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MESHLESS METHODS FOR SOLVING REACTION-DIFFUSION PROBLEMS-A BRIEF REVIEW

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Abstract – Reaction-diffusion equations represent many important and critical applications in engineering and science. Numerical techniques play an important role for solving such equations accurately and efficiently. This paper presents a brief review of meshless methods for solving general diffusion equations, including reaction-diffusion systems.

Keywords: Diffusion; reaction-diffusion system; engineering and science; numerical modelling; meshless methods.

1. Introduction

Modeling and analysis of thermodynamics and reaction-diffusion problems are frequently indispensable in many design and technological applications such as in heated cylinder and plate (Wang and Mai, 2005; Ootao and Tanigawa, 2005), pipe of vapor transport (Wu et al., 2007), quenching molten materials by rapid contact with a cold surface or material joining process (Bag et al., 2009). Modeling of transient heat conduction with non-homogeneous and time dependent heat sources is of particular interest as the domain heat sources can produce a temperature rise which is not always uniform inside a material, while precise knowledge of temperature distribution and variation with respect to time is crucial in the analysis. Numerical analysis is preferred for such thermodynamics problems in particular due to complexity of geometries involved and the non-homogeneity of heat sources as well as material properties. In addition to well-known numerical methods such as finite difference (FD), finite element (FE), finite volume (FV) and boundary element (BE) methods which are commonly employed, in recent years the so-called meshless or meshfree methods have been introduced as versatile tool for numerical analysis of thermal problems. Different with the aforementioned mesh-based methods, meshless methods rely only on nodes instead of mesh. As a result, rigid connectivity of mesh in a problem domain is simply replaced by distribution of nodes in which a group of nodes can be simply added or removed. It is hence obvious that meshless methods can offer several potential advantages and flexibilities than the mesh-based methods.

2. Meshless Methods for Diffusion Problems

Meshless methods may be traced back to the smoothed particle hydrodynamics (SPH) method by Lucy (1977) and Gingold and Monaghan (1977), and diffused element method (DEM) by Nayroles *et al.* (1992). Since then, a number of meshless methods have been developed such as element-free Galerkin (EFG) method (Belytschko *et al*., 1994), reproducing kernel particle (RKP) method (Liu *et al.*, 1995), meshless local Petrov-Galerkin (MLPG) method (Atluri and Zhu, 1998; Atluri and Shen, 2002) and point interpolation methods-PIM (Liu *et al.*, 2004).

Following the introduction of meshless methods, advancement and implementations of meshless methods in various applications are growing tremendously in literature. For instances, the element-free method has been employed by Li *et al*. (2003) for free surface seepage analysis. Local RBF collocation methods have been developed by Shu et al. (2003), Tolstykh and Shirobokov (2003) and further discussed by Shan *et al*. (2009). RBF collocation method, pioneered by Kansa (1990), has been investigated for bending of FGM plates using a sinusoidal plate formulation by Neves *et al*. (2011). Moreover, Roque *et al*. (2011) employed the RBF-FD method for analyzing composite plates. In the field of heat transfer, Wang *et al.* (2006) presented a meshless model for transient heat conduction in FGM. Gao (2006) employed a meshless BEM for isotropic heat conduction problems with heat generation and spatially varying conductivity. MLPG method for 2D steady-state heat conduction problems of irregular domains was investigated by Wu *et al.* (2007). Meshless EFG method for nonlinear heat conduction problems was presented by Singh *et al.* (2007). Singh and Tanaka (2006), Sladek *et al.* (2008) and Li *et al*. (2013) presented heat transfer analyses in 3D applications. Li *et al*. (2011) employed the MLPG method for transient heat conduction analysis with modified precise time step integration method. In a separate study, Soleimani *et al.* (2011) employed the RBF-DQ method for 2D transient heat conduction in complex geometries.

Development of new classes of meshless method, including the search for more favourable basis functions for meshless method, has been also an active research area in recent years. Development of the meshless Hermite–Cloud method for structural mechanics applications has been presented by Lam *et al*. (2006). A meshfree differential reproducing kernel (DRK)-based collocation method has been introduced by Wu *et al*. (2008) for coupled analysis of functionally graded magneto-electro-elastic shells and plates. Le *et al.* (2010) has proposed a collocation method based on one-dimensional RBF interpolation scheme for solving PDEs. Khosravifard *et al*. (2011) presented improved meshless RPIM for the analysis of nonlinear transient heat conduction in FGM. Chen and Liew (2011) presented local Kriging interpolation for transient heat conduction problems. Numerical solution of transient heat conduction problems using improved MLPG was presented by Dai *et al.* (2013). Ren *et al*. (2012) introduced the complex variable interpolating MLS method. Zhang *et al.* (2013) presented an improved EFG method with almost interpolation property for isotropic heat conduction problems.

3. Meshless Methods for Reaction-Diffusion Problems

Reaction-diffusion equations represent a wide range of important phenomena in many branches of science and engineering (Quintela *et al.*, 2017). Turing (1952) showed that pattern formation is related to the occurrence of chemical instability called as diffusion-driven instability and the emergence process could be described by a simple system of coupled reaction-diffusion equations. Surprisingly, the equations are able to describe many dynamical processes in nature. They also represent a wide range of behaviors by interactions and mechanisms in chemical and biological systems. The extension covers chemical reactions and combustion (Lucchesi *et al*., 2019), pollution and concentration spreads (Ivorra *et al*., 2017), bi-stable systems and material growth process (Liu *et al*., 2015; *Sgura et al*., 2012), heat and mass transfer, population dynamics (Wen and Fu, 2009; Rattanakul *et al*., 2019), predator-prey problems (Guin *et al*., 2012; Macías-Díaz and Vargas-Rodríguez, 2021), chemotaxis (Sarra, 2012; Ma *et al*., 2019), cell growth processes and other biological problems (Murray, 2003; Bellomo *et al*., 2007). The reaction-diffusion mechanisms are also a robust paradigm to represent many biological and physical phenomena over multiple spatial scales (Smith and Yates, 2021) and growing domains such as skin scales (Fofonjka and Milinkovitch, 2021). Other applications also cover multicomponent diffusion and phase transformation (Matychack *et al*., 1998), micro and nanotechnology (Grzybowski *et al*., 2005), microscale structures/devices/functional systems (Malchow *et al*., 2019) as well as synthesis of materials with periodic microstructure (Shevchenko *et al*., 2021).

Cross-diffusion and Turing systems are two important classes of reaction-diffusion systems. In cross-diffusion systems, transport process is influenced by the gradient of concentration in which the concentration gradient of one chemical or biological species induces a flux of another species (Vanag and Epstein, 2009; Lou and Martínez, 2009; Madzvamuse *et al*., 2015). In the equations, positive cross-diffusion coefficient represents the species movement in the direction of another species of lower concentration, and vice versa. In the absence of cross-diffusion, reaction-diffusion equations also represent many interesting systems such as Turing systems. Turing systems in fact belong to a wide class of reaction-diffusion systems. Turing systems can be regarded as models of complex pattern formation (Barrio, 2008; Shakeri and Dehghan, 2011). In phenomena of pattern formation, the presence of cross-diffusion in reaction-diffusion systems can induce greater effects on the emergence of patterns compared with the process of pattern formation by self-diffusion (Gui-Quan *et al*., 2008; Xie, 2012; Yang *et al*., 2013; Iqbal and Wu, 2019). Due to their significance and importance in describing so many important phenomena of process dynamics and behaviors, accurate solutions for the systems are of great interest and importance, in which computational mathematics and numerical simulations play an important role and indispensable (Ruiz-Baier and Tian, 2013; Sebestyén *et al*., 2016; Giunta *et al*., 2020).

Many numerical studies have been devoted in order to obtain their solutions stably and accurately. Unfortunately, obtaining their numerical solutions accurately is challenging for several reasons. Firstly, their solutions exhibit numerical oscillations/steep fronts and requiring stable approximation schemes. Secondly, pursuing for numerical stability can lead to severe restriction in time step size. Consequently, simulation will take longer time and costly. Thirdly, as a matter of fact, important chemistry and physics of the problems are lying within the featured steep fronts of solutions and they need to be captured accurately. The solutions have to be therefore tracked precisely in order to avoid loss of information due to the presence of numerical oscillations. Traditional numerical methods such as finite difference (FD), finite element (FE) and finite volume (FV) methods are often used to solve the reaction-diffusion systems. However, devising more efficient and robust numerical scheme is still of great interest and importance in numerical studies of the reaction-diffusion systems (Settanni and Sgura, 2016). For examples, a proper orthogonal decomposition (POD) method was employed to establish a POD-based reduced-order FD extrapolating model with few degrees of freedom for solving 2D shallow water equations with sediment concentration (Luo *et al*., 2015). Reduced order modelling with principal decomposition framework in time-windowed form was presented for analysis of nonlinear cross-diffusion systems in (Karasözen *et al*., 2021). An AFC-stabilized implicit FE method has been presented for partial differential equations on evolving-in-time surfaces (Sokolov *et al*., 2015). The proposed FE method can avoid nonphysical oscillations in the numerical solution of the problem. In other works, extended procedures (Boffi *et al*., 2013) have been developed to increase numerical simulation effectiveness allowing robust implementation of numerical method for challenging problems, even for multiscale problems (Efendiev *et al*., 2021). In (Rossinelli *et al*., 2008; Lo and Mao, 2019), accelerated stochastic and hybrid methods were presented for simulation of reaction-diffusion systems, while mathematical modeling of time fractional reaction–diffusion systems has been discussed in (Gafiychuk *et al*., 2008; Garrappa and Popolizio, 2021).

Evidently, complexities in the simulation problems have urged rising demands for reliable and efficient computational methods in order to obtain accurate solutions in a faster computational time. Recently, meshless methods have appeared as emerging numerical techniques besides the mentioned numerical methods. The attractiveness of the methods comes from their less dependence and even no dependence at all on grid or mesh. Bottlenecks due to the presence of grid or mesh can be eliminated seamlessly. The meshless methods have gained increasing popularity in recent years. The methods are shown to be robust and attractive solvers for many challenging problems in engineering and science, including reaction-diffusion problems (Cheng et al., 2014; Shivanian and Jafarabadi, 2020; Ahmad *et al*., 2017).

Advantage in using meshless methods is obvious that there is a greater flexibility in choosing basis function or shape function to be used for a numerical analysis. As pointed out in (Batra and Zhang, 2008; Divo *et al.*, 2014; Gerace *et al.*, 2016), such a flexibility opens up a large variety of classes of meshless methods based upon different constructions of basis/shape functions, such as moving least square (MLS) approximation (Shirzadi *et al.*, 2013a; Shirzadi *et al.*, 2013b), polynomial basis functions (Abd-Elhameed and Youssri, 2018; Heydari *et al.*, 2021; Pandey and Gómez-Aguilar, 2021), radial basis functions (Mesmoudi *et al*., 2020; Mohebbi and Evans, 2020; Watson *et al*., 2020; Chen *et al*., 2021) and B-spline basis functions (Arora *et al*., 2020), among others. It is also no doubt that selection of appropriate basis function or shape function will determine accuracy and efficiency of a meshless method.

4. Conclusions

In the present paper, a brief review of meshless methods for solving general diffusion equations, including reaction-diffusion systems has been presented. It is highlighted that selection of appropriate basis function or shape function will determine accuracy and efficiency of a meshless method. Investigation of new classes of meshless method, including the search for more favourable basis functions, would have been an active research area in forthcoming meshless method developments and applications.

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