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A moving least squares based meshless local petrov-galerkin method for the simulation of contaminant transport in porous media

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ABSTRACT

Contamination of soil, surface and subsurface water resources through direct or indirect sources is a major problem in many parts of the world. To understand the contamination process in the porous media, we have to simulate the contaminant transport mechanism and predict its behaviour with respect to space and time. The contaminant transport process can be simulated by solving the well posed advection-dispersion partial differential equation by using numerical techniques with appropriate initial and boundary conditions. The transport equation is generally solved using grid based techniques like Finite Difference Method (FDM) and Finite Element Method (FEM). The Meshless methods are alternatively developed numerical methods to overcome the limitations of aforementioned grid based techniques. This paper presents a newly developed Meshless Local Petrov-Galerkin (MLPG) model based on the moving least squares (MLS) method for numerical simulation of contaminant transport equation in porous media. The Meshless MLPG-MLS model has been developed for one- and two- dimensional problems in MATLAB. These models are investigated and verified with available analytical and numerical solutions for its accuracy and efficiency. The models gave quiet promising results showing the efficacy and applicability of the method for the simulation of contaminant transport in porous media.

1. Introduction

Contaminant transport in the porous media has been one of the most important research topics in the hydro-geological sciences and geo-environmental engineering for the past many decades. Once a contaminant is released into the soil, it will interact hydrologically, physically and chemically with both the water present and the soil matrix [1]. It is essential to develop an accurate numerical model for predicting the movement and transfer of contaminants in the porous media, for proper management and remediation of the contaminated sites. Numerical modelling plays an important role in the real life management of groundwater systems [2]. Any successful application of numerical schemes for engineering solutions to these problems demands a firm comprehension of the principles of contaminant transport through porous media. The effect of individual governing mechanisms which control the fate of contaminants in the porous media and the movement of the contaminant plume are usually complex to assess, as the entire process is the outcome of interactions of many factors like dispersion, advection, sorption, reaction, degradation, etc., [3–5].

Many analytical solutions for the contaminant transport problems in which the boundary conditions and geometries are simplified are available in the literature [6–8]. However, there is no way of computing the behaviour of the real field case studies unless it is a full-scale experiment actually subjected to the real conditions. Construction of a full-scale experimental set up for every field study would be restrictive, costly and time consuming. The only feasible substitute, therefore, is to develop a numerical model, which reasonably represents and simulates the relevant problem scenario and can predict the possible significant outcomes of the transport phenomena [4,7].

Contaminant transport in the porous media is modeled using mathematical techniques wherein the processes under simulation are expressed by a set of governing equations defined over a specific domain with Dirichlet and/or Neumann boundary conditions [6]. The most frequently used numerical techniques are namely analytic, boundary element, finite difference, finite element and finite volume methods [9]. However, they rely on grids/elements that are connected together by nodes in a proper manner leading to high cost of meshing and re-meshing. These techniques can model problems with complex geometries, complicated boundary conditions, heterogeneity and non-linearity. However, they have some difficulties when dealing with problems where there are high advective velocities, low dispersivities and/or high contrast in dispersivity [10].

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In case of modelling advection-dominated transport phenomena, the main difficulty arises due to the presence of advective operators in the formulation of transport problems which are based on kinematical descriptions other than Lagrangian [11]. Advection operators are, in fact, non-symmetric and thus the approximation property of Galerkin finite element method (FEM), which is the basis for success in symmetric cases, is lost when advection dominates the transport process [4,11]. In practice, solutions to advection-dominant transport problems by the Galerkin FEM are often corrupted by spurious node-to-node oscillations. These can be removed by mesh and time step refinement schemes. To overcome the aforementioned shortcomings and to develop a more robust method has prompted for the development of alternative numerical techniques such as Meshless methods [4,12].

In the past two decades, a group of new methods called Meshless methods has been developed, whose main aim is to get rid of the mesh and to compute approximate solutions for the unknown variables in the governing equation entirely using only a set of nodes [12]. Meshless methods such as the element-free Galerkin [13], meshless local Petrov–Galerkin (MLPG) [14], hp-clouds [15], the reproducing kernel particle [16], the smoothed particle hydrodynamics [17], the diffuse element [18], the partition of unity finite element [19], the natural element [20] and the meshless using radial basis functions [21] for seeking approximate solutions of partial differential equations have become popular because of the flexibility of placing nodes at arbitrary locations and the ability to simulate even for complicated conditions. So far only limited amount of research is done regarding the potential usage of these meshless methods for modelling contaminant transport in porous media [11,22–26].

The Meshless Local Petrov-Galerkin (MLPG) was originally proposed by Atluri and Zhu [14], for solving linear and non-linear boundary problems. The MLPG methodology of domain representation is such that of local weak based formulation wherein the sub-domain lies within the global problem domain and these sub-domains can overlap each other, rather than forming a continuous mesh. Generally, in MLPG method, the nodal trial/shape and test functions are taken different to reduce the computational cost and number of points required to obtain a converged result [27]. The MLPG method has been successfully used for solving numerous boundary value problems related to various fields of study [28–35]. Even though MLPG has been used for many engineering problems in the last decade, to the knowledge of authors, it was not applied for contaminant transport problems. Earlier [36,37], an attempt was made to use this method for groundwater flow simulation wherein, trial and test functions are taken such that it belongs to the same function spaces with Exponential/Gaussian Radial basis function (EXP-RBF). Although encouraging results were reported, there were still some technical issues in using RBF when dealing with high advective velocities, low dispersivities and/or high contrast in dispersivity, and functional issues like, the determination of suitable RBF shape parameters, the optimal shape and size of the sub-domain which are to be determined subjectively through parametric studies in aforementioned cases. Hence, the moving least squares (MLS) approximation [38], which is one of the most widely used methods for the construction of meshless shape functions is alternatively undertaken. It has been found that the MLS is accurate and stable for arbitrarily distributed nodes [12] for many problems in computational mechanics. However, to the best of author's knowledge, the MLS Meshless Local Petrov Galerkin technique for solving the contaminant transport in porous media was not attempted earlier.

The objective of this paper is to develop a Meshless Local Petrov Galerkin model based on MLS for the numerical simulation of contaminant transport in porous media. Few numerical examples with different problem domains and different nodal distributions are used to validate and investigate the efficiency of the newly developed Meshless formulation.

2. Meshless Local Petrov Galerkin method

In this study, a Meshless Local Petrov Galerkin technique based on the MLS for the numerical simulation of contaminant transport equation in porous media is developed. The moving least square (MLS) approximant is formulated [12,38–42] to approximate the function $c(\boldsymbol{x})$ with $c^h(\boldsymbol{x})$, in which $c(\boldsymbol{x})$ represents the contaminant concentration and $c^h(\boldsymbol{x})$ is the nodal concentration at $\mathbf{x}$, where $\mathbf{x}$=(x, y) is a position vector.

2.1. Moving Least Squares (MLS) scheme

The trial function in Meshless methods is approximated with the help of randomly distributed nodes in a local domain about the point of interest. Consider a sub-domain Ω_*, which is the neighbourhood of a point $\mathbf{x}$ and is denoted as the domain of definition of the MLS approximation for the trial function at $\mathbf{x}$, which is located within the problem domain Ω. To approximate the distribution of function c in Ω_*, over a number of randomly located nodes $\{\mathbf{x}_i\}$, i =1, 2 .... N, the Moving Least Squares approximation $c^h(\boldsymbol{x})$ of c, for all x ϵ Ω_*, can be defined as [12,39].

$$c(\boldsymbol{x}) \cong \ c^h(\boldsymbol{x}) = \boldsymbol{p}^{\boldsymbol{T}}(\boldsymbol{x})\boldsymbol{a}(\boldsymbol{x}) for\ all\ x \in \Omega_* \tag{1}$$

where $\boldsymbol{p}^{\boldsymbol{T}}(\boldsymbol{x})$=[$p_1(\boldsymbol{x})$, $p_2(\boldsymbol{x})$, …$p_m(\boldsymbol{x})$]is a complete monomial basis, m is the number of terms in the basis; if we denote by t the highest order polynomial which is completely included in the basis, the relation between m and t can be described as: m =(t+1)(t+2)/2 in two dimensions, while m =(t+1)(t+2)(t+3)/6 in three dimensions and $\boldsymbol{a}(\boldsymbol{x})$ is a vector containing coefficients $\boldsymbol{a_j}(\mathbf{x})$, j=1,2,....$m$ which are functions of the spatial coordinates.

In the present work, we use the linear basis $\boldsymbol{p}^{\boldsymbol{T}}(\boldsymbol{x}) = [1,x^1, x^2]$; m =3, which assures linear completeness. Thus, it can reproduce any smooth function and its first derivative with arbitrary accuracy, as the approximation is refined.

The coefficient vector $\boldsymbol{a}(\boldsymbol{x})$ is determined by minimizing a weighted discrete norm, which is defined as [12,39]:

$$\boldsymbol{J}(\boldsymbol{a}(\boldsymbol{x})) = \sum_{i=1}^{N} w_i(\boldsymbol{x})[\boldsymbol{p}^{\boldsymbol{T}}(\boldsymbol{x}_i)\boldsymbol{a}(\boldsymbol{x}) - \hat{c}_i]^2 = [\boldsymbol{P}.\ \boldsymbol{a}(\boldsymbol{x}) - \hat{c}]^T.\ \boldsymbol{W}.\ [\boldsymbol{P}.\ \boldsymbol{a}(\boldsymbol{x}) - \hat{c}] \tag{2}$$

where, $\boldsymbol{x}_i$ denotes the position vector of node i; $w_i(\boldsymbol{x})$ is the weight function associated with the node i, with $w_i(\boldsymbol{x}) > 0$ for all $\mathbf{x}$ in the support of $w_i(\boldsymbol{x})$; N is the number of nodes in Ω_* for which the weight functions $w_i(\boldsymbol{x}) > 0$ and the matrices $\mathbf{P}$ and $\mathbf{W}$ are defined as

$$P = \begin{bmatrix} p^T(x_1) \\ p^T(x_2) \\ \cdots \\ p^T(x_N) \end{bmatrix} (N \times m)\ matrix \tag{3}$$

$$W = \begin{bmatrix} w_1(\boldsymbol{x}) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & w_N(\boldsymbol{x}) \end{bmatrix} (N \times N)\ matrix \tag{4}$$

$$\text{And } \hat{c} = [\hat{c}_1\ \ \hat{c}_2\ \ \ldots\ \ \hat{c}_N]\ (1 \times N)\ vector \tag{5}$$

It should be noted that $\hat{c}_i$, i=1, 2,....,N in Eqs. (2) and (5) are fictitious. The stationarity of $\mathbf{J}$ in Eq. (2) with respect to $\mathbf{a(x)}$ leads to the following linear system:

$$\boldsymbol{A}(\boldsymbol{x})\,\boldsymbol{a}\,(\boldsymbol{x}) = \boldsymbol{B}(\boldsymbol{x})\,\hat{c} \tag{6}$$

where the matrices $\mathbf{A(x)}$ and $\mathbf{B(x)}$ are defined by

$$A(x) = \boldsymbol{P}^{\boldsymbol{T}}WP \ \equiv B(x)\,P = \sum_{i=1}^{N} w_i(x)p(\boldsymbol{x}_i)\,\boldsymbol{p}^{\boldsymbol{T}}(\boldsymbol{x}_i) \tag{7}$$