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Application of implicit sub-time stepping to simulate flow and transport in fractured porous media

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ABSTRACT

In general, the accuracy of numerical simulations is determined by spatial and temporal discretization levels. In fractured porous media, the time step size is a key factor in controlling the solution accuracy for a given spatial discretization. If the time step size is restricted by the relatively rapid responses in the fracture domain to maintain an acceptable level of accuracy in the entire simulation domain, the matrix tends to be temporally over-discretized. Implicit sub-time stepping applies smaller sub-time steps only to the sub-domain where the accuracy requirements are less tolerant and is most suitable for problems where the response is high in only a small portion of the domain, such as within and near the fractures in fractured porous media. It is demonstrated with illustrative examples that implicit sub-time stepping can significantly improve the simulation efficiency with minimal loss in accuracy when simulating flow and transport in fractured porous media. The methodology is successfully applied to density-dependent flow and transport simulations in a Canadian Shield environment, where the flow and transport is dominated by discrete, highly conductive fracture zones.

1. Introduction

Groundwater flow and contaminant transport in fractured porous media is controlled by rapid flow and mass transport through the highly conductive interconnected fractures, the slower but persistent fluid and mass exchange between the fractures and the rock matrix, and the storage in the matrix blocks [3,4,16]. For example, fractured reservoirs have been conceptualized as double porosity media, to evaluate the rate at which water or petroleum stored in the matrix could be withdrawn from the subsurface through the fracture domain [2,9,32]. If an external stress such as the injection/withdrawal of a fluid is introduced into a fractured porous medium, the pressure response typically propagates mainly through the fracture domain, but interacts with the surrounding matrix with increasing time. Also, for contaminant migration, rapid advective-dispersive transport in the fractures together with slower but persistent diffusion into or out of the matrix are considered to be the dominant physical processes (e.g. [15,23]). It is generally understood that the early-time responses in flow and transport behavior are dominated by the fracture network properties, while the long-term responses are determined by the matrix properties. Difficulties arise in performing long-term numerical simulations of fluid flow and solute transport in fractured porous media because the characteristic response time can be orders-of-magnitude different in the fracture and matrix domains.

For a given spatial discretization, the accuracy of transient numerical solutions is determined by the temporal discretization level (time step size): in general, a smaller time step size produces more accurate solutions but with a higher computational cost (more time steps). The standard finite difference approximation of the temporal derivative utilizes a fixed value of a given time step size for the entire computational domain. Therefore, in order to achieve a suitable level of accuracy throughout the entire domain, the time step size needs to satisfy the least tolerant accuracy requirement. In fractured porous media, the selection of a time step size is therefore restricted by the relatively quick responses in the fracture domain, while the matrix domain tends to be temporally over-discretized. This is noteworthy because the fracture domain usually constitutes a smaller portion of the physical system.

A hybrid implicit–explicit approach, suggested by VanderKwaak [29], is an attempt to apply implicit time marching only to the part of the domain where the stability requirements are more strict, with the explicit scheme being applied to the remainder of the domain. VanderKwaak [29] demonstrated that the hybrid approach

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could reduce the needed computational effort by decreasing the number of discrete equations to be solved implicitly at each time step. Sub-time stepping is an alternative fully-implicit numerical strategy that applies different time step sizes to one or more sub-domains with each having different accuracy requirements [1,7,20,21]. By applying smaller sub-time steps to the sub-domain with relatively rapid responses and utilizing larger time steps in the remainder of the domain, the accuracy requirement is satisfied in the entire domain with minimal temporal over-discretization. In the method of sub-timing suggested by Singh and Bhallamudi [20,21], the time step size is constrained by a stability condition because of its explicit nature (for example, diffusion or Courant number constraints, depending on the nature of the problem), as well as the accuracy requirements. Bhallamudi et al. [1] suggested an implicit sub-time stepping approach, which is unconditionally stable. Although stable implicit sub-time stepping can generally address the temporal over-discretization issue, additional unknowns arise in the sub-timed nodes in each time step. Thus, this approach is most suitable for problems where the system response is high in only a small portion of the computational domain, such as in fractured porous media (see [1] for additional details).

In this paper, a Galerkin finite element formulation is derived for the implicit sub-time stepping approach based on Bhallamudi et al.'s generic formulation [1] and then it is applied to the transient simulation of flow and transport in fractured porous media. An automated adaptive sub-time stepping strategy is suggested to improve its efficiency. The performance and efficiency of the sub-time stepping approach will be demonstrated with a set of illustrative examples, followed by an application to a large-scale density-dependent flow and transport problem involving a discretely-fractured rock in a Canadian Shield setting.

2. Finite element formulation

Fig. 1 is a schematic of the spatio-temporal discretization for the implicit sub-time stepping approach. In a standard finite element (FE) formulation, only one unknown arises at each node for time $t+\Delta t$, given the knowns at t, resulting in n equations for the n nodes. In the implicit sub-time stepping approach, a smaller sub-time step ($\Delta t_s = \Delta t/M$) is applied to a prescribed set of nodes (s_i's in Fig. 1), where the response is expected to be rapid. Thus, more than one unknown ($M = \Delta t/\Delta t_s$) arise at each sub-timed node s_i but only one unknown arises at fully-timed nodes f_i. Fig. 1 indicates that an element can have either fully-timed nodes (e_1 and e_6 in Fig. 1), sub-timed nodes (e_3 and e_4), or both fully- and sub-timed nodes (e_2 and e_5).

The Galerkin finite element approach is a popular numerical method used for conducting groundwater flow and solute transport simulations [10,31,11]. In the following sections, (1) the elemental coefficient matrices for the groundwater flow equation are derived based on Bhallmudi et al.'s generic formulation [1] for three types of elements: those with only fully-timed nodes, those with only sub-timed nodes, or those with both fully- and sub-timed nodes, (2) the structure and characteristics of the FE coefficient matrices are examined, and (3) an automated adaptive sub-time stepping is suggested to maximize the efficiency of the method, where the sub-timed nodes and the number of sub-time steps applied can be determined from the results of the previous time step. Expansion of the approach to solute transport in discretely-fractured porous media is then straightforward once the elemental conductance and capacitance matrices are given for the flow problem [26,27].

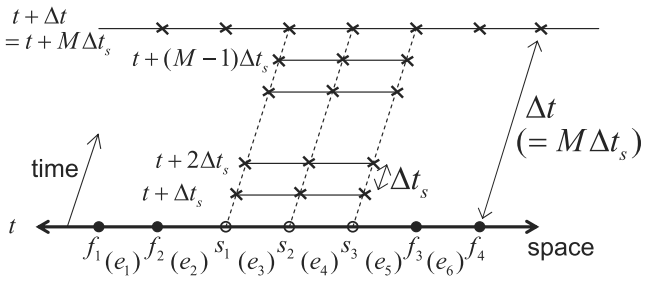

Fig. 1. Schematics of implicit sub-time stepping in space-time coordinate system (modified from [1]). Open and closed circles represent knowns for sub- and fully-timed nodes respectively and crosses are unknowns.

2.1. Formulation for an element with only fully- or sub-timed nodes

Groundwater flow is described by the continuity principle and Darcy's law in saturated porous media

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_j}\right) + Q = S_s\frac{\partial h}{\partial t} \tag{1}$$

where $x_i (i = 1,2,3)$ represents the spatial coordinate system, t is the time, K_{ij} is the saturated hydraulic conductivity tensor, h is the hydraulic head, Q is an external source or sink, and S_s is the specific storage. In the standard FE approach, the Galerkin weighted residual technique leads to the following discrete matrix equation (see [10,31,11] for details):

$$(1-\omega)[K^e]_{IJ}\{h\}_J^t + \omega[K^e]_{IJ}\{h\}_J^{t+\Delta t} = [C^e]_{IJ}(\{h\}_J^{t+\Delta t} - \{h\}_J^t) + \{f\}_I^{t+\Delta t} \tag{2a}$$

$$[K^e]_{IJ} = -\int_{V_e} K^e_{kl}\left[\frac{\mathrm{d}N_I}{\mathrm{d}x_k}\frac{\mathrm{d}N_J}{\mathrm{d}x_l}\right]\mathrm{d}V_e, \quad k,l = 1,2,3 \tag{2b}$$

$$[C^e]_{IJ} = \begin{cases} \int_{V_e} S^e_s N_I N_J \,\mathrm{d}V_e/\Delta t \\ \quad \text{for the consistent mass-matrix formulation} \\ \int_{V_e} S^e_s \delta_{IJ}\,\mathrm{d}V_e/n_e\Delta t = S^e_s V_e \delta_{IJ}/n_e\Delta t \\ \quad \text{for the lumped mass-matrix formulation} \end{cases} \tag{2c}$$

$$\{f\}_I = -\int_{V_e} QN_I\,\mathrm{d}V_e - \int_{\Gamma_e} N_I q_n\,\mathrm{d}\Gamma_e \tag{2d}$$

where $[K^e]_{IJ}$ and $[C^e]_{IJ}$ are the $n_e \times n_e$ elemental conductance and capacitance matrices, derived from the elemental hydraulic conductivity K^e and specific storage S^e_s, respectively (n_e is the number of unknowns in the element), $\{h\}_J^t$ is the hydraulic head at node J at time t, Δt is the time step size, ω is a time weighting factor ($\omega = 1$ for a fully-implicit scheme and $\omega = 0.5$ for a Crank–Nicholson scheme), δ_{IJ} is an identity matrix, and $\{f\}_I$ is the flux vector, derived from the source/sink term (Q) and boundary flux (q_n) over the elemental volume V_e and along the boundary Γ_e. If all the nodes in an element are fully-timed (e.g., e_1 and e_6 in Fig. 1), the elemental coefficient matrices can be directly computed from (2) to be assembled in the global coefficient matrices.

$$\begin{aligned}&(1-\omega)[K^e]_{IJ}\{h_f\}_J^t + \omega[K^e]_{IJ}\{h_f\}_J^{t+\Delta t} \\ &\quad = C^e_{II}(\{h_f\}_I^{t+\Delta t} - \{h_f\}_I^t) + \{f\}_I^{t+\Delta t}\end{aligned} \tag{3}$$

where subscript f represents a fully-timed node and the lumped mass formulation is used for simplicity ($C^e_{II} = S^e_s V_e/n_e\Delta t$). When all the nodes in an element are sub-timed (e_3 and e_3 in Fig. 1), the elemental coefficient matrices can be calculated at each sub-time step as

$$\begin{aligned}&(1-\omega)[K^e]_{IJ}\{h_s\}_J^{t+(m-1)\Delta t_s} + \omega[K^e]_{IJ}\{h_s\}_J^{t+m\Delta t_s} \\ &\quad = C^e_{sII}(\{h_s\}_I^{t+m\Delta t_s} - \{h_s\}_I^{t+(m-1)\Delta t_s}) + \{f\}_I^{t+m\Delta t_s}, \quad m = 1,2,\ldots,M\end{aligned} \tag{4}$$

where the subscript s represents a sub-timed node with a given number of sub-time steps M, the sub-time step size is $\Delta t_s = \Delta t/M$