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On continuous and discontinuous approaches for modeling groundwater flow in heterogeneous media using the Numerical Manifold Method: Model development and comparison

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ABSTRACT

One major challenge in modeling groundwater flow within heterogeneous geological media is that of modeling arbitrarily oriented or intersected boundaries and inner material interfaces. The Numerical Manifold Method (NMM) has recently emerged as a promising method for such modeling, in its ability to handle boundaries, its flexibility in constructing physical cover functions (continuous or with gradient jump), its meshing efficiency with a fixed mathematical mesh (covers), its convenience for enhancing approximation precision, and its integration precision, achieved by simplex integration. In this paper, we report on developing and comparing two new approaches for boundary constraints using the NMM, namely a continuous approach with jump functions and a discontinuous approach with Lagrange multipliers. In the discontinuous Lagrange multiplier method (LMM), the material interfaces are regarded as discontinuities which divide mathematical covers into different physical covers. We define and derive stringent forms of Lagrange multipliers to link the divided physical covers, thus satisfying the continuity requirement of the refraction law. In the continuous Jump Function Method (JFM), the material interfaces are regarded as inner interfaces contained within physical covers. We briefly define jump terms to represent the discontinuity of the head gradient across an interface to satisfy the refraction law. We then make a theoretical comparison between the two approaches in terms of global degrees of freedom, treatment of multiple material interfaces, treatment of small area, treatment of moving interfaces, the feasibility of coupling with mechanical analysis and applicability to other numerical methods. The newly derived boundary-constraint approaches are coded into a NMM model for groundwater flow analysis, and tested for precision and efficiency on different simulation examples. We first test the LMM for a Dirichlet boundary and then test both LMM and JFM for an idealized heterogeneous model, comparing the numerical results with analytical solutions. Then we test both approaches for a heterogeneous model and compare the results of hydraulic head and specific discharge. We show that both approaches are suitable for modeling material boundaries, considering high accuracy for the boundary constraints, the capability to deal with arbitrarily oriented or complexly intersected boundaries, and their efficiency using a fixed mathematical mesh.

1. Introduction

Heterogeneity is a basic, ubiquitous property within various groundwater systems, one frequently associated with features such as different geological materials, inclusions, or fractures. In numerical modeling of groundwater flow in heterogeneous geological media, material interfaces (including fractures) and typical Dirichlet, Neumann, or Cauchy boundary conditions are boundary constraints influencing the existence, uniqueness, and stability of the numerical solution. A schematic of a groundwater problem involving strong heterogeneity, including material interfaces and various boundary conditions, is shown in Fig. 1. The main challenges for modeling such a problem are: (1) accurately satisfying the continuity of both hydraulic head and normal flux across material interfaces, known as the refraction law [1,2], and (2) the difficulties related to mesh discretization and numerical convergence associated with singular points, especially if the interfaces

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Notations

$f(h)$	boundary constraints, as a function of hydraulic head h
h	hydraulic head
h_0	given hydraulic head
$h_i(x,y)$	hydraulic head function of physical cover i
h_{ij}	jth degree of freedom of physical cover i
k_n	permeability coefficient in the n direction
k_n^ζ	permeability coefficient of the material type ζ in the n direction
m	number of degrees of freedom of physical cover i
n_x and n_y	2D components of the cosine of the normal vector of the boundary relative x- and y-axes, respectively
n^+ and n^-	influx to and outflux from a boundary, respectively
n_d	total number of degrees of freedom related to material interfaces
$n_{e(r)}$	number of material interfaces in a physical cover.
q_n	normal flux across a boundary
$\bar{q}_x$ and $\bar{q}_y$	known flux components
s_j	coefficient of the jth degree of freedom
$\mathbf{v}$	velocity vector
$w_i(x,y)$	weight function of physical cover i on element e
C_{ij}	component of the conductivity matrix
$F_j(x,y)$	function with the features of gradient jump and head continuity
J_{ij}	element of matrix $\mathbf{J}$, representing the contribution of jth on the ith degree of freedom as jump terms
$\mathbf{K}$	tensor of permeability coefficient
L_{ij}	element of matrix $\mathbf{L}$, representing the contribution of jth degree of freedom as jump on ith degree of freedom as hydraulic head
$N_{pc}^{(e)}$	number of physical covers related to element e
Q_i	flux term
U_i	geometric range of physical cover i
W_D	work done by water flow through Dirichlet boundaries
W_M	work done by fluid flow through material interfaces
W_N	work done by fluid flow through Neumann boundaries
α	contains coefficients of compressibility of media or water
λ	Lagrange multiplier
ζ	material type ζ of a material domain
β_i	element of matrix $\boldsymbol{\beta}$, representing the flux term related to the ith degree of freedom as jump term
$\omega_j(x,y)$	jump shape function
$\psi_j(x,y)$	jth jump function
$\varphi_j\,(x,y)$	jump amplitude to be solved
$\phi_j(x_i,y_i)$	normal distance from the "star" of physical cover i to a material boundary
Γ	material or domain boundary
Γ_D	Dirichlet boundary
Γ_M	material interface

are geometrically complex and intersecting. According to a recent review by Cainelli et al. [3], standard continuous methods such as finite element [4,5] and finite volume [6–8] methods (FEM and FVM) suffer from accuracy limitations when modeling heterogeneous media, including difficulties in the need for continuity of normal flux across material interfaces. This difficulty has been addressed by using post-processing techniques (such as in [9–11]) to enforce the continuity of normal flux after hydraulic head calculations, though such techniques require several iterations to achieve convergence. Mathematically, the difficulty in satisfying the refraction law in standard continuous methods is rooted in limitations related to continuous, nodal-based approximation. In geological media, the material interfaces may intersect or even move under deformation, making discretization with a numerical grid (including adaptive gridding) more complex and computationally demanding. In this context, new mixed continuous/discontinuous methods with fixed meshes are promising and might provide a long-sought breakthrough in modeling groundwater flow in strongly heterogeneous geological media.

As proposed by Shi [12,13], the Numerical Manifold Method (NMM) is a promising numerical method for modeling such continuous/discontinuous media. Development of this method was motivated by the urgent need for modeling the dynamic processes of rock deformations spanning both continuous and discontinuous media using a unified approach, an approach not possible using continuous methods (such as FEM) or discontinuous methods (such as the distinct element method). In response to this need, NMM, based on the theory of mathematical manifolds, has recently been successfully applied to rock-mechanics analysis of both continuous and discontinuous geologic media [14]. Numerical grids (or meshes) in the NMM consist of mathematical and physical covers. These mathematical covers overlay the entire material domain and determine the approximation precision by the mesh density, whereby a finer mesh can achieve a higher precision in the solution.

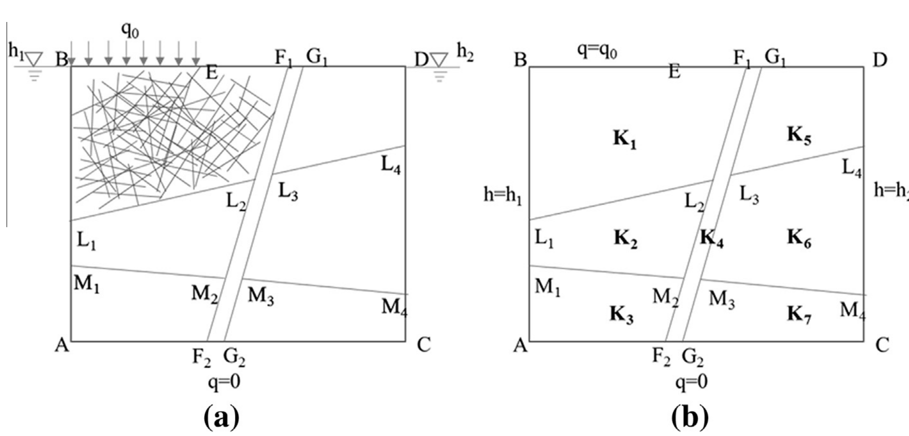

Fig. 1. (a) A 2D model of water flow under certain boundary conditions in a heterogeneous geological media, consisting of different material domains separated by different material interfaces, possibly containing a dominant fault or an area with dense fractures; (b) mathematical expressions of the material properties and boundary conditions.