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The local integral equation method for pattern formation simulations in reaction–diffusion systems

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ABSTRACT

A meshless local integral equation (LIE) method is proposed for numerical simulation of 2D pattern formation in nonlinear reaction diffusion systems. The method uses weak formulation of the differential governing equations on local sub-domains with using the Green function of the Laplace operator as the test function. The moving least square (MLS) approximation is employed for spatial variations of field variables while the time evolution is discretized by using suitable finite difference approximations. The effect of parameters and conditions are studied by considering the well known Schnakenberg model.

1. Introduction

It is well known a homogenizing influence of diffusion in nature. Alan Turing was the first who discovered that spatial patterns would be formed by a reaction–diffusion system combining local activation with long range inhibition [1]. He demonstrated how a simple model system of coupled reaction–diffusion equations could give rise to spatial patterns in chemical concentrations through a process of chemical instability (diffusion driven instability). Turing also pointed out the role of such patterns in biological pattern formation. The first experimental evidence supporting the Turing instability was found in chemistry rather recently [2,3]. A large variety of pattern formation with various applications has been explained by Turing type models. It is not the aim of this paper to give a review of such application and modeling of pattern formation [4,5]. Recall that several Turing models have been developed such as the Gierer–Meinhardt model [6], Gray–Scott model [7], Lengyel–Epstein model [8], Brusselator model [9], Schnakenberg model [10] and Selkov model [11].

A typical Turing system is a reaction–diffusion system consisting of at least two chemical species (activator and inhibitor) exhibiting a steady state which is stable to small perturbations in the absence of diffusion, but becomes unstable when diffusion is present (Turing instability). The formation of spatial patterns is principally a nonlinear phenomenon. Otherwise the unstable modes would grow unlimitedly. Linear theory does determine conditions under which spontaneous pattern formation is allowed for certain parameter ranges [4]. Initial and boundary conditions, the shape and size of the domain yield various forms of patterns. To determine which of the various possible patterns will be stable or which conversion takes place, one has to go beyond linear theory. Various numerical methods have been used to solution of nonlinear reaction–diffusion systems and computer simulations of pattern formation. In [12], the authors applied a moving grid finite element method to some models of the Turing problem, where the mesh movement was prescribed to mimic the growth that is observed in nature. Shakeri and Dehghan [13] combined the spectral element method and finite volume technique for numerical solution of the Turing model, Zhu et al. [14] applied Discontinuous Galerkin method to reaction–diffusion systems in developmental biology.

In recent decades, various mesh-free methods have been successful in solution of many scientific and engineering problems. Besides avoiding mesh generation, one could name other advantages such as elimination of re-meshing, elimination of failure of numerical stability due to large distortions of finite elements, convenient modeling of separable media and problems with moving boundaries. Therefore one can expect the mesh-free methods to become attractive also in numerical simulations of nonlinear coupled reaction–diffusion problems [15,16]. In these works, the authors developed weak formulations of general reaction–diffusion problems on local subdomains with using meshless approximation for field variables. The test functions have been utilized either as the Heaviside function or the Green's function. The accuracy of the proposed methods has been verified on examples with analytical benchmark

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solutions. In [20], the authors modified the formulation given in [15] by simple replacement of the MLS-approximation by moving Kriging interpolation and verified the technique on the same numerical examples as used in [16]. The strong mesh-free formulations have been developed and applied to reaction-diffusion [21] and advection–diffusion–reaction equations [22]. In [21], the effects of various geometries on resulting patterns have been studied in Schankenberg as well as in Gierer–Meinhardt model. In [21], the MLS approximation is used for spatial variations of field variables while the radial basis functions in view of multiquadrics in [22].

In this paper, the formulation given in [16] is extended to numerical simulations of pattern formation in nonlinear reaction–diffusion systems exhibiting diffusion driven instability after spatial perturbation of homogeneous steady state initial conditions. The local integral equation (LIE) method is developed for numerical simulations of 2-d pattern formation in reaction–diffusion systems. The method is truly meshless, since no elements are required either for approximations or for integration in the analyzed domain. The moving least square (MLS) approximation is employed for spatial variations of field variables while the time evolution is discretized by using the one-step θ method. The nodal points are distributed freely inside the analyzed domain and on its boundary without using any connectivity among nodes. The LIE is a weak formulation of the differential governing equations on local sub-domains considered around each interior node with using the Green function of the Laplace operator as the test function. Thus the integral form of the governing equations is the integral representation of field variables at interior nodes. The appropriate choice of the shape of sub-domains enables us to find the Green function vanishing on the boundary of the sub-domain and so eliminate the normal derivatives of the field variables from the formulation. This is valuable achievement since the accuracy of approximations for derivatives is lower than for primary fields and also the evaluation of derivatives at integration points prolongs the computation. The nonlinear terms are treated iteratively within each time step. The paper is organized as follows. In Section 2, mathematical formulation of reaction–diffusion problems is summarized and the main results of the linear theory of stability analysis [4] are overviewed. In Section 3, the LIE formulation for solution of initial-boundary value problems in reaction-diffusion systems is presented. Section 4 is devoted to numerical simulations in order to verify the developed method. Attention is paid to illustrate the dependence of pattern shape on the initial conditions, size and shape of the analyzed domain. Our conclusions are summarized in Section 5.

2. Mathematical formulation of reaction–diffusion problems

The governing equations for the concentrations of two chemicals $u(\mathbf{x},t)$and $v(\mathbf{x},t)$subjected to reaction–diffusion processes are given as follows [4]:

$$\frac{\partial u}{\partial t}=\nabla^2 u+\gamma f(u,v),\ \ \frac{\partial v}{\partial t}=d\nabla^2 v+\gamma g(u,v)\ \text{ in }\ \Omega[0,T]. \tag{1}$$

These equations must be completed with prescription of the initial values $\{u(\mathbf{x},0),\ v(\mathbf{x},0)\}$ and the boundary conditions which are usually taken as the Neumann type

$$\frac{\partial u}{\partial \mathbf{n}}=0,\ \ \frac{\partial v}{\partial \mathbf{n}}=0 \text{ on } \partial\Omega \tag{2}$$

The zero flux conditions imply no external input. If we imposed fixed boundary conditions on u and v, the spatial patterning could be a direct consequence of the boundary conditions (as it can be seen in ecological problems).

The relevant homogeneous steady state $(u_0,\ v_0)$ of (1) is the positive solution of

$$f(u,v)=0,\ \ g(u,v)=0.$$

Since we are concerned with diffusion-driven instability, the steady state must be homogeneous and satisfy the following equations:

$$\frac{\partial u}{\partial t}=\gamma f(u,v),\ \ \frac{\partial v}{\partial t}=\gamma g(u,v), \tag{3}$$

which becomes

$$\frac{\partial w}{\partial t}=\gamma A\, w,\ \ A=\begin{pmatrix} f_{,u} & f_{,v} \\ g_{,u} & g_{,v}\end{pmatrix} \tag{4}$$

for $w=(u-u_0,\ v-v_0)^T$, assuming linear stability about the steady state $(u_0,\ v_0)$. The partial derivatives of $f$and $g$are taken to be evaluated at the steady state. Looking for the time evolution in the form $w\sim e^{\omega t}$, where ω is the eigenvalue, we get the condition $\mathrm{Re}\,\omega<0$for requirement of linear stability of the steady state $w=0$. It can be shown [4] that the linear stability is guaranteed if

$$f_{,u}+g_{,v}<0,\ \ f_{,u}g_{,v}-f_{,v}g_{,u}>0. \tag{5}$$

The solution of the linearized full reaction–diffusion system (1),

$$\frac{\partial w}{\partial t}=D\nabla^2 w+\gamma A\, w,\ \ D=\begin{pmatrix}1 & 0\\ 0 & d\end{pmatrix}, \tag{6}$$

can be expanded as follows:

$$w(\mathbf{x},t)=\sum_k c_k e^{\omega t}W_k(\mathbf{x}), \tag{7}$$

with $W_k(\mathbf{x})$ being the eigenfunction of the Laplace operator corresponding to the eigenvalue k^2. The expansion coefficients c_k being determined by a Fourier expansion of the initial conditions in terms of $W_k(\mathbf{x})$. The eigenvalue ωdetermines temporal growth of the linearized solution. For particular k^2, the values $\omega(k^2)$ are determined by the roots of the characteristic equation

$$\omega^2+\omega\left[k^2(1+d)-\gamma(f_{,u}+g_{,v})\right]+h(k^2)=0 \tag{8}$$

with

$$h(k^2)=k^4 d-k^2\gamma(df_{,u}+g_{,v})+\gamma^2(f_{,u}g_{,v}-f_{,v}g_{,u}) \tag{9}$$

In the absence of any spatial effects $(k^2=0)$ we have already imposed constraints resulting from the requirement of the linear stability of the homogeneous steady state solution. For the steady state to be unstable to spatial disturbances we require $\mathrm{Re}\,\omega(k^2)>0$ for some $k^2\neq 0$. This can happen only if $h(k^2)<0$ for some $k^2\neq 0$, since the roots are given by the following equation:

$$\omega=-\frac{1}{2}\left[k^2(1+d)-\gamma(f_{,u}+g_{,v})\right]\pm\frac{1}{2}\left\{\left[k^2(1+d)-\gamma(f_{,u}+g_{,v})\right]^2-4h(k^2)\right\}^{1/2} \tag{10}$$

and $[k^2(1+d)-\gamma(f_{,u}+g_{,v})]>0$ because $f_{,u}+g_{,v}<0$, $k^2(1+d)>0$ for $k^2\neq 0$.

Since $(f_{,u}g_{,v}-f_{,v}g_{,u})>0$, the only possibility for $h(k^2)$ to be negative is if $(df_{,u}+g_{,v})>0$. This implies that $d\neq 1$ and $f_{,u}g_{,v}<0$ because $f_{,u}+g_{,v}<0$ from (5).

$$(df_{,u}+g_{,v})>0, d\neq 1 \tag{11}$$

The conditions are necessary but not sufficient for $\mathrm{Re}\,\omega(k^2)>0$. For $h(k^2)$ to be negative for some $k^2\neq 0$, the minimum h_{min} must be negative, hence and from (9)

$$h_{\min}=\gamma^2(f_{,u}g_{,v}-f_{,v}g_{,u})-dk_m^4,\ \ k_m^2=\gamma\frac{df_{,u}+g_{,v}}{2d}. \tag{12}$$

Thus, the condition that $h(k^2)<0$ for some $k^2\neq 0$ is as follows:

$$\frac{(df_{,u}+g_{,v})^2}{4d}>(f_{,u}g_{,v}-f_{,v}g_{,u}). \tag{13}$$