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Remediation of contaminated groundwater by meshless local weak forms

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ABSTRACT

In this paper, four meshless local weak form methods such as direct meshless local Petrov–Galerkin method (DMLPG), meshless local Petrov–Galerkin method (MLPG), local weak radial point interpolation method (LWRPIM) and local weak moving kriging method (LWMK) are applied to find the numerical solution of coupled non-linear advection–diffusion–reaction system arising in the prevention of groundwater contamination problem. A comparison between these methods is done from the perspective of accuracy and computational efficiency. An efficient fourth-order exponential time differencing Runge–Kutta method is utilized for the time discretization. The computational efficiency is the most significant advantage of the DMLPG method in comparison with the other meshless local weak form methods, because DMLPG reduces the computational costs, significantly. This is due to the fact that DMLPG shifts the numerical integrations over low-degree polynomials rather than over complicated shape functions. The main aim of this paper is to show that the meshless local weak form methods can be used for solving the system of non-linear partial differential equations especially coupled non-linear advection–diffusion–reaction system. The numerical results confirm the good efficiency of the proposed methods for solving our model.

1. Introduction

1.1. Mathematical model for prevention and control of groundwater contaminant

With the microbiological technology, a mathematical model for prevention and control of groundwater contaminant can be considered as a coupled nonlinear advection–diffusion–reaction system. This model, which is taken from [1], can be described as follows

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$$\begin{cases} S_t + v(\mathbf{x}) \cdot \nabla S - \nabla \cdot (D(\mathbf{x}) \nabla S) + e_1 M_p \cdot \dfrac{S}{K_s + S} \cdot \dfrac{A}{K_a + A} = 0, \\ A_t + v(\mathbf{x}) \cdot \nabla A - \nabla \cdot (D(\mathbf{x}) \nabla A) + e_2 M_p \cdot \dfrac{S}{K_s + S} \cdot \dfrac{A}{K_a + A} = 0, \\ (M_s)_t + v(\mathbf{x}) \cdot \nabla M_s - \nabla \cdot (D(\mathbf{x}) \nabla M_s) + e_3 M_s \cdot \dfrac{S}{K_s + S} \cdot \dfrac{A}{K_a + A} + r(\mathbf{x}) M_s = 0, \\ S|_{\partial\Omega} = A|_{\partial\Omega} = M_s|_{\partial\Omega} = 0, \\ S(\mathbf{x}, 0) = S_0(\mathbf{x}), \qquad A(\mathbf{x}, 0) = A_0(\mathbf{x}), \qquad M_s(\mathbf{x}, 0) = (M_s)_0(\mathbf{x}), \end{cases} \tag{1.1}$$

where $\Omega \subset \mathbb{R}^2$ is a bounded domain with a Lipschitz continuous boundary $\partial\Omega$. S, A and M_s denote the concentration of the main ground substance, aqueous solution electrolyte concentration and concentration of microorganism (e.g. bacteria), respectively [1]. The vector $v(\mathbf{x}) = (v_1(\mathbf{x}), v_2(\mathbf{x}))$ is the average linearized groundwater velocity, $D(\mathbf{x})$ is a hydrodynamic diffusion function, M_p is the total concentration of active microorganism and $M_s = M_p/R_M$ with a positive constant R_M. e_i $(i = 1, 2, 3)$, K_s and K_a are positive constants. We refer to [2] for the meaning of these notations. The variable coefficients $v(\mathbf{x})$, $D(\mathbf{x})$ and $r(\mathbf{x})$ are assumed to satisfy [1]

$$\begin{cases} 0 < k_1 \le D(\mathbf{x}) \le k_2, & D(\mathbf{x}) \in W_\infty^1(\Omega), \\ |v_i(\mathbf{x})| \le \alpha_i, & v_i(\mathbf{x}) \in W_\infty^1(\Omega), \\ r(\mathbf{x}) \le r_1, \end{cases} \tag{1.2}$$

where r_1 and k_i, α_i $(i = 1, 2)$ are positive constants.

1.2. Meshless local weak form methods

The weak forms are used to derive a set of algebraic equations through a numerical integration process over the domain of the problem, globally or locally. The use of the global weak-form requires the system of equations in the global integral form to be satisfied over the entire problem domain, and hence, a set of background cells has to be used for the numerical integration [3]. Therefore these methods are not truly meshless methods [3]. To avoid the use of global background cells, the so-called local weak-form methods have been developed. This concept was first proposed by Atluri and Shen [4], and later discussed in depth in [5,6]. The most significant difference between this method and the finite element method or any other meshless method is that the local weak forms are generated on overlapping local sub-domains, instead of using the global weak form. Integration of the weak form is performed in local sub-domains with simple geometrical shapes, therefore no elements or background cells are necessary either for interpolation purposes or for integration purposes. Any integration technique can be used for these local sub-domain integrals.

In the MLPG method, due to Petrov–Galerkin formulation being used, the trial and test function spaces can be different, and the classical Galerkin formulation is just one of its special cases. This yields an additional generality and advantage over other meshless methods.

A wide range of problems has been solved by MLPG method. It shows that the MLPG method is very promising for solving various boundary value problems. In recent years, many problems have been solved using MLPG method such as elasto-statics problems [7], continuously nonhomogeneous linear viscoelastic solids [8], two-dimensional sine–Gordon equations [9], Maxwell equations [10], system of n-coupled nonlinear Schrodinger equations [11], Brusselator model [12,13], spike dynamics in the Gierer–Meinhardt system [12], inverse heat conduction problems [14], transient heat conduction problems [15] and etc. A review on application of MLPG in engineering and sciences is provided in [16].

In MLPG and other local weak form methods based on trial approximation, numerical integrations are traditionally done over some shape functions and their derivatives [17]. Such shape functions are complicated and have no closed form. To get accurate results, numerical quadratures with many integration points are required. Thus the subroutines for evaluating the shape functions must be called very often and this leads to high computational costs. In contrast to this, the stiffness and mass matrices in finite element methods (FEMs) are constructed by integrating over polynomial basis functions which are much cheaper to evaluate [18].

For overcoming this disadvantage a tricky and simple modification has been applied to MLPG in [18]. This modification uses the concept of generalized moving least squares (GMLS) approximation [19] and shifts the numerical integrations over low-degree polynomial basis functions rather than complicated MLS shape functions. Since we have a direct approximation of local weak functionals, the new technique is called direct MLPG (DMLPG). Ignoring the costs of mesh generation and mesh refinement, we can roughly say DMLPG reduces the computational cost of MLPG to the level of that in classical FEM [20]. Because both FEM and DMLPG lead to sparse final linear systems, and in both methods numerical integrations are done over low-degree polynomial basis functions [20].

The direct meshless local Petrov–Galerkin method can be a very attractive scheme for computer modeling and simulation of problems in engineering and sciences, as it significantly uses less computational time in comparison with the classical meshless local Petrov–Galerkin method. For example, the authors of [21] numerically analyzed the solution of 2D and 3D potential problems via DMLPG. In [22], DMLPG method is applied for solving elliptic interface problems. In [23], the DMLPG technique is applied for solving 3D Poisson problems. The author of [24], developed DMLPG method for solving two and

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