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INVERSE MODELING OF GROUNDWATER SYSTEM USING COUPLED PSO- MLPG TECHNIQUES

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The effective management of groundwater systems relies on the adequate knowledge of its hydro-geological parameters. In large aquifer systems, it is often computationally expensive to estimate the spatially distributed aquifer parameters. Inverse modeling of these parameters are usually required in simulation of flow and contaminant transport in the problem domain for its meaningful system prediction. In the present study, a new approach for inverse modeling is adopted based on Meshless Local Petrov Galerkin (MLPG) flow simulation model which is coupled with Particle Swarm Optimization (PSO) model. MLPG is one of the meshless techniques, which are recently developed to solve many partial differential governing equations in various engineering fields. Here, without using a pre-defined mesh, the system of equations are established for the entire domain. In MLPG, only appropriate distribution of nodes is utilized in the modeling. The nodes are used for approximation of the governing equations by using support domain. This alleviates the huge efforts required in pre-processing for groundwater modeling, as in mesh based methods. The numerical model is developed in 2 dimensions using MATLAB. The standard PSO algorithm is used for optimization and both simulation optimization models are coupled. The model is applied to a hypothetical confined aquifer to compute transmissivity in different zones of the aquifer. The stability of the estimated parameter is investigated by considering different sets of head data, assuming error free head and different sets involving measurement errors. The solutions are compared with other inverse models using the Levenberg-Marquardt Algorithm (LMA) and Genetic Algorithm (GA). The PSO results are comparable with LMA and are better compared to GA estimates. From the results we can say that the model can be applied to obtain optimal estimates of the aquifer parameters in the regional groundwater systems.

Keywords: Inverse modeling, Groundwater flow, Meshless method, Particle swarm optimization

INTRODUCTION

Efficient and effective management of groundwater systems primarily depends on the sufficient knowledge of its hydro-geologic parameters such as transmissivity, hydraulic conductivity, specific yield and aquifer recharge. For the hydraulic head prediction in the flow domain, these parameters are essential. These parameters are generally worked out only at few different locations in the aquifers; thus the information on their spatial distribution is often inadequate. Estimation of these hydro-geologic parameters in large aquifer systems often involves considerable time, human efforts and financial resources [12]. Inverse modeling of the system helps in the adequate assessment of these parameters for a meaningful system simulation. Auto-calibration of the optimal parameter values is the basic benefit from inverse modeling for a given regional aquifers that fit best between the observed and simulated hydraulic heads [3,11,14,15]. Inverse modeling for any problem includes simulation of the system and then optimization.

In the present work, a new simulation model based on Meshless Local Petrov Galerkin (MLPG) has been developed that predicts the head in the flow domain [13]. Further, the hydro-geological parameters of the system are estimated by coupling the simulation model with Particle Swarm optimization model [4]. Further the coupled model is applied for a hypothetical case study.

SIMULATION MODELING BY MLPG

The 2D groundwater flow governing equation for a heterogeneous, isotropic confined aquifer [2] is considered as

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y}\right) = S\,\frac{\partial h}{\partial t} + Q_w\,\delta(x - x_i)(y - y_j) - q \qquad (1)$$

For transient state flow analysis, the initial condition used is $h(x, y,0) = h_o(x, y)$ for $x, y \in \Omega$ and the boundary conditions of the Dirichlet boundary condition or Neumann boundary condition. They can be taken as: $h(x, y, t) = h_1(x, y, t)$ for $x, y \in \partial\Omega_1$ and $T\frac{\partial h}{\partial n} = q(x, y, t)$ for $x, y \in \partial\Omega_2$ respectively.

Here, $h(x, y, t)$ = Hydraulic head (m); $T(x, y)$ = Transimissivity (m^2/d); S = Storage coefficient; x, y = Horizontal space variables (m); Q_w = Source or sink function ($-Q_w$ source, Q_w = Sink) ($m^3/d/m^2$); t = Time in days; Ω = Flow region; $\partial\Omega$ = The boundary region ($\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$); $\frac{\partial}{\partial n}$ = Normal derivative; $h_o(x, y)$= Initial head in the flow domain (m); $h_1(x, y, t)$ = Known head value of the boundary head (m); $q(x, y, t)$ = Known inflow rate (m^3/d/m); δ is Dirac delta function, δ = 1 if $x = x_i$, $y = y_i$ or δ = 0 if $x \neq x_i, y \neq y_i$

The groundwater flow is generally described by a partial differential equation (Eq. 1), which commonly been solved using numerical techniques like Finite Difference Method (FDM) and Finite Element Method (FEM) [8]. However, they have inherent shortcomings of relying on meshes that are connected together by mesh in a predefined manner. High costs in creating an FDM/FEM mesh, low accuracy of prediction, difficulty in adaptive analysis are few shortcomings of these methods. The root of these problems is the use of grid or elements in the formulation stage. The idea of getting rid of these meshes in the process of numerical treatments has naturally evolved and the concepts of Meshless Methods have been shaped up [6].

Meshless method is best described as a numerical method used to establish a system of algebraic equations for the entire problem domain without using a predefined mesh for the domain discretization [6]. Meshless methods use a set of nodes within the problem domain as well as on the boundaries of the domain to represent (not discretize) the problem. As these nodes do not form a mesh and thereby they do not require prior information on the relationship between the nodes for the interpolation or approximation of the unknown functions of the field variables.

Many Meshless methods have found many applications and shown high potential to become powerful numerical tools in various fields of engineering. However, the Meshless methods are still in developing stage, and there are technical problems that need to be resolved before the methods can become efficient tools for complex engineering problems [6].

In this paper, the Galerkin's equivalent of MLPG [1] with Gaussian Radial basis function is assumed. In MLPG formulation, the first step is to define the trial solution $\hat{h}(x,y,t)$ as $\hat{h}(x,y,t) = \sum_{i=1}^{n} h_i(t)\, R_i(x,y)$, where, h_i *is* the unknown head, R_i *(x, y)* is the shape function at node *i* and n is the total number of nodes in the support domain. In the present study, the shape function R_i *(x. y)* is taken as [9]

$$R_i(x,y) = \exp[-\alpha_c(\frac{r_i}{d_c})^2\,] = = \exp[-Cs * r_i^2] \tag{2}$$

Where, $r_i = \sqrt{(x - x_i)^2 + (y - y_i)^2}$ and $Cs = \alpha_c/{d_c}^2$, α_c is the dimensionless size of support domain, and d_c is the nodal spacing near the node *i*, x_i and y_i are nodal co-ordinates.

Simplified from eq. (1), the MLPG principle of local residual formulation, the equation is written as

$$\iint_{\Omega_s} \left[\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} - \frac{S}{T}\frac{\partial h}{\partial t}\right] R_i(x,y)\, dx\, dy = 0 \tag{3}$$

To account for the time derivative an implicit finite difference approximation was used. The complete formulation for solving Groundwater equation using MLPG technique can be referred from Swathi and Eldho [13]. The resulting set of simultaneous equations are expressed in the matrix form as

$$\left\{[K_1] + \left(\frac{\Delta t}{S}\right)\left(T_x[K_2] + T_y[K_3]\right)\right\}\{h_i\}^{t+\Delta t} = [K_1]\{h_i\}^t \pm \left(\frac{\Delta t}{S}\right)([K_1]Q_w) \tag{4}$$

Where $[K_1]$ is a global matrix for square of shape function; $[K_2]$ is global matrix for square of first derivative of shape function with respect to x; $[K_3]$ is global matrix for square of first derivative of shape function with respect to y; Δt is time step size; $\{h_i\}^{t+\Delta t}$is the unknown head vector and $\{h_i\}^t$the known head vector. Such that,

$$[K_1] = \iint_{\Omega_s}\left(R_i(x,y)\right)^2 dx\,;\ [K_2] = \iint_{\Omega_s}\left(\frac{\partial R_i(x,y)}{\partial x}\right)^2 dx\,dy\ ;\ [K_3] = \iint_{\Omega_s}\left(\frac{\partial R_i(x,y)}{\partial y}\right)^2 dx\,dy \tag{5}$$

The $[K_1]$, $[K_2]$ and $[K_3]$ are calculated for every support domain initially and global matrices later on are formed and the Eq. (4) is solved using the Gauss-Jordan method.

Based on the MLPG formulation [13], 2D flow model for confined aquifer is developed for transient conditions. For the given problem, entire domain is represented using nodes. Here, depending on the problem, equidistant nodes or irregular nodes may be used which are added in the aquifer domain and on the boundary. The value of shape parameter, for 2D cases, α_c (dimensionless size of the support domain) should have the value between 2.5 and 3.5 [6] for accuracy as well as stability of the results. Hence for present study, square support domain is considered such that the dimension of support size, α_c will be 3 in all directions as shown in Fig. 2. The following are the brief steps to be followed. (1) Domain Representation with nodes, (2) Function Approximation of the unknown, (3) Formation of System of Equations and (4) Solving Global Equations

INVERSE MODELING BY PARTICLE SWARM OPTIMIZATION (PSO)

PSO is an optimization technique introduced by Kennedy and Eberhart [4] based on the flocking behavior of birds, fish and other animals. The "particle" in PSO is related with three main parameters: position, velocity and fitness. Position represents the unknown variable of the problem, the rate of change of position (or change of variable) is given by velocity and the fitness is a measure of how well the particle solves the objective function optimally [7].

The first step of the algorithm is to create the initial swarm of particles. Each particle's position consists of m variables where m is the number of unknowns in the optimization problem. The particles will search this m-dimensional space to find the optimum solution. Well within the search space, the variable is initialized randomly. An initial velocity which is determined randomly is assigned to all particles. Each particle moves towards its best previous position and towards the best particle in the whole swarm. The number of particles in a swarm is called as population. The objective function is a measure of the quality of a solution and here PSO, minimizes the objective function.

Further, "pbest" is the coordinates in the search space which are associated with the best solution (fitness) the particle has achieved so far and "lbest" is the best value obtained so far by any neighboring particle. When a particle takes all the population as its neighbors, the best value is a global best "gbest". The PSO concept consists of, at each time step, changing the particle (velocity) towards its pbest and lbest locations. Acceleration is weighted by a random term, with separate random numbers being generated for acceleration toward pbest and lbest locations. The individual particle position is updated as follows [4, 5]:

$$x_{k+1}^i = x_k^i + v_{k+1}^i \qquad (6)$$

Where, velocity calculated as:

$$v_{k+1}^i = wv_k^i + c_1 r_1 \left(p_k^i - x_k^i\right) + c_2 r_2 \left(p_k^g - x_k^i\right) \qquad (7)$$

Where, x_k^i is the particle position; v_k^i is the particle velocity**;** p_k^i is the best remembered individual particle position**;** p_k^g is the best remembered swarm position**;** $c_1 c_2$ are the cognitive and social parameters**;** $r_1 r_2$ are the random numbers between 0 and 1**;** w is the constriction factor.

The steps involved in the PSO computation process are (1) Initialize particle swarm, (2) Evaluate optimization function, (3) Modify particle's best value, (4) Modify overall best value, (5) Move each particle to new position, and (6) Termination condition.

MODEL STUDY

To study the PSO-MLPG model for inverse modeling, a hypothetical confined aquifer of 36 sq. km area [10] is considered for the present study. The flow domain (Fig. 1) is bounded by a Dirichlet boundary condition in the south with a constant head value of 100 m, Neumann boundary condition in the west with an inflow rate of 0.25m^3/day/m, and no flow boundaries in the east and north. Some portion in the north of the aquifer is recharged at the rate of 0.15 x 10^{-3} m/day through some aquitard. Three pumping wells P1, P2 and P3 at the rates of 6000, 3000 and 800m^3/day, respectively, are considered in the flow domain. The storativity of the entire aquifer is taken as 0.001 and the aquifer is parameterized into three zones (Fig.1) with transmissivity values varying from 50 to 200m^2/day. The considered flow problem is solved using MLPG, 2D model with 169 nodes with Δx = Δy = 500m and 9 nodes in the support domain (Fig. 2). The time step of 1 day is considered and the value of $\alpha_c = 3$ and therefore, *Cs* is taken as 1.2x10^{-5}.

The hydraulic heads obtained from MLPG model for the known transmissivity values for the flow problem are taken as observed heads in the inverse modeling.

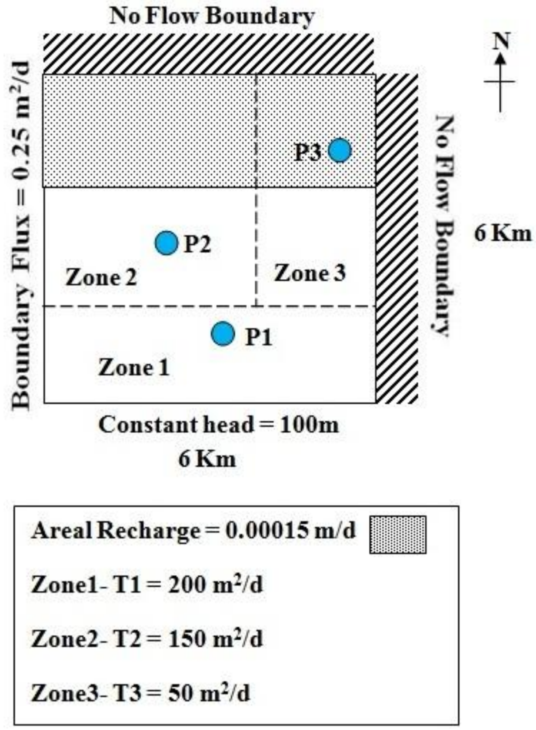

Fig. 1: Aquifer Configuration (Not to scale)

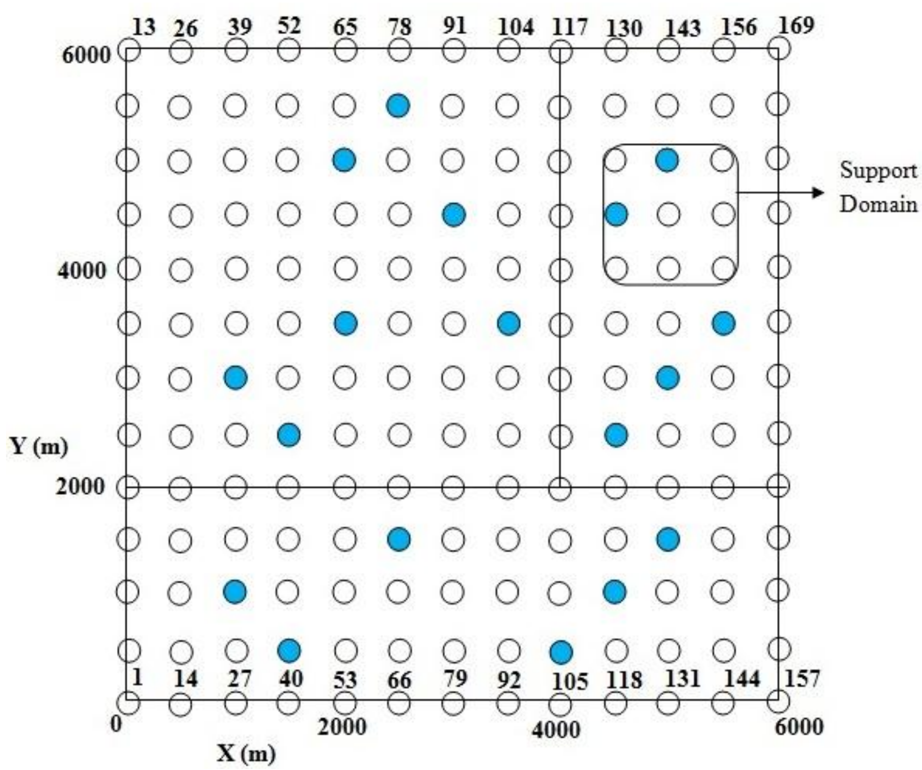

Fig. 2: Nodal Arrangement for the problem with observation points (Not to scale)

The objective function (J) considered involving weighted least squares criterion, and the functional to be minimized [10, 12] is

$$\underset{T_l \ldots T_M}{Min} \; J = \sum_{l=1}^{L} \sum_{t=t_0}^{t_f} \omega_{l,t} \left[h_{l,t}^{c} - h_{l,t}^{ob} \right]^2 \tag{8}$$

Subject to lower and upper bounds of the parameter: $T_i^l \le T_i \le T_i^u$.

Where $h_{l,t}^{c}$ is MLPG head for assumed parameter; $h_{l,t}^{ob}$ is the MLPG head for true parameter, (these are replaced by observed head values in the field case studies); T_i is transmissivity at block i; M is the parameter dimension; L, the number of observation wells; and t_0 and t_f , beginning and ending times of observations. Superscripts l and u are used to denote the lower and upper bounds of parameters and $\omega_{l,t}$ is the weighting coefficient = 1.

Generally, the weights are decided based on the poorer or better hydraulic head observations. Here, the weighting coefficient is considered as unity as the observed heads are taken from the MLPG solution. The initial parameter value is considered to be ranging from 2 to 200m^2/day.

For inverse modeling, different data sets of observed head are obtained by adding certain noise to the MLPG solutions. Data set 1 represents the error free head data whereas Data sets 2 to 4 are obtained by adding normally distributed random errors with zero mean and standard deviations of 0.01, 0.1, and 1, respectively to the Data set 1.This analysis is carried on to know the influence of the quality of head measurement in estimation of parameters. Initially, the transient state head data at 18 observation points in the problem domain are considered for four different sets and are used for evaluating the zonal transmissivity in different zones of the problem. The data sets with noise are considered to be equivalent for the observation heads with measurement errors, which are common in the field cases. Also the PSO model characteristics considered are: population = 100; maximum number of generations = 400; c_1, c_2 are 0.5 each**;** w is the constriction factor = 1.2.

The observed head data at 100 days of pumping is obtained from MLPG model at these eighteen observation points. From Table 1, the results from the model show that the parameter values are estimated satisfactorily for all four data sets. Also for data sets with noise, the PSO solutions are better with respect to the GA estimates (GA-FEM model, [10]) and are comparable to LMA. Also, to check the robustness of the developed model the observation points are reduced to nine and six. Head values are simulated at 100, 200 days, and 50, 100 and 200 days, respectively, which together give 18 head data values to evaluate the objective function. From Tables 2 and 3, the estimated transmissivities using the model in both cases are closer to true values and are better for noisy head data sets too, demonstrating its applicability for field studies.

CONCLUSIONS

In the present work, simulation model based on Meshless Local Petrov-Galerkin (MLPG) is used for groundwater head prediction. The model is coupled with Particle Swarm optimization for parameter estimation in a hypothetical confined aquifer. The aquifer parameter of transmissivity is computed for transient states using error free data and different sets of noisy data this indicates that the model can be applied to regional aquifers where the data available may be sparse and with errors. The robustness of the model is checked by computing the parameters by considering head data at different times.

Table 1: Transmissivity (m^2/day) values estimated in the aquifer using different data sets for t=100 days and number of observation points: 18

Method		True Value	PSO	GA	LMA
Data Set 1	Zone 1	200	200	200.041	200
	Zone 2	150	150.112	150.062	150
	Zone 3	50	49.955	49.810	50
Data Set 2	Zone 1	200	200	199.456	199.964
	Zone 2	150	149.955	149.769	150.028
	Zone 3	50	50.007	50.103	49.999
Data Set 3	Zone 1	200	200	202.379	199.866
	Zone 2	150	150.198	149.769	150.391
	Zone 3	50	50.05	50.687	50.001
Data Set 4	Zone 1	200	200	219.039	200
	Zone 2	150	155.107	149.185	155.151
	Zone 3	50	50.681	48.349	50.668

Table 2: Transmissivity (m^2/day) values estimated in the aquifer using different data sets for t=100, 200 days and number of observation points: 9 for each time

Method		True Value	PSO	GA	LMA
Data Set 1	Zone 1	200	200	199.749	200
	Zone 2	150	150.013	150.062	150
	Zone 3	50	50.001	49.810	50
Data Set 2	Zone 1	200	200	200.626	199.929
	Zone 2	150	149.999	150.646	150.117
	Zone 3	50	50.001	49.810	49.978
Data Set 3	Zone 1	200	200	201.210	200
	Zone 2	150	149.610	150.062	149.644
	Zone 3	50	49.907	50.395	49.892
Data Set 4	Zone 1	200	200	202.087	200
	Zone 2	150	144.937	152.692	145.057
	Zone 3	50	51.058	49.518	51.024

Table 3: Transmissivity (m^2/day) values estimated in the aquifer using different data sets for t=50, 100, 200 days and number of observation points: 6 for each time

Method		True Value	PSO	GA	LMA
Data Set 1	Zone 1	200	200	200.041	200
	Zone 2	150	149.992	150.062	150
	Zone 3	50	49.999	50.103	50
Data Set 2	Zone 1	200	200	200.041	199.974
	Zone 2	150	149.982	150.062	150.102
	Zone 3	50	49.954	49.810	49.940
Data Set 3	Zone 1	200	200	200.918	200
	Zone 2	150	150.417	150.354	150.469
	Zone 3	50	50.401	50.103	50.416
Data Set 4	Zone 1	200	200	211.148	200
	Zone 2	150	149.452	152.4	149.378
	Zone 3	50	53.079	50.687	53.102

The comparison study of the model results with the GA-FEM technique shows that the PSO-MLPG results are better and comparatively good results are obtained when compared with LMA-MLPG. The study demonstrates the effectiveness of the PSO-MLPG coupled model, and suggests its application in inverse modeling.

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