Comparison between local and global Mesh-free methods for Ground-Water modeling

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Abstract

Ground water pollution is a serious environmental problem that may damage human health, destroy the ecosystem and cause water shortage. In all situations, we need tool to predict the pollutant distribution in ground water. The only tool that we can use is mathematical modeling.

Recently, very intensive efforts have been devoted to develop meshless or element free methods that eliminate the need of element connectivity. The motivation is to cut down modeling costs in industrial applications by avoiding the labor intensive step of mesh generation. In this paper we develop and compare two types of a meshfree method for modeling groundwater contaminant transport: globally supported multiquadric radial basis function (MQRBF) and locally supported compactly supported radial basis functions (CSRBF). The algorithm uses collocation method with radial basis functions. RBF is a truly meshfree method and can be used to solve complex geometry and high dimensional problems very easily compared to other classical numerical method. Numerical results are presented for 1-D, 2-D and 3-D groundwater contaminant transport models. The results show that the method is very simple and accurate.

Keywords: Meshl-free, Radial Basis Function, Multiquadric, Compactly supported, Groundwater Equation, Contaminant Transport.

1. Introduction

The demand for water resources is increasing day by day due to ever increasing population. Groundwater plays a major role in the livelihood of mankind by providing water for drinking, irrigation and industrial purposes. The rapid population growth in the last three decades all over the globe resulted in exploiting more groundwater [12]. A ground water model is thus a simplified version of the real system that approximately simulates the input-output stresses and response relations of the system. One has to understand here that normally the real system is simplified to model the system as such there is no unique model for a given groundwater system. Normally, models are classified as predictive, interpretive and generic models. Predictive models are used to predict the future response of the aquifer, which needs a calibrated and validated model. Interpretive models are used for studying system dynamics and it is generally used for optimal data network design. Generic models are used to understand the flow dynamics in hypothetical situations [12].

Groundwater contamination and soil pollution have been recognized as critical environment problems throughout the world for many years. In the protection and improvement of groundwater quality, two challenging problems are evident for uncontaminated aquifers, one must assess the potential dangers of pollution and for contaminated aquifers, it is necessary to develop and implement remediation strategies. In both situations, a predictive tool is needed to estimate the pollutant distribution in groundwater [7].

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Ne Zheng sun shows in [16] that the only tool that we can use is mathematical modeling. Over the past decade, mesh reduction techniques (Meshless or Mesh-free methods) have emerged as effective numerical techniques for solving science and engineering problems. The motivation is to cut down modelling costs in industrial applications by avoiding the labor intensive step of mesh generation. In this study, we consider the collocation formulation to solve a system of groundwater model. The numerical solution is evaluated at scattered collocation points and the spatial partial derivatives are formed directly from partial derivatives of the radial basis functions without using any difference scheme.

Applications of radial basis functions have gained quite some importance over the past years. They have been successfully applied to large variety of problems [1, 2, 3, 4, 5, 15]. A major advantage with using RBFs is that the points on the grid do not need to be uniformed in anyway. To increase the computational efficiency of the numerical solution two different kind of radial basic functions are used: Multiquadric (MQRBF) and Wendland's function (CSRBF). Compared to other mesh-free methods, the radial basis function methods have the following advantages: they require neither domain nor boundary discretization, domain or boundary integration is not required, in some cases, they converge exponentially for smooth solutions, since RBFs are univariate functions which depend only on the distances between points, RBFs are attractive to high dimensional problems, the implementation and coding are very easy. In [7, 15] they shown that computed results by RBF are quit steady as observed in some finite element method (FEM), Larsson and Formberg shown in [10] that RBF collocation method can easily achieved much higher-order accuracy than the finite difference method (FDM).

In this paper we develop and compare two types global and local radial basis function mesh-free method for modeling groundwater contaminant transport. This paper is organized as follows. Section 2 describes the modeling aspects of time-dependent 3D governing equations of groundwater contaminant transport. In Section 3 we discuss the application of compactly supported RBFs and multiquadric RBFs. Section 4 discusses some numerical results. The paper ends with a conclusion.

2. Governing Equations

The governing equations of groundwater contaminant transport modeling can be described as:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V_x \frac{\partial C}{\partial x} - V_y \frac{\partial C}{\partial y} - V_z \frac{\partial C}{\partial z} - \lambda C \qquad (2.1)$$

the initial and boundary conditions are chosen accordingly so that the exact solution is :

$$C(x,y,z,t) = e^{-\lambda t}(c1 + c2 e^{\frac{V_x}{D_x}} x)(c3 + c4 e^{\frac{V_y}{D_y}} y)(c5 + c6 e^{\frac{Vz}{D_z}} z) \qquad (2.2)$$

where C is the concentration of the contaminant. $V = (V_x, V_y, V_z)$ is the seepage velocity, D_x, D_y and D_z are the dispersion coefficients in the x, y and z direction, respectively, λ is the rate of decay, $c_1, c_2, c_3, c_4, c_5, c_6$ are parameters constant. This problem was also considered in [11].

3. Global and Local Radial Basis Functions

Following Kansa's formulation scheme [8], the application of collocation radial basis functions to a system equation (2.1) and its boundary conditions start by first selecting a set of boundary points $\{(x_1, y_1, z_1), \ldots, (x_b, y_b, z_b)\}$ and $\{(x_{b+1}, y_{b+1}, z_{b+1}), \ldots, (x_{d+b}, y_{d+b}, z_{d+b})\}$ domain nodes. The unknown solution of the problem at each time t can be determined under the form

$$C = \sum_{j=1}^{d+b} \alpha_j \varphi_j(x,y,z), \qquad (3.1)$$

where $\{\alpha_j\}_1^N$ are unknown coefficients to be determined and $\varphi_j(x,y,z)$ is the selected radial basis function. The most commonly used mesh-free radial basis functions are given in Table [1] for global radial basis function, Table [2] for local radial basis function and indicated in Figures (1, 2, 3).

Table 1: Some commonly used Global (Kansa) RBFs

$\phi(r)(r \geq 0)$	***Type of basis function***
$\sqrt{\varepsilon^2 + r^2}$	Multiquadric (MQ)
$(\varepsilon^2 + r^2)^{-1/2}$	Inverse Multiquadric (IMQ)
$e^{-(r/\varepsilon)^2}$	Gaussian (GA)
$r^2 \log r$	Thin Plate Spline (TPS)
r	Linear
r^3	Cubic

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Table 2: Some commonly used Local (Wendland) RBFs [13]

Dimenso l	CSRBFs	Smoothness
$l=1$	$\phi_{1,0}(r) = (1-r)_+$ $\phi_{1,1}(r) = (1-r)_+^3(3r+1)$ $\phi_{1,2}(r) = (1-r)_+^5(8r^2+5r+1)$	C^0 C^2 C^4
$l \le 3$	$\phi_{3,0}(r) = (1-r)_+^2$ $\phi_{3,1}(r) = (1-r)_+^4(4r+1)$ $\phi_{3,2}(r) = (1-r)_+^6(35r^2+18r+3)$ $\phi_{3,3}(r) = (1-r)_+^8(32r^2+25r^2+8r+1)$	C^0 C^2 C^4 C^6
$l \le 5$	$\phi_{5,0}(r) = (1-r)_+^3$ $\phi_{5,1}(r) = (1-r)_+^5(5r+1)$ $\phi_{5,2}(r) = (1-r)_+^7(16r^2+7r+1)$	C^0 C^2 C^4

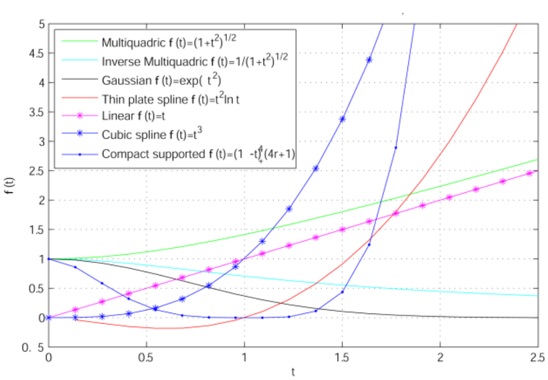

Fig. 1 The most commonly used radial functions.

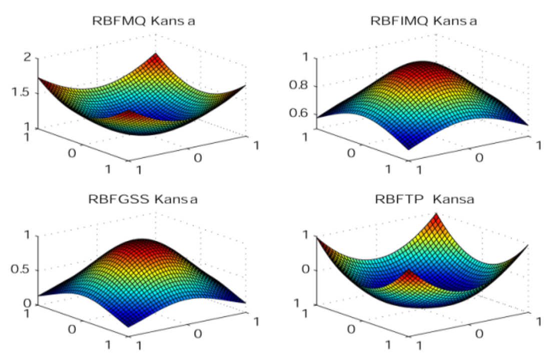

Fig. 2 The most commonly used Kansa's radial functions 3D.

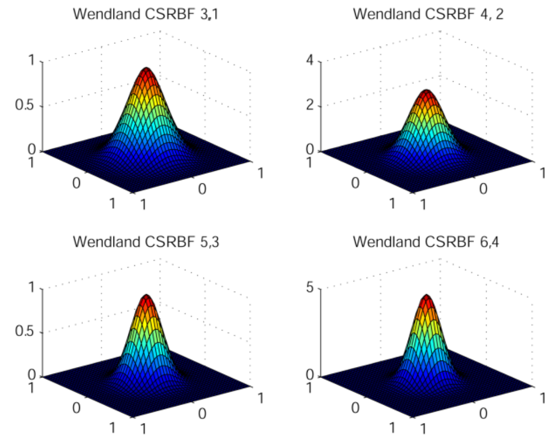

Fig. 3 The most commonly used Wendland's Compact supported radial functions 3D.

To solve the three-dimensional time-dependent differential equations given by equation (2.1), we start the time integration scheme with implicit scheme using Θ weighted; therefore equation (2.1) will be of the form:

$$\frac{C^{n+1}}{\Delta t} = \frac{C^n}{\Delta t} + \Theta\left(D_x\frac{\partial^2 C^{n+1}}{\partial x^2} + D_y\frac{\partial^2 C^{n+1}}{\partial y^2} + D_z\frac{\partial^2 C^{n+1}}{\partial z^2} - V_x\frac{\partial^2 C^{n+1}}{\partial x^2} - V_y\frac{\partial^2 C^{n+1}}{\partial y^2} - V_z\frac{\partial^2 C^{n+1}}{\partial z^2} - \lambda C^{n+1}\right) + (1-\Theta)\left(D_x\frac{\partial^2 C^n}{\partial x^2} + D_y\frac{\partial^2 C^n}{\partial y^2} + D_z\frac{\partial^2 C^n}{\partial z^2} - V_x\frac{\partial^2 C^n}{\partial x^2} - V_x\frac{\partial^2 C^n}{\partial x^2} - V_z\frac{\partial^2 C^n}{\partial z^2} - \lambda C\right), \quad (3.2)$$

where Δt is the time step, C_i^{n+1} is the solution vector at points (x_i, y_i, z_i) in time $(n+1)\Delta t$. The values of the interpolant C^n are given by collocating equation (3.2) at the interior points $(x_i, y_i, z_i)_{i=b+1}^{b+d}$ and by the boundary conditions at $\{(x_1, y_1, z_1), \ldots, (x_b, y_b, z_b)\}$.
This yields the system of N linear equations which can be expressed in matrix form $A\vec{\alpha} = \vec{Q}$. where $A = \left[\varphi_j(x_i, y_i, z_i)\right]$ is a $N \times N$ coefficient matrix $\vec{\alpha} = [\alpha_j^n]$ and $\vec{Q} = [Q_j^n]$ are $N \times 1$ matrices. The numerical values of the corresponding spatial derivatives of $C^n(x_i, y_i, z_i)$ can be determined using equation (3.1) and the solution of the variable C computed by substituting the partial derivatives into the equation (3.2) with its given boundary conditions.

Two different type of radial basic functions are used, the multiquadric function φ^{MQ} given as: $\varphi_j^{MQ} = \sqrt{r_j^2 + \varepsilon^2}$

and Wendland's functions (CSRBF) φ^{CS} given as:

$$\varphi_j^{CS}(x,y,z) = \left(1 - \frac{r_j}{\delta}\right)_+^6 \left(35\left(\frac{r_j}{\delta}\right)^2 + 18\frac{r_j}{\delta} + 3\right),$$

where $r_j = \sqrt{(x-x_j)^2 + (y-y_j)^2 + (z-z_j)^2}$, ε is the shape parameter, δ is the support of the function and $\left(1 - \frac{r_j}{\delta}\right)_+ = \sup\left\{0, \left(1 - \frac{r_j}{\delta}\right)\right\}$.

A free shape parameter _ in global RBFs or _ in local RBFs plays an important role for the accuracy of the method and that can be tuned by the user. To the best of our knowledge, the optimal choice of the constant shape parameter is still an open question, and it is most often selected by trial and error. In order to overcome these shortcomings, many efforts have been made to find a new computational method that is capable of circumventing the ill-conditioning problems using linear solvers. The effort reported in the literature to reduce the ill-conditioning problems include: (1) Using variable shape parameters. (2) Pre-conditioning the coefficient matrix. (3) Using domain decomposition methods in over lapping or non overlapping schemes that decompose a very large ill-conditioned problem in to many subproblems with better conditioning. (4) Optimizing the center locations by the Greedy algorithm. (5) Using an improved numerical solver based on affine space decomposition, for more (see [9, 14, 15] and references therein and references therein).

4. Numerical results

We present here the simulation numerics by two RBF methods MQRBF and CSRBF and compare between these types of RBFs see Figures 4, 5. Using 11×11 uniformly distributed collocation points, Figures 6-10 plots the contours, surface and the errors of the numerical results of 2D concentration contaminant equation by both MQRBFs and CSRBFs, with the error between analytical and numerical simulation. While the Figures 11-12 given the solution of 3D using $11 \times 11 \times 11$ uniformly distributed collocation points. We presented the simulation at the time steps $nt = 100$ for 2D and at $nt = 200$ for 3D, with $\varepsilon = 1, \delta = 100$, $\Delta t = 0.01s$, φ^{MQ} and φ^{CS} for both 2D and 3D. The optimal maximum norm error is 0.0194 by MQRBF and 0.0053 by CSRBF

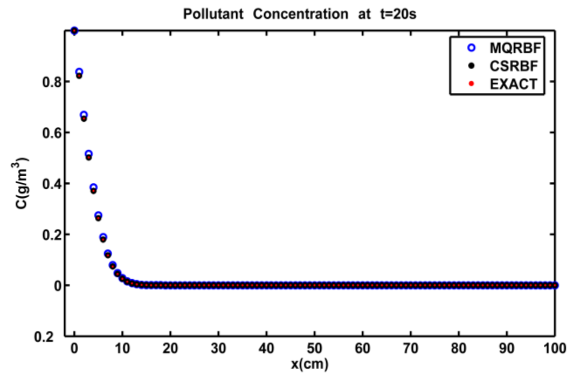

Fig. 4 Pollutant Concentration in 1-D, nt=20, $\Delta t = 0.01s$, ε=1, $\delta = 1000$.

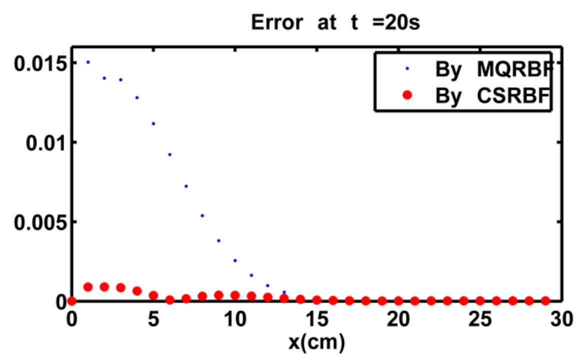

Fig. 5 Error by MQRBF and CSRBF in 1-D.

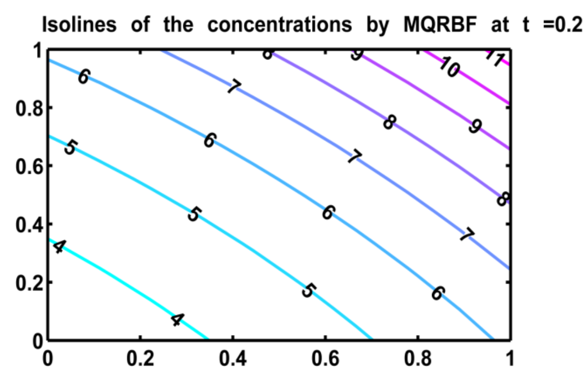

Fig. 6 Pollutant Concentration in 2-D, $nt = 20$, $\Delta t = 0.01s$, ε=1, $\Theta = 1$.

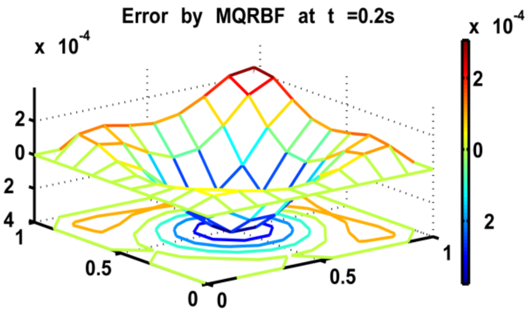

Fig. 7 Error of 2-D by MQRBF at $nt = 20$,

$\Delta t = 0.01s$, ε=1, $\Theta = 1$.

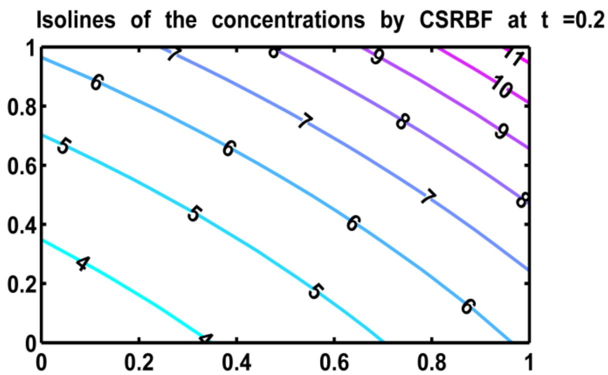

Fig. 8 Pollutant Concentration in 2-D, $nt = 20$,

$\Delta t = 0.01s$, $\delta = 100$, $\Theta = 1$.

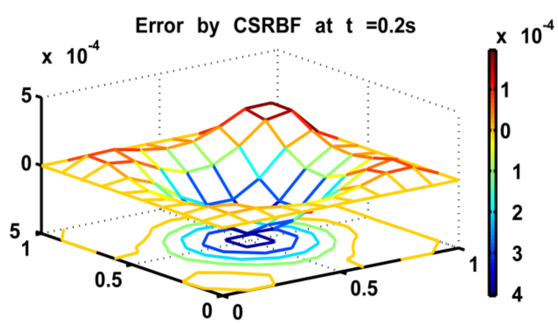

Fig. 9 Error of 2-D by CSRBF at $nt = 20$, $\Delta t = 0.01s$,

$\delta = 100$, $\Theta = 1$.

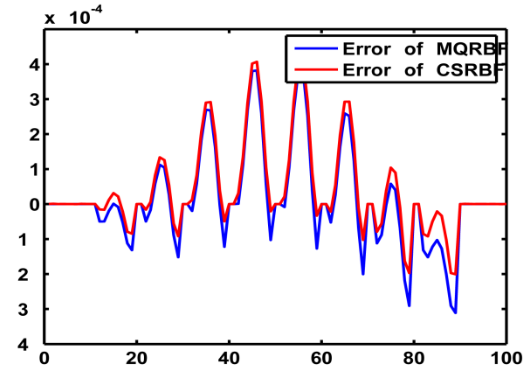

Fig. 10 Error of 2-D by MQRBF and CSRBF at $nt = 20$,

$\Delta t = 0.01s$, $\Theta = 1$.

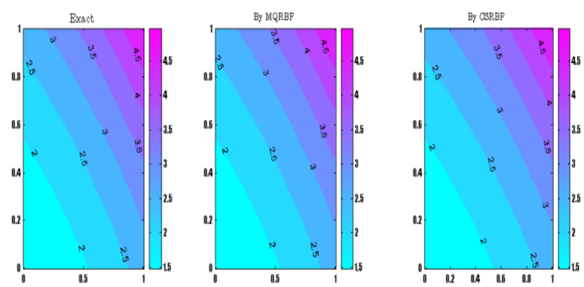

Fig. 11 Contours of 3-D on plane $z = 1/2$, $nt = 20$,

$\Delta t = 0.01s$, $\Theta = 0.5$.

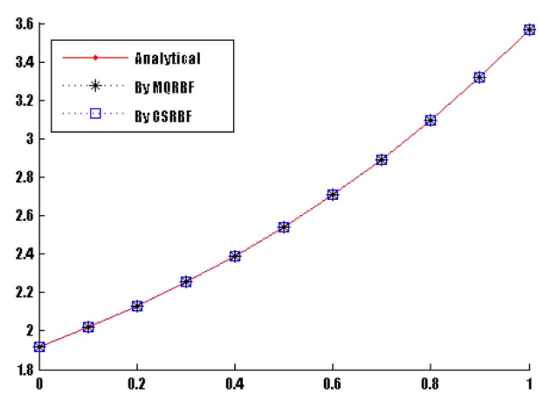

Fig. 12 Analytical and numerical solution of 3-D on

$y = 1/2$, $z = 1/2$, $nt = 20$, $\Delta t = 0.01s$, $\Theta = 0.5$.

5. Conclusions

Our experiments have shown that CSRBFs with a suitable choice of scaling factor δ would perform better than global MQRBFs. We have shown that the condition number of MQs scheme increased rapidly with the increase in the number of data points. Using CSRBF technique which enable one to work with sparse banded matrices the problem of ill-condition was reduced and improve the conditioning of the matrices. A meshfree method does not require a mesh to discretise the domain of the problem under consideration, and the approximate solution is constructed entirely based on a set of scattered nodes. Without using meshferr radial basis functions it would be difficult to solve 3-D problems by traditional method as FDM, FEM and FVM. Since it is a meshless method implementation is simple contrary to the others methods.

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