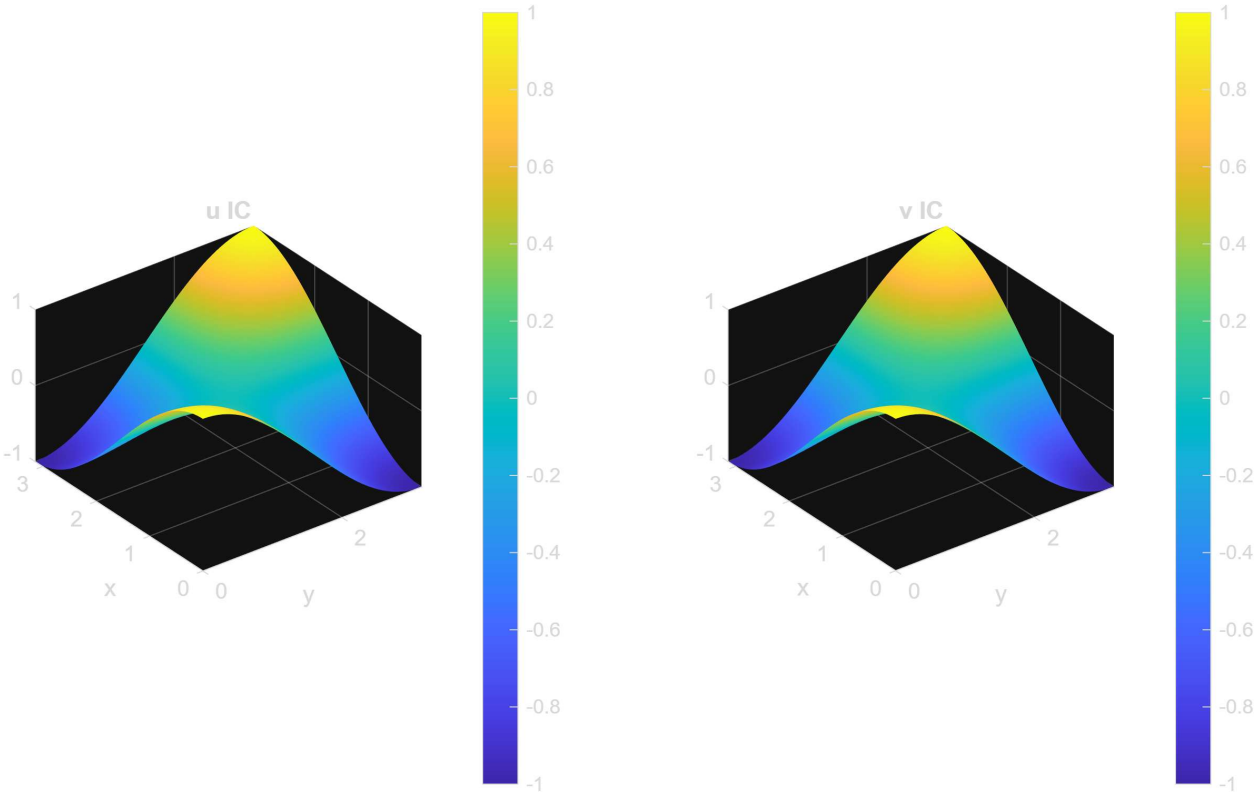

Figure 1: u and v at Initial Condition

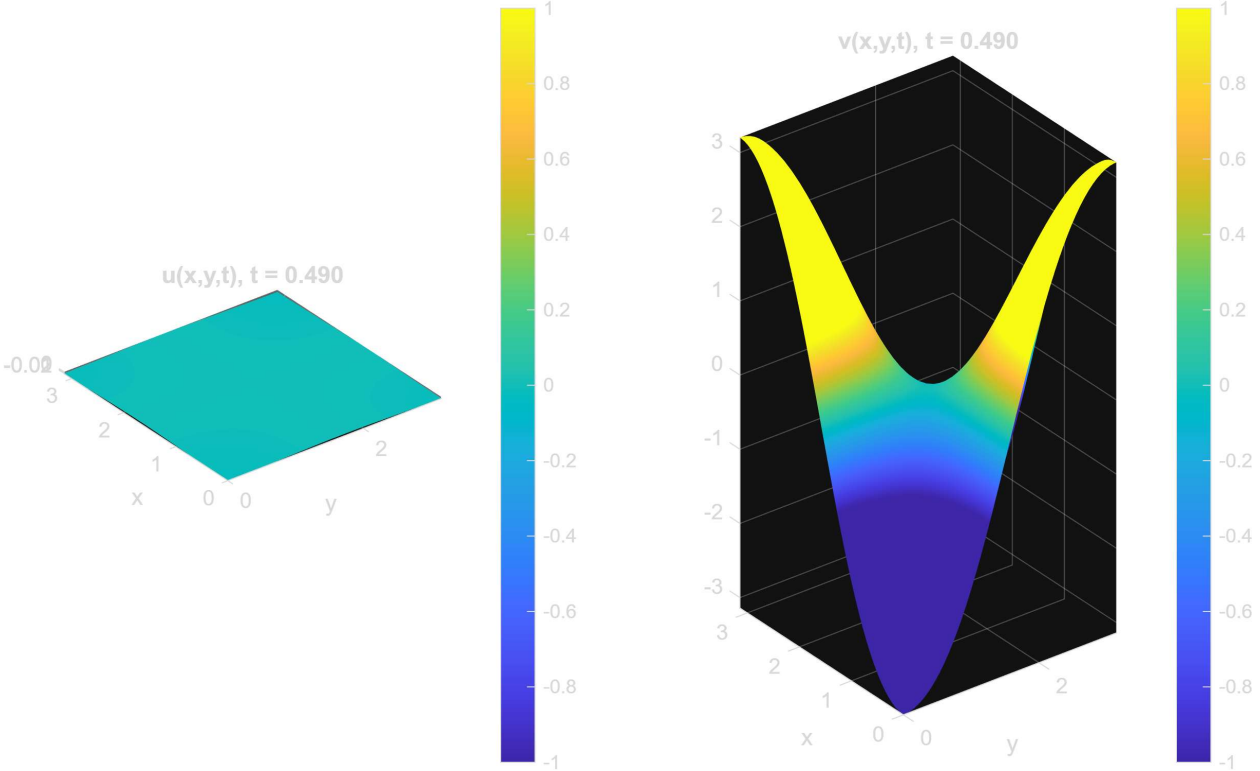

Figure 2: u and v at T=0.5

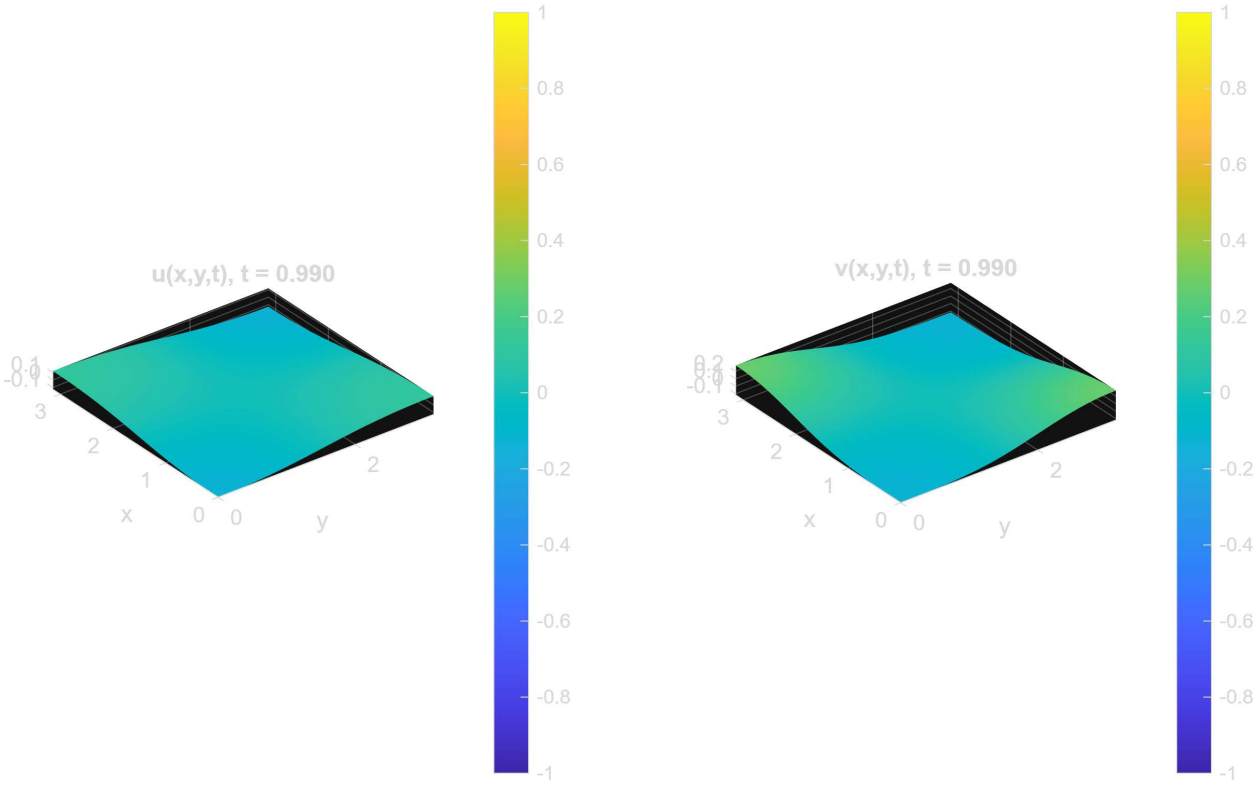

Figure 3: u and v at T=1.0

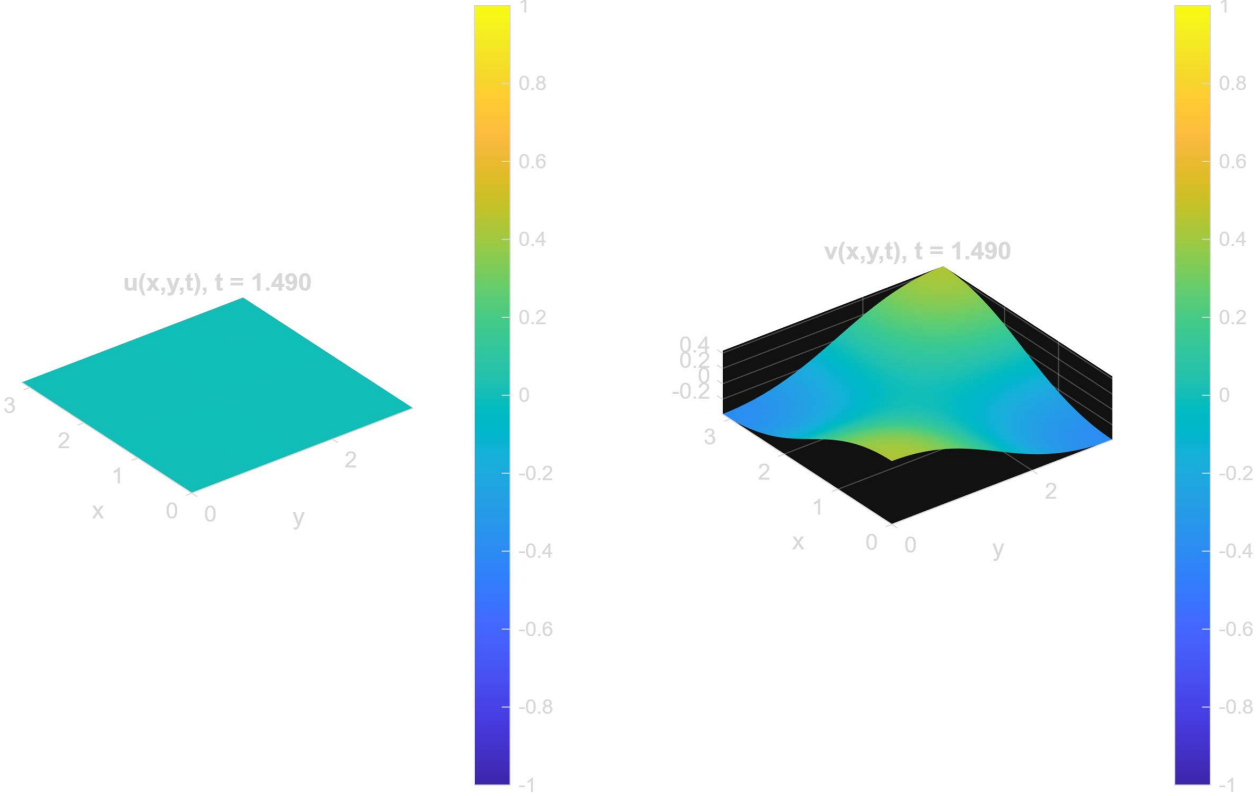

Figure 4: u and v at T=1.5

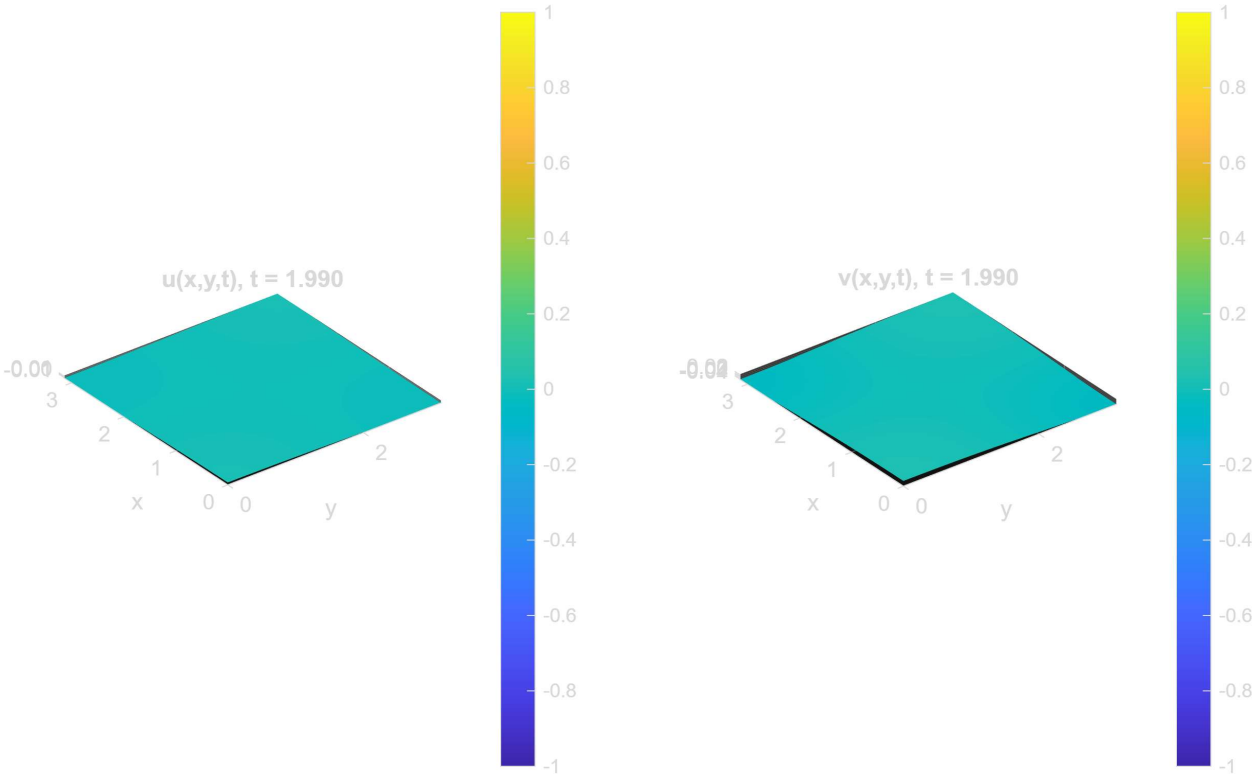

Figure 5: u and v at T=2.0

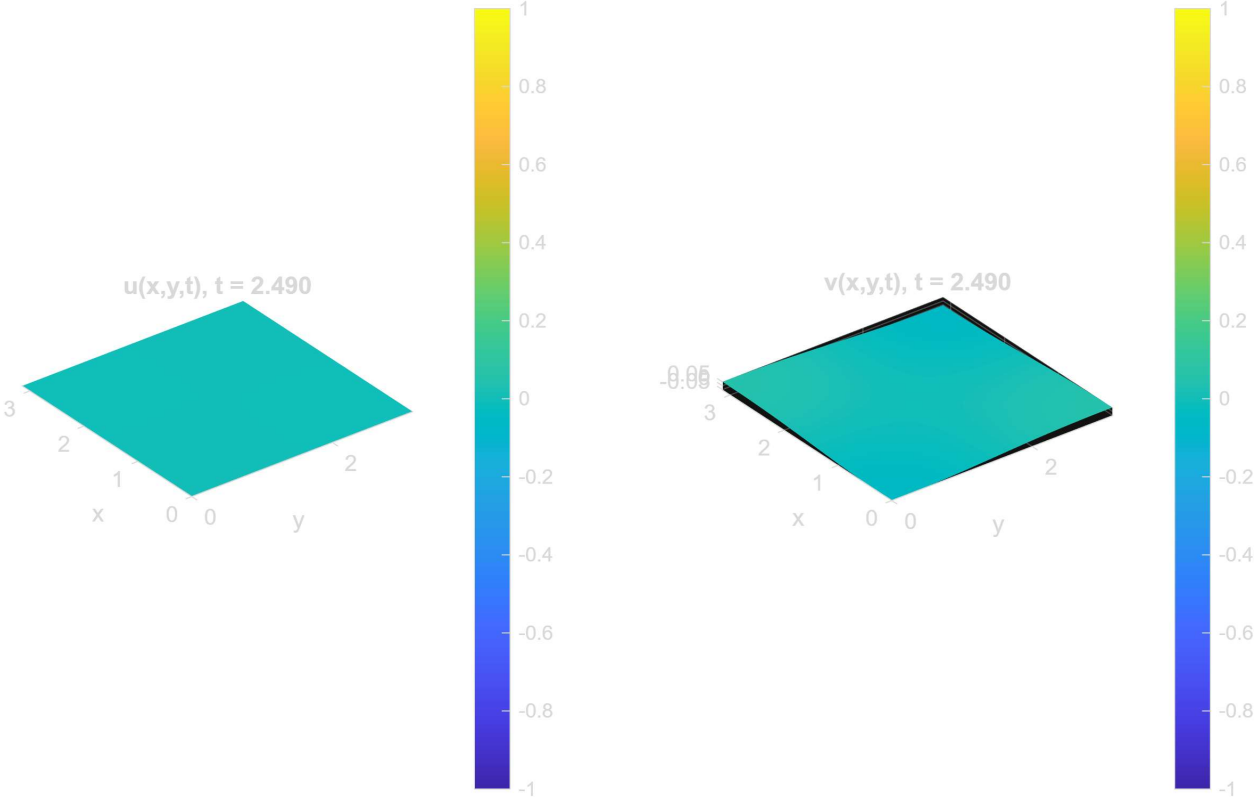

Figure 6: u and v at T=2.5

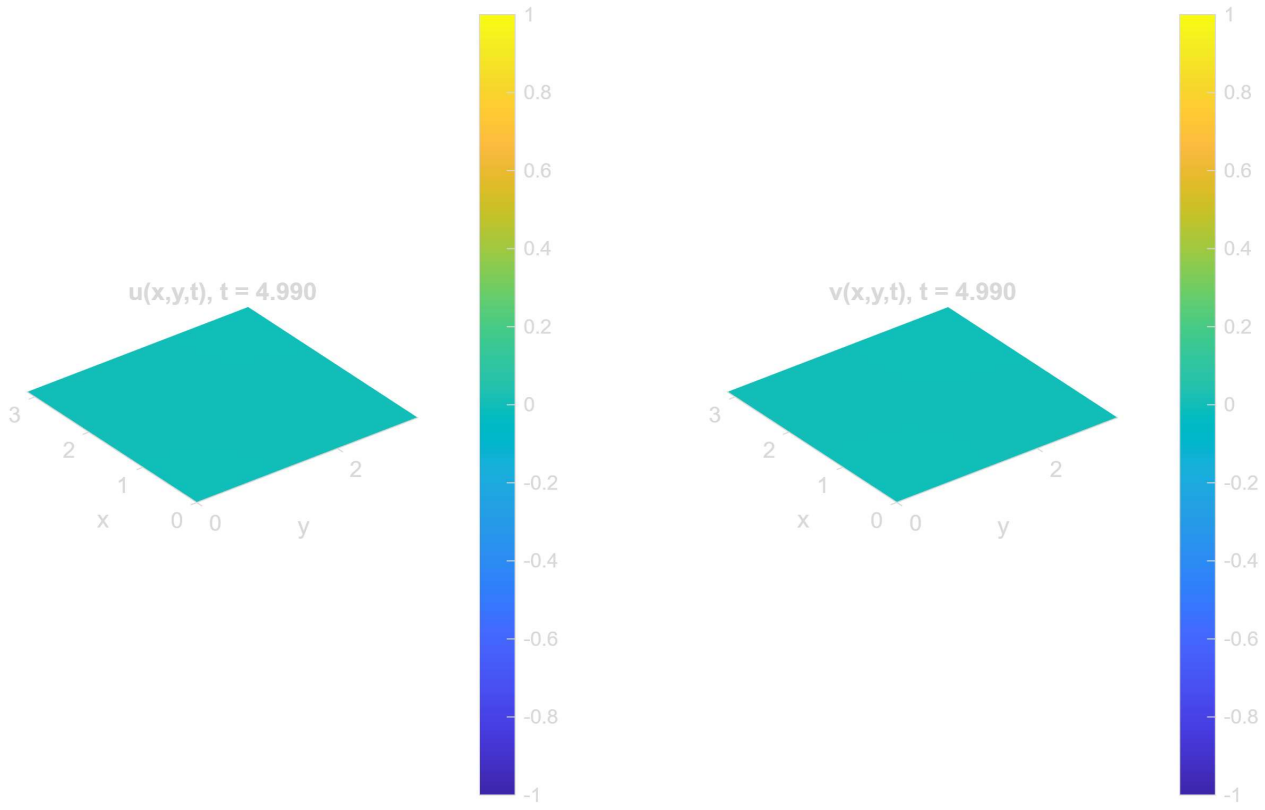

Figure 7: u and v at T=5

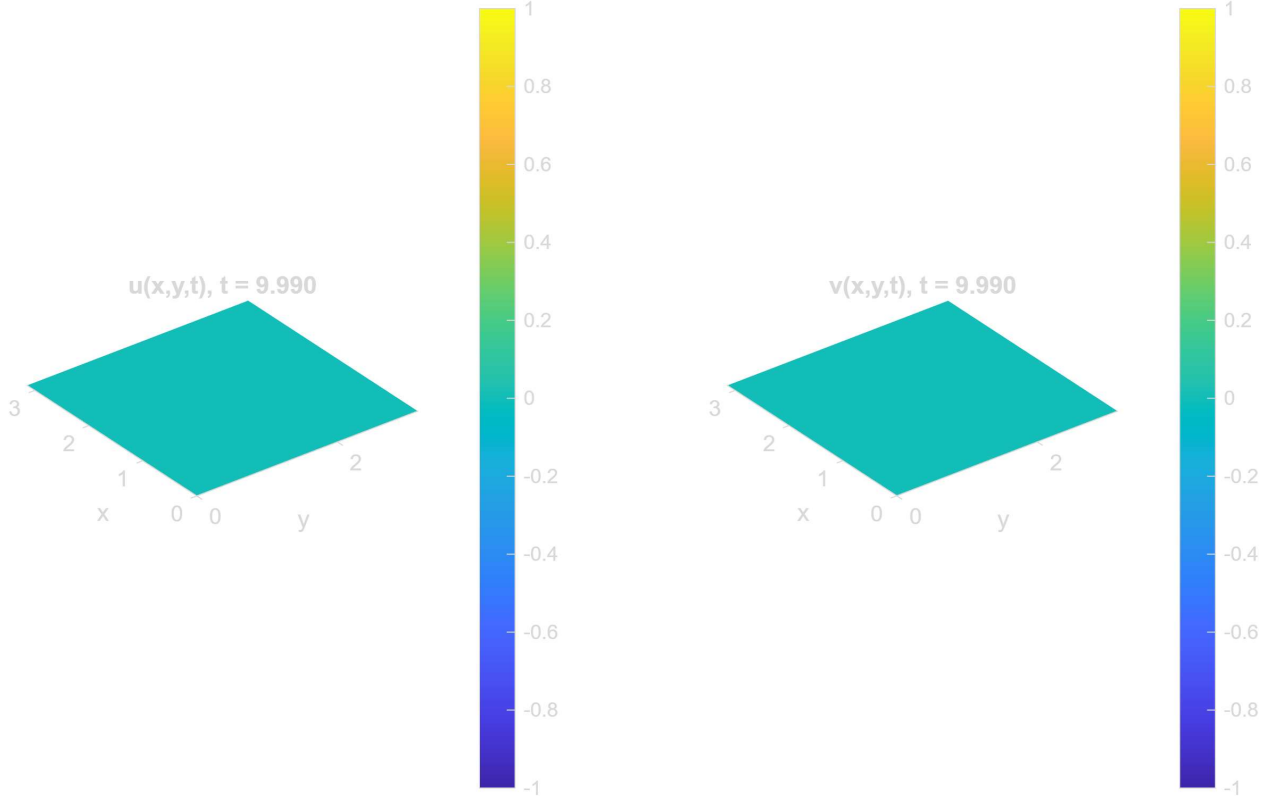

Figure 8: u and v at T=10

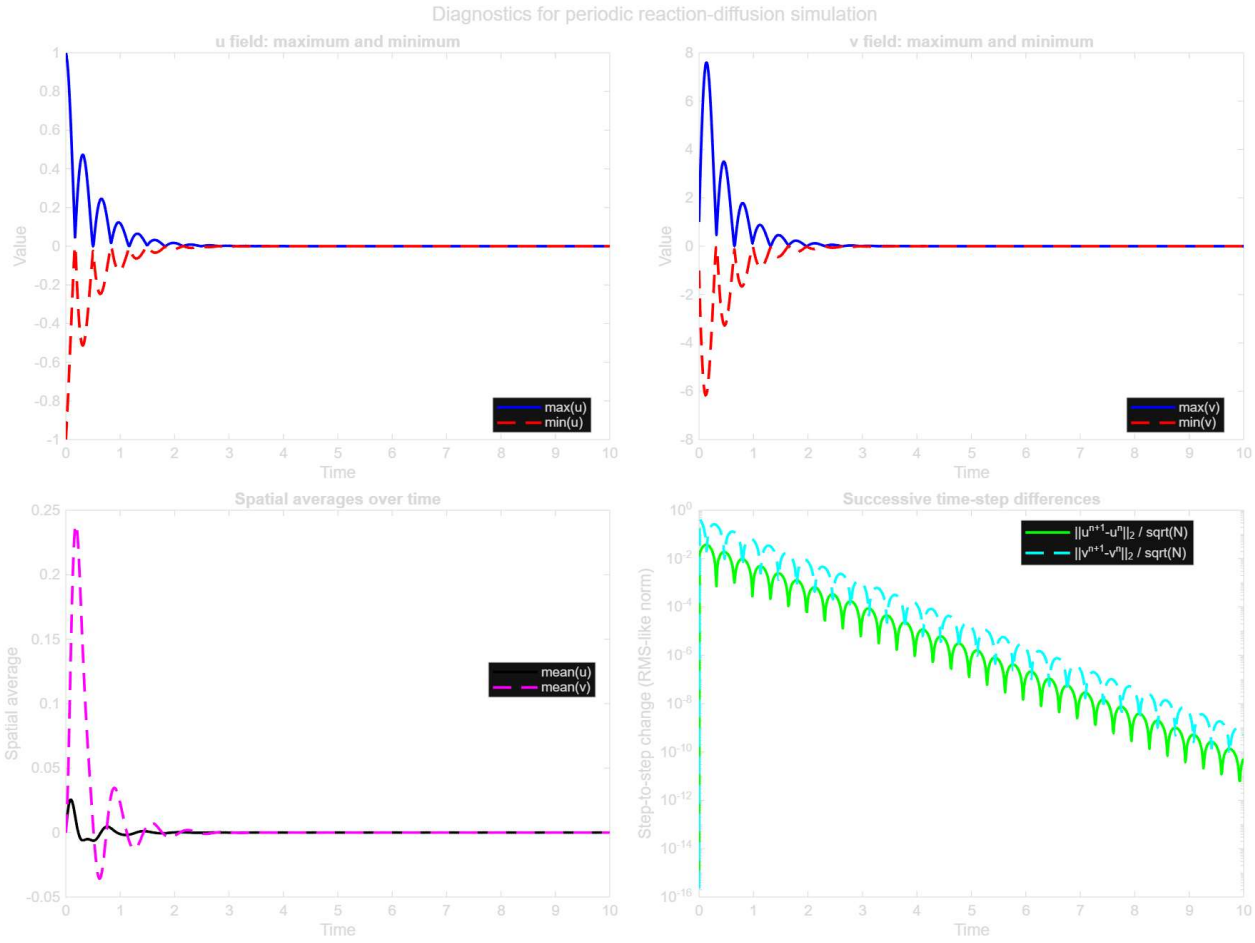

Figure 12: Top - The minimum and maximum of u and v are flattening out, indicating a steady state. Bottom Left - Spatial averages over time and shows that the behavior diffuses out. Bottom Right - Successive time-step differences plot measures the change in solution from one time step to the next using a norm. The curve is decreasing towards 0, indicating that the solution is settling.

Conclusion

To conclude, we were able to solve the 2D reaction diffusion system with periodic boundary conditions using the MOLE library for spatial discretization and applying a semi-implicit and explicit time-stepping scheme to the system. The Laplacian operator was replaced by a sparse mimetic matrix L, allowing the diffusion terms to be computed efficiently on the grid. The diagnostic plots shows that the solution remains stable and exhibits a dampening oscillator behavior that converges to a near-steady equilibrium state. Overall, this computation demonstrates that MOLE provides an effective framework for solving 2D reaction diffusion equations with periodic boundary conditions.

References

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[2] J. Corbino and J.E. Castillo, High-order mimetic finite-difference operators satisfying the extended Gauss divergence theorem, J. Comput. Appl. Math., vol. 364, 2020.

[3] J.E. Castillo and R.D. Grone, A matrix analysis approach to higher-order approximations for divergence and gradients satisfying a global conservation law, SIAM J. Matrix Anal. Appl., 2003.