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A Numerical Method for Diffusion and Cahn-Hilliard Equations on Evolving Spherical Surfaces

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Abstract**—**In this paper, we present a simple effective numerical geometric method to estimate the divergence of a vector field over a curved surface. The conservation law is an important principle in physics and mathematics. However, many well-known numerical methods for solving diffusion equations do not obey conservation laws. Our presented method in this paper combines the divergence theorem with a generalized finite difference method and obeys the conservation law on discrete closed surfaces. We use the similar method to solve the Cahn-Hilliard equations on evolving spherical surfaces and observe stability results in our numerical simulations.

Keywords**—**Conservation laws, diffusion equations, Cahn-Hilliard Equations, evolving surfaces.

I. Introduction

FINDING numerical methods to compute partial differential equations on evolving surfaces is an interesting and difficult problem. These methods have many important applications in fluid dynamics, magnetohydrodynamics, image processing, and so on. See more details in [1], [2], [9]. In this note, we shall introduce a new numerical method for solving the diffusion equation on evolving closed surfaces that we proposed in 2016. This method is an intrinsic geometric method to deal with the discrete conservation law on evolving regular surfaces, and we shall improve the Cahn-Hilliard equation on evolving spherical surfaces by this method.

The Cahn-Hilliard equation with a variable mobility on a regular closed surface Σ takes the form:

$$\frac{\partial u(x,t)}{\partial t} = \nabla\cdot[M(u(x,t))\nabla\mu(u(x,t))],$$

$$x\in\Sigma\,,0<t\le T. \text{ and } \mu(u(x,t)) = F'(u(x,t)) - \varepsilon^2\Delta_\Sigma u(x,t)$$

where the quantity $u(x,t)$ is the difference between the mole fractions of binary mixtures. The function $F(u)=\frac{1}{4}(u^2-1)^2$ is the Helmholtz free energy per unit volume of a homogeneous fluid, and ε is a positive constant. See [10], [11] for more details.

II. Preliminaries

First, we introduce a discrete Laplace-Beltrami operator on a stationary surface that we proposed in 2013 and 2014 [3], [4].

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A. The Local Tangential Method [3]

Let $S=(V,F)$ be a triangular mesh with $V=\{p_i \mid 1\le i\le n_V\}$ the list of vertices and $F=\{T_k \mid 1\le k\le n_F\}$ the list of triangles. We introduce the approximating tangent plane $TS(p)$ at the vertex p of as:

1. The unit normal vector $N_A(p)$ at the vertex p in S is given by the weighted normal vector

$$N_A(p) = \sum_{k\in I(p)} w_{T_k} N_{T_k} \Big/ \left\| \sum_{k\in I(p)} w_{T_k} N_{T_k} \right\|, \tag{1}$$

where N_{T_k} is the unit normal vector of the triangle T_k including a vertex p. We refer to [3] for more details.

2. The approximating tangent space $TS(p)$ of S at p is now determined by

$$TS(p) = \left\{ w\in\mathbf{R}^3 \mid w\perp N_A(p) \right\}. \tag{2}$$

We can choose an orthonormal basis e_1, e_2 for the tangent plane $TS(p)$ of S at p. Hence, $\{e_1, e_2 N_A(p)\}$ forms an orthonormal basis for $\mathbf{R}^3$ and every $q\in\Sigma$ around p can be assigned a new xyz -coordinate by

$$x(q)e_1 + y(q)e_2 = (q-p) - \big((q-p)\cdot N_A(p)\big)N_A(p) \tag{3}$$

and

$$z(q) = h(x(p),y(p)) = (q-p)\cdot N_A(p). \tag{4}$$

Obviously, the new coordinate of p is $(0,0,0)$.

B. Discrete Tangential Gradient Vector

Since the gradient $\nabla_\Sigma f$ of a smooth function f on a regular surface Σ with a parametrization $\mathbf{x}(u,v)$ is given by

$$\nabla_\Sigma f = \frac{f_u G - f_v F}{EG-F^2}\mathbf{x}_u + \frac{f_v E - f_u F}{EG-F^2}\mathbf{x}_v \tag{5}$$

where *E, F,* and *G* are the coefficients of the 1st fundamental form of Σ and $f_u = \frac{\partial}{\partial u} f\big(\mathbf{x}(u,v)\big)$ and $f_v = \frac{\partial}{\partial v} f\big(\mathbf{x}(u,v)\big)$, we need to approximate the local parametrization of Σ around p and the differential quantities of the function f.

We shall construct a local parametrization by representing the regular surface Σ as locally a graph surface around the vertex p. Consider the triangular mesh $S=(V,F)$ 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 $p_0=p_n$. Suppose that the new coordinate of p_j is (x_j,y_j,z_j), and we denote $h(x_j,y_j)=z_j$. We use the polynomial fitting for the height function h of Σ around p. By the Taylor expansion, one has

$$\begin{aligned}&h(x_j,y_j)-h(0,0)=x_jh_x(0,0)+y_jh_y(0,0)\\&+\frac{1}{2}\left(x_j^2h_{xx}(0,0)+2x_jy_jh_{xy}(0,0)+y_j^2h_{yy}(0,0)\right)\\&+\cdots+O(r_j^m).\end{aligned}\tag{6}$$

for each $j=1,\cdots,n$.

Set $A=\begin{pmatrix}x_1&\cdots&x_n\\y_1&\cdots&y_n\\x_1^2&\cdots&x_n^2\\x_1y_1&\cdots&x_ny_n\\y_1^2&\cdots&y_1^2\end{pmatrix}$ and α_j, $j=1,\cdots,n$ is a set of real numbers. Then, we have

$$h_u(0,0)=\sum_{j=1}^{n}\alpha_j\left(h(u_j,v_j)-h(0,0)\right)+O(r^3)\tag{7}$$

if $A\begin{pmatrix}\alpha_1\\\vdots\\\alpha_n\end{pmatrix}=\begin{pmatrix}1&0&0&0&0\end{pmatrix}'$ and

$$h_v(0,0)=\sum_{j=1}^{n}\alpha_j\left(h(u_j,v_j)-h(0,0)\right)+O(r^3)\tag{8}$$

if $A\begin{pmatrix}\alpha_1\\\vdots\\\alpha_n\end{pmatrix}=\begin{pmatrix}0&1&0&0&0\end{pmatrix}'$.

Similarly, we can also approximate the differential quantities of the function f on Σ. Therefore, the gradient vector $\nabla_\Sigma f$ at p can be approximated by

$$\nabla_A f(p)=\frac{1}{1+h_u^2+h_v^2}\begin{pmatrix}f_u\left(1+h_u^2\right)-f_vh_uh_v\\f_v\left(1+h_v^2\right)-f_uh_uh_v\\f_u+f_v\end{pmatrix}.\tag{9}$$

We refer to [5] for the detail of the high-order approach.

Theorem 1. Using above notations, one has

$$\nabla_\Sigma f(p)=\nabla_A f(p)+O(r^2)\tag{10}$$

where

$$\nabla_A f(p)=\frac{1}{1+h_u^2+h_v^2}\begin{pmatrix}f_u\left(1+h_u^2\right)-f_vh_uh_v\\f_v\left(1+h_v^2\right)-f_uh_uh_v\\f_u+f_v\end{pmatrix}.\tag{11}$$

C. Discrete Laplace-Beltrami Operator

If X is a local vector field $X=A\mathbf{x}_u+B\mathbf{x}_v$ on $\mathbf{x}(U)\subset\Sigma$. The 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

$$Div_\Sigma X=\frac{1}{\sqrt{EG-F^2}}\left[\frac{\partial}{\partial u}\left(A\sqrt{EG-F^2}\right)+\frac{\partial}{\partial v}\left(B\sqrt{EG-F^2}\right)\right].\tag{12}$$

Note that the divergence theorem gives

$$\int_U Div_\Sigma X=\int_{\partial U}X\cdot\mathbf{n}\tag{13}$$

where $\mathbf{n}$ is the unit outward normal vector on ∂U.

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

$$\begin{aligned}\Delta_\Sigma f=\frac{1}{\sqrt{EG-F^2}}\Bigg[&\frac{\partial}{\partial u}\left(\frac{G}{\sqrt{EG-F^2}}f_u\right)\\&-\frac{\partial}{\partial u}\left(\frac{F}{\sqrt{EG-F^2}}f_v\right)+\frac{\partial}{\partial v}\left(\frac{E}{\sqrt{EG-F^2}}f_v\right)\\&-\frac{\partial}{\partial v}\left(\frac{F}{\sqrt{EG-F^2}}f_u\right)\Bigg].\end{aligned}\tag{14}$$

See [7], [8] for details.

We use the divergence theorem to give a discrete approximation of the divergence of a vector field X defined on a triangular surface mesh $S=(V,F)$. Consider a vertex $p\in V$ and let p_j, $j=0,1,\cdots,n$, be the neighboring vertices of p with $p_0=p_n$. These vertices p_j are labeled counterclockwise about the normal vector $N_A(p)$. Let T_j be the triangle with vertices p, p_j, and p_{j+1}. We define the approximating outer normal vectors $n(T_j,p_j)$ and $n(T_j,p_{j+1})$ of the triangle T_j at the vertex p_j and p_{j+1} in Σ by

$$n(T_j,p_j)=\frac{(p_{j+1}-p_j)\wedge N_A(p_j)}{\left\|(p_{j+1}-p_j)\wedge N_A(p_j)\right\|}\tag{15}$$

and

$$n(T_j, p_{j+1}) = \frac{(p_{j+1} - p_j) \wedge N_A(p_{j+1})}{\left\|(p_{j+1} - p_j) \wedge N_A(p_{j+1})\right\|}. \tag{16}$$

Since

$$\begin{aligned}\int_{\partial U} X \cdot \mathrm{n} = \sum_{j=0}^{n-1} \Bigg\{ & \frac{\|p_{j+1} - p_j\|}{6} (1 + O(r^2)) \big[2X(p_j) \cdot n(T_j, p_j) \\ & + X(p_{j+1}) \cdot n(T_j, p_j) + 2X(p_{j+1}) \cdot n(T_j, p_{j+1}) \\ & + X(p_j) \cdot n(T_j, p_{j+1})\big](1 + O(r))\Bigg\}\end{aligned} \tag{17}$$

and

$$\int_{\mathrm{U}} Div_\Sigma X = \left(\sum_{j=0}^{n-1} |T_j| (1 + O(r^2)) \right) (Div_\Sigma X(p) + O(r)). \tag{18}$$

We can now define the discrete divergence $Div_A X$ of a vector field on the triangular surface mesh $\mathbf{S}$ by

$$\begin{aligned}Div_A X(p) = \frac{1}{\sum_{k=0}^{n-1} |T_k|} \Bigg[& \sum_{j=0}^{n-1} \frac{\|p_{j+1} - p_j\|}{6} \big((2X(p_j) + X(p_{j+1})\big) \cdot n(T_j, p_j) \\ & + \big(X(p_j) + 2X(p_{j+1})\big) \cdot n(T_j, p_{j+1}) \Bigg]\end{aligned} \tag{19}$$

where $|T_k|$ denotes the area of the triangle T_k.

Theorem 2. Let f be a smooth function defined on a regular surface Σ and the vector field $\nabla_A f$ on S satisfy

$$\nabla_\Sigma f = \nabla_A f + O(r^2) \tag{20}$$

where $\nabla_\Sigma f$ is the gradient vector field of f on Σ. Then, we have

$$\Delta_\Sigma f(p) = Div_A(\nabla_A f)(p) + O(r). \tag{21}$$

III. Discrete Algorithms of PDEs on Evolving Surfaces

Next, we discuss the discrete algorithms about the diffusion equation and Cahn-Hilliard equation on evolving surfaces.

A. Diffusion Equations on Evolving Surfaces

Let $\{\Sigma(t)\}$, $t \in [0,T]$, denote a moving oriented regular surfaces in $\mathbf{R}^3$. Suppose that these regular surfaces are moving with prescribed velocity field $X(t)(p(t))$, $p(t) \in \Sigma(t)$. We want to solve the surface diffusion equation:

$$\partial_t^* h + h \nabla_{\Sigma(t)} \cdot X - \Delta_{\Sigma(t)} h = 0 \tag{22}$$

on evolving surfaces $\Sigma(t)$. Here, $\partial_t^* = \partial_t + X \cdot \nabla$ is the material derivative. See Elliott and Ranner [11] for more details.

After some direct computations, one has

$$\begin{aligned}\frac{dh(t)}{dt}(u,v) + \frac{1}{2} h(t)(u,v)[div_{\Sigma(t)} V(t)(u,v) \\ - 4c(t)(u,v)H(t)(u,v)] = \Delta_{\Sigma(t)} h(t)(u,v),\end{aligned} \tag{23}$$

where $H(t)(u,v)$ is the mean curvature on the surface $\Sigma(t)$.

The is the equation for the conservation law on the evolving surface $\Sigma(t)$ with the velocity field $X(t)(u,v) = V(t)(u,v) + c(t)(u,v)N(t)(u,v)$. See [6] about these computations.

Since the divergence theorem, integrating (22) on a portion $U(t) \subset \Sigma(t)$, one has

$$\int_{U(t)} \partial_t^* h + h \nabla_{\Sigma(t)} \cdot X = \int_{U(t)} \Delta_{\Sigma(t)} h \tag{24}$$

and this is equivalent to

$$\frac{d}{dt} \int_{U(t)} h = \int_{U(t)} \Delta_{\Sigma(t)} h = \int_{\partial U(t)} \nabla_{\Sigma(t)} h \cdot \mathbf{n}(t). \tag{25}$$

After an explicit time discretization, (25) becomes

$$\frac{1}{\tau^n} \left(\int_{U^{n+1}} h^{n+1} - \int_{U^n} h^n \right) = \int_{U^n} \Delta_{\Sigma^n} h^n = \int_{\partial U^n} (\nabla_{\Sigma^n} h^n) \cdot \mathbf{n}(t) \tag{26}$$

or

$$\left(\int_{U^{n+1}} h^{n+1} \right) = \int_{U^n} h^n + \tau^n \int_{U^n} \Delta_{\Sigma^n} h^n \tag{27}$$

After space discretization, (27) yields

$$h^{n+1}(p^{n+1}) = \frac{\sum_{p^n \in T_k^n} |T_k^n|}{\sum_{p^{n+1} \in T_k^{n+1}} |T_k^{n+1}|} \left[\left(h^n(p^n) + \tau^n \Delta_{\Sigma^n} h^n(p) \right) \right] \tag{28}$$

Now our two-step algorithm can be stated as follows.

Step 1: For each p, use the above method to compute the Laplae-Beltrami operator $\Delta_A h^j(p^j)$ and set

$$\bar{h}^j(p^j) = h^j(p^j) + \tau^j \Delta_A h^j(p^j) \tag{29}$$

Step 2: Let p_k^j, $k = 0,1,\cdots,n$, be the neighboring vertices of p^j with $p_0^j = p_n^j$. These vertices p_k^j are labeled counterclockwise about the normal vector $N_A(p^j)$ of the surface Σ^j at the vertex p^j in the space $\mathbf{R}^3$. Let T_k^j be the triangle with vertices p^j, p_k^j and p_{k+1}^j, $j \geq 0$. We set

$$h^{j+1}(p^{j+1}) = \frac{\sum_k |T_k^j|}{\sum_k |T_k^{j+1}|} \bar{h}^j(p^j). \tag{30}$$

One can find the proofs of the convergence and conservation law of this method in [6].

B. Cahn-Hilliard Equation on Evolving Surfaces

We solve the Cahn-Hilliard equation

$$u_t = \Delta_{\Sigma(t)}\left(u^3 - u - \varepsilon^2 \Delta_{\Sigma(t)} u\right) \tag{31}$$

on an evolving surface $\Sigma(t)$.

Set $\phi = u^3 - u - \varepsilon^2 \Delta_{\Sigma(t)} u$, then (31) can be rewritten as

$$\begin{cases} u_t = \Delta_{\Sigma(t)}\phi, \\ \phi = u^3 - u - \varepsilon^2 \Delta_{\Sigma(t)} u. \end{cases} \tag{32}$$

Using the explicit time discretization, the first equation in (28) becomes

$$\frac{u^{n+1} - u^n}{\tau^n} = \Delta_{\Sigma^n}\phi^n \tag{33}$$

or

$$u^{n+1} = u^n + \tau^n \Delta_{\Sigma^n}\phi^n. \tag{34}$$

The function ϕ^n is given by

$$\phi^n = (u^n)^3 - u^n - \varepsilon^2 \Delta_{\Sigma^n} u^n. \tag{35}$$

IV. Simulations

Now we solve (32) with $\varepsilon = 0.1$ on two different evolving surfaces. All initial conditions of our simulations are the same random numbers in $[-0.5, 0.5]$, and the time step is $\frac{r^2}{100}$.

We solve (32) on the unit sphere moving with a prescribed velocity

$$\mathbf{X}(t,p) = \begin{pmatrix} 0.5s\pi\cos(st\pi)\sin(0.5z\pi) \\ 0 \\ 0 \end{pmatrix} \tag{36}$$

and

$$\mathbf{Y}(t,p) = \begin{pmatrix} 0.5s\cos(st\pi)\cos(0.5z\pi) \\ 0 \\ 0 \end{pmatrix} \tag{37}$$

where $p = (x, y, z)$ in the unit sphere and s is a nonzero real number. We show all solution of (34) at times are 0.75 and 1.

Fig. 1 shows the solution of (32) on a stationary unit sphere. Figs. 2-7 present the numerical solutions of (32) with $s = 1, 2, 10, 50, 250,$ and 500. Fig. 8 is the solution with $\mathbf{X}(t,p) = (500\pi\cos(500t\pi)\sin(0.5z\pi) \quad 0 \quad 0)$. Fig. 9 shows the Ginzberg-Landau free energy of (32) on the moving surfaces with different s in (36).

Figs. 10-15 show the numerical solution on a unit sphere with velocity field $\mathbf{Y}$.

V. Conclusion

Conservation laws play important key roles in the partial differential equation on surfaces. An efficient numerical method should at least obey the conservation law. Our proposed method obeys the discrete conservation law. Furthermore, the Ginzberg-Landau free energy is decreasing in our simulations.

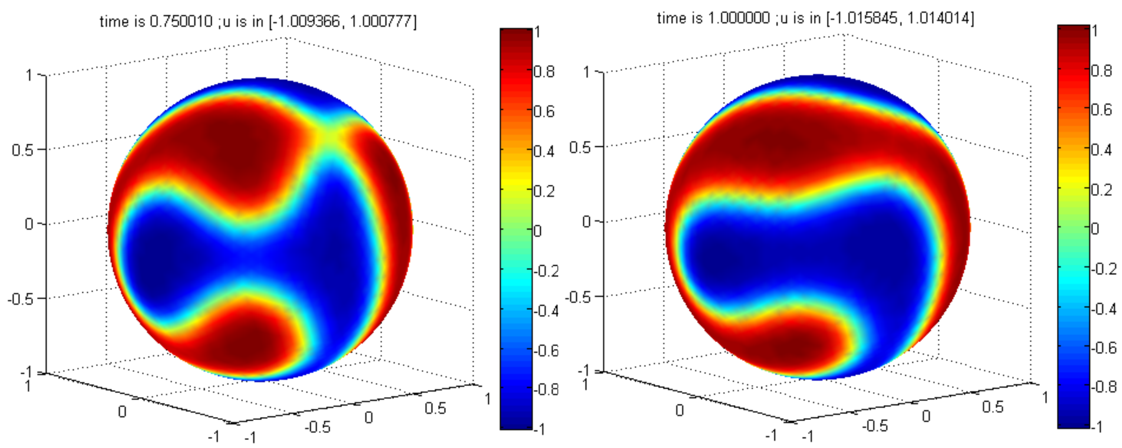

Fig. 1 The solution of (26) on a unit sphere

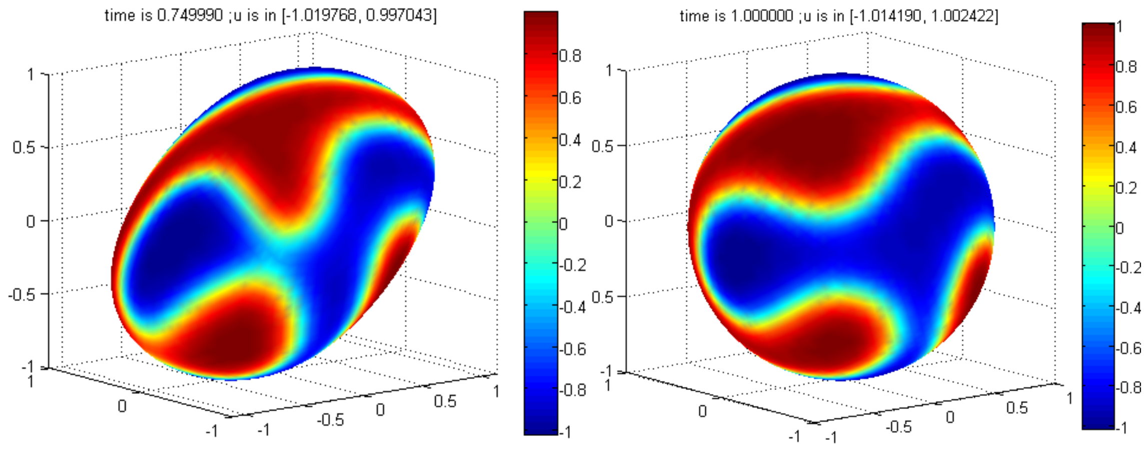

Fig. 2 The solution of (26) with $s=1$ in the velocity field $\mathbf{X}$

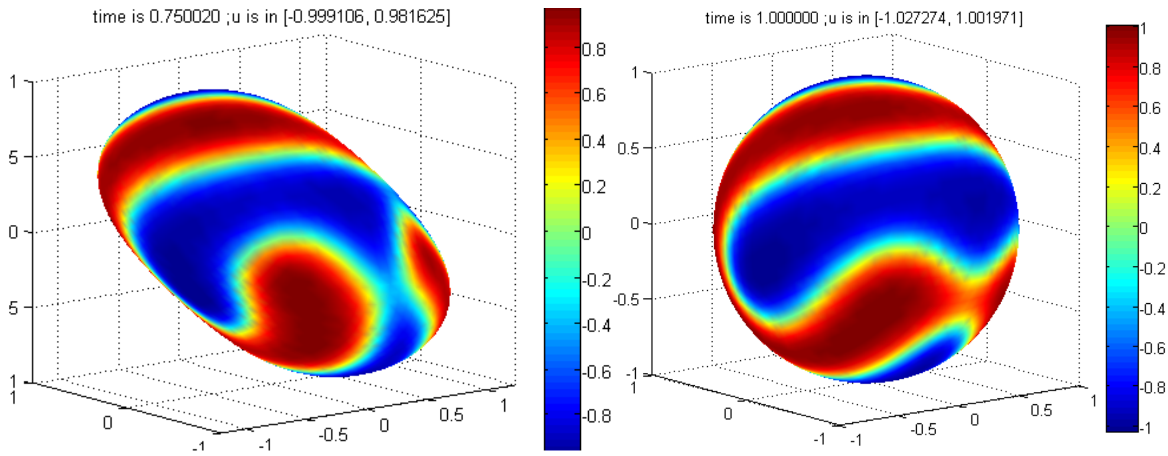

Fig. 3 The solution of (26) with $s=2$ in the velocity field $\mathbf{X}$

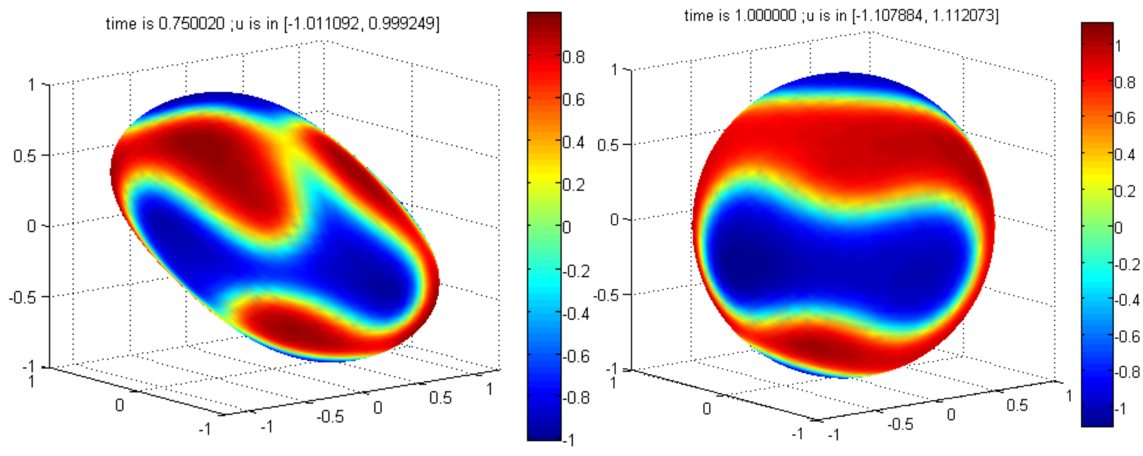

Fig. 4 The solution of (26) with $s=10$ in the velocity field $\mathbf{X}$

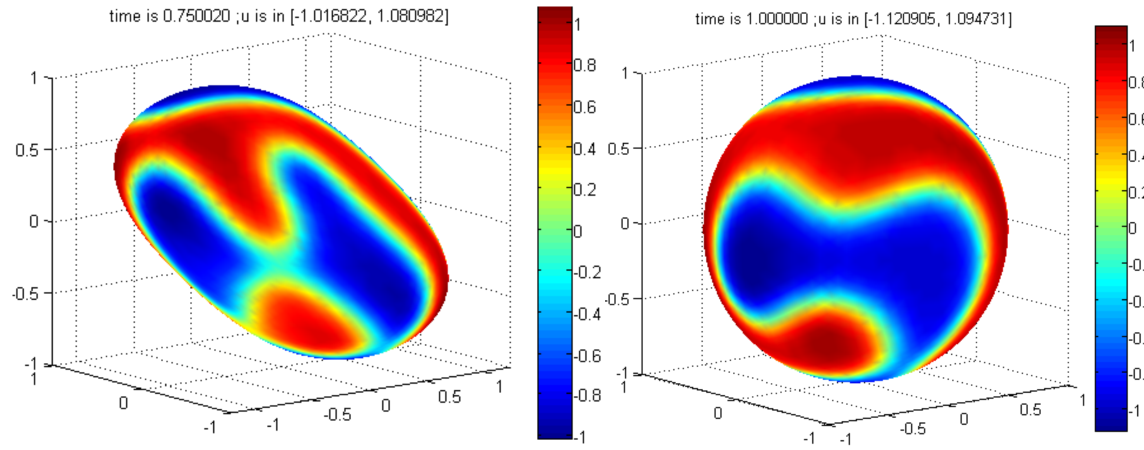

Fig. 5 The solution of (26) with $s = 50$ in the velocity field $\mathbf{X}$

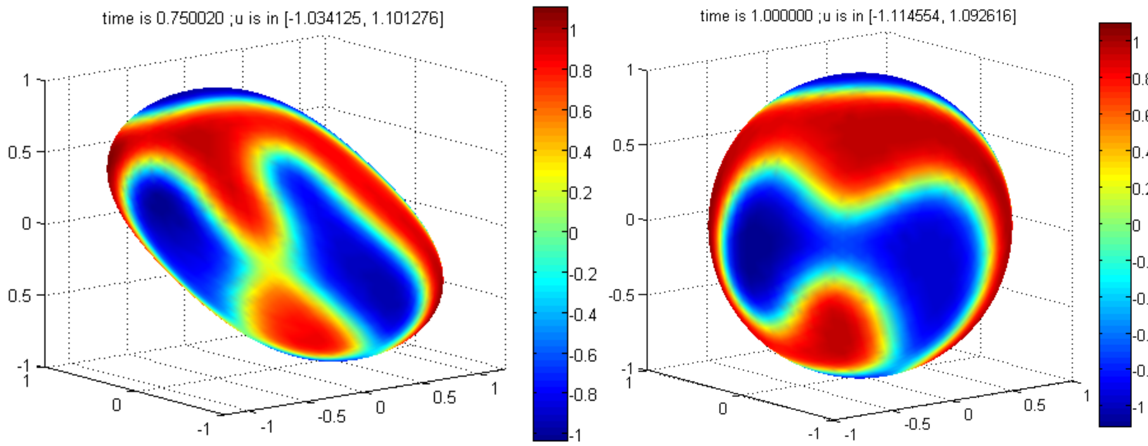

Fig. 6 The solution of (26) with $s = 250$ in the velocity field $\mathbf{X}$

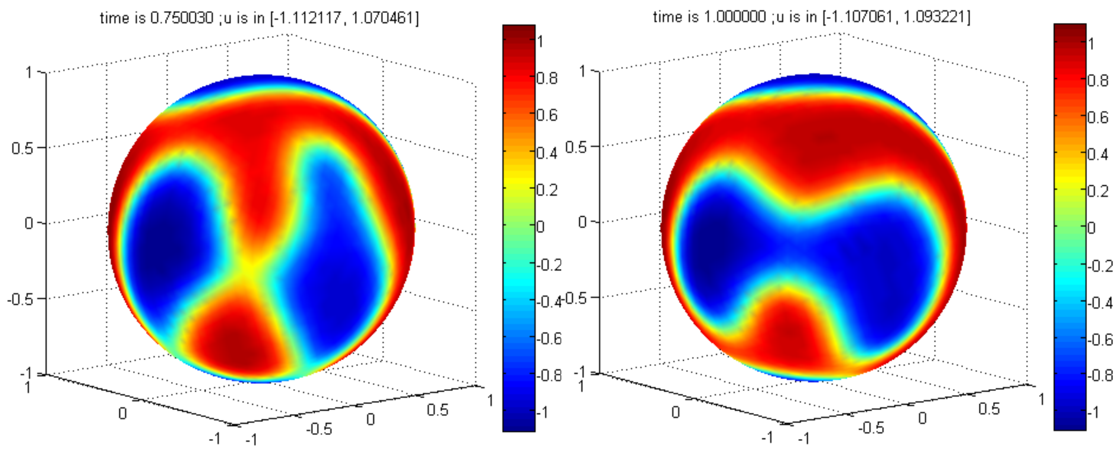

Fig. 7 The solution of (26) with $s = 500$ in the velocity field $\mathbf{X}$

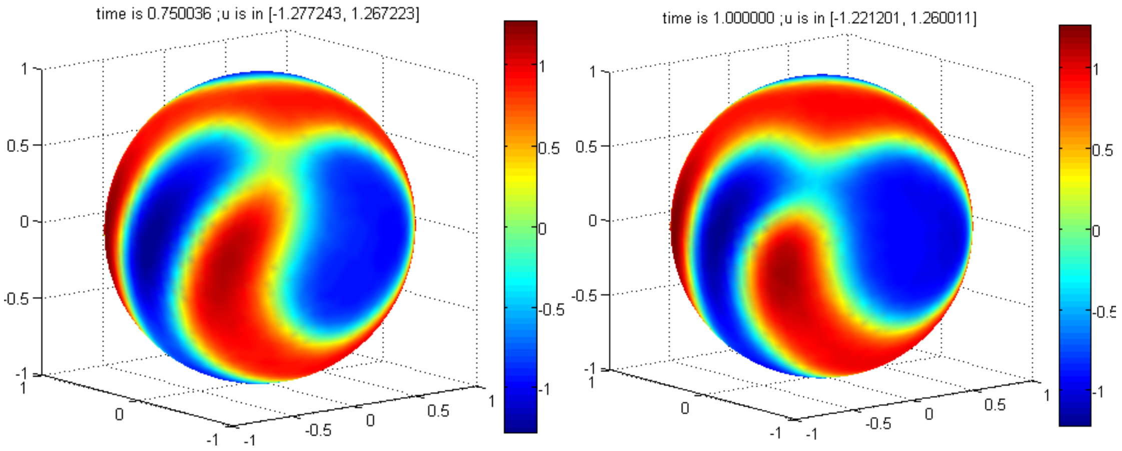

Fig. 8 The solution of (26) with $\mathbf{X}(1) = 500\pi\cos(500t\pi)\sin(0.5z\pi)$

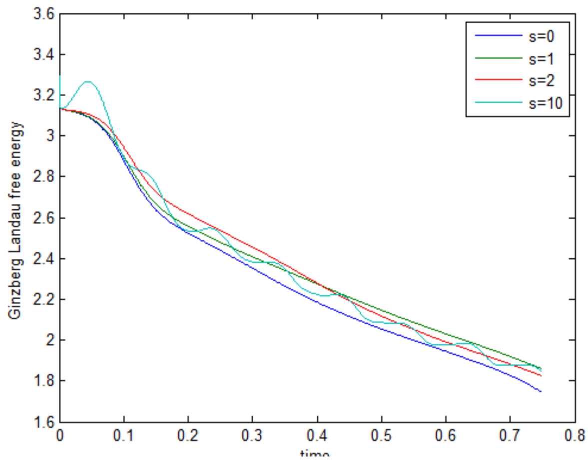

Fig. 9 The Ginzberg-Landau free energy with different s

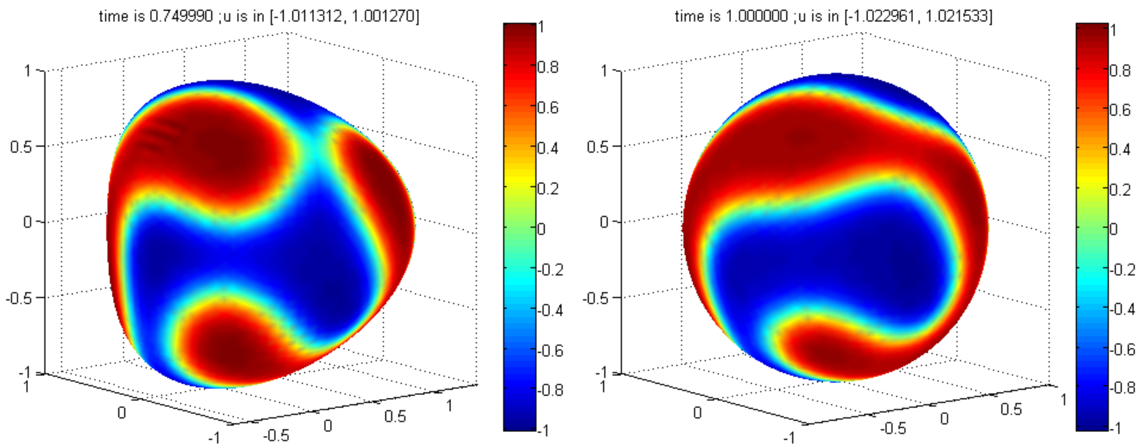

Fig. 10 The solution of (26) with $s = 1$ in the velocity field $\mathbf{Y}$

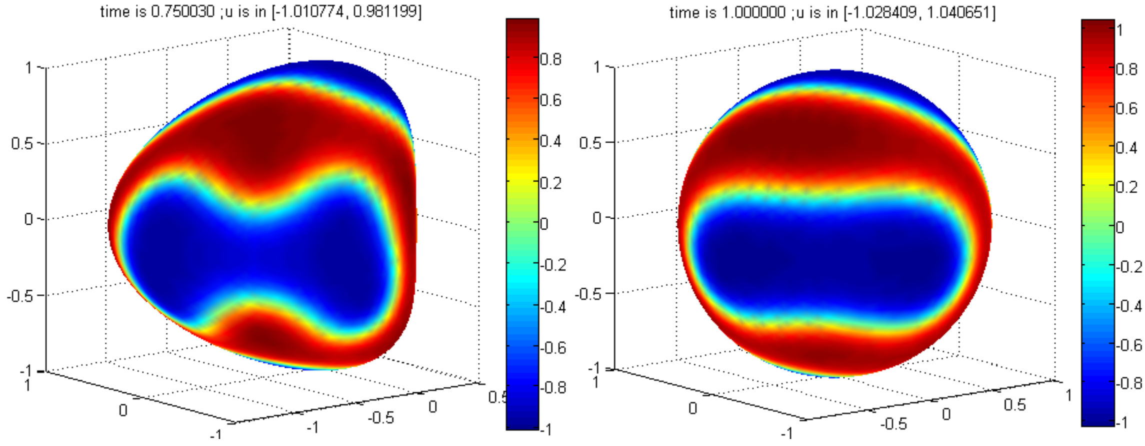

Fig. 11 The solution of (26) with $s = 2$ in the velocity field $\mathbf{Y}$

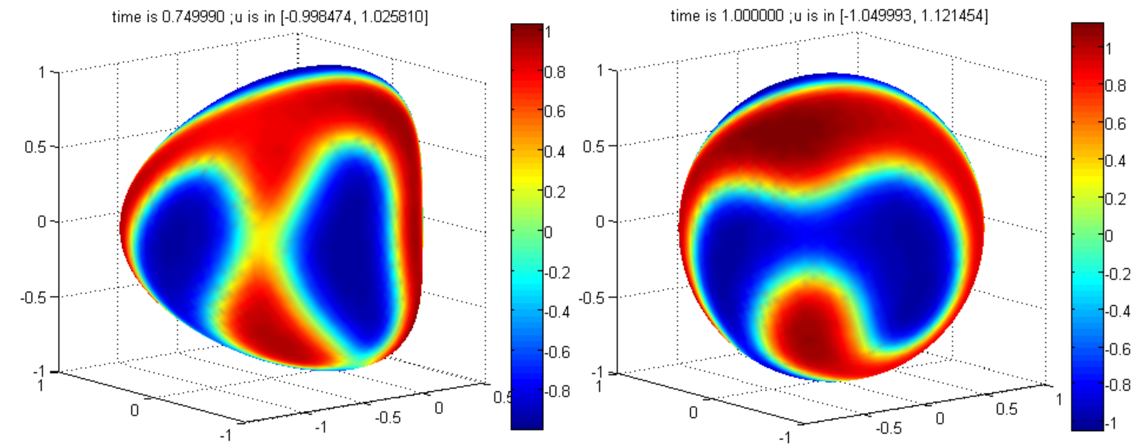

Fig. 12 The solution of (26) with $s = 10$ in the velocity field $\mathbf{Y}$

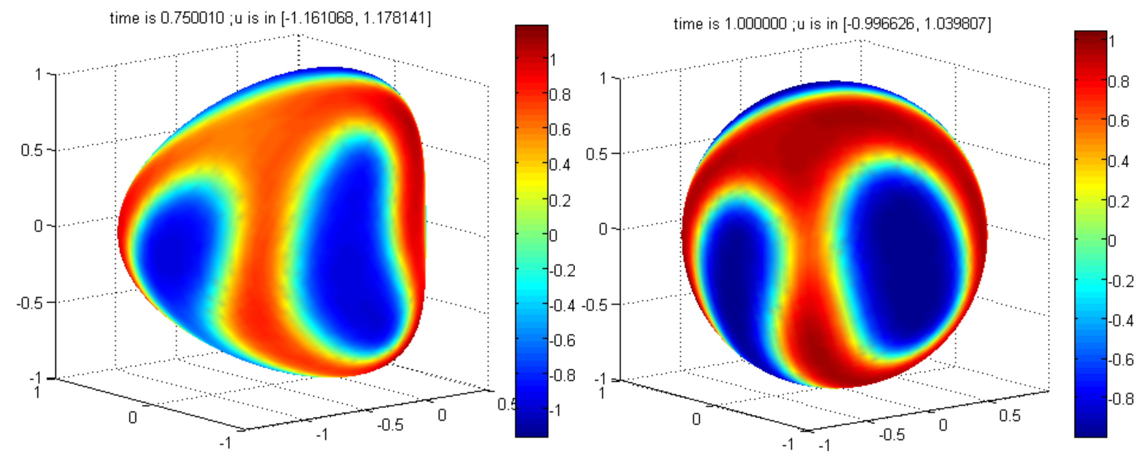

Fig. 13 The solution of (26) with $s = 50$ in the velocity field $\mathbf{Y}$

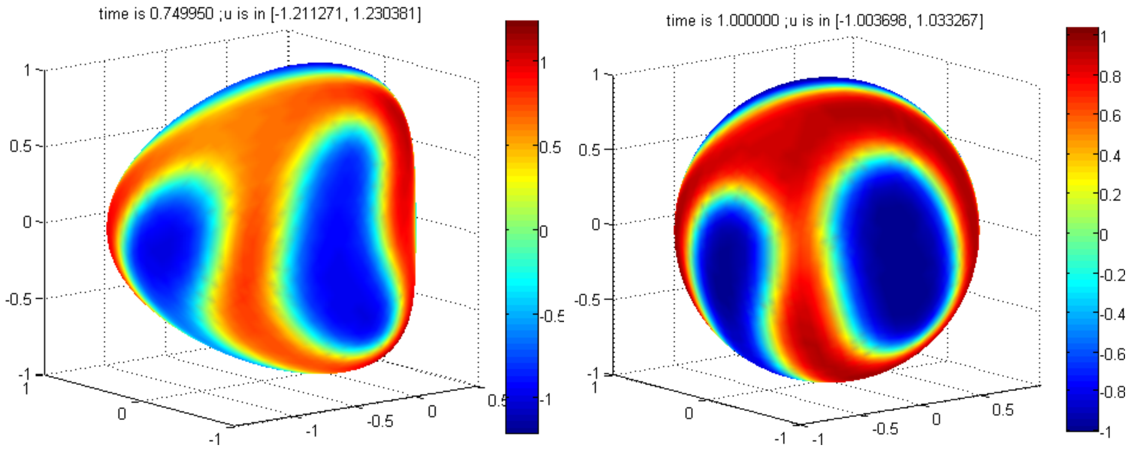

Fig. 14 The solution of (26) with $s = 250$ in the velocity field $\mathbf{Y}$

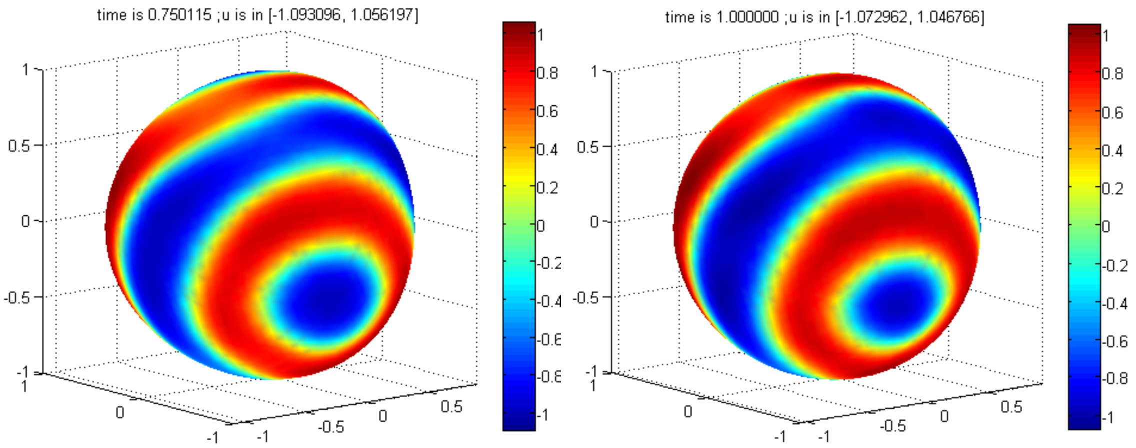

Fig. 15 The solution of (26) with $s = 500$ in the velocity field $\mathbf{Y}$

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