On Continuous and Discontinuous Approaches for Modeling Groundwater Flow in Heterogeneous Media Using the Numerical Manifold Method: Model Development and Comparison

Mengsu Hu^{1,2}, Yuan Wang^{1,2}, and Jonny Rutqvist^{2,*}

¹College of Civil and Transportation Engineering, Hohai University,
Nanjing, 210098, China

²Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720,
USA

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 Figure 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 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. The physical covers are divided from the mathematical covers by boundaries and define the integration domain. The global function of an element is the weighted average of the function on each physical cover overlapping the element. Based on this definition framework, NMM appears to be a promising method for modeling flow in strongly heterogeneous media, superior to that of nodal-based methods. Specifically, the following features of the NMM can be highlighted for solving continuous/discontinuous problems:

- (1) The NMM is based on finite covers that the modeler can flexibly define and move. The mathematical covers can be split and easily removed or added. A split of mathematical covers can be used to model discontinuous processes, and the removal or addition of covers can be used to define multiple physical fields or to change the approximation precision.
- (2) In NMM, the global approximation field is not defined by a nodal weighted average as in standard FEM, but by the cover functions, which could be spatially constant, linear, or an arbitrary user-defined function.
- (3) As will be shown in this paper, the unique definition of physical covers in NMM makes it possible to model material interfaces using either continuous or discontinuous approaches.
- (4) Because of the cover-weighted global approximation used in NMM, the computation precision can be easily enhanced by increasing the order of the physical cover functions [17].
- (5) With the fixed mathematical covers used in NMM, the meshing effort can be substantially reduced, especially in the case of moving boundaries [12, 14-16].
- (6) The simplex integration used in NMM [13] achieves exact analytical solutions in polygons with complex shapes, avoiding errors caused by Gaussian integration as used in standard FEM models.

These features of the NMM make it particularly promising for modeling of groundwater flow in strongly heterogeneous geologic media—media that includes material interfaces, fractures, and boundary conditions that can be modeled as boundary constraints.

In previous studies of mechanical analysis with NMM, several methods for boundary constraints have been proposed and applied, including the penalty method [12, 18], the Lagrange Multiplier Method (LMM) [19], the Augmented Lagrange Method (ALM) [20], and the Jump Function Method (JFM) [15-16]. The penalty method, LMM, and ALM all regard a material interface as a discontinuity bounding different elements across it, while the JFM regards a material interface as an internal boundary inside an element. In groundwater flow modeling using NMM, Ohnishi et al. [21] suggested a node-adjustment method for boundaries. Recently, Wang et al. [22- 23] applied the penalty method and a pipe model for boundaries, whereas Zheng et al. [24], proposed and applied a mixed head-flux formulation to analyze unconfined water flow.

In this study, we develop and compare two new approaches for boundary constraints in groundwater flow modeling based on NMM, i.e., a continuous approach using JFM and a discontinuous approach using LMM. In Section 2, we introduce and interpret the refraction law for both continuous and discontinuous approaches (Section 2.1), and then present the basic concepts of finite covers and elements and global approximations defined in NMM (Section 2.2). Based on two different interpretations of refraction law for continuous and discontinuous fields, in Section 3 we derive the new discontinuous approach using LMM (Section 3.1) and the new continuous approach using JFM (Section 3.2) for boundary constraints, and make a theoretical comparison between these two approaches (Section 3.3). In Section 4, we demonstrate the accuracy and efficiency of the new approaches through comparison to analytical solutions, and finally compare the two approaches for a heterogeneous case.

2 Mathematical statement of boundary constraints and NMM for groundwater flow in heterogeneous media

In this section, we first briefly introduce the concepts of boundary constraints for groundwater flow in heterogeneous media, find the similarity between various types of boundary constraints, and interpret the refraction law in two different ways (Section 2.1). Then, from the basic concepts defined in NMM, we construct an outline of modeling boundary constraint in NMM for both continuous and discontinuous approaches (Section 2.2).

2.1 Boundary constraints of groundwater flow in heterogeneous media

Figure 1a shows a schematic of groundwater flow 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. In this problem, water flow follows mass conservation:

$$\text{div}(\mathbf{v}) + \alpha \frac{\partial h}{\partial t} = 0 \quad (1)$$

and Darcy's law:

$$\mathbf{v} = -\mathbf{K} \text{grad}(h) \quad (2)$$

where $\mathbf{v}$ is the velocity vector, α contains coefficients of compressibility of media or water, h is the hydraulic head, and $\mathbf{K}$ is the tensor of permeability coefficient. If the fracture area $BL_1L_2F_1$ in Figure 1a could be regarded as an equivalent continuum, and the dominant fault conducts water as a different material with much higher permeability, the problem could be simplified to a 2D model with seven different material domains, as shown in Figure 1b. The boundaries are categorized as Dirichlet boundaries (such as AB and CD), Neumann boundaries (such as AC and BE), and material interfaces (such as F_1F_2 , G_1G_2 , L_1L_2 , M_1M_2 , L_3L_4 , and M_3M_4). The corresponding mathematical boundary constraints are expressed as

$$h = h_0 \quad (3)$$

for Dirichlet boundary conditions,

$$q_n = \bar{q}_x n_x + \bar{q}_y n_y \quad (4)$$

for Neumann boundary conditions, and

$$h^- = h^+ \text{ and } q_n^- = q_n^+ \quad (\mathbf{K}^- \neq \mathbf{K}^+) \quad (5)$$

for material interfaces satisfying the refraction law, where h_0 is the given hydraulic head, q_n is the normal flux across a boundary, $\bar{q}_x$ and $\bar{q}_y$ are the known flux components, n_x and n_y are the 2D components of the cosine of the normal vector of the boundary relative x - and y -axes, and $-$ and $+$ are the negative and positive directions of the normal vector of a boundary, respectively.

Examining Equations (3)-(5), we find that mathematically the Dirichlet and Neumann boundary conditions expressed by Equations (3) and (4) are special cases of the refraction law for material interfaces expressed by Equation (5). Specifically, when the hydraulic head is given on one side of a material interface, the interface is simplified as a Dirichlet boundary. The same is true when the flux is given: the interface becomes a Neumann boundary. With this recognition, we are able to model the three types of boundary constraints using a unified approach.

As for the refraction law (Equation (5)), we could interpret this in two different ways, depending on whether we are considering continuous or discontinuous fields. If considering a

continuous field, the hydraulic gradient across the interface in the direction normal to the interface is discontinuous due to a change in material properties (permeability). If considering a discontinuous field, continuity across the interface should be satisfied for both hydraulic heads and fluxes in the direction normal to the interface. Following this reasoning, here we develop and compare both continuous and discontinuous approaches for boundary constraints based on NMM.

2.2 Fundamentals of NMM

The NMM is based on a finite cover system with independent mathematical and physical covers. The mathematical covers, which define numerical precision by mesh density and are chosen by users, consist of finite overlapping covers that occupy the entire material domain. Conventional meshes such as regular finite difference grids, finite elements, or convergence regions of series can be used as mathematical covers. The physical covers are divided by boundaries or joints from mathematical covers, defining the integration fields. The global behavior can be computed by functions defined in local physical covers. Based on finite covers, the NMM is flexible and general enough to include and combine well-developed analytical methods, the widely used FEM, and block-oriented discontinuous deformation analysis (DDA), all in a unified form.

Figure 1 introduces (in schematic form) the basic concept of NMM in the context of groundwater flow modeling in heterogeneous geological media. It is an “extreme” case—a groundwater flow problem including several boundary intersections and a major discontinuity, which may represent a fracture, a material interface, or a moving water-free surface. In order to model such a problem, we first need to choose mathematical covers to occupy the entire material domain. For a 2D problem, usually simplex such as triangles or rectangles could be used for the mathematical covers. Here, we use triangular elements for mathematical covers, because these have proven to perform better [26].

Figure 2 shows in principal how such a problem could be discretized in NMM, including the mathematical covers, physical covers, and elements defined with uniform triangles as the fixed mathematical mesh. As shown in Figure 2, all the triangles sharing a certain node (marked as stars) form a mathematical cover (i.e., a hexagon such as P_1 , P_2 , and P_3 , distinguished by different colors). The corresponding physical covers (P_1^1 and P_1^2 , P_2^1 and P_2^2 , and P_3^1 and P_3^2) are divided from the mathematical covers by the outer boundaries or the inner discontinuity. The overlapping areas of physical covers are defined as elements (such as elements $P_1^1 P_2^1 P_3^1$ and $P_1^2 P_2^2 P_3^2$, distinguished by different patterns of shadow). From Figure 2, we can see that the physical covers and elements are not necessarily regular grids. Once a mathematical cover is divided into different physical covers, the processes involving both continuous to discontinuous behavior can be modeled [12, 14, 15]. For problems with moving interfaces such as free surface flow, complex re-meshing is not necessary, because the mathematical covers could be fixed and the physical covers updated by changing their integration area [22].

The hydraulic head at a point (x, y) within element e is the weighted average hydraulic head of all physical covers overlapping the element:

$$h(x, y) = \sum_{i=1}^{N_{pc}^{(e)}} w_i(x, y) h_i(x, y) \quad (6)$$

where $N_{pc}^{(e)}$ is the number of physical covers related to element e , $h_i(x, y)$ is the hydraulic head function of physical cover i and $w_i(x, y)$ is the weight function of physical cover i on element e . For an individual physical cover i , we have

$$\begin{cases} w_i(x, y) > 0 & (x, y) \in U_i \\ w_i(x, y) = 0 & (x, y) \notin U_i \end{cases} \quad (7)$$

where U_i is the geometric range of physical cover i .

The hydraulic head $h_i(x, y)$ (i.e., cover function) of physical cover i can be a constant, linear, or locally defined series:

$$h_i(x, y) = \sum_{j=1}^m s_j h_{ij} = \begin{pmatrix} 1 & x & y & \cdots & s_m \end{pmatrix} \begin{pmatrix} h_{i1} \\ h_{i2} \\ h_{i3} \\ \vdots \\ h_{im} \end{pmatrix} \quad (8)$$

where m and h_{ij} are the number of degrees of freedom and the j th degree of freedom of physical cover i , respectively, and s_j is the coefficient of the j th degree of freedom. For 2-D flow analysis, m is 1 or 3 when the hydraulic head is 0-order (constant), or first-order (linear), respectively. For a complete N -order physical cover function, $m = (N+1)(N+2)/2$. The contribution of each physical cover to all corresponding elements is summed to form the global approximation over the entire domain.

In this paper, we use linear weight functions and linear physical cover functions ($m=3$) with triangular mesh for groundwater flow analysis. When deactivating the linear part of the cover function, the global approximation is reduced to linear with constant cover functions. As studied in [25] and [26], the rank deficiency caused by linear dependence for a triangular mesh with linear cover functions is very small (only three), which could be easily overcome by different ways to impose boundary conditions (such as the approaches presented in this study). The details of second-order NMM approximation for water flow analysis and its application were derived and demonstrated by Wang et al. [23].

According to the above definitions of independent mathematical covers, physical covers, and global approximations, combined with the two different ways of interpreting the refraction law from Section 2.1, we can regard a material interface either as a discontinuity or an inner “weak discontinuity.” As for discontinuity, it divides one mathematical cover into different physical covers and the continuity constraints of the refraction law could be imposed by numerical approaches, such as the LMM described in Section 3.1; as for an inner “weak discontinuity”, it is contained in a physical cover, whereas the normal hydraulic gradient discontinuity of the refraction law could be imposed by constructing special physical cover functions, such as the JFM described below in Section 3.2.

3 Derivation and theoretical comparison of two different new approaches for modeling boundaries in NMM

In this section, we will present two different new approaches for boundary constraints in NMM, i.e., the discontinuous LMM for both Dirichlet boundaries and material interfaces in Section 3.1, and the continuous JFM for material interfaces in Section 3.2—and make a thorough theoretical comparison of these two approaches in Section 3.3.

3.1 A discontinuous approach- Lagrange Multiplier approach for modeling boundaries in NMM

In discontinuous fields, where different material domains are separated by material interfaces, the continuity of hydraulic heads or normal fluxes can be realized by Lagrange multipliers functioning as numerical “links.” The application of a Lagrange multiplier to boundary constraints was introduced by Kikuchi and Ando [27] for structural mechanics analysis and comprehensively described by Zienkiewicz et al. [28] and Belytschko et al. [29]. With the physical verification of a Lagrange multiplier as negative normal flux, the Nitsche method was proposed for the heat equation [30]. The Nitsche concept was later extended for multidomain discontinuous analysis known as Discontinuous Galerkin (DG) or Interior Penalty (IP) methods, with theory and mathematical formulations derived in [31- 34] and applied in neutron transport [35], heat transport [36] and diffusion [37- 39]. The selection of numerical flux for diffusion problems such as in [34, 37- 39] was compared and analyzed in [40- 41], and the limitation of the DG approach was studied by [42]. As discussed by Cainelli et al. [3], the DG approach was developed to better handle discontinuous solutions and is therefore not suitable for solving elliptical equations whose solutions cannot be discontinuous, regardless of the nature of the parameters (smooth or discontinuous). As a result, DG has not been successfully applied in the simulation of groundwater flow in heterogeneous geological media, which should satisfy the refraction law as in Equation (5). In this section, we will present a discontinuous approach in NMM using a Lagrange multiplier for boundary constraints with an energy-work seepage model [22].

3.1.1 Definition of Lagrange multiplier in NMM according to an energy-work seepage model

According to the above description of NMM in Section 2, if a material interface were regarded as a discontinuity, it divides mathematical covers into different physical covers, as shown in Figure 3. The definitions of mathematical covers, physical covers, and elements are the same as in Figure 2. The created overlapping physical covers form two elements. In special cases such as when the element boundary is an outer boundary (e.g., a Dirichlet boundary), only one element within the computation domain is taken into account. To realize the boundary constraints according to Equations (3)-(5), a numerical “link” is required to satisfy the given head for a Dirichlet boundary or the continuity of normal flux and hydraulic head for material interfaces. Wang et al. (in press) [22] used the penalty method with a pipe model to impose the boundary, achieving accurate results with a good estimation of the penalty. To avoid estimating the penalty value, in this new approach we introduce Lagrange multipliers between divided physical covers, as shown in Figure 3.

According to the energy-work seepage model [22], the work done by water flow related to the boundary constraints is expressed as:

$$W = -\int_{\Gamma} \lambda f(h) d\Gamma \quad (9)$$

where λ is the Lagrange multiplier to be determined, Γ is a material or domain boundary, and $f(h)$ represents the boundary constraints, as a function of hydraulic head h in Equations (3) and (5). According to the energy-work seepage model [22], we can derive the physical meaning of the Lagrange multiplier via:

$$\lambda = -\gamma q_n \big|_{\Gamma} \quad (10)$$

i.e., the negative specific discharge in the direction normal to a boundary Γ multiplies the unit weight of the fluid.

However, the normal flux q_n across boundary Γ is unknown. According to Darcy's law:

$$q_n(x, y)|_{\Gamma} = -k_n \frac{\partial h(x, y)}{\partial n} \Big|_{\Gamma} \quad (11)$$

where n is the direction normal to the boundary Γ and k_n is the permeability coefficient in the n direction.

Corresponding to the expression of q_n , we derive the Lagrange multiplier λ at location (x, y) :

$$\lambda(x, y) = \gamma k_n \frac{\partial h(x, y)}{\partial n} \Big|_{\Gamma} \quad (12)$$

3.1.2 Derivation of a new LMM for modeling water flow in heterogeneous media

From Equations (3), (9), and (12), we have the work related to Dirichlet boundary conditions:

$$W_D = -\gamma \int_{\Gamma_D} k_n^{\zeta} \frac{\partial h(x, y)}{\partial n} [h(x, y) - h_0(x, y)] d\Gamma \quad (13)$$

where W_D is the work done by water flow through Dirichlet boundaries, ζ denotes the material type ζ of a material domain, Γ_D is the Dirichlet boundary, and k_n^{ζ} is the permeability coefficient of the material type ζ in the n direction. According to our energy-work seepage model [22], we obtain:

$$C_{ij} = \gamma \int_{\Gamma_D} k_n^{\zeta} \left[\frac{\partial w_i(x, y)}{\partial n} w_j(x, y) + \frac{\partial w_j(x, y)}{\partial n} w_i(x, y) \right] d\Gamma \quad (14)$$

$$Q_i = \gamma \int_{\Gamma_D} k_n^{\zeta} \frac{\partial w_i(x, y)}{\partial n} h_0(x, y) d\Gamma \quad (15)$$

where C_{ij} is the component of the conductivity matrix and Q_i is the flux term.

For material interfaces, a mathematical cover is divided into different independent physical covers with different cover functions; thus, the corresponding global approximations are different. Following Equation (6), we express the global approximations of hydraulic heads on the different sides of a material interface as follows:

$$h^-(x, y) = \sum_{i=1}^{N_{pc}^{(e)}} w_i(x, y) h_i(x, y) \quad (16)$$

$$h^+(x, y) = \sum_{i=1}^{N_{pc}^{(e)'}} w_i'(x, y) h_i'(x, y) \quad (17)$$

where $w_i(x, y)$ and $w_i'(x, y)$ are the weight functions of the independent physical covers and $h_i(x, y)$ and $h_i'(x, y)$ are the corresponding cover functions.

How to express the work at each side of the interface as functions of hydraulic heads is a delicate issue. In [34, 37-41] using the DG method, different techniques for imposing numerical flux were proposed and compared from a mathematical perspective. The common basic idea in those studies was to relax the continuity requirements at the interelement boundaries, supposing that jumps of both hydraulic heads and normal fluxes exist, but are limited by certain techniques. However, in the presence of abrupt boundaries, the solution is not stable [37].

In this study, we assume that a material interface consists of two Dirichlet boundaries. As shown in Figure 4, there are two material domains with permeability coefficients k^1 and k^2 , separated by a material interface AB and hydraulic head functions $h^-(x, y)$ and $h^+(x, y)$, respectively. The normal flux across the interface is $q_n(x, y)$. Regarding the material interface as

two connected Dirichlet boundaries, the problem becomes flow out of domain 1, where the hydraulic head $h^-(x, y)$ is to be solved with given hydraulic head $h^+(x, y)$ out of the boundary AB, plus flow in to domain 2, where hydraulic head $h^+(x, y)$ is to be solved with a given hydraulic head $h^-(x, y)$ out of the boundary AB. Considering the continuity of fluxes and hydraulic heads across the material interfaces, we could divide the work into two parts: (1) the work for flux out of the material domain 1 (in the negative direction) and (2) the work for flux into the material domain 2 (in the positive direction). Since the corresponding fluxes and pressure differences are equivalent in the two work components, it is evenly divided as follows:

$$W_M = -\frac{1}{2}\gamma \int_{\Gamma_M} k_n^\zeta \frac{\partial h^-(x, y)}{\partial n^-} [h^-(x, y) - h^+(x, y)] d\Gamma - \frac{1}{2}\gamma \int_{\Gamma_M} k_n^{\zeta'} \left(-\frac{\partial h^+(x, y)}{\partial n^+}\right) [h^-(x, y) - h^+(x, y)] d\Gamma \quad (18)$$

where W_M is the work done by fluid flow through material interfaces, ζ and ζ' denote material type ζ and material type ζ' on the different sides of a material interface, Γ_M is the material interface, k_n^ζ and $k_n^{\zeta'}$ are the corresponding permeability coefficients, n^+ and n^- denote the influx to and outflux from a boundary, respectively. Equation (18) can be further expressed as:

$$W_M = \frac{1}{2}\gamma \int_{\Gamma_M} k_n^\zeta \frac{\partial h^-(x, y)}{\partial n^+} [h^-(x, y) - h^+(x, y)] d\Gamma + \frac{1}{2}\gamma \int_{\Gamma_M} k_n^{\zeta'} \frac{\partial h^+(x, y)}{\partial n^+} [h^-(x, y) - h^+(x, y)] d\Gamma \quad (19)$$

Considering the special case when $h^+(x, y)$ is solved, we have the following expression for a Dirichlet boundary condition:

$$W_D = -\gamma \int_{\Gamma_D} k_n^\zeta \frac{\partial h^-(x, y)}{\partial n^-} [h^-(x, y) - h^+(x, y)] d\Gamma \quad (20)$$

and considering the special case when $h^-(x, y)$ is solved, we have the following expression:

$$W_D = -\gamma \int_{\Gamma_D} k_n^{\zeta'} \frac{\partial h^+(x, y)}{\partial n^+} [h^+(x, y) - h^-(x, y)] d\Gamma \quad (21)$$

Considering Equations (19-21), because the material interfaces are regarded as connected Dirichlet boundaries, the continuity of hydraulic heads is naturally imposed; because the flux is evenly divided, the continuity of both normal fluxes is naturally imposed.

According to our energy-work seepage model, we derive the components of the conductivity matrix as:

$$\begin{aligned} C_{ij} &= -\frac{1}{2}\gamma \int_{\Gamma_M} k_n^\zeta \left[\frac{\partial w_i(x, y)}{\partial n^+} w_j(x, y) + \frac{\partial w_j(x, y)}{\partial n^+} w_i(x, y) \right] d\Gamma \\ C_{ij'} &= \frac{1}{2}\gamma \int_{\Gamma_M} \left[k_n^\zeta \frac{\partial w_i(x, y)}{\partial n^+} w_{j'}'(x, y) - k_n^{\zeta'} \frac{\partial w_{j'}'(x, y)}{\partial n^+} w_i(x, y) \right] d\Gamma \\ C_{i'j} &= \frac{1}{2}\gamma \int_{\Gamma_M} \left[k_n^\zeta \frac{\partial w_j(x, y)}{\partial n^+} w_{i'}'(x, y) - k_n^{\zeta'} \frac{\partial w_{i'}'(x, y)}{\partial n^+} w_j(x, y) \right] d\Gamma \\ C_{i'j'} &= \frac{1}{2}\gamma \int_{\Gamma_M} k_n^{\zeta'} \left[\frac{\partial w_{i'}'(x, y)}{\partial n^+} w_{j'}'(x, y) + \frac{\partial w_{j'}'(x, y)}{\partial n^+} w_{i'}'(x, y) \right] d\Gamma \end{aligned} \quad (22)$$

3.2 A continuous approach: jump function approach for modeling boundaries in NMM

In continuous fields, material interfaces in heterogeneous media are interpreted as “weak discontinuities,” i.e., inner discontinuities with a gradient jump. From this point of view, the implementation of gradient jumps as the enrichment of the approximation functions is a promising approach for modeling material interfaces to reduce meshing efforts. The idea of using jump functions to incorporate discontinuities in derivatives was first proposed by Krongauz et al. [43] for the application of the element-free Galerkin method in mechanical analysis. Then, different forms of jump terms were constructed in extended finite element (XFEM) [44-46] and numerical manifold [16] methods, based on the level set method [47], and successfully applied to mechanical problems with holes or inclusions. However, the linearized approximation of the nonlinear distance functions derived in these jump-term formulations for circular interfaces in 2D or 3D leads inevitably to errors. Furthermore, the lack of consideration for cases in which interfaces that may be arbitrarily oriented, or intersect with multiple other boundaries and interfaces, limits the applicability of these formulations to model heterogeneous media. Herein, we derive a new approach with an accurate jump function, one that accounts for intersections with Dirichlet or Neumann boundaries and other interfaces.

3.2.1 The fundamentals of physical covers containing jumps for groundwater flow modeling using NMM

Instead of dividing the mathematical covers into different physical covers (as described in Section 2), in our new JFM approach we construct special physical covers containing gradient jumps. It is expressed as:

$$h(x, y) = \sum_{i=1}^{N_{pc}^{(e)}} w_i(x, y) h_i(x, y) + \sum_{j=1}^{n_d} \omega_j(x, y) \psi_j(x, y) \quad (23)$$

where $\omega_j(x, y)$ is the jump shape function, $\psi_j(x, y)$ is the j th jump function, and n_d is the total number of degrees of freedom related to material interfaces. The jump function $\psi_j(x, y)$ should satisfy the following conditions: (1) it should have a compact support and (2) the approximation of Equation (23) should be able to reproduce the continuity of hydraulic heads as well as the discontinuity of their gradients normal to the interface, which are inversely proportional to the coefficients of permeability.

The jump covers could partly or fully cover the element with special assignment of the weight functions from the regular covers. For simplicity, we choose the jump covers to share the same approximation field with the regular physical covers, as shown in Figure 5. Then the jump shape functions are in the same form as the weight functions of the hydraulic head:

$$\omega_j(x, y) = w_i(x, y) \quad (24)$$

Therefore, one jump cover and its corresponding regular cover are merged into one cover, and the hydraulic head in the elements associated with material interfaces are further expressed as:

$$h(x, y) = \sum_{i=1}^{N_{pc}^{(e)}} w_i(x, y) \left[h_i(x, y) + \sum_{j=1}^{n_d} \psi_j(x, y) \right] \quad (25)$$

where $n_{e(r)}$ is the number of material interfaces in a physical cover. Then, the function of a physical cover which contains material interfaces becomes the summation of the **continuous function of** hydraulic head $h_i(x, y)$ and the **function associated with the** jump term $\sum_{j=1}^{n_{e(r)}} \psi_j(x, y)$.

3.2.2 The NMM approximation with jump function for material interfaces in **groundwater flow analysis**

We further express the jump function as:

$$\psi_j(x, y) = F_j(x, y)\phi_j(x, y) \quad (26)$$

where $F_j(x, y)$ is a function with the features of gradient jump and head continuity, and $\phi_j(x, y)$ is the jump amplitude to be solved. There are several ways to construct the function $F_j(x, y)$, **as** have been studied **by** Sukumar et al. [44], Belytschko et al. [45] and Moes et al. [46]. In this paper, we choose $F_j(x, y)$ **to have a** similar form as in [16, 46]:

$$F_j(x, y) = \sum_{i=1}^q w_i(x, y) \left| \phi_j(x_i, y_i) \right| - \left| \sum_{i=1}^q w_i(x, y) \phi_j(x_i, y_i) \right| \quad (27)$$

where $\phi_j(x_i, y_i)$ denotes the normal distance from the “star” of physical cover i located at $P_i(x_i, y_i)$ to the material boundary intersecting at points $P_1(x_1, y_1)$ and $P_2(x_2, y_2)$ with the triangle mesh. Instead of using a circle-based distance as in [16, 46], we express $\phi_j(x_i, y_i)$ by:

$$\phi_j(x, y) = \frac{1}{\sqrt{(x_1^j - x_2^j)^2 + (y_1^j - y_2^j)^2}} \begin{vmatrix} 1 & x & y \\ 1 & x_1^j & y_1^j \\ 1 & x_2^j & y_2^j \end{vmatrix} \quad (28)$$

where the superscript j means the j th material interface in a physical cover. From Equation (28) we can see that:

- (1) The direction of the distance is expressed through the relative location of P_i to P_1P_2 (anticlockwise is positive), distinguishing the material domains;
- (2) The distance is a linear function of the coordinates of P_i once P_1P_2 is determined, leading to:

$$\phi_j(x, y) = \sum_{i=1}^q w_i(x, y) \phi_j(x_i, y_i) \quad (29)$$

which corresponds to a level set function, denoting the distance from a node located at (x, y) to the boundary P_1P_2 . It is the exact 2D approximation compared with the circle-based distance and is flexible to represent polygons or curves in arbitrary shapes approximated by straight line segments.

- (3) The jump $F(x, y)$ reduces to 0 when reaching the “star” of a physical cover, i.e., the triangle nodes.

Following our energy-work seepage model [22] and combining **it** with Equation (25), we derive the equilibrium equations as:

$$\begin{pmatrix} \mathbf{C} & \mathbf{L} \\ \mathbf{L}^T & \mathbf{J} \end{pmatrix} \begin{pmatrix} \mathbf{h} \\ \boldsymbol{\phi} \end{pmatrix} = \begin{pmatrix} \mathbf{Q} \\ \boldsymbol{\beta} \end{pmatrix} \quad (30)$$

where L_{ij} is the element of matrix $\mathbf{L}$, representing the contribution of **the** j th degree of freedom as **a** jump on the i th degree of freedom as hydraulic head, J_{ij} is the element of matrix $\mathbf{J}$, representing

the contribution of j th on the i th degree of freedom as jump terms, and β_i is the element of matrix $\mathbf{\beta}$, representing the flux term related to the i th degree of freedom as jump term, derived by:

$$L_{ij} = \frac{\partial^2 \Pi}{\partial h_i \partial \varphi_j} \quad (31)$$

$$J_{ij} = \frac{\partial^2 \Pi}{\partial \varphi_i \partial \varphi_j} \quad (32)$$

$$\beta_i = -\frac{\partial \Pi}{\partial \varphi_i} \quad (33)$$

With a fixed mathematical mesh, we also need to consider cases in which the material interfaces share the same cover with Dirichlet or Neumann boundaries, including a special case in which the interfaces intersect Dirichlet or Neumann boundaries. Following the energy-work seepage model [22] and combining Equations (13) and (25), for the Dirichlet boundary condition, we have:

$$C_{ij} = \gamma \int_{\Gamma_D} k_n^\varepsilon \left[\frac{\partial w_i(x, y)}{\partial n} w_j(x, y) + \frac{\partial w_j(x, y)}{\partial n} w_i(x, y) \right] d\Gamma \quad (34)$$

$$L_{ij} = \gamma \int_{\Gamma_D} k_n^\varepsilon \left[\frac{\partial w_i(x, y)}{\partial n} w_j(x, y) F_j(x, y) + \frac{\partial (w_j(x, y) F_j(x, y))}{\partial n} w_i(x, y) \right] d\Gamma \quad (35)$$

$$J_{ij} = \gamma \int_{\Gamma_D} k_n^\varepsilon \left[\frac{\partial [w_i(x, y) F_i(x, y)]}{\partial n} w_j(x, y) F_j(x, y) + \frac{\partial (w_j(x, y) F_j(x, y))}{\partial n} w_i(x, y) F_i(x, y) \right] d\Gamma \quad (36)$$

$$Q_i = \gamma \int_{\Gamma_D} k_n^\varepsilon \frac{\partial w_i(x, y)}{\partial n} h_0(x, y) d\Gamma \quad (37)$$

$$\beta_i = \gamma \int_{\Gamma_D} k_n^\varepsilon \frac{\partial [w_i(x, y) F_i(x, y)]}{\partial n} h_0(x, y) d\Gamma \quad (38)$$

According to the energy-work seepage model [22], the work related to a Neumann boundary condition is:

$$W_N = \gamma \left(\int h \bar{q}_x dy + \int h \bar{q}_y dx \right) \quad (39)$$

where W_N is the work done by fluid flow through Neumann boundaries and $(\bar{q}_x, \bar{q}_y)$ are the known flux components. Correspondingly, we have:

$$Q_i = \gamma \left[\int_{\Gamma_D} \bar{q}_x dy + \int_{\Gamma_D} \bar{q}_y dx \right] \quad (40)$$

$$\beta_i = \gamma \left[\int_{\Gamma_D} \bar{q}_x dy + \int_{\Gamma_D} \bar{q}_y dx \right] \quad (41)$$

3.2.3 Modeling groundwater flow in heterogeneous geological media

Furthermore, we need techniques to deal with material interfaces of arbitrary orientation, and possibly with multiple intersections, to model real cases of groundwater flow in heterogeneous geological media. As shown in Figure 6, there are three possible cases in which a physical cover contains two material interfaces. In Case 1, the material interfaces do not intersect within the cover, which could represent different material compositions, including a fracture when the distance between the two interfaces is relatively small. In Case 2, the two material interfaces intersect and divide the whole domain into three or four material domains. In Case 3, the two

material interfaces intersect and **split** the cover into **two** different material domains, which could represent part of an inclusion.

In Figure 6, the “+” and “-” **signify** the positive and negative value of the normal distance $\phi_j(x, y)$ from a certain material interface, whereas “++”, “+-”, “-+” and “--” represent the positive and negative values of normal distances $\phi_1(x, y)$, $\phi_2(x, y)$ from a point (x, y) to the two material interfaces within the same cover. From Equations (26)-(28), we can see that the jump function $\psi_j(x, y)$ is a piecewise linear function. The superposition of different jump functions could exactly represent different material properties with multiple material interfaces on an integral domain within **the** same physical cover. In cases with more than **two** material interfaces in one physical cover, the algorithm is the same as dealing with **two** material interfaces.

3.3 Theoretical comparison of the two approaches

Despite **the** different interpretations of material interfaces as **continuities or discontinuities**, the two approaches have something in common. The two approaches are both derived **based on** NMM for boundary constraints, and both approaches inherit the advantages of NMM. First, the definition of **the** NMM **finite cover** system enables us to reduce meshing efforts **by using a fixed mathematical mesh** for complex geometries **or moving interfaces**. On the other **hand**, **using** the definitions of the two-cover-meshing system and the global approximation expressed by Equations (6)-(8), we have the option of **enhancing the approximation precision by** increasing the approximation order expressed in Equation (8), or introducing additional degrees of freedom in the physical cover, such as the jump terms expressed by Equation (25). Moreover, **as shown by An et al. [16]**, the **simplex** integration enhances the accuracy of the numerical results, especially for irregular or complex geometries.

Comparing the continuous JFM and discontinuous LMM approaches, the different definitions of physical covers (depending on **whether** material interfaces are regarded as discontinuities or inner interfaces) lead to the differences listed in Table 1. While Table 1 indicates some advantages and disadvantages with **each** method, both methods are applicable for modeling material interfaces, although the ultimate choice of method may depend on the problem to be solved—that is, if numerical accuracy can be assured. This will be investigated by simulation examples in the next section.

4 Demonstration examples

Based on the above formulation, the two approaches were coded into a NMM **model for groundwater flow analysis**. In the following subsections, we will first demonstrate the accuracy of LMM for Dirichlet boundary conditions, and then demonstrate the accuracy of both approaches for **groundwater flow** across a region intersected by an idealized fault, with comparison to an analytical solution. Last, we present applications of the two approaches **for** modeling fluid flow in heterogeneous media with two material interfaces, and compare the results **for** hydraulic head and specific discharge.

4.1 Example 1: Demonstration of LMM for Dirichlet boundary conditions

In order to demonstrate the accuracy of NMM with LMM **for Dirichlet boundary conditions**, we simulate a $1 \text{ m} \times 1 \text{ m}$ rectangular model with the following boundary conditions:

$$h(0, y) = h(x, 0) = 1; h(x, 1) = 1-x; h(1, y) = 1-y;$$

The analytical solution for this example is: $h = 1-xy$.

As shown in Figure 7a, we calculate this problem with 28 elements and plot the overall distribution of hydraulic head. Specifically, in Figure 7b, we compare the solutions of 21 points from profile $y=x$ with the analytical solution. From Figure 7, we observe that LMM achieves good accuracy for Dirichlet boundary conditions, even with a relatively coarse mesh.

4.2 Example 2: demonstration of the two approaches for material interfaces

In the explicit modeling of faults or dominant fractures, faults could be regarded as a media containing different material from the surrounding rock [48-49]. To demonstrate the accuracy and efficiency of our model for material interfaces, we simulate groundwater flow in a $10 \text{ m} \times 4 \text{ m}$ model domain with a single fault located at $x \in [4.75, 4.85] \text{ (m)}$, modeled as thin as a factor of 0.01 of the whole domain width. The boundary conditions are: $h(0, y) = 2 \text{ m}$, $h(1, y) = 12 \text{ m}$; with impermeable upper and bottom boundaries. The coefficients of permeability for the three material domains are: $k_{xx}=k_{yy}=2 \times 10^{-8} \text{ m/s}$, $k_{xy}=k_{yx}=0$, $x \in [0, 4.75]$; $k_{xx}=k_{yy}=1 \times 10^{-7} \text{ m/s}$, $k_{xy}=k_{yx}=0$, $x \in [4.75, 4.85]$; $k_{xx}=k_{yy}=1 \times 10^{-8} \text{ m/s}$, $k_{xy}=k_{yx}=0$, $x \in [4.85, 10]$. We solve this problem using NMM with LMM and JFM, respectively, with the same number of mathematical covers, and compare the results with analytical solutions available in [48]. The computation parameters for NMM analysis using LMM and JFM are listed in Table 2. As shown in Figure 8a-c, the numerical results using both LMM and JFM with a very coarse mesh are in agreement with the analytical solution, still showing excellent accuracy and efficiency.

4.3 Example 3: comparison of the two approaches for material interfaces

We apply the two approaches to a rectangular heterogeneous domain for groundwater flow analysis. As shown in Figure 9, the left and right boundaries are Dirichlet boundaries with hydraulic heads of 1 m and 0 m, respectively. The top boundary is a Neumann boundary with 1 m/s discharge, and the bottom boundary is impermeable. There are two material interfaces located at $y=20 \text{ m}$ and $y=x+40 \text{ m}$, dividing the model into three material domains with permeability ratios of 10:1:10.

As shown in Figure 10a, we use 538 mathematical covers in both approaches to analyze the water flow. Respective computation parameters are listed in Table 3. The distribution of hydraulic head calculated by NMM with LMM and JFM are shown in Figures 10b and 10c, respectively. From these figures, we can observe that the hydraulic heads calculated by the two approaches agree well with each other.

We further extract two profiles at $y=80 \text{ m}$ and $x=40 \text{ m}$ and calculate the hydraulic head and specific discharge in both x and y directions with the two approaches, respectively, as shown in Figure 11.

We find a good agreement between the two approaches according to Figure 11. Specifically, at profile $y=80 \text{ m}$ (Figure 11d-f), the discontinuity of the specific discharge at both x and y directions occurs at $(40, 80)$, which is located at the material interface $y=x+40$. There is a slight deviation in the calculated q_x and q_y by JFM from those by LMM, owing to the different number of degrees of freedom along the material interface. The profile $x=40$ intersects both material interfaces (Figure 11a-c), leading to discontinuity of horizontal specific discharge at the two intersections $(40, 20)$ and $(40, 80)$. For the vertical specific discharge, both approaches yield continuous results at the intersection located at $(40, 20)$, indicating that normal flux continuity for the material interface $y=20$ is well satisfied. From this example, we can see that the two different approaches arrive at consistent results, reflecting continuity of hydraulic head and normal flux.

5 Conclusions

The NMM, based on a finite cover system with independent mathematical covers and physical covers, is an ideal method for modeling flow in heterogeneous media (including the complexity of intersected boundaries or abrupt media material property changes) in both continuous and discontinuous ways. The advantages of NMM include its flexibility in constructing physical cover functions (continuous or with gradient jump), its meshing efficiency with fixed mathematical covers, the convenience of increasing the approximation precision, and the high integration precision provided by simplex integration. In this study, we interpreted the refraction law in both continuous and discontinuous ways. From these two interpretations based on the NMM, we were able to develop two new approaches for boundary constraints, i.e., a continuous approach with jump functions and a discontinuous approach with Lagrange multipliers, and then made comparisons between these two approaches. In the discontinuous LMM, Dirichlet boundaries or material interfaces are regarded as discontinuities which separate mathematical covers into different physical covers. We defined and derived stringent forms of Lagrange multipliers to link the divided physical covers to satisfy the continuity requirement by the refraction law. In the continuous JFM, the material interfaces are regarded as inner interfaces, contained by physical covers. We constructed jump terms to represent the discontinuity of a head gradient in the direction normal to the interface to satisfy the refraction law. Both continuous and discontinuous approaches can consider multiple interface intersections and are accurate from stringent physical interpretation and mathematical derivation. Besides, they were developed for a uniform triangular mesh, to reduce meshing efforts. On top of that, we made a thorough theoretical comparison of 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 were coded into an NMM model for groundwater flow analysis and tested for precision and efficiency on different examples. We first tested the LMM for modeling Dirichlet boundary conditions and then tested both LMM and JFM for an idealized heterogeneous model, comparing the results with analytical solutions. Then we tested both approaches for a heterogeneous model and compared the results of hydraulic head and specific discharge. Despite the differences of computation parameters (the required number of physical covers, elements, and degrees of freedom), the two approaches agree well with each other, arriving at results of hydraulic heads and fluxes accurately satisfying the refraction law. We showed that NMM using both boundary-constraint approaches is very suitable for modeling groundwater flow in heterogeneous media considering its accuracy and ability to satisfy boundary constraints, its capability for dealing with arbitrarily oriented or complexly intersected boundaries, and its efficiency with a fixed mathematical mesh.

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Tables

Table 1 Comparison and contrast between LMM and JFM

	LMM	JFM	Comparison and Contrast
The global number of degrees of freedom	$3m(n_{ce} - 1)$, where m is defined as in Section 2 and n_{ce} is the number of elements cut by interfaces.	$3n_i$, where n_i is the number of material interfaces within an element	When material interfaces do not intersect such as Case 1 in Figure 6, $n_i = n_{ce} - 1$; when material interfaces intersect such as Case 2 in Figure 6, $n_i < n_{ce} - 1$ or case 3 in Figure 6, $n_i = n_{ce}$
The treatment of multiple material interfaces in the same triangle	In LMM, multiple interfaces divide the triangle into different elements, which may involve small integration areas	In JFM, the contribution of multiple interfaces are related to different degrees of freedom in a physical cover	Both approaches are able to model multiple material interfaces within the same mathematical mesh.
The treatment of small integration area	LMM treats small area as independent elements and calculate integration independently on the small area	JFM calculates the integration on small areas and add to the corresponding physical covers	The global equilibrium equations established by JFM are numerically more stable, avoiding small numbers in the diagonal elements
The treatment of moving interfaces	In LMM, the moving interfaces are considered by updating the normal directions and integral lengths in Equation (22) and element geometric data for integration.	In JFM, the moving interfaces are considered by updating jump functions according to Equation (28) and integral data.	As a level-set method, JFM is more straightforward for moving interfaces. However, the numerical efforts in the two approaches are equivalent. With simplex integration, the updated areas related to the moving interfaces are readily integrated by updated geometric coordinates of vertices.
The capability of being coupled with mechanical analysis	LMM requires different choices of numerical flux for mechanical analysis when the Poisson's ratio is not 0 to guarantee the boundary constraints.	JFM is straightforward to be coupled with mechanical analysis by constructing jump degrees of freedom representing strain jumps	Both methods are promising for modeling coupled process in fractured rock, in which fractures are considered as strong discontinuities for mechanical analysis while a different material composition for water flow analysis.
The application to other numerical methods	With stringently defined Lagrange multiplier for water flow analysis, LMM can be applied to FEM, DG as a promising approach to overcome the errors on continuity of hydraulic head or flux, being an alternative to the approach proposed by Zhou et al. in [11] but avoiding iterative adjustment.	JFM could also be applied to the XFEM for water flow modeling similar to the existing XFEM mechanical analysis [46]. Compared with existing JFM in XFEM, the constructed JFM in this paper has the following advantages: (1) it is able to model arbitrarily heterogeneous media, without limitation to a closed shape; (2) simplex integration enables higher precision with arbitrary polygons.	LMM can be applied to other methods as a discontinuous approach for material interfaces, such as FEM or DG, whereas JFM can be applied to continuous numerical methods, such as XFEM.

Table 2 Computation parameters for NMM analysis using LMM and JFM of demonstration example 2.

	LMM	JFM
Number of mathematical covers	17	17
Triangular mesh side length (m)	2.75	2.75
Number of physical covers	29	17
Number of elements	26	18
Number of degrees of freedom	29	29

Table 3 Computation parameters for NMM analysis using LMM and JFM of demonstration example 3.

	LMM	JFM
Number of mathematical covers	538	538
Triangular mesh side length (m)	5.077	5.077
Number of physical covers	625	538
Number of elements	1067	984
Number of degrees of freedom	1875	1701

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}	j th 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 j th 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 j th on the i th degree of freedom as jump terms
$\mathbf{K}$	Tensor of permeability coefficient
L_{ij}	Element of matrix $\mathbf{L}$, representing the contribution of j th degree of freedom as jump on i th 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 $\mathbf{\beta}$, representing the flux term related to the i th degree of freedom as jump term
$\omega_j(x, y)$	Jump shape function
$\psi_j(x, y)$	j th 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

Figure 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 expression of the material properties and boundary conditions.

Figure 2 Mathematical covers, physical covers and elements defined in NMM with uniform triangles as mathematical mesh

Figure 3 Illustration of Lagrange multipliers applied in discontinuous physical covers

Figure 4 Illustration of a material interface related to Dirichlet boundaries

Figure 5 Physical covers containing jump terms related to a material interface

Figure 6 Three cases of two material interfaces in the same element

(a)

(b)

Figure 7 Demonstration example 1: (a) computed contour map of hydraulic head using NMM with LMM; (b) Comparison of computed and analytical solution at profile $y=x$.

Figure 8 Demonstration example 2: (a) computed hydraulic head distribution using NMM with LMM and JFM; (b) The comparison of solutions computed by LMM and JFM with an analytical solution along a profile located at $y=1\text{m}$; (c) The local comparison between computed and analytical solutions in the fault area at $x \in [4.5, 5.5]$.

Figure 9 Demonstration example 3: model geometry and boundary conditions

Figure 10 Demonstration example 3: (a) the modeling mesh for both NMM with LMM and JFM; contour of hydraulic head calculated by (b) NMM with LMM and (c) NMM with JFM.

Figure 11 Demonstration example 3: comparison of hydraulic heads, horizontal and vertical specific discharges by NMM with LMM and JFM (a) - (c) at profile $x=40\text{m}$ and (d) - (f) at profile $y=80\text{m}$.