CAPTER 1 INTRODUCTION

1.1 Rationale

Systems of reaction-diffusion have a long history since the pioneering work by Alan Turing (1952). They have many important applications in mathematical physics, chemistry and biology. Turing presented that a chemistry state is stable against perturbations in the absence of diffusion and may become unstable to perturbations in the presence of diffusion. Arbitrary random deviations of the stationary state and results in stationary spatially periodic variations in concentration initiated Turing or diffusion driven, i.e., chemical patterns. The reaction-diffusion equation is often solved by numerical methods and usually diffusion is thought to be stabilizing. The viewpoint that diffusion could make a stable and uniform chemical state unstable was innovative.

The classical subject of linear stability theory analyzes disturbance to an equilibrium state for a governing system of equations by omitting all nonlinear terms in the perturbation quantities. The idea of linear theory is the determination of the critical conditions for the onset of instability to initially infinitesimal disturbances and the wavelength associated with those disturbances. If the effect of finite amplitude perturbations is to be estimated, or if the long-time behavior of growing disturbances is to be ascertained, then the nonlinear terms must be taken into account (David, 1994). Considering the long-range effects of the chemicals, which are not equal due to the difference in the pace of diffusion, an instability arises called Turing instability (Leppänen, 2004).

Shirzadi et al. (2013) developed the MLPG formulation for numerical solutions of the nonlinear reaction-diffusion equations. The spatial variations are approximated by moving least squares and the nonlinear terms are treated iteratively within each time step. The developed formulation is verified into two accurate numerical results.

Constructing of shape functions is one of the most important issues in the MLPG method. Development of more effective methods for constructing shape functions have been one of the most active areas of research. There are many methods for constructing a shape function such as the moving least square (MLS) and the weighted least square (WLS) method. The most popular method is the moving least square. Although the MLPG method and many other meshless methods have been gradually applied to different fields, there exists an inconvenience because of the difficulty in implementing some essential boundary conditions; the shape function constructed by MLS approximation does not satisfy the Kronecker delta function property. Recently, we have tried to use the moving Kriging approximation technique to construct meshless shape functions. The moving Kriging approximation procedure was originally employed in geostatistics by using known values and a semivariogram to determine unknown values. This mathematical model is named after Krige (Sacks, 1989) who introduced the initial version of this spatial prediction process. The moving Kriging

approximation has two advantages; (1) the Kronecher delta property and (2) the consistency property.

In this thesis, we shall develop the MLPG formulation for numerical solutions with the test function in view of the Heaviside step function on local sub-domains. The system of two nonlinear partial differential equations of the parabolic type is proposed to be solved by the local integral equation formulation and one-step time discretization method by using the Euler, Runge-Kutta and Crank-Nicolson methods. The shape functions are approximated by the moving Kriging approximation. Moreover, there are some methods for constructing shape functions, that satisfies the Kronecher delta property such as the radial point interpolation method (RPIM) Its property is the same as the moving Kriging approximation. The radial point interpolation method which was proposed by Chen et al. (2010), is presumed to provide the numerical results similar to the developed method based on moving Kriging approximation. The boundary and domain integrals are calculated using the Gauss-Legendre quadrature method. Two numerical examples are considered in order to verify the proposed method with testing its convergence and accuracy.

1.2 Literature Review

1.2.1 The chemical basis of morphogenesis (Turing, 1952)

It is suggested that a system of chemical substances, called morphogens, reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis. Such a system, although it may originally be quite homogeneous, may later develop a pattern or structure due to an instability of the homogeneous equilibrium, which is triggered off by random disturbances. Such reaction-diffusion systems are considered in some detail in the case of an isolated ring of cells, a mathematically convenient, though biologically unusual system. The investigation is chiefly concerned with the onset of instability. It is found that there are six essentially different forms which this may take. In the most interesting form stationary waves appear on the ring. It is suggested that this might account, for instance, for the tentacle patterns on Hydra and for whorled leaves. A system of reactions and diffusion on a sphere is also considered. Such a system appears to account for gastrulation. Another reaction system in two dimensions gives rise to patterns reminiscent of dappling. It is also suggested that stationary waves in two dimensions could account for the phenomena of phyllotaxis. The purpose of this paper is to discuss a possible mechanism by which the genes of a zygote may determine the anatomical structure of the resulting organism. The theory does not make any new hypotheses; it merely suggests that certain well-known physical laws are sufficient to account for many of the facts. The full understanding of the paper requires a good knowledge of mathematics, some biology, and some elementary chemistry. Since readers cannot be expected to be experts in all of these subjects, a number of elementary facts are explained, which can be found in text-books, but whose omission would make the paper difficult reading.

1.2.2 Design and analysis of computer experiments (Sacks, 1989)

Many scientific phenomena are now investigated by complex computer models or codes. A computer experiment is a number of runs of the code with various inputs. A feature of many computer experiments is that the output is deterministic--rerunning the code with the same inputs gives identical observations. Often, the codes are computationally expensive to run, and a common objective of an experiment is to fit a cheaper predictor of the output to the data. Our approach is to model the deterministic output as the realization of a stochastic process, thereby providing a statistical basis for designing experiments (choosing the inputs) for efficient prediction. With this model, estimates of uncertainty of predictions are also available. Recent work in this area is reviewed, a number of applications are discussed, and we demonstrate our methodology with an example**.**

1.2.3 Weakly nonlinear stability analysises of prototype reaction-diffusion model equations (David, 1994**)**

Comparisons are made between the results obtained by the application of various methods of weakly nonlinear stability analysis to several prototype reaction-diffusion equations which among them reproduce most of the salient features representative of such investigations of model systems for dissipative phenomena. Emphasis is placed upon the subtleties involved in scaling these equations and deducing asymptotically valid solutions. Phenomenological interpretations of the bifurcation behavior of the model equations are offered, based on the pattern formational aspects of convective instabilities in hydrodynamics, morphological instabilities in solidification, and diffusive instabilities inecology.

1.2.4 Computational studies of pattern formation in turing system (Leppänen, 2004)

This thesis is an analytical and computational treatment of Turing models, which are coupled partial differential equations describing the reaction and diffusion behavior of chemicals. Under particular conditions, such systems are capable of generating stationary chemical patterns of finite characteristic wave lengths even if the system starts from an arbitrary initial configuration. The characteristics of the resulting dissipative patterns are determined intrinsically by the reaction and diffusion rates of the chemicals, not by external constraints. Turing patterns have been shown to have counterparts in natural systems and thus Turing systems could provide a plausible way to model the mechanisms of biological growth. Turing patterns grow due to diffusion-driven instability as a result of infinitesimal perturbations around the stationary state of the model and exist only under non-equilibrium conditions. Turing systems have been studied using chemical experiments, mathematical tools and numerical simulations.

In this thesis a Turing model called the Barrio-Varea-Aragon-Maini (BVAM) model is studied by employing both analytical and numerical methods. In addition to the pattern formation in two-dimensional domains, also the formation of three-dimensional structures is studied extensively. The scaled form of the BVAM model is derived from first principles. The model is then studied using the standard linear stability analysis, which reveals the parameter sets corresponding to a Turing instability and the resulting

unstable wave modes. Then nonlinear bifurcation analysis is carried out to find out the stability of morphologies induced by two-dimensional hexagonal symmetry and various three-dimensional symmetries (SC, BCC, FCC). This is realized by employing the center manifold reduction technique to obtain the amplitude equations describing the reduced chemical dynamics on the center manifold. The main numerical results presented in this thesis include the study of the Turing pattern selection in the presence of bi-stability, and the study of the structure selection in three-dimensional Turing systems depending on the initial configuration. Also, the work on the effect of numerous constraints, such as random noise, changes in the system parameters, thickening domain and multi-stability on Turing pattern formation brings new insight concerning the state selection problem of non-equilibrium physics.

1.2.5 A local Petrov-Galerkin approach with moving Kriging interpolation for solving transient heat conduction problems (Chen, 2011)

A meshless Local Petrov-Galerkin approach based on the moving Kriging interpolation (Local Kriging method; LoKriging hereafter) is employed for solving partial different equations that govern the heat flow in two- and three-dimensional spaces. The method is developed based on the moving Kriging interpolation for constructing shape functions at scattered points, and the Heaviside step function is used as a test function in each sub-domain to avoid the need for domain integral in symmetric weak form. As the shape functions possess the Kronecker delta function property, essential boundary conditions can be implemented without any difficulties. The traditional two-point difference method is selected for the time discretization scheme. For computation of 3D problems, a novel local sub-domain from the polyhedrons is used for evaluating the integrals. Several selected numerical examples are presented to illustrate the performance of the Lo-Kriging method.

1.2.6 MLPG method for two-dimensional diffusion equation with Neumann's and non-classical boundary conditions (Abbasbandy, 2011)

In this paper, a meshless local Petrov–Galerkin (MLPG) method is presented to treat parabolic partial differential equations with Neumann's and non-classical boundary conditions. A difficulty in implementing the MLPG method is imposing boundary conditions. To overcome this difficulty, two new techniques are presented to use on square domains. These techniques are based on the finite differences and the Moving Least Squares (MLS) approximations. Non-classical integral boundary condition is approximated using Simpson's composite numerical integration rule and the MLS approximation. Two test problems are presented to verify the efficiency and accuracy of the method.

1.2.7 A local integral equation formulation to solve coupled nonlinear reaction-diffusion equations by using moving least square approximation (Shirzadi, 2013).

A new procedure is developed for the numerical solution of the nonlinear reaction-diffusion equations responsible for appearance of diffusion driven instabilities. The system of two nonlinear partial differential equation of the parabolic type is proposed to be solved by the local integral equation formulation and one-step time discretization method. The spatial variations are approximated by moving least squares and the nonlinear terms are treated iteratively within each time step. The developed formulation

is varified in two numerical test examples while investigating the convergence accuracy of numerical results.

1.3 Objective of Research

To develop a procedure for the numerical solution of the nonlinear reaction - diffusion problem by meshless method with moving Kriging approximation.

1.4 Scope of Research

1. The equations are needed to be studied as the coupled nonlinear reaction-diffusion equations and Brusselator system.

2. A procedure for the numerical solution is developed by the local integral equation to solve coupled nonlinear reaction-diffusion equations by using moving Kriging approximation and radial point interpolation method.

1.5 Advantage of Research

The meshless method, which is developed, is a specific numerical method, no mesh generation for solving coupled nonlinear reaction-diffusion equations. Moreover, the developed formulation corresponds to the boundary conditions problem.