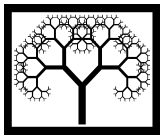
Paper 16



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The Local Discontinuous Galerkin Method for Coupled Unsaturated Flow and Chemical Transport in Porous Media

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Abstract

The local discontinuous Galerkin (LDG) method offers many advantages over conventional finite element solutions of transport and mechanics problems in soils, namely more accurate simulation of sharp fronts, easier representation of domain discontinuities, algorithms that are more suited to *h* and *p* adaptivities and better mass balances between elements. The LDG has been applied to a large number of problems in soils, saturated and unsaturated, including the Richard's equation, diffusion-advection equation and elastic and non-elastic mechanics. However, its application to coupled problems in porous media is much less widespread. When it has been used to solve problems such as poro-elasticity [1,2] and thermo-elasticity [3], it has been found to be computationally efficient. Coupled problems, thermal, mechanical, hydraulic and chemical, single or multi-phase have become highly significant in the last two decades and are indispensable to a number of current engineering challenges in waste management, biomedical engineering, mining, pollution control, and water resources management, among others.

Multiphase thermo-chemo-hydro-mechanical problems frequently occur in problems of waste management and groundwater quality. A number of engineering material and subsurface environments experience unsaturated conditions where both air and water are present in the pores, with or without thermal gradients (*e.g.* exothermally decaying waste over clay liners, solar ponds, brine ponds). This paper presents an LDG solution to the problem of hydro-chemical transport in an undeformable, three-phase medium containing solid, water and air. We build a weak formulation of the non-linear coupled equations of water flow (Richards' equation) and chemical transport (diffusion-advection equation), in terms of the incremental variables. We present results for the one-dimensional, steady-state case. We implement both linear and higher order elements. We validate the formulation by comparing its predictions to known analytical solutions. We compare the performance of the LDG to that of a continuous Galerkin variant, and identify conditions under which the former is superior to the latter. The work is a prelude for the development of an hp adaptive

LDG solution to the problem of multi-phase chemo-poro-elasticity in multiple dimensions and its application to the solution of problems of environmental containment systems based on compacted and geosynthetic clay liners.

Keywords: local discontinuous Galerkin, coupled analysis, unsaturated flow, chemical transport, unsaturated porous media.

1 Introduction

Solving coupled equations in geomechanics is essential for tackling a number of problems such as contaminant transport, water infiltration and soil deformation, slope stability, thermal and isothermal consolidation, etc. The numerical analysis of coupled problems is more expensive in terms of computational time and memory resources. Particularly, for some of 2D and many 3D finite element models the cost can be prohibitive [4-6]. One way of dealing with this problem is by implementing adaptive finite element methods (FEM) to find the optimum discretization, in time or space or both.

Recently, spatial optimization using discontinuous Galerkin (DG) FEM has received increasing attention from researchers [7]. Due to their local nature, the DG methods can handle discontinuities at element boundaries. Also these methods are highly suitable for both h-adaptive and p-adaptive techniques in which neighbouring elements might have different orders of approximation. The main advantage of DG methods are their extremely high parallelizability and their high-order accuracy [8]. However, the application of these methods to coupled problems in geomechanics remains limited. The accuracy and ability of DG methods to approximate some linear and non-linear problems arising in contaminant transport in porous medium were examined by Aizinger [9]. These problems were investigated for transient flow in heterogeneous media with abrupt variations of velocity present, using a standard FEM to solve the mixed form of Richards' equation and a DG method for the advection terms [10]. In another work by Sun et al. [11], optimal convergences were obtained for coupled flow and reactive transport models (under saturated conditions) based on the DG method. In a recent study [12], the accuracy and efficiency of local discontinuous Galerkin (LDG) method to solve Richards' equation (for flow in unsaturated porous media) was compared for a wide variety of permeability and quadrature approximations. However, to the best of our knowledge, no DG method for solving the coupled Richards' and reactive diffusion-advection equation (flow and contaminant transport in unsaturated porous media) has been developed. This paper presents such a formulation and compares the performance of standard continuous Galerkin (CG) and the LDG methods. In the next section, we present the governing equations, then the LDG formulation is described. Finally, we discuss then present our results and conclusions.

2 Governing equations

2.1 Water flow model

Flow in porous media is widely described by Darcy's equation. This equation was extended to unsaturated medium by Richards [13]. The head pressure form of Richard's equation for steady state (without source/sink) and horizontal flow (non-gravity flow) is:

$$\frac{\partial}{\partial x}\left(k(h)\frac{\partial h}{\partial x}\right) = 0 \tag{1}$$

where h is the head pressure ($h > 0$ under saturated conditions and $h < 0$ under unsaturated conditions), $k(h)$ is the hydraulic conductivity of the soil layer and x is the horizontal coordinate. The hydraulic conductivity for saturated soil is independent of the pressure head:

$$k(h) = k_s \tag{2}$$

For unsaturated soils, we use the Gardner's exponential relation [14]:

$$k(h) = k_s . k_r \tag{3}$$

$$k_r = e^{ah} \tag{4}$$

where α is an experimentally-determined parameter. Tracy states [15] that some soils can be modelled by experimental Irmay's equation as following:

$$k_r = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^m \tag{5}$$

where θ is the volumetric moisture content, θ_r is the residual volumetric moisture content, θ_s is at the saturated volumetric moisture content and m is an experimentally-determined parameter. Substituting (4) in (5) gives an exponential form of moisture content:

$$\theta = \theta_r + (\theta_s - \theta_r) e^{\alpha h / m} \tag{6}$$

2.3 Chemical transport equation

The steady state form of Fickian solute transport (without source/sink) in a porous medium is:

$$\frac{\partial}{\partial x}\left(\theta D\frac{\partial C}{\partial x}\right)=0 \tag{7}$$

D is the hydrodynamic dispersion coefficient, representing both mechanical dispersion and molecular diffusion. In a standard formulation, $\theta D=\lambda_L|v|+\theta D_m\tau$ where λ_L is the longitudinal pore-scale dispersivity, $|v|$ is the magnitude of Darcy's velocity, D_m is the molecular diffusion coefficient in free water and τ is the tortuosity. We start with this simplified version of the diffusion – advection equation in view of later incorporating the advective and reactive terms. The coupling of equation (1) and (7) clearly occurs through θ.

3 The LDG Method

The LDG method falls into the general category of weighted residual methods. The same space function is used in both continuous Galerkin method and discontinuous Galerkin method, with the later providing relaxed continuity at inter-element boundaries. In this method, discontinuity of either field variables or their derivatives, usually both, is allowed while the continuity of computational domain is maintained. As a result, the LDG can deal with elements independently of each other or, in other words, at a local level, hence the title of the method. In addition, the method does not require elements to be conforming at their interfaces. This makes the LDG highly suitable for both h-adaptive and p-adaptive methods in which neighbouring elements might have different orders of approximation. In addition, the local nature of the method creates excellent conditions for generating parallelised algorithms. From a theoretical perspective, the LDG method can be seen as a more general method which encompasses both the continuous finite element method or continuous Galerkin (CG) and the finite difference (FDM) or finite volume methods: the FDM is recovered from the LDG by adopting a constant element; enforcing cross-boundary continuity will lead to the CG.

3.1 The LDG formulation

We use both CG and LDG methods to solve the coupled flow and chemical transport in unsaturated porous media. The formulation for the CG method is available in the literature [16], [17]. We focus here on the LDG formulation. Equations (1) and (7) are elliptic. We can rewrite them as a system of first order differential equations for a one-dimensional domain Ω where $0<x<L$.

$$v=-k(h)\frac{dh}{dx};\quad \frac{dv}{dx}=0 \qquad \in\Omega \tag{8a}$$

$$q=-\theta D\frac{dC}{dx};\quad \frac{dq}{dx}=0 \qquad \in\Omega \tag{8b}$$

Figure 1: Illustration of element j quantities (modified from [18])

The mixed weak formulation considering Equations (8) over a typical element $\Omega_e = (x_a, x_b)$ gives:

$$\int_{\Omega_e} \varphi v dx - \int_{\Omega_e} \frac{d}{dx}(\varphi k(h)) h dx + \left[\varphi k(\hat{h})\hat{h}\right]_{xa}^{xb} = 0 \tag{9a}$$

$$\int_{\Omega e} \frac{d\psi}{dx} v dx - \left[\psi \hat{v}\right]_{xa}^{xb} = 0 \tag{9b}$$

$$\int_{\Omega_e} \eta q dx - \int_{\Omega_e} \frac{d}{dx}(\eta \theta D) C dx + \left[\eta \theta D \hat{C}\right]_{xa}^{xb} = 0 \tag{9c}$$

$$\int_{\Omega e} \frac{d\omega}{dx} q dx - \left[\omega \hat{q}\right]_{xa}^{xb} = 0 \tag{9d}$$

where φ, ψ, η, and ω are test functions and $\hat{h}$, $\hat{v}$, $\hat{C}$, and $\hat{q}$ are LDG numerical field and flux variables which can be derived from [8] as follows:

$$\hat{h} = \underline{\{h\}} + C_{12}\underline{[h]} \tag{10a}$$

$$\hat{v} = \underline{\{v\}} - C_{11}\underline{[h]} - C_{12}\underline{[v]} \tag{10b}$$

$$\hat{C} = \underline{\{h\}} + C_{12}\underline{[h]} \tag{10c}$$

$$\hat{q} = \underline{\{q\}} - C_{11}\underline{[C]} - C_{12}\underline{[q]} \tag{10d}$$

where C_{11} and C_{12} are LDG coefficients with:

$$\underline{\{h\}} = 0.5\left(h^+ + h^-\right), \quad \underline{[h]} = h^+.n^+ + h^-.n^- \tag{11a}$$

$$\underline{\{v\}} = 0.5\left(v^+ + v^-\right), \quad \underline{[v]} = v^+.n^+ + v^-.n^- \tag{11b}$$

$$\underline{\{C\}} = 0.5\left(C^+ + C^-\right); \quad \underline{[C]} = C^+.n^+ + C^-.n^- \tag{11c}$$

$$\underline{\{q\}} = 0.5\left(q^+ + q^-\right); \quad \underline{[q]} = q^+.n^+ + q^-.n^- \tag{11d}$$

We assume that h, v, C, and q vary over an element, according to the space shape functions:

$$h = \sum_{j=1}^{Ne} \varphi_j h_j = \phi^T \underline{h}; \quad v = \sum_{j=1}^{Ne} \varphi_j v_j = \phi^T \underline{v} \tag{12a}$$

$$C = \sum_{j=1}^{Ne} \varphi_j C_j = \phi^T \underline{C}; \quad q = \sum_{j=1}^{Ne} \varphi_j q_j = \phi^T \underline{q} \tag{12b}$$

Other quantities used in the formulation are defined in Figure 1. The choice of numerical fluxes in discontinuous Galerkin method is vital and it is discussed for diffusion problems by [19]. A substitution of Equation (10) in (9) yields a matrix formulation and a discrete algebraic system of equations. Li [18] presents the equations for a steady state heat transfer problem in 2D. We extend it here to coupled flow and chemical transport in 1D as follows:

$$\begin{bmatrix} E_f & H_f \\ J_f & 0 \end{bmatrix} \begin{pmatrix} \underline{v} \\ \underline{h} \end{pmatrix} + \sum_{i=1}^{2} \begin{bmatrix} 0 & H_{f,i} \\ J_{f,i} & G_{f,i} \end{bmatrix} \begin{pmatrix} \underline{v} \\ \underline{h} \end{pmatrix} - \sum_{i=1}^{2} \begin{bmatrix} 0 & H_{f,B,i} \\ J_{f,B,i} & G_{f,B,i} \end{bmatrix} \begin{pmatrix} \underline{v} \\ \underline{h} \end{pmatrix}_{(NB,i)} = 0 \tag{13a}$$

$$\begin{bmatrix} E_C & H_C \\ J_C & 0 \end{bmatrix} \begin{pmatrix} \underline{q} \\ \underline{C} \end{pmatrix} + \sum_{i=1}^{2} \begin{bmatrix} 0 & H_{C,i} \\ J_{C,i} & G_{C,i} \end{bmatrix} \begin{pmatrix} \underline{q} \\ \underline{C} \end{pmatrix} - \sum_{i=1}^{2} \begin{bmatrix} 0 & H_{C,B,i} \\ J_{C,B,i} & G_{C,B,i} \end{bmatrix} \begin{pmatrix} \underline{q} \\ \underline{C} \end{pmatrix}_{(NB,i)} = 0 \tag{13b}$$

where subscript NB refers to the neighbouring element quantities and the matrices are calculated as follows:

$$E_f = E_C = \int_{\Omega e} \phi\phi^T dx \tag{14a}$$

$$H_f = \int_{\Omega e} \frac{d\left(\phi k(h)\right)}{dx} \phi^T dx \tag{14b}$$

$$H_C = \int_{\Omega e} \frac{d\left(\phi\theta D\right)}{dx} \phi^T dx \tag{14c}$$

$$J_f = J_C = \int_{\Omega e} \frac{d\phi}{dx} \phi^T dx \tag{14d}$$

$$H_{f,i} = -\left(\tfrac{1}{2} + C_{12}\right)\left[k(h)\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14e}$$

$$H_{f,B,i} = -\left(\tfrac{1}{2} - C_{12}\right)\left[k(h)\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14f}$$

$$H_{C,i} = -\left(\tfrac{1}{2} + C_{12}\right)\left[\theta D\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14g}$$

$$H_{C,B,i} = -\left(\tfrac{1}{2} - C_{12}\right)\left[\theta D\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14h}$$

$$J_{f,i} = J_{C,i} = -\left(\tfrac{1}{2} - C_{12}\right)\left[\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14i}$$

$$J_{f,B,i} = J_{C,B,i} = -\left(\tfrac{1}{2} + C_{12}\right)\left[\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14j}$$

$$G_{f,i} = -G_{f,B,i} = G_{C,i} = -G_{C,B,i} = C_{11}\left[\phi\phi^T\right]_{xa}^{xb}, \quad i = 1,2 \tag{14k}$$

To obtain the fully coupled formulation, we can combine equations (13a) and (13b) whereby hydraulic pressure and chemical concentrations are mutually dependent. On the other hand, these equations could be treated separately with only chemical concentrations dependent on hydraulic pressure but not vice versa. In this paper we choose the later treatment. Details of numerical implementation are described next.

4 Numerical implementation

Dealing with nonlinear differential equations requires an iterative scheme. We use a well-known procedure, called Picard iteration method of successive substitution (direct iteration procedure), for both CG and LDG methods in order to solve the nonlinear Richards' equation (Equation (1)) and the diffusion equation (Equation (7)).

The iterative scheme is also useful in handling linear equations. Introducing the scheme to CG method for a linear problem is straight-forward and only one cycle of iterations is sufficient. On the other hand, two possible approaches can be followed for the DG methods: (1) assembling all the element equations and constructing the global matrices in the same way as for the CG method; (2) starting from boundaries and solving the equations are tentatively element by element. A major disadvantage of the first approach is the loss of the localised nature of the DG method and the considerable memory requirements, in comparison with CG method, that arise from this. In this paper, we followed the second approach. For more details on iterative schemes, the reader is referred to [18, 20].

We develop a FORTRAN code using Intel® Visual FORTRAN Composer XE 2011. Figures 2 and 3 show flowcharts for the CG and LDG procedures. The integrals of equations (14) are evaluated numerically using Gauss quadrature schemes with variable number of Gauss integration points.

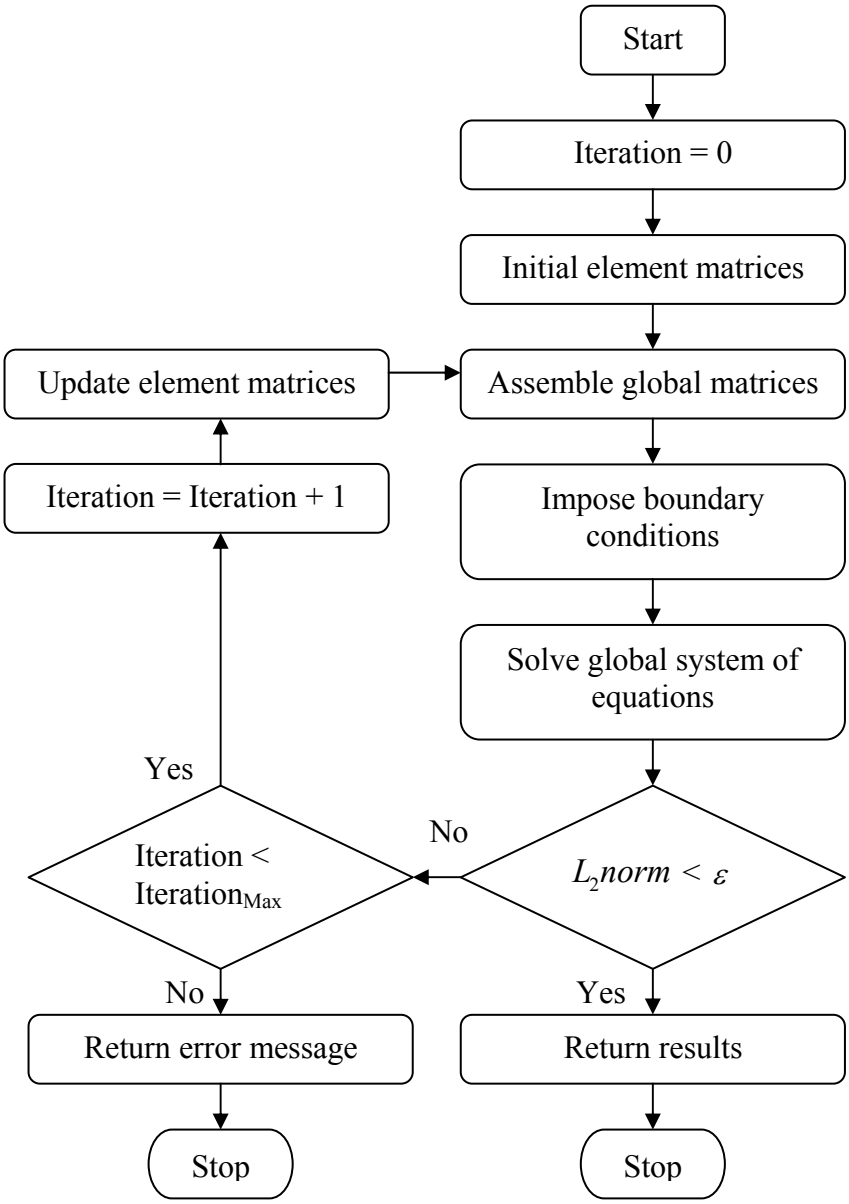

Figure 2: Iterative CG method flowchart for both linear and nonlinear problems

5 Analytical solution for a one layer Gardner soil

In order to validate numerical results, we consider an analytical solution for the problem of coupled unsaturated flow and chemical transport for a one layered Gardner soil. Warrick et al. [21] solved the Richards' equation for horizontal flow through a homogenous Gardener soil:

$$h \approx h_1 + \frac{1}{\alpha}\ln\left\{1 - \frac{x}{L} + \exp\left[\alpha\left(h_2 - h_1\right)\right]\frac{x}{L}\right\} \tag{15}$$

where h is hydraulic head pressure, h_1 and h_2 are specified hydraulic pressure head at boundaries, x is the horizontal coordinate, L is the domain length. Now, integrating equation (7) twice and separating variables yields:

$$\frac{C}{A_1} + A_2 = \int D^{-1}\theta^{-1} dx \tag{16}$$

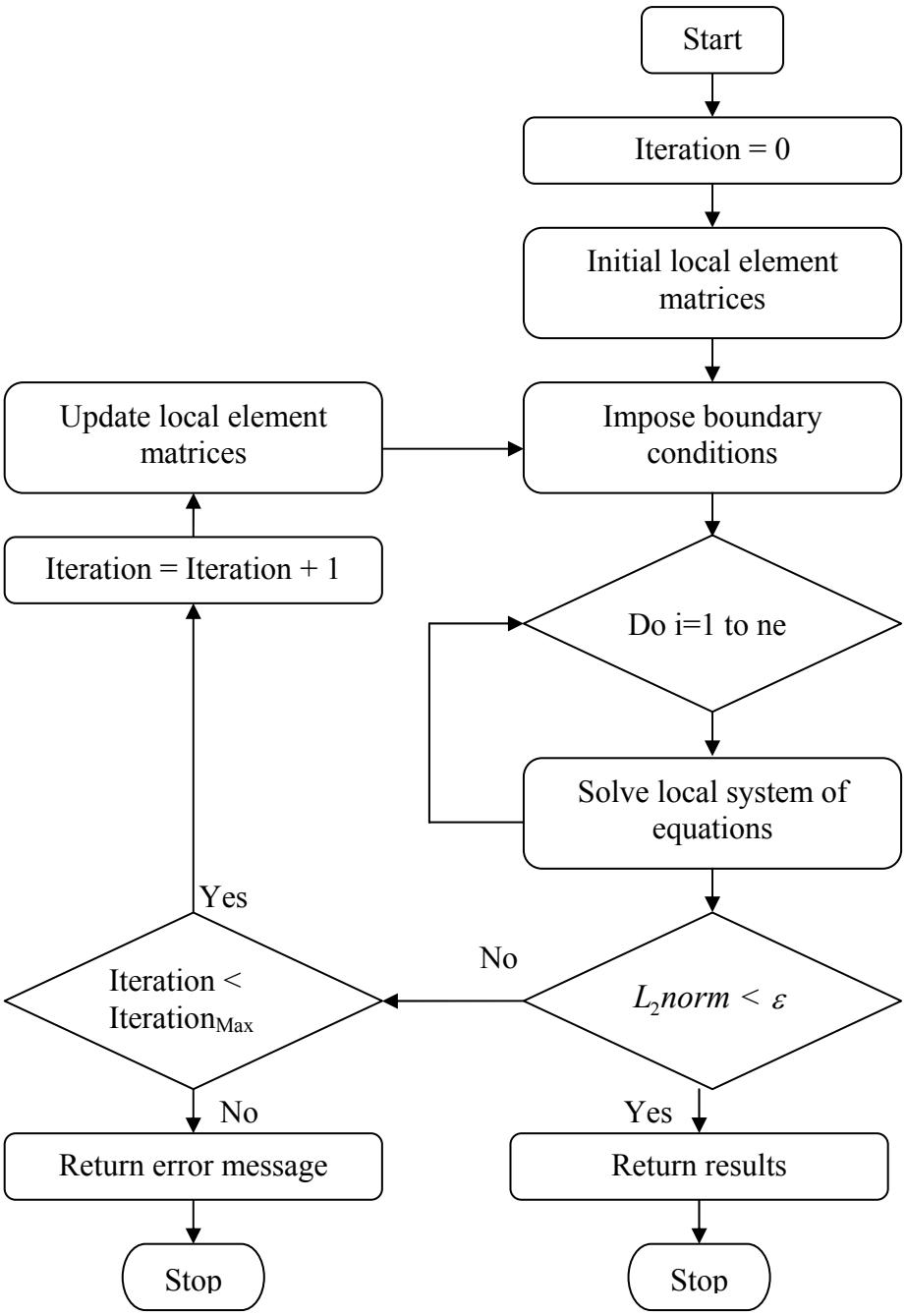

Figure 3: Iterative LDG method flowchart for both linear and nonlinear problems

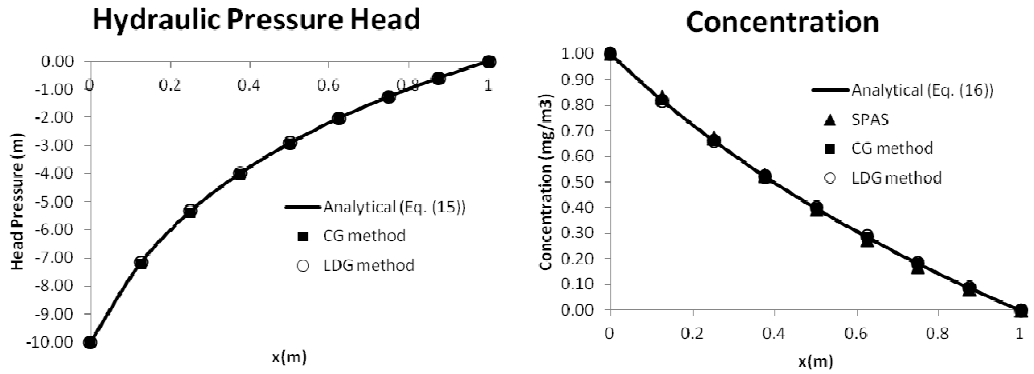

Figure 4: Comparison of CG and LDG method solutions with Analytical solution (Equations (15) and (16)) and SPAS: (a) Hydraulic Pressure Head, (b) Concentration (h_1=-10m, h_2=0m, α=0.19m, L=1m, θ_s=0.45, θ_r=0.15, m=1, D=0.05m^2.year^{-1}, k_s=0.001m.year^{-1})

where A_1 and A_2 are integration constants to be determined from chemical boundary conditions.

6 Results

6.1 Validation and comparison

Figure 4 shows a comparison of predictions generated by the LDG with results from the analytical solution shown earlier, the CG method developed here, as well as those of a 2D finite element software, the Soil Pollution Analysis System (SPAS) [22] based on an earlier multiple-porosity analysis framework [23]. There is clearly excellent agreement between the predictions of all four sources.

Performances of CG and LDG method are compared in terms of accuracy and processing time hereafter. Figure 5 compares performance of CG and LDG methods

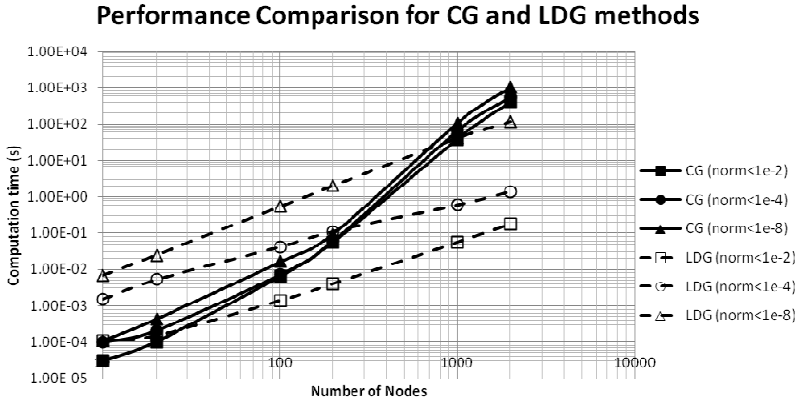

Figure 5: Performance of CG and LDG for different number of nodes and accuracy

for different number of nodes and required degree of accuracy (calculated by an *a posteriori* energy norm estimation) for same domain and processing conditions. The processing time is the average of running each problem for 100 times. This is to ensure the CPU measurements are not overly affected by variable factors related to other jobs the computer may be performing.

As expected, the processing time for both methods increases for higher accuracy and density of nodes. The LDG method performs significantly better for larger problems (e.g., more than 200 nodes for a norm of 10^{-4}), while the CG method requires less computation time for low density problems. This is in agreement with Kubatco et al. [24] who performed a similar comparison and reached similar conclusions for the generalised wave continuity equation. More generally, the growth of CPU requirements with meshing refinement appears to be quasi-exponential for the CG method and linear for the LDG method. The graph also reveals that the execution time for the CG method is less sensitive to the required level of accuracy than for the LDG method.

7 Conclusions

Multiphase thermo-chemo-hydro-mechanical problems occur frequently in problems of waste management and groundwater quality. However, few studies have applied the LDG method to such coupled problems. In this paper, we presented an LDG solution for the coupled unsaturated flow and chemical transport (diffusion only) problem in porous media. We also presented an analytical solution for these problems in one dimensional domain for a one-layer Gardner soil to validate the new numerical model. We found that the LDG method achieves better performance than the CG method in solving this coupled problem for refined meshes with a higher number of nodes. This is an encouraging preliminary finding as our research aim is to incorporate the advective and reactive terms of the diffusion-advection equation in the solution and extend the method to deformable soils, i.e. chemo-hydro-mechanical couplings in multiple dimensions.

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