Multiphase Groundwater Flow and Transport using a New Localized Collocation Method (LOCOM)

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Multi-phase groundwater flow and transport problems can be solved accurately using the classical collocation method with Hermite cubic basis functions. However, because of inefficiencies inherent in the classical collocation method, the computational time required to solve large-scale problems limit its widespread use. However, when this complex model is modified to utilize a new numerical concept based upon a localized collocation formulation, the computational efficiency of the code is significantly enhanced. Solutions to the groundwater flow and transport equations obtained using the classical and new formulation were compared for accuracy as well as efficiency. An increase in speed of more than 100 percent has been observed for large problems.

1. Introduction

The classical collocation approach to the solution of differential equations has been known since at least 1937 [1]. However, it was largely through work conducted in the early 1970's that the method was popularized for the solution of second-order partial-differential equations. While it was evident that the inherent simplicity of the approach held promise as a computationally efficient algorithm, the popularity of the method was limited.

In this paper we investigate what appears to be a new numerical approach that builds upon the classical collocation method. The formulation leads to a single-degree of freedom at each node as opposed to the classical approach that requires two degrees of freedom in one space dimension, four in two space dimensions and eight in three space dimensions. We investigate its application to an existing classical-collocation code for the solution of the multi-phase flow and transport equations.

2. Localized Collocation Method (LOCOM)

Let us consider for simplicity in presentation the one-dimensional advective-diffusive equation

$\mathbf{L}(u) = 0$

with $\mathbf{L} = \frac{\partial}{\partial t} + c\frac{\partial}{\partial x} - D\frac{\partial^2}{\partial x^2}$

as the advective-diffusive operator. Consider the grid $\Omega_x = \{x_i, 1 < i < N_x\}$ with Δx =L/N$_x$, in which L is the length of the domain. When Hermite collocation is applied, the derived discretization of the operator is based on the value of the unknown function u and its first derivative du/dx for each node. The purpose of this new method is to derive a different collocation approach, which involves only one unknown for each node. The new method is based on two fundamental steps:

Step 1: Consider the generic node x_i and its surrounding intervals: the left interval $[x_{i-1}, x_i]$ and the right one $[x_i, x_{i+1}]$. In each of these intervals we approximate the unknown $u(x,t)$ using Hermite basis functions as follows:

$$u(x,t)\Big|_{[x_{i-1},x_i]} \cong U^L = H_{0,i-1}(x)u_{i-1} + H_{1,i}(x)u_i + \frac{\Delta x}{2}\overline{H}_{0,i-1}(x)\left(\frac{\partial u}{\partial x}\right)_{i-1} + \frac{\Delta x}{2}\overline{H}_{1,i}(x)\left(\frac{\partial u}{\partial x}\right)_i \quad (1)$$

$$u(x,t)\Big|_{[x_i,x_{i+1}]} \cong U^R = H_{0,i}(x)u_i + H_{1,i+1}(x)u_{i+1} + \frac{\Delta x}{2}\overline{H}_{0,i}(x)\left(\frac{\partial u}{\partial x}\right)_i + \frac{\Delta x}{2}\overline{H}_{1,i+1}(x)\left(\frac{\partial u}{\partial x}\right)_{i+1} \quad (2)$$

Step 2: The elimination of the unknown derivatives from the equations is undertaken by deriving an appropriate approximation for the derivatives present in equations (1) and (2). For this purpose, we consider the 2^{nd}order Lagrange polynomial ($\mathfrak{L}$) as an interpolator for the function u inside the double interval $[x_{i-1}, x_{i+1}]$:

$$U(x,t)\Big|_{[x_{i-1},x_{i+1}]} = \mathfrak{L}_{i-1}(x)u_{i-1} + \mathfrak{L}_i(x)u_i + \mathfrak{L}_{i+1}(x)u_{i+1}$$

The Lagrangian interpolator allows us to evaluate the first derivative of u as the following:

$$\frac{\partial u}{\partial x} \cong \frac{\partial U}{\partial x} = \frac{d\mathfrak{L}_{i-1}}{dx}u_{i-1} + \frac{d\mathfrak{L}_i}{dx}u_i + \frac{d\mathfrak{L}_{i+1}}{dx}u_{i+1}$$

Therefore, for equal grid spacing, the expressions for the nodal approximation of the derivatives are:

$$\left(\frac{\partial u}{\partial x}\right)_{i-1} \cong \frac{-3u_{i-1} + 4u_i - u_{i+1}}{2\Delta x} \quad (3)$$

$$\left(\frac{\partial u}{\partial x}\right)_i \cong \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad (4)$$

$$\left(\frac{\partial u}{\partial x}\right)_{i+1} \cong \frac{u_{i-1} - 4u_i + 3u_{i+1}}{2\Delta x} \quad (5)$$

The approximation of the derivatives using Lagrange polynomials as interpolators is equivalent to using the 2^{nd} order central difference approximation for the derivative at the i^{th} node, the forward difference approximation for the derivative at the $(i-1)^{th}$ node and backward approximation at the $(i+1)^{th}$ node. Substitution of expressions (3) through (5) into equations (1) and (2) leads to the following final interpolator of the function u inside the left and right interval respectively:

$$\begin{aligned} U^L(x,t) &= f_1(x)u_{i-1} + f_2(x)u_i + f_3(x)u_{i+1} \\ U^R(x,t) &= g_1(x)u_{i-1} + g_2(x)u_i + g_3(x)u_{i+1} \end{aligned}$$

where:

$$\begin{aligned} f_1 &= H_{0,i-1} - \frac{3\overline{H}_{0,i-1} + \overline{H}_{1,i}}{4} & g_1 &= \frac{\overline{H}_{1,i+1} - \overline{H}_{0,i}}{4} \\ f_2 &= H_{1,i} + \overline{H}_{0,i-1} & g_2 &= H_{0,i} - \overline{H}_{1,i+1} \\ f_3 &= \frac{\overline{H}_{1,i} - \overline{H}_{0,i-1}}{4} & g_3 &= H_{1,i+1} + \frac{\overline{H}_{0,i} + 3\overline{H}_{1,i+1}}{4} \end{aligned}$$

3. Application to Multi-phase Flow and Transport

3.1. Existing Classical Collocation Code

The existing multi-phase code can accommodate as many as three fluid phases, identified as a water-phase, a NAPL-phase and a gas-phase, and can model flow of either one, two or three phases in any combination [2]. The governing equations for this simulator consist of two species equations, NAPL species in water and NAPL species in gas, as well as the three fluid-phase mass balance equations.

The two species equations are represented by:

$$\frac{\partial\left(\varepsilon S_\beta \rho_n^\beta\right)}{\partial t} + \nabla\cdot\left[\varepsilon S_\beta \rho_n^\beta v^\beta\right] - \nabla\cdot\left[\varepsilon S_\beta \rho^\beta D^\beta \cdot \nabla\left(\frac{\rho_n^\beta}{\rho^\beta}\right)\right] + \varepsilon S_\beta \kappa_n^\beta \rho_n^\beta = \rho_n^\beta Q^\beta + \widehat{\rho}_n^\beta \tag{6}$$

The three fluid-phase mass balance equations are given by:

Water-phase:

$$\frac{\partial\left(\varepsilon S_W \rho^W\right)}{\partial t} + \nabla\cdot\left[\varepsilon S_W \rho^W v^W\right] = \rho^W Q^W + E_n^W - E_{n/W}^G - E_{n/W}^S \tag{7}$$

NAPL-phase:

$$\frac{\partial\left(\varepsilon S_N \rho^N\right)}{\partial t} + \nabla\cdot\left[\varepsilon S_N \rho^N v^N\right] = \rho^N Q^N - E_n^W - E_n^G \tag{8}$$

Gas-phase:

$$\frac{\partial\left(\varepsilon S_G \rho^G\right)}{\partial t} + \nabla \cdot \left[\varepsilon S_G \rho^G v^G\right] = \rho^G Q^G + E_n^G + E_{n/W}^G \tag{9}$$

where:
α is the phase (W-water, N-NAPL, G-gas)
β is the phase (W-water, G-gas)
ε is the porosity of the porous medium
S_α and S_β are the saturations of the α and β-phases
ρ_n^β is the mass concentration of NAPL in the β-phase [M/L^3]
ν^α and ν^β are the mass average velocities of the α and β-phases [L/T]
ρ^α and ρ^β are the densities of the α and β-phases [M/L^3]
D^β is the dispersion coefficient for the β-phase, a symmetric second-order tensor [L^2/T]
κ_n^β is the decay coefficient for NAPL in the β-phase [1/T]
Q^α and Q^β are the point source (+) or sink (-) for the α and β-phases [1/T]
$\widehat{\rho}_n^\beta$ is the source or sink of mass for NAPL in the β-phase due to interphase mass exchange [M/L^3T]
E_n^W is the dissolution mass transfer of the NAPL species from the NAPL phase to the water phase
$E_{n/W}^G$ is the volatilization mass transfer of the NAPL species from the water phase to the gas phase
E_n^G is the volatilization mass transfer of the NAPL species from the NAPL phase to the gas phase
$E_{n/W}^S$ is the adsorption mass transfer of the NAPL species from the water phase to the soil

The existing code solves these equations using an implicit-in-time classical collocation finite element method with Hermite cubic basis functions. It is a physically complete subsurface flow and transport model that was previously developed to study the movement and fate of NAPL contaminants in near-surface granular soils [2].

3.2. Addition of LOCOM

3.2.1. General Method - Lagrangian Boundary Conditions

In our formulation, we apply LOCOM to equations (6) through (9) in a similar manner. For each partial-differential equation, the classical-collocation equations are generated as in the original method, with the exception of the treatment of boundary conditions. As a first step in our method, the four collocation equations within each element are averaged to form an elemental equation. Then for every internal node, the four elemental equations surrounding the nodes are averaged to form one equation for each node. We then use Lagrangian finite-difference approximations to represent each of the unknown derivative functional values, thereby reducing the system of equations so that only functional values remain unknown.

Boundary nodes are handled differently based on whether the node is a Neumann or a Dirichlet condition. In the general method, for each Neumann boundary condition,

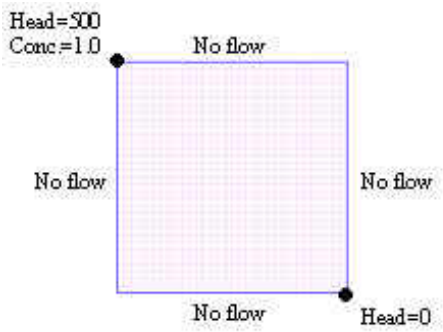

Figure 1. Sample problem run using the new LOCOM code and the classical collocation code.

a Lagrangian finite-difference approximation is written as the equation for that node. If the new finite-difference expression contains Dirichlet nodes, the known information is applied to the equation. Equations are not created at Dirichlet boundary nodes as the functional value at that location is known.

3.2.2. Alternative Method - Hermite Boundary Conditions

In the general method for treating boundary conditions we ignore the continuity equations on the boundary. In an attempt to retain the continuity equations at the boundaries, a second method was developed. In this method, all known boundary-condition information is applied initially to the system of collocation equations. Again, equations are not written at Dirichlet boundary nodes as they are unnecessary for solution of the problem. At corner Neumann-boundary nodes, the corner elemental equation is directly applied to that node. The side Neumann-boundary nodal equations are created by averaging the two elemental equations that surround the node. The unknown nodal derivatives are then approximated using the Lagrangian basis functions, similar to the method used for internal nodes. Again, known Dirichlet information at the nodes is applied to the system of equations.

4. Results & Discussion

To date, LOCOM has been applied to the solution of the flow, gas phase transport and water phase transport equations. The LOCOM code and the original classical collocation code were run using the sample problem shown in Figure 1. The results were compared for computational efficiency, as well as accuracy.

4.1. Computational Efficiency

The sample problem (Figure 1)was run for 200 time steps with a variety of different mesh sizes. Both codes were run on a Dell Optiplex GX1p, 450 MHz. Computation times are presented in Table 1.

Number of Nodes	Classical Collocation	LOCOM
81 (9x9)	88	80
289 (17x17)	205	140
1089 (33x33)	895	422
4225 (65x65)	4972	1802

Table 1
A comparison of computation time versus the number of nodes in the system (in seconds).

4.2. Accuracy of Solution

The sample problem (Figure 1) was run for 1500 seconds for two different mesh sizes. The results can be seen in Figures 2 and 3. For the 9x9 mesh size (Figure 2), the LOCOM solution has more numerical diffusion than the classical approach due to the lower order accuracy solutions of the LOCOM. In addition, one can see that the LOCOM concentration front is slightly behind that of the classical collocation method.

However, as the mesh density is increased to 33x33 (Figure 3), the LOCOM solution approaches the classical collocation solution. The front is steeper (less diffusive), though still slightly lagging the classical approach. From these two figures, one can see the effects of round-off error for lower order solutions and how they can be overcome through mesh refinement.

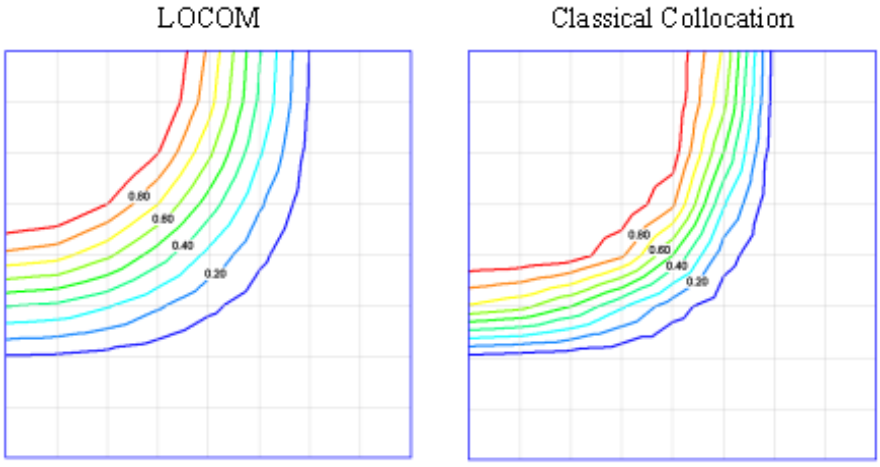

Figure 2. Comparison of LOCOM and classical collocation for a concentration front propogation on a 9x9 nodal mesh

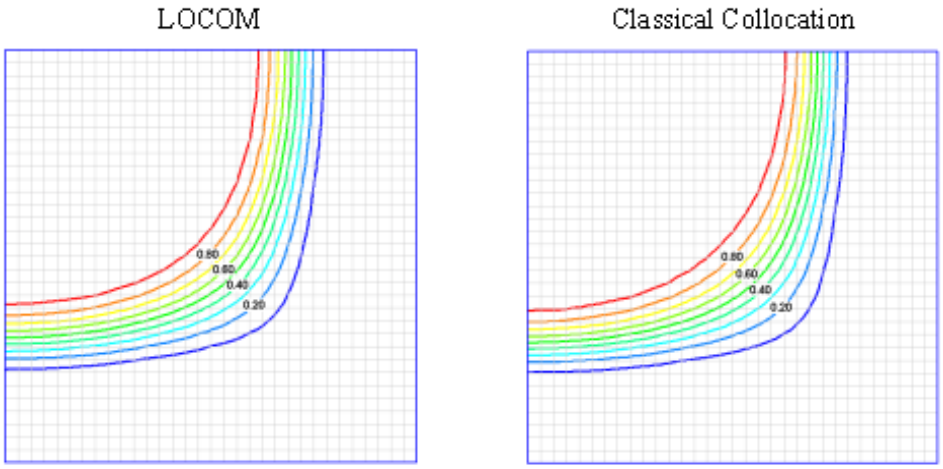

Figure 3. Comparison of LOCOM and classical collocation for a concentration front propogation on a 33x33 nodal mesh.

4.3. Comparison of Treatment of Boundary Conditions

Differences can be seen in solutions depending on whether boundary conditions are represented using Hermite polynomials, or by standard Lagrangian finite-difference approximations. Both cases were run for the sample problem (Figure 1) and the results were compared with the original classical-collocation code, as seen in Figure 4. The three panels show that the Lagrangian boundary condition solution most closely resembles the results from the classical collocation approach.

In addition, as seen in Figure 5, the Lagrangian boundary condition approach yields a method of order 2.33, while the Hermite boundary condition approach is only of order 1.86.

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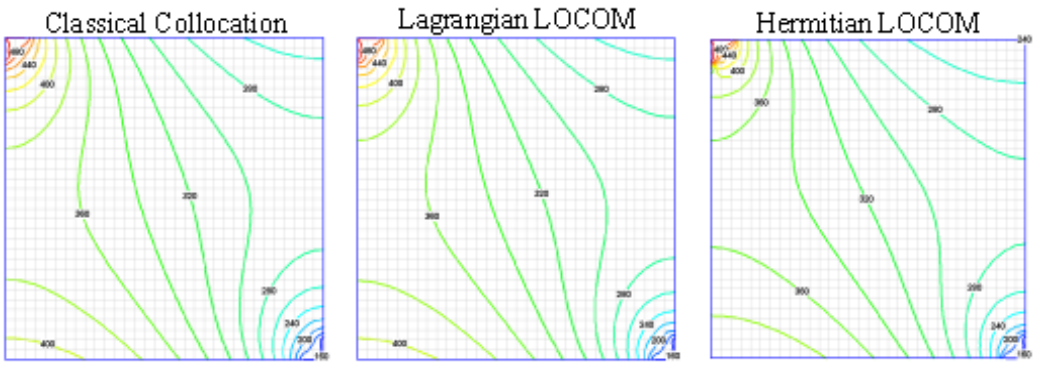

Figure 4. Comparison of head values obtained via the LOCOM method using Lagrangian boundary conditions versus Hermitian. Both results are compared with that of the classical-collocation approach.

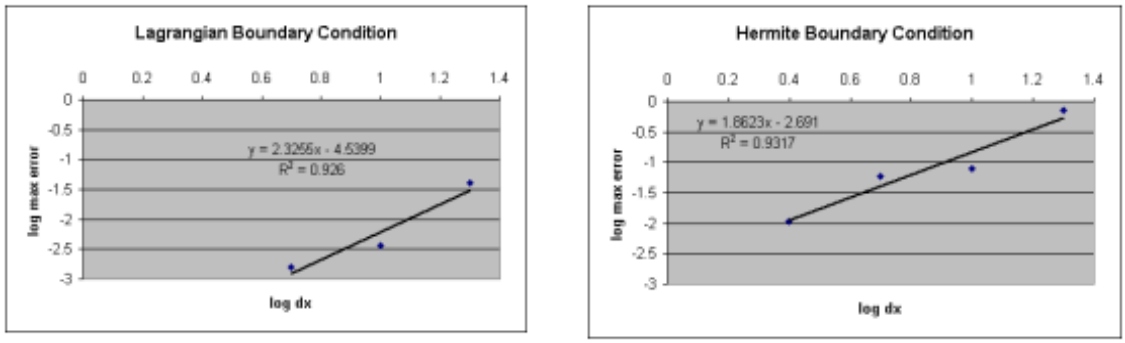

Figure 5. Comparison of order of solution accuracy for the Lagrangian and Hermitian boundary condition approaches.