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A Meshfree Technique for Numerical Simulation of Reaction-Diffusion Systems in Developmental Biology

Zahra Jannesari[1] and Mehdi Tatari[1,2,*]

[1] *Department of Mathematical Sciences, Isfahan University of Technology, Isfahan, 84156-83111, Iran*
[2] *Institute for Research in Fundamental Sciences (IPM), P.O. Box: 19395-5746, Tehran, Iran*

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Abstract. In this work, element free Galerkin (EFG) method is posed for solving nonlinear, reaction-diffusion systems which are often employed in mathematical modeling in developmental biology. A predicator-corrector scheme is applied, to avoid directly solving of coupled nonlinear systems. The EFG method employs the moving least squares (MLS) approximation to construct shape functions. This method uses only a set of nodal points and a geometrical description of the body to discretize the governing equation. No mesh in the classical sense is needed. However a background mesh is used for integration purpose. Numerical solutions for two cases of interest, the Schnakenberg model and the Gierer-Meinhardt model, in various regions is presented to demonstrate the effects of various domain geometries on the resulting biological patterns.

AMS subject classifications: 65M99, 92B99

Key words: Element free Galerkin (EFG) method, reaction-diffusion systems, meshfree methods, MLS approximation, developmental biology.

1 Introduction

1.1 Reaction-diffusion equations

One of the important class of partial differential equations, are reaction-diffusion equations. These equations are frequently encountered in mathematical biology, ecology, chemistry and physics. This type of equations leads to interesting phenomena, such as pattern formation far from equilibrium, shading and pulse splitting. Biologists and

*Corresponding author.
Email: z.jannesari@math.iut.ac.ir (Z. Jannesari), mtatari@cc.iut.ac.ir (M. Tatari)

mathematicians have explored stable patterns, like spots and stripes by several reaction-diffusion systems. Alan Turing in [41], created a mathematical model describing the growing embryo's sequential changes that occur from fertilization to birth. He defined the mechanism in the context of biological morphogenesis, which showing that reactions between two diffusible chemicals (morphogens) could give rise to spatially heterogeneous concentrations through an instability driven by diffusion. Turing [41], Madzvamuse [24–27] have proposed numerical simulations considering growing dominion conditions and particular geometries modifying distribution patterns. The simplest and most typical Turing reaction-diffusion system consists of two chemical species, usually referred to as activator and inhibitor u and v as follows:

$$\frac{\partial u}{\partial t} = \gamma f(u,v) + \nabla^2 u, \tag{1.1a}$$

$$\frac{\partial v}{\partial t} = \gamma g(u,v) + d\nabla^2 v, \tag{1.1b}$$

where $d = d_v/d_u$ is the relationship between these species diffusion coefficients, while γ is a non-dimension coefficient associated with reactive processes f and g [15] that is proportional to the length of the domain.

In 1952, Turing in [41] suggested that chemicals can react and diffuse to produce patterns. Therefore, the formation of patterns in an organism can be modeled by a series of reaction-diffusion equations for the interacting species. Some authors have been studying another biological situations like animal skin pattern formation [13, 26, 28, 31], bone, tissue and tumor formation [7, 12, 14], animal population distribution [5, 42]. Therefore, different numerical techniques for solution of the reaction-diffusion problem have been implemented, like finite difference methods [4, 8, 20, 31], finite element methods [7, 24, 25], spectral element methods [19], finite volume spectral element method [37] and meshfree finite point method [39]. Many initial studies on Turing pattern formation have been devoted to work on fixed meshes.

The growing nature of reaction-diffusion problems (in a biological context) have led to studies on growing meshes. For example, Madzvamuse [26] has studied the incidence of mesh growth in diffusion formation of pattern. In this seminal work, Madzvamuse suggested an algorithm for 2D diffusion-reaction problem solution using a continuously growing Eulerian dominion. For example, [25] introduced a mesh growing finite element technique application for biological problems.

In this study, a meshfree method for solving the reaction-diffusion system in complex domains is considered.

1.2 A brief review on meshfree methods

Conventional numerical methods such as finite element method (FEM) and finite volume method (FVM) need an a priori definition of the connectivity of the nodes, i.e., these methods rely on a mesh. Mesh generation has always posed challenges for computational scientists, because of its complication and time consuming.