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A Study of Numerical Reaction-Diffusion Systems on Closed Surfaces

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***Abstract*—**The diffusion-reaction equations are important Partial Differential Equations in mathematical biology, material science, physics, and so on. However, finding efficient numerical methods for diffusion-reaction systems on curved surfaces is still an important and difficult problem. The purpose of this paper is to present a convergent geometric method for solving the reaction-diffusion equations on closed surfaces by an O(r)-LTL configuration method. The O(r)-LTL configuration method combining the local tangential lifting technique and configuration equations is an effective method to estimate differential quantities on curved surfaces. Since estimating the Laplace-Beltrami operator is an important task for solving the reaction-diffusion equations on surfaces, we use the local tangential lifting method and a generalized finite difference method to approximate the Laplace-Beltrami operators and we solve this reaction-diffusion system on closed surfaces. Our method is not only conceptually simple, but also easy to implement.

***Keywords*—**Close surfaces, high-order approach, numerical solutions, reaction-diffusion systems.

I. Introduction

THE reaction-diffusion system has been an important model in biology, image processing, material science, physics and mathematics since 1942 [9]. There are many elegant numerical methods for the reaction-diffusion problem in $\mathbf{R}^n$, but this problem on closed surfaces is much less understood. Recently, more and more numerical methods for solving the reaction-diffusion system on surfaces have been proposed. In 2010, Landsberg and Voigt [7] solved this problem by a multigrid finite element method. Fuselier and Wright [6] proposed a high-order kernel method in 2013 and Tuncer et al. [10] developed the projected finite elements for this problem on stationary closed surfaces. And Bergdorf et al. [1] solved the reaction-diffusion systems on deforming surfaces by the Lagrangian particle method in 2010. In 2015, we presented a general convergent geometric method to estimate the differential quantities on surfaces [2]. In this note, we shall use our proposed method to solve numerically the reaction-diffusion systems on stationary closed surfaces.

II. The Gradient and Laplace-Beltrami Operator on Surfaces

In this section, we introduce the gradient, divergence, and Laplace-Beltrami operator over functions and vector fields on a regular surface. Let Σ be a regular surface in $\mathbf{R}^2$ and a parametrization $\mathbf{x}: U \to \Sigma$ at a point p, where $U \subset \mathbf{R}^2$ is an open subset. The gradient $\nabla_\Sigma \phi$ of a smooth function ϕ on Σ is given by

$$\nabla_\Sigma \phi = \frac{\phi_u G - \phi_v F}{EG - F^2}\mathbf{x}_u + \frac{\phi_v E - \phi_u F}{EG - F^2}\mathbf{x}_v \tag{1}$$

where E, F and G are the coefficients of the 1st fundamental form of Σ, $\phi_u = \frac{\partial}{\partial u}\phi(\mathbf{x}(u,v))$ and $\phi_v = \frac{\partial}{\partial v}\phi(\mathbf{x}(u,v))$. If X is a local vector field, $X = A\mathbf{x}_u + B\mathbf{x}_v$ on $\mathbf{x}(U) \subset \Sigma$. The (surface) divergence $Div_\Sigma X$ of X is defined as a function $Div_\Sigma X : \mathbf{x}(U) \to \mathbf{R}$ given by the trace of the linear map $Y(p) \to \nabla_{Y(p)} X$ for p in Σ. A direct computation yields:

$$Div_\Sigma X = \frac{1}{\sqrt{EG - F^2}}\left[\frac{\partial}{\partial u}\left(A\sqrt{EG - F^2}\right) + \frac{\partial}{\partial v}\left(B\sqrt{EG - F^2}\right)\right]. \tag{2}$$

The Laplace-Beltrami operator $\Delta_\Sigma \phi$ acting on the function ϕ is defined by $\Delta_\Sigma \phi = Div_\Sigma(\nabla_\Sigma \phi)$ and has the local representation

$$\Delta_\Sigma \varphi = \frac{1}{\sqrt{EG - F^2}}\left[\frac{\partial}{\partial u}\left(\frac{G}{\sqrt{EG - F^2}}\varphi_u\right) - \frac{\partial}{\partial u}\left(\frac{F}{\sqrt{EG - F^2}}\varphi_v\right) + \frac{\partial}{\partial v}\left(\frac{E}{\sqrt{EG - F^2}}\varphi_v\right) - \frac{\partial}{\partial v}\left(\frac{F}{\sqrt{EG - F^2}}\varphi_u\right)\right]. \tag{3}$$

See [4], [5] for more details.

III. Numerical Algorithms for Reaction-Diffusion Equations on Surfaces

A. Model Equations

In this study, we restrict (u,v) to be a vector of two chemical pieces which are resident on a closed stationary surface Σ. The evolution equations for reaction-diffusion on the stationary closed surfaces can be obtained from the law of mass conservation, and are in the form [6]-[8] of

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$$\begin{cases} u_t - \Delta_\Sigma u = \gamma f(u,v) \\ v_t - d\Delta_\Sigma v = \gamma g(u,v), \end{cases} \tag{4}$$

where $u, v : \Sigma \to \mathbf{R}$.

Let $\mathbf{U} = \begin{pmatrix} u \\ v \end{pmatrix}$, $\mathbf{L} = \begin{pmatrix} u \\ d \cdot v \end{pmatrix}$, and $\mathbf{F}(u,v) = \begin{pmatrix} f(u,v) \\ g(u,v) \end{pmatrix}$. Equation (4) can be rewritten as

$$\mathbf{U}_t - \Delta_\Sigma \mathbf{L} = \gamma \mathbf{F}, \tag{5}$$

where Δ_Σ is the vector Laplace-Beltrami operator.

B. Time Discretization

After an explicit time discretization, the model function (5) becomes

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\tau^n} = \Delta_\Sigma \mathbf{L}^n + \gamma \mathbf{F}^n, \tag{6}$$

or

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \tau^n \left(\Delta_\Sigma \mathbf{L}^n + \gamma \mathbf{F}^n \right) \tag{7}$$

where $\tau^n = t^{n+1} - t^n$ is the step of time, $\mathbf{U}^n = \begin{pmatrix} u^n \\ v^n \end{pmatrix}$, $\mathbf{L}^n = \begin{pmatrix} u^n \\ dv^n \end{pmatrix}$ and $\mathbf{F}^n = \begin{pmatrix} f(u^n, v^n) \\ g(u^n, v^n) \end{pmatrix}$. If we use the implicit time discretization, (5) becomes:

$$\mathbf{U}^{n+1} - \tau^n \Delta_\Sigma \mathbf{L}^{n+1} = \mathbf{U}^n + \tau^n \gamma \mathbf{F}^n. \tag{8}$$

Both in (7) and (8), we only need to estimate the vector Laplace-Beltrami operator.

C. Space Discretization

We shall use our high-order approach method in [2] that we proposed in 2015 to improve the problem of space discretization of (5).

To estimate the vector Laplace-Beltrami operator on Σ, we propose a two-step algorithm:

Step 1. Obtain a high-order approximation of the underlying surface Σ around a vertex p on Σ.

Step 2. Find a high-order approximation (at least $O(r^2)$) of the function ϕ on Σ around the vertex p.

To obtain the approximation of Σ around p, we shall construct a local parametrization by representing Σ as a graph surface around p locally. Let $S = (V, F)$ be a triangular mesh of a closed surface Σ with mesh size $r > 0$. Given a vertex $p \in V$, let p_j, $j = 0,1,\cdots,n$ be the neighboring vertices of p with $p_0 = p_n$. Let $N_A(p)$ be the weighted normal vector of S given in [3] by the centroid weights. The approximating tangent plane $TS(p)$ of S at p is given by $TS(p) = \{w \in \mathbf{R}^3 \mid w \perp N_A(p)\}$. We choose an orthonormal basis $\{e_1, e_2\}$ for $TS(p)$. Obviously, every vector w in $TS(p)$ has a unique coordinate (x, y) with $w = xe_1 + ye_2$. Therefore, each q on Σ around p can be assigned a new coordinate (x, y, z) on the base $\{e_1, e_2, N_A(p)\}$ as follows,

$$x(q)e_1 + y(q)e_2 = (q - p) - \big((q - p) \cdot N_A(p)\big) N_A(p) \tag{9}$$

and

$$z(q) = h(x(p), y(p)) = (q - p) \cdot N_A(p). \tag{10}$$

The neighboring vertices p_j of p is now given as

$$x_j = x(p_j),\ y_j = y(p_j) \text{ and } z_j = h(x_j, y_j).$$

Hence, the new coordinate of p is $(0,0,0)$. Next, we want to find a suitable polynomial fitting for the height function h of Σ around p. By the 3rd order Taylor formula, we have

$$\begin{aligned} h(x,y) - h(0,0) &= x h_x(0,0) + y h_y(0,0) \\ &+ \frac{1}{2}\left(x^2 h_{xx}(0,0) + 2xy h_{xy}(0,0) + y^2 h_{yy}(0,0) \right) + O(r^3). \end{aligned} \tag{11}$$

Let α_j, $j = 1, \cdots, n$ be a set of real numbers, one has

$$\begin{aligned} \sum_{j=1}^n \alpha_j \left(h(x_j, y_j) - h(x_j, y_j) \right) &= h_x(0,0) \sum_{j=1}^n \alpha_j x_j \\ &+ h_y(0,0) \sum_{j=1}^n \alpha_j y_j + h_{xx}(0,0) \sum_{j=1}^n \alpha_j x_j^2 \\ &+ h_{xy}(0,0) \sum_{j=1}^n \alpha_j x_j y_j + \frac{1}{2} h_{yy}(0,0) \sum_{j=1}^n \alpha_j y_j^2 + O(r^3). \end{aligned} \tag{12}$$

Set $A = \begin{pmatrix} x_1 & \cdots & x_n \\ y_1 & \cdots & y_n \\ x_1^2 & \cdots & x_1^2 \\ x_1 y_1 & \cdots & x_n y_n \\ y_1^2 & \cdots & y_1^2 \end{pmatrix}$ and $\alpha = \begin{pmatrix} \alpha_1^1 & \alpha_1^2 & \alpha_1^3 & \alpha_1^4 & \alpha_1^5 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \alpha_n^1 & \alpha_n^2 & \alpha_n^3 & \alpha_n^4 & \alpha_n^5 \end{pmatrix}$.

If

$$A\alpha = I_{5\times 5}, \tag{13}$$

we have

$$\begin{cases} h_x(0,0) = \sum_{j=1}^n \alpha_j^1 \left(h(x_j, y_j) - h(0,0) \right) + O(r^3), \\ h_y(0,0) = \sum_{j=1}^n \alpha_j^2 \left(h(x_j, y_j) - h(0,0) \right) + O(r^3), \\ h_{xx}(0,0) = \sum_{j=1}^n \alpha_j^3 \left(h(x_j, y_j) - h(0,0) \right) + O(r^3), \\ h_{xy}(0,0) = \sum_{j=1}^n \alpha_j^4 \left(h(x_j, y_j) - h(0,0) \right) + O(r^3), \\ h_{yy}(0,0) = \sum_{j=1}^n \alpha_j^5 \left(h(x_j, y_j) - h(0,0) \right) + O(r^3). \end{cases} \tag{14}$$

When the number of neighboring vertices of p is at least 6, (13) is underdetermined and hence, it always has a solution.

Similarly, the partial differentials of a function ϕ on Σ around p can also be approximated by

$$\begin{cases} \phi_x(0,0) = \sum_{j=1}^{n} \alpha_j^1 \big(\phi(x_j, y_j) - \phi(0,0)\big) + O(r^3), \\ \phi_y(0,0) = \sum_{j=1}^{n} \alpha_j^2 \big(\phi(x_j, y_j) - \phi(0,0)\big) + O(r^3), \\ \phi_{xx}(0,0) = \sum_{j=1}^{n} \alpha_j^3 \big(\phi(x_j, y_j) - \phi(0,0)\big) + O(r^3), \\ \phi_{xy}(0,0) = \sum_{j=1}^{n} \alpha_j^4 \big(\phi(x_j, y_j) - \phi(0,0)\big) + O(r^3), \\ \phi_{yy}(0,0) = \sum_{j=1}^{n} \alpha_j^5 \big(\phi(x_j, y_j) - \phi(0,0)\big) + O(r^3). \end{cases} \quad (15)$$

Using (3), we obtain a convergent approximation of the Laplace-Beltrami operator of ϕ on Σ. In this way, the Laplace-Beltrami operator on Σ is corresponding to a square matrix, denoted as $\mathbf{M}$. Equation (7) becomes

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \tau^n \left(\mathbf{M}\mathbf{L}^n + \gamma \mathbf{F}^n\right) \quad (16)$$

and (8) can also be rewritten as

$$\begin{cases} (\mathrm{I} - \tau^n \mathrm{M}) u^{n+1} = u^n + \tau^n \gamma f(u^n, v^n) \\ (\mathrm{I} - \tau^n d\mathrm{M}) v^{n+1} = v^n + \tau^n \gamma g(u^n, v^n). \end{cases} \quad (17)$$

IV. Simulations

We solve the Schnakenberg model [5] by (16). The functions corresponding reaction kinetics are

$$\begin{cases} f(u,v) = a - u + uv^2 \\ g(u,v) = b - u^2 v. \end{cases} \quad (18)$$

A. Convergence Test

First, we solve the system

$$\begin{cases} u_t - \Delta_\Sigma u = \gamma f(u,v) + F(u,v,t) \\ v_t - d\Delta_\Sigma v = \gamma g(u,v) + G(u,v,t), \end{cases} \quad (19)$$

on a sphere. We compute the functions F and G in (19) such that $u(p) = (1 + \exp(10t))x$ and $v(p) = (1 + \exp(10t))y$ are the exact solution of (11), where $p = (x, y, z)$ on the sphere. We estimate the $L^\infty(L^\infty)$ error by

$$L^\infty L^\infty(u) = \max_{t^n \in [0,1]} \left(\max_{p \in V} \left| u^n(p) - u(p) \right| \right),$$

and

$$L^\infty L^\infty(v) = \max_{t^n \in [0,1]} \left(\max_{p \in V} \left| v^n(p) - v(p) \right| \right),$$

where $u(p), v(p)$ are the exact solutions of (19) at p. Table I shows the $L^\infty(L^\infty)$ errors of u and v at time $t = 1$.

TABLE I
$L^\infty(L^\infty)$ Error of u and v

Mesh size	The error $L^\infty L^\infty(u)$	The error $L^\infty L^\infty(v)$
0.6180	3.1e-2	8.2e-2
0.3249	2.5e-3	6.5e-3
0.1646	2.2e-4	5.8e-4
0.0813	3.2e-5	4.7e-5

B. Spherical Surfaces

Let $a = 0.1$, $b = 0.9$, $d = 10$, $\gamma = 5000$, and $\tau^n = 0.1r^2$. We solve (4) and (18) by our proposed method on three different spherical surfaces.

Figs. 1-4 show the values of u (left figure) and v (right figure) at time about 10^{-6}, 10^{-3}, 0.05, and 0.1 on the sphere with radius 0.25. Figs. 5-8 show the numerical solution on a bean surface with parametrization

$$x(u,v) = \left(r \sin u \sin v \quad r \sin u \cos v \quad r \cos u\right) \quad (20)$$

with $r = 1 + a \sin u \sin v + b \sin u \cos v \sin^2 v$ and $a = 0.61$, $b = 0.4$. Fig. 9 is the numerical solution on the bean surface at time 0.1 in another viewpoint.

Figs. 10-13 present the numerical solutions on the peanut surface with parametrization

$$x(u,v) = \left(r \sin u \sin v \quad r \sin u \cos v \quad r \cos u\right) \quad (21)$$

with $r = \sqrt{\cos 2u + \sqrt{1 - \sin^2 2u}}$

V. Conclusion

The high-order approach presents an efficient method for estimating the differential quantities and solving the system of reaction-diffusion equations on surfaces. In our simulations, we only use 3rd order Taylor formula. However, we can also obtain higher accurate approaches by this method. Furthermore, this method can also be used to improve many kinds of partial differential equations on surfaces.

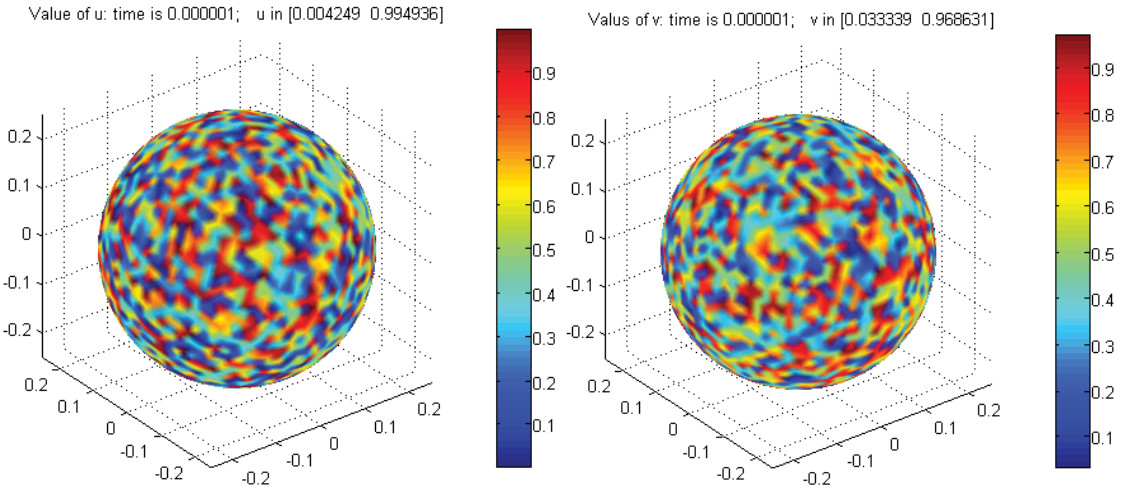

Fig. 1 Simulation of (4) and (21) on sphere at time 10^{-6}

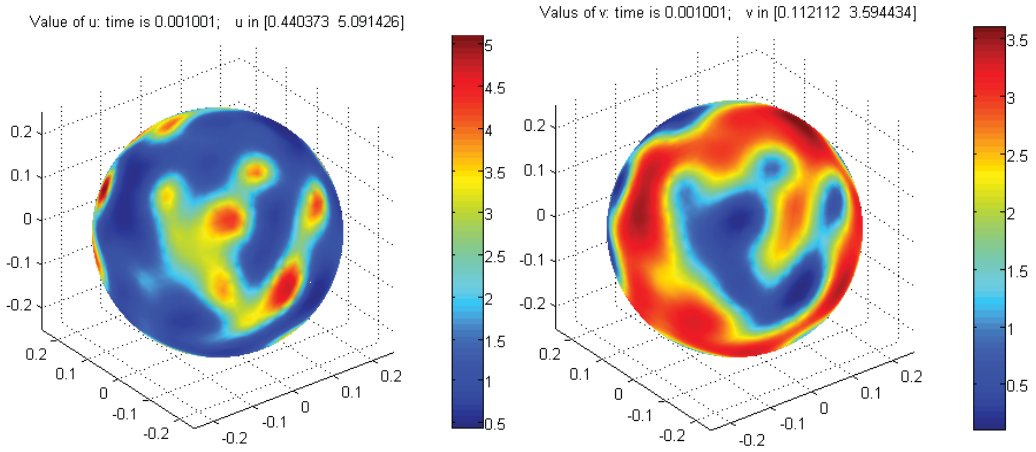

Fig. 2 Simulation of (4) and (21) on sphere at time 10^{-3}

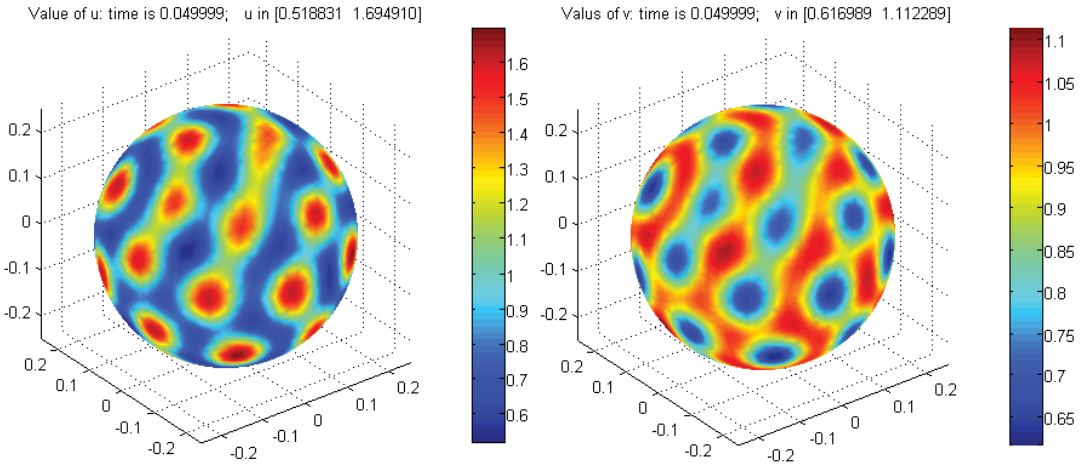

Fig. 3 Simulation of (4) and (21) on sphere at time 0.05

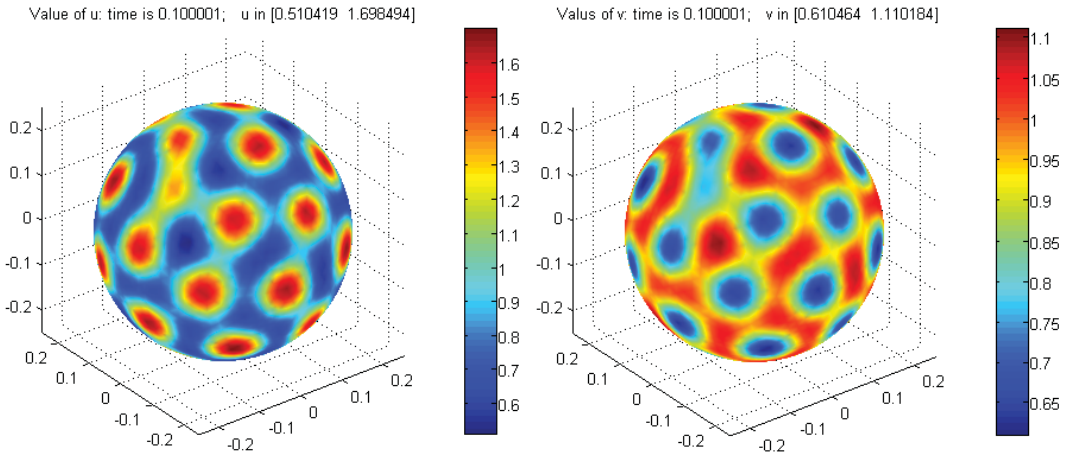

Fig. 4 Simulation of (4) and (21) on sphere at time 0.1

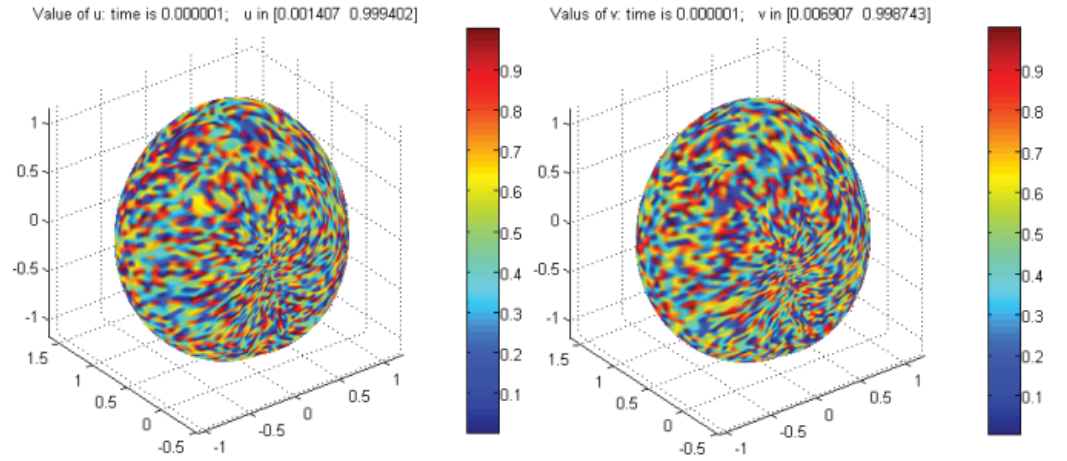

Fig. 5 Simulation of (4) and (21) on bean at time 10^{-6}

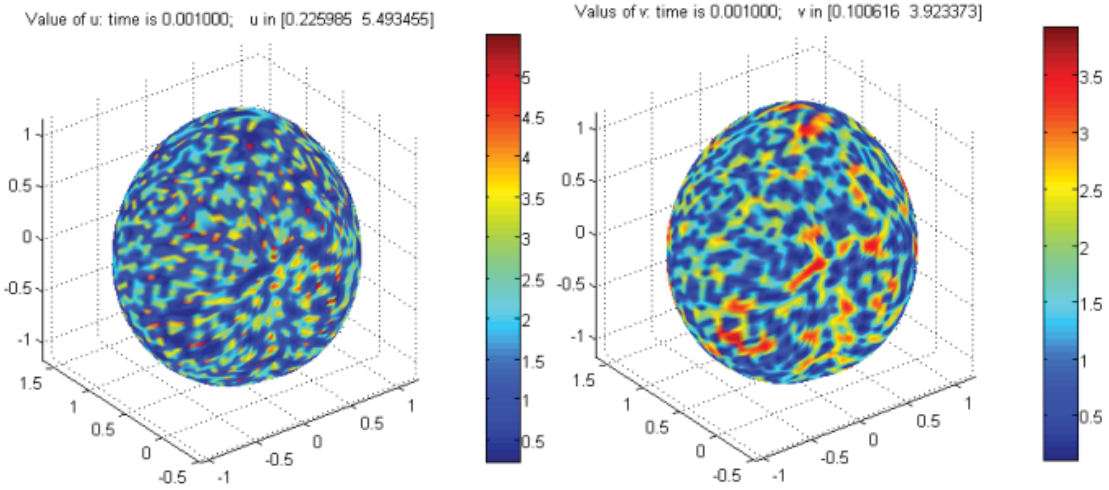

Fig. 6 Simulation of (4) and (21) on bean at time 10^{-3}

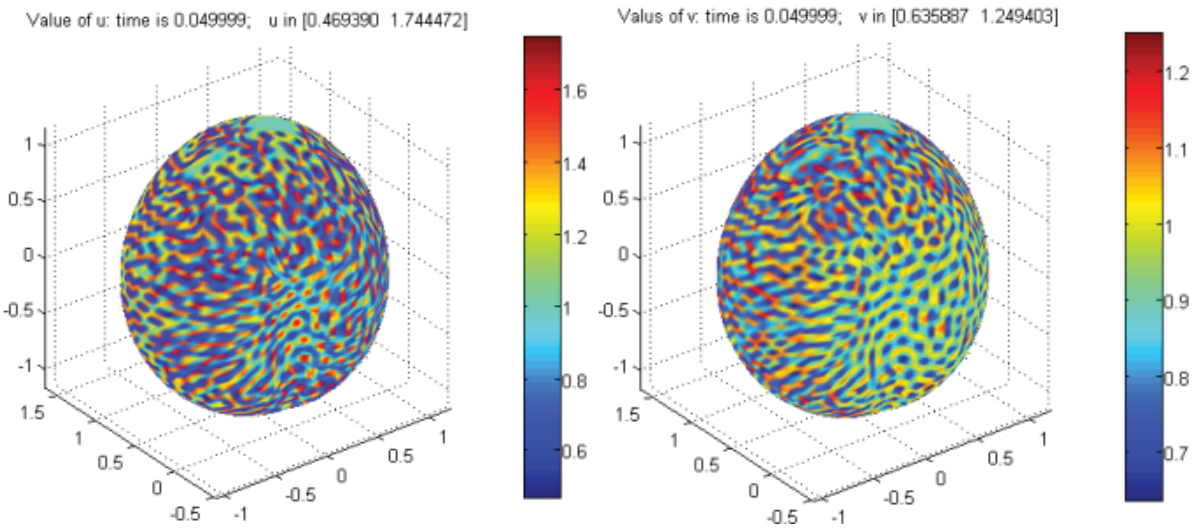

Fig. 7 Simulation of (4) and (21) on bean at time 0.05

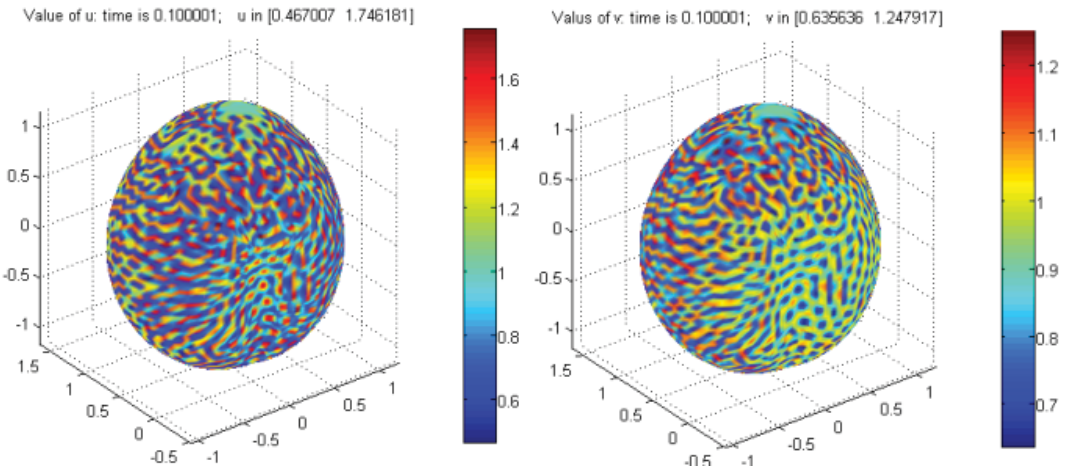

Fig. 8 Simulation of (4) and (21) on bean at time 0.1

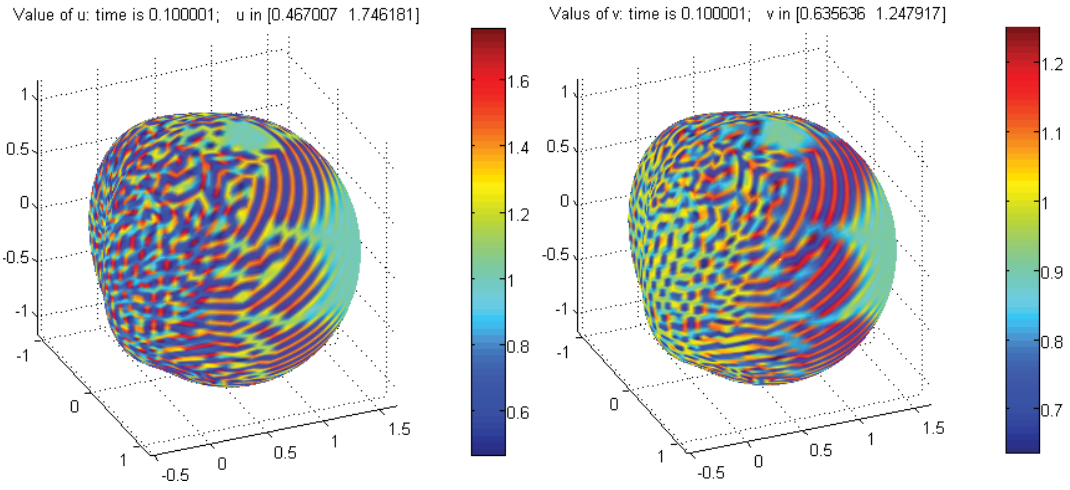

Fig. 9 Simulation of (4) and (21) on bean at time 0.1

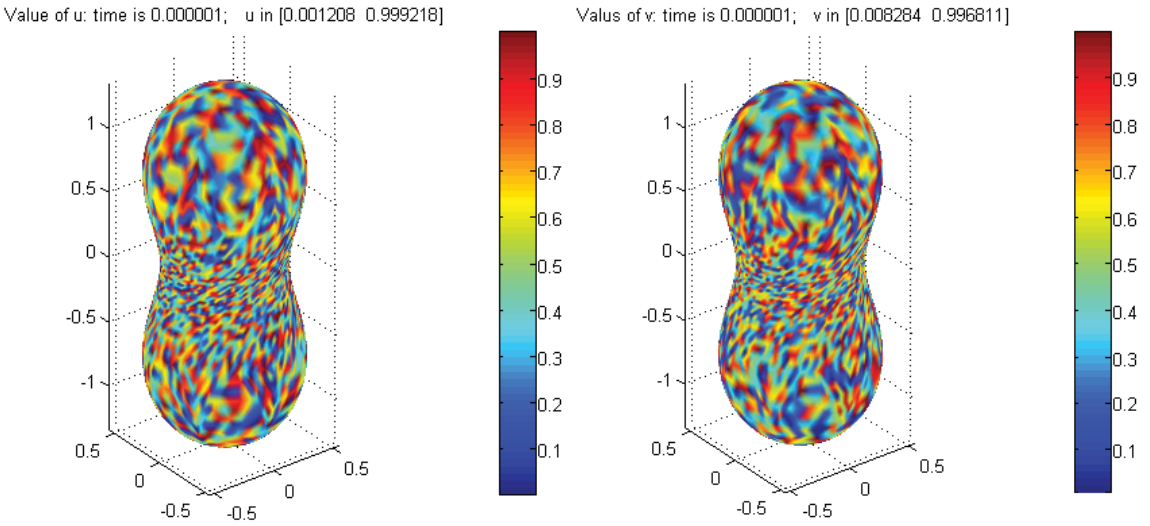

Fig. 10 Simulation of (4) and (21) on peanut at time 10^{-6}

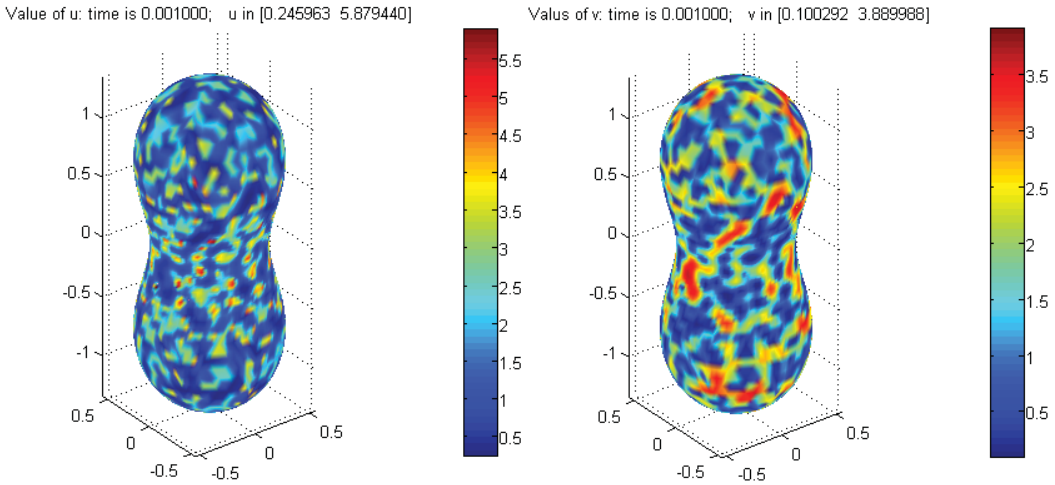

Fig. 11 Simulation of (4) and (21) on peanut at time 10^{-3}

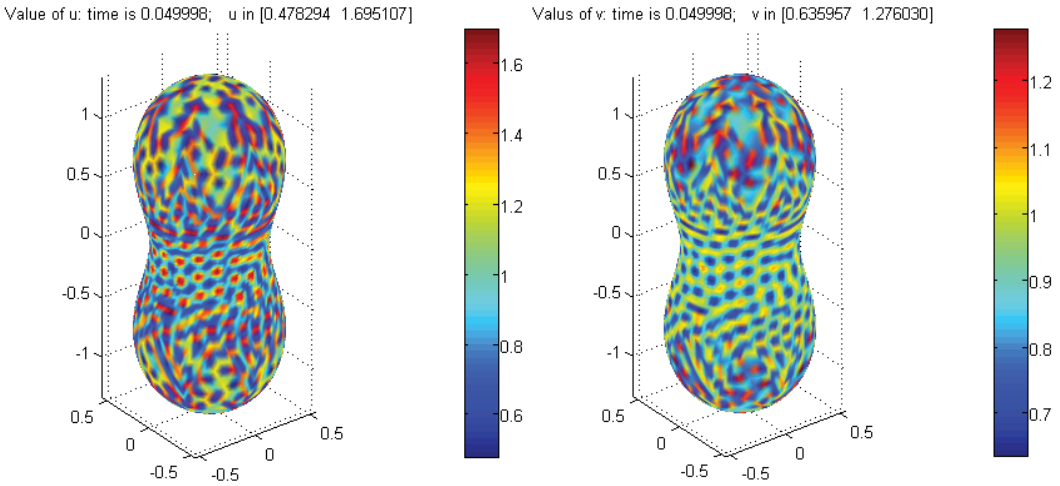

Fig. 12 Simulation of (4) and (21) on peanut at time 0.05

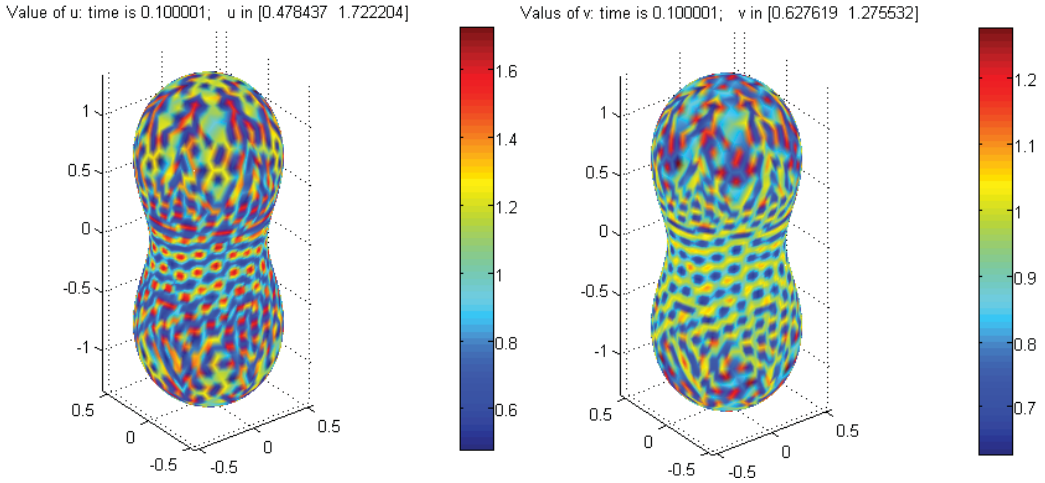

Fig. 13 Simulation of (4) and (21) on peanut at time 0.1

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