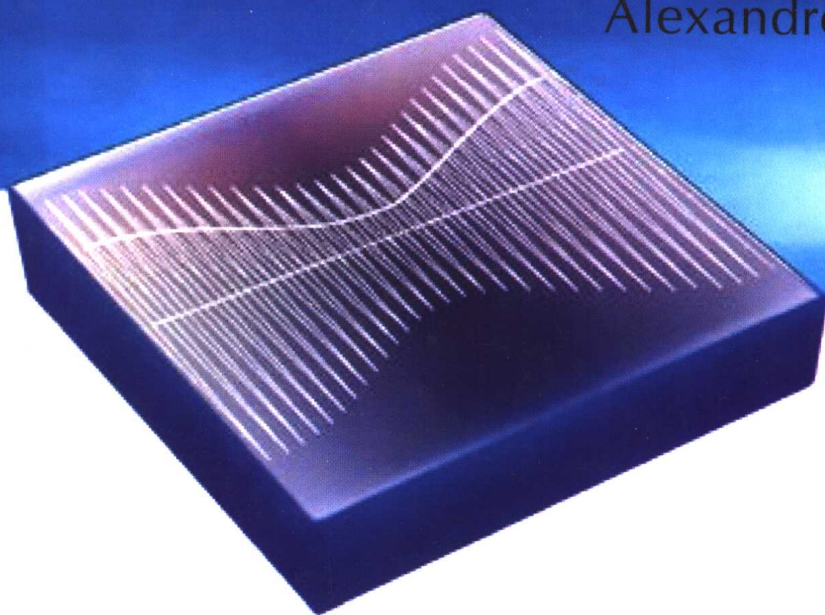


Series in Contemporary Applied Mathematics
CAM 7

Mathematical Methods for Surface and Subsurface Hydrosystems

Deguan Wang
Christian Duquennoi
Alexandre Ern

editors



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CERMICS ENPC, France



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Preface

The ISFMA Symposium on Mathematical Models for Surface and Subsurface Hydrosystems was held on September 13—17, 2004 at Hohai University, Nanjing, China. With the increasing awareness of the heavy burden placed on environmental resources and the need of industry and public institutions to cope with more stringent regulations, the scope of the Symposium was to focus on some specific, but very important, environmental problems, namely surface and subsurface hydrosystems. The purpose was to present state-of-the-art techniques to model such systems, to promote the exchange of scientific ideas between French and Chinese experts, and to foster new collaborations between France and China in this field. Approximately 70 participants, including five French representatives attended the Symposium.

The activities of the Symposium included five 3-hour keynote lectures elaborating from the basics to recent advances in hydrosystem modeling and several contributed presentations dealing with more specific problems. This volume collects the material presented in the keynote lectures and some selected contributed lectures. The topics covered include mixed finite element method, finite volume formulation, sharp front modeling, biological process modeling, red tide simulation, and contaminant transfer in coastal waters. As such, this volume should be useful to graduate students, post-graduate fellows and researchers both in applied mathematics and in environmental engineering.

As organizers of this Symposium, we would like to express our gratitude to various institutions for their supports: National Nature Science Foundation of China, Mathematical Center of Ministry of Education of China, Hohai University, French Embassy in Beijing, Consulate General of France in Shanghai, ISFMA (Institut Sino-Français de Mathématiques Appliquées) and SOGREAH. We also thank all the lecturers and participants for their contributions. Our deepest appreciation goes to Professor Li Tatsien for his support in launching this Symposium. Special thanks also to Matthieu Jouan for his instrumental help in the organization.

Deguan Wang, Christian Duquennoi, and Alexandre Ern
October 2005

Contents

Preface

Series Talks

<i>P. Ackerer, A. Younes: A Finite Volume Formulation of the Mixed Finite Element Method for Triangular Elements</i>	1
<i>Alexandre Ern: Finite Element Modeling of Hydrosystems with Fully Saturated, Variably Saturated, and Overland Flows</i>	19
<i>Patrick Goblet: Sharp Front Modeling</i>	60
<i>Catherine Gourlay, Marie-Hélène, Tusseau-Vuillemin: Numerical Modeling of Biological Processes: Specificities, Difficulties and Challenges</i>	75
<i>Deguan Wang: Ecological Simulation of Red Tides in Shallow Sea Area</i>	99
<i>Ling Li: Subsurface Pathways of Contaminants to Coastal Waters: Effects of Oceanic Oscillations</i>	126

Invited Talks

<i>Tingfang Wang, Sixun Huang, Huadong Du, Gui Zhang: Studies on Retrieval of the Initial Values and Diffusion Coefficient of Water Pollutant Advection and Diffusion Process</i>	174
<i>Jing Chen, Zhifang Zhou: Application of Tabu Search Method to the Parameters of Groundwater Simulation Models</i>	191
<i>Xiaomin Xu, Deguan Wang: Several Problems in River Networks Hydraulic Mathematics Model</i>	201

Jue Yang, Deguan Wang, Ying Zhang: Study on the Character of
Equilibrium Point and Its Impact on the Changing Rate of
Phytoplankton Concentration Using a Simple Nutrient-
Phytoplankton Model 211

Jie Zhou, Deguan Wang, Haiping Jiang, Xijun Lai: A Numerical
Simulation of Thermal Discharge into Tidal Estuary with FVM 223

A Finite Volume Formulation of the Mixed Finite Element Method for Triangular Elements

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1 Introduction

Numerous mathematical models are based on conservation principles and constitutive laws, which are formulated by,

$$s \frac{\partial u}{\partial t} + \nabla \cdot \mathbf{q} = f \quad (1.1)$$

$$\mathbf{q} = -\mathbf{K} \nabla u \quad (1.2)$$

where s is a storage coefficient, \mathbf{K} is the flux related parameter and \mathbf{q} is the flux of the associated state variable u . Equation (1.1) states for the conservation principle and (1.2) states for the constitutive law like Fourier's law (u is the temperature), Fick's law (u is the concentration of a solute), Ohm's law (u is the electric potential) or Darcy's law (u is the hydraulic head). The associated initial and boundary conditions are of Dirichlet or Neumann type,

$$\begin{aligned} u(x, 0) &= u_0(x) & x &\in \Omega \\ u(x, t) &= g_1(x, t) & (x \in \partial\Omega^1, t > 0) \\ (-\mathbf{K} \nabla u) \cdot \mathbf{n}_{\partial\Omega} &= g_2(x, t) & (x \in \partial\Omega^2, t > 0) \end{aligned} \quad (1.3)$$

where Ω is a bounded, polygonal open set of \mathbb{R}^2 , $\partial\Omega^1$ and $\partial\Omega^2$ are partitions of the boundary $\partial\Omega$ of Ω corresponding to Dirichlet and Neumann boundary conditions and $\mathbf{n}_{\partial\Omega}$ the unit outward normal to the boundary $\partial\Omega$.

This system is often solved by finite volumes (FV) or finite elements (FE) methods of lower order (see LeVeque [1] and Ern & Guermond [2] among others). FV ensures an exact mass balance over each element and continuous fluxes across common element boundaries. FE ensures an exact mass balance on a dual mesh but leads to discontinuous fluxes at common elements edges. However, finite element is considered as

more flexible because of its high capacity of discretizing domains with complex geometry.

The mixed finite element method (MFE) keeps the advantages of both methods: accurate mass balance at the element level, continuity of the flux from one element to its neighbors one and mesh flexibility. Moreover, the method solves simultaneously the state variable and its gradient with the same order of accuracy (Babuska *et al.* [3], Brezzi & Fortin [4], Girault & Raviart [5] and Raviart & Thomas [6]). Therefore, MFE has received a growing attention and some numerical experiments showed the superiority of the mixed finite element method with regard to the other classic methods (Darlow *et al.* [7], Durlofsky [8], Kaaschieter [9] and Mosé *et al.* [10]).

However, its implementation leads to a system matrix with significantly more unknowns than FV and FE methods. When the lowest-order Raviart-Thomas space [6, 11] is used, which is very often the case, the resolution of (1.1) and (1.2) leads to a system with one scalar unknown per edge for the hybrid formulation of the MFE [6, 11].

Attempts to reduce the number of unknowns have been investigated by various authors. For rectangular meshes, mixed finite elements of lowest order reduce to the standard cell-centered finite volume method [11] provided that numerical integration is used. Baranger *et al.* [12] provides similar results for triangles and Cordes & Kinzelbach [13] showed the equivalence between mixed finite element and finite volumes without any numerical integration. However, such equivalence is restricted to steady state and without sink/source terms inside the domain. Moreover, the mixed finite element method does not require a Delaunay triangulation [9] unlike a finite volume scheme.

We present here an alternative formulation of the MFE which leads to a system matrix with only one unknown per element without any approximation. In the first part, the steady state formulation is derived in details for the MFE, FV and the alternative formulation. In the second part, the main results concerning the general formulation for the elliptic PDE (steady state) will be described. The detailed developments can be found in Younes *et al.* [14, 15] and Chavent *et al.* [16]. The last part is dedicated to the parabolic PDE.

2 Resolution of the elliptic case with a scalar flux related parameter

Assuming that the system is in equilibrium, the storage term in (1.1) vanishes. The system of equations (1.1) and (1.2) leads to an elliptic

partial differential equation. The finite volume formulation of yields,

$$\sum_{i=1}^3 Q_i = Q_s \quad (2.1)$$

2.1 The mixed finite element formulation

In the lowest-order MFE formulation for triangular elements, the flux is approximated with vector basis functions that are piecewise linear along both coordinate directions. In any point inside element A , \mathbf{q}^A is approximated by (e.g. [9]):

$$\mathbf{q}^A = \sum_{i=1}^3 \mathbf{w}_i^A Q_i^A \quad (2.2)$$

where Q_i are the fluxes across the element edges A_i taken positive outwards and $\mathbf{w}_i(L^{-1})$ are the three vectorial basis functions for the element A (Figure 2.1) defined by:

$$\int_{A_j} \mathbf{w}_i \cdot \mathbf{n}_j^A = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (2.3)$$

For a triangular element, the vectorial basis function is given by:

$$\mathbf{w}_i^A = \frac{1}{2|A|} \begin{pmatrix} x - x_i \\ y - y_i \end{pmatrix} \quad (2.4)$$

where (x_i, y_i) are the coordinates of the vertices of A and $|A|$ is its area.

In addition, they satisfy

$$\nabla \cdot \mathbf{w}_i = \frac{1}{|A|} \quad (2.5)$$

and, on the edge A_j ,

$$\mathbf{w}_i \cdot \mathbf{n}_j^A = \begin{cases} \frac{1}{|A_i|} & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (2.6)$$

where $|A_i|$ is the length of the edge A_i .

Using properties (2.5) and (2.6) of the vectorial basis functions, the flux's law (1.2) is written in a variational form

$$\begin{aligned} \int_A (K^{-1} \mathbf{q}^A) \cdot \mathbf{w}_i &= - \int_A (\nabla u) \cdot \mathbf{w}_i \\ &= \int_A u \nabla \cdot \mathbf{w}_i - \sum_{j=1}^3 \int_{A_j} u \mathbf{w}_i \cdot \mathbf{n}_j^A = \frac{q}{|A|} \int_A u - \frac{1}{|A_i|} \int_{A_i} u \end{aligned} \quad (2.7)$$

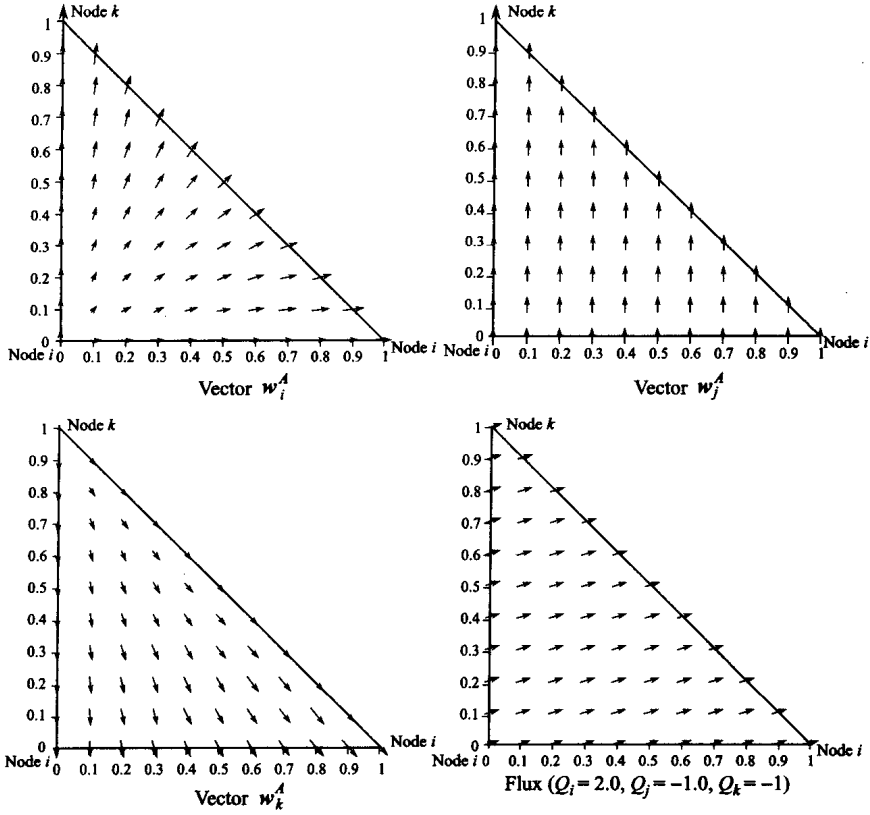


Figure 2.1 Vectorial basis function and related flux.

which can be written as

$$\sum_{j=1}^3 B_{ij}^A Q_j^A = u^A - u_i^A \quad (2.8)$$

with $B_{ij}^A = \frac{1}{K^A} \int_E \mathbf{w}_i^A \cdot \mathbf{w}_j^A$, u^A is the average value of the state variable over A and u_i^A is the average value of the state variable on element edge A_i . K^A is a scalar and represents the average value of K on element A .

We define \mathbf{r}_{ij} as the edge vector from node i toward node j and L_{ij} as its length ($L_{ij} = \|\mathbf{r}_{ij}\|$). As shown by Cordes & Kinzelbach [13], applying the scalar product $\mathbf{r}_{ij} \cdot \mathbf{r}_{ik} = \frac{1}{2}(L_{ij}^2 + L_{ik}^2 - L_{jk}^2)$ leads to the

following relation:

$$\sum_{j=1}^3 B_{ij}^A = (r_{ij}^2 + r_{jk}^2 + r_{ki}^2)/48K^A|A| = L \quad (2.9)$$

The previous properties of the discretized flux law is used to build a system of equations with average edge value as unknown. The system of equations (2.8) gives

$$L \sum_{i=1}^3 Q_i = 3u^A - \sum_{i=1}^3 u_i^A \quad (2.10)$$

Equation (2.10) is inserted in (2.1), which leads to:

$$u = \frac{1}{3} \left(\sum_{i=1}^3 u_i^A + LQ_s \right) \quad (2.11)$$

System (2.8) is inverted and u is replaced by the previous formulation (2.11),

$$Q_i^A = -\frac{K^A}{|A|} r_{jk} [r_{jk} u_i^A + r_{ki} u_j^A + r_{ij} u_k^A] + \frac{Q_s^A}{3} \quad (2.12)$$

Using the continuity of the fluxes between two adjacent elements A and say B (Figure 2.2)

$$Q_i^A + Q_j^B = 0 \quad (2.13)$$

leads then to the equation:

$$\begin{aligned} & \left[\frac{K^A}{|A|} r_{jk} [r_{jk} u_i^A + r_{ki} u_j^A + r_{ij} u_k^A] + \frac{Q_s^A}{3} \right] \\ & + \left[\frac{K^B}{|B|} r_{jk} [r_{jk} u_i^B + r_{ki} u_j^B + r_{ij} u_k^B] + \frac{Q_s^B}{3} \right] = 0 \end{aligned} \quad (2.14)$$

For continuity reasons, we have

$$u_i^A = u_i^B \quad (2.15)$$

This equation is written for each edge of the mesh which is not a Dirichlet type boundary. If a Neuman boundary conditions is applied on edge i , (2.14) becomes:

$$\left[\frac{K^A}{|A|} r_{jk} [r_{jk} u_i^A + r_{ki} u_j^A + r_{ij} u_k^A] + \frac{Q_s^A}{3} \right] + Q_N = 0 \quad (2.16)$$

Equation (2.14) is the discretized form of equations (1.1) and (1.2) using the mixed finite element method in its hybrid form.

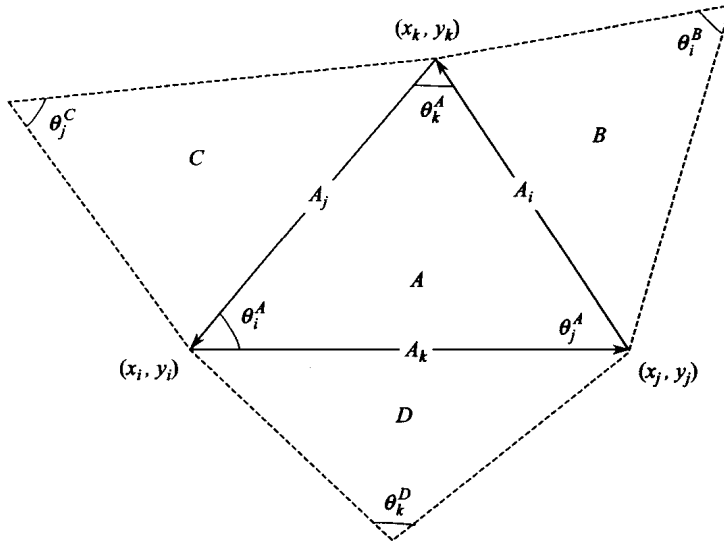


Figure 2.2 Triangular element A and its three neighbors.

2.2 The finite volume formulation

The main idea of the finite volume formulation consists in defining the flux by

$$Q_i^A = -K^A(u_C^A - u_i) \frac{L_{A_i}}{L_{C_i}^A} \quad (2.17)$$

where u_C^A is the value of the state variable at the circumcenter of A , L_{A_i} is the length of the edge i , and $L_{C_i}^A$ is the distance from edge i to the circumcenter of the element A (Figure 2.3).

Writing flux and variable continuity at the common edge of element A and one of its neighbors noted B yields

$$u_i = \frac{\frac{L_{C_i}^A}{K^A} u_C^A + \frac{L_{C_i}^B}{K^B} u_C^B}{\frac{L_{C_i}^A}{K^A} + \frac{L_{C_i}^B}{K^B}} \quad (2.18)$$

and therefore,

$$Q_i = L_{A_i} \left(\frac{L_{C_i}^A}{K^A} + \frac{L_{C_i}^B}{K^B} \right)^{-1} (u_C^A - u_C^B) = K_{AB} (u_C^A - u_C^B) \quad (2.19)$$

where K_{AB} is the harmonic mean of the flux related parameter multiplied by the length of the edge and is called the stiffness coefficient.

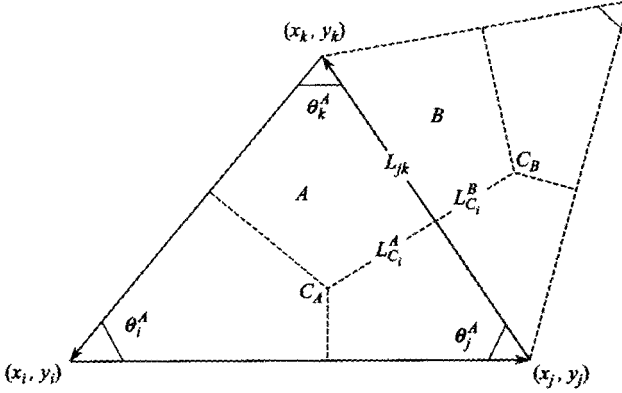


Figure 2.3 A triangular finite volume and its neighbor.

The finite volume discretization of equations (2.1) and (2.2) is obtained by plugging (2.19) into (2.1):

$$K_{AB}(u_C^A - u_C^B) + K_{AC}(u_C^A - u_C^C) + K_{AD}(u_C^A - u_C^D) = Q_s \quad (2.20)$$

This equation is written for each element. The finite volume requires significantly less unknowns than the mixed formulation (one per element against one per edge) and leads to a more sparse system matrix (4 non zero values per line against 5).

2.3 The re-formulation of the mixed finite element

The main idea of the reformulation is first to define a linear interpolate of the state variable by,

$$U^A = \sum_{i=1}^3 \pi_i^A u_i^A \quad (2.21)$$

where U is the value of the state variable somewhere (in or outside the element A , not necessarily the average value over the element or the value at the circumcenter of the element), and second, to use a very generic finite volume formulation of the flux,

$$Q_i^A = \xi_i^A (U^A - u_i^A) + \gamma_i^A \quad (2.22)$$

Building an equation with unknowns U is then straightforward. The continuity of the fluxes between two adjacent elements and of the state variable on the common edge yields:

$$\begin{cases} Q_i^A + Q_i^B = 0 \\ u_i^A = u_i^B \end{cases} \quad (2.23)$$

and therefore

$$u_i = \frac{\xi_i^A U^A + \xi_i^B U^B}{\xi_i^A + \xi_i^B} + \frac{\gamma_i^A + \gamma_i^B}{\xi_i^A + \xi_i^B} \quad (2.24)$$

Equation (2.24) is plugged in equation (2.22) which leads to

$$Q_i^A = \frac{\xi_i^A \xi_i^B}{\xi_i^A + \xi_i^B} (U^A - U^B) + \frac{\xi_i^B \gamma_i^A - \xi_i^A \gamma_i^B}{\xi_i^A + \xi_i^B} \quad (2.25)$$

Equation (2.25) is then plugged in the discretized mass balance equation, which leads to an equation with one unknown per element, if, of course, the values of π_i^A , ξ_i^A and γ_i^A can be determined.

Replacing (2.21) in (2.22) and comparing with (2.12) allows the identification of these coefficients,

$$\begin{cases} \pi_i^A = \frac{(\mathbf{r}_{ik} \mathbf{r}_{jk})(\mathbf{r}_{ij} \mathbf{r}_{kj})}{4|A|^2} \\ \xi_i^A = -\frac{4K^A |A|}{\mathbf{r}_{ij} \mathbf{r}_{ik}} = \frac{2K^A}{\cot(\theta_i)} = K^A \frac{L_{A_i}}{L_{A_i}^A} \\ \gamma_i^A = \frac{Q_s^A}{3} \end{cases} \quad (2.26)$$

and the discretized form of (1.1) and (1.2) is then

$$\begin{aligned} & \frac{\xi_i^A \xi_i^B}{\xi_i^A + \xi_i^B} (U^A - U^B) + \frac{\xi_j^A \xi_j^C}{\xi_j^A + \xi_j^C} (U^A - U^C) + \frac{\xi_k^A \xi_k^D}{\xi_k^A + \xi_k^D} (U^A - U^D) \\ &= Q_s^A - \left[\frac{\xi_i^B \gamma_i^A - \xi_i^A \gamma_i^B}{\xi_i^A + \xi_i^B} + \frac{\xi_i^C \gamma_i^A - \xi_i^A \gamma_i^C}{\xi_i^A + \xi_i^C} + \frac{\xi_i^D \gamma_i^A - \xi_i^A \gamma_i^D}{\xi_i^A + \xi_i^D} \right] \end{aligned} \quad (2.27)$$

Note that $\frac{\xi_i^A \xi_i^B}{\xi_i^A + \xi_i^B} = K_{AB}$ and therefore, the system equation (2.27) of the mixed reformulation differs from the system equation of the finite volume formulation (equation (2.20)) only by the sink/source term. Without sink/source terms, both formulations are identical. Moreover, the variable U is then the state variable at the circumcenter since, from equations (2.26) and (2.21):

$$\begin{aligned} U = \frac{1}{4|A|^2} [& (\mathbf{r}_{ik} \mathbf{r}_{jk})(\mathbf{r}_{ij} \mathbf{r}_{kj}) u_i + (\mathbf{r}_{ij} \mathbf{r}_{ik})(\mathbf{r}_{ik} \mathbf{r}_{jk}) u_j \\ & + (\mathbf{r}_{ij} \mathbf{r}_{ik})(\mathbf{r}_{ij} \mathbf{r}_{kj}) u_k] = u_C^A \end{aligned} \quad (2.28)$$

With sink/source terms, both formulations are different, except for equilateral triangles and homogeneous domain. Moreover, in that case, the velocity derived from the MFE approach varies linearly and therefore, the linear interpolation of the state variable is no more valid.

3 General 2D formulation for the elliptic case

We treat here the case where \mathbf{K} is a full tensor. With the FV method, the computation of accurate fluxes with a full parameter tensor is a difficult issue, especially for discontinuous coefficient. For these methods, recent developments have been done to improve the flux computation by using locally additional constraints on the continuity of the state variable and fluxes [17–20].

With MFE method, the case of full parameter tensor is treated in an elegant way leading to a system with as many unknowns as the total number of edges. Reduction of the number of unknowns can be obtained for rectangular meshes when using appropriate quadrature rules with a variant of the MFE method, the “expanded mixed method” [21, 22]. For general geometry, enhanced cell-centered finite difference method was obtained from a quadrature approximation of the expanded mixed method [23]. This method is improved by adding Lagrange multiplier for non smooth meshes or abrupt changes in \mathbf{K} [23].

The parameter tensor \mathbf{K} is generally symmetric [24]. It commonly arises from a rotation of the locally diagonal tensor from its principal axes with respect to the computational grid and is therefore always symmetric and positive definite.

\mathbf{K}^A is defined by

$$\mathbf{K}^A = \begin{pmatrix} k_x^A & k_{xy}^A \\ k_{xy}^A & k_y^A \end{pmatrix} \quad (3.1)$$

The principal components of \mathbf{K}^A are constant and positive over each element A , therefore

$$\det(\mathbf{K}^A) = k_x^A k_y^A - (k_{xy}^A)^2 > 0 \quad (3.2)$$

3.1 The mixed finite element formulation

We define now l_{ij} by $l_{ij} = \mathbf{r}_{ij}^T (\mathbf{K}^A)^{-1} \mathbf{r}_{ij}$ where $(\mathbf{K}^A)^{-1}$ is the parameter tensor defined over element A . The variational form of equation (1.2) leads now to:

$$\begin{aligned} \int_A ((\mathbf{K}^A)^{-1} \mathbf{q}^A) \cdot \mathbf{w}_i^A &= - \int_A \nabla u \cdot \mathbf{w}_i^A \\ &= \int_A u \nabla \cdot \mathbf{w}_i^A - \sum_{j=1}^3 \int_{A_j} u \mathbf{w}_i^A \cdot \mathbf{n}_j^A \end{aligned} \quad (3.3)$$

Written in a matrix form yields

$$\sum_{j=1}^3 B_{ij}^A Q_j^A = u^A - u_i^A \quad \text{with} \quad B_{ij}^A = \int_A \mathbf{w}_i^{A,T} (\mathbf{K}^A)^{-1} \mathbf{w}_j^A \quad (3.4)$$

The matrix \mathbf{B} is given by

$$\mathbf{B} = \frac{1}{48|A|} \begin{pmatrix} 3l_{12} + 3l_{13} - l_{23} & -3l_{12} + l_{13} + l_{23} & l_{12} - 3l_{13} + l_{23} \\ -3l_{12} + 3l_{13} + l_{23} & 3l_{12} - l_{13} + 3l_{23} & l_{12} + l_{13} - 3l_{23} \\ l_{12} - 3l_{13} + l_{23} & l_{12} + l_{13} - 3l_{23} & -l_{12} + 3l_{13} + 3l_{23} \end{pmatrix} \quad (3.5)$$

with

$$\sum_{j=1}^3 B_{ij}^A = \frac{1}{48|A|} (l_{12} + l_{13} + l_{23}) = L^A \quad (3.6)$$

where L^A can be seen as the inverse of the parameter tensor scaled by the shape of the element. Therefore, we obtain the same equations than and (2.11), *i.e.*

$$L^A \sum_{i=1}^3 Q_i = 3u^A - \sum_{i=1}^3 u_i^A \quad \text{and} \quad u = \frac{1}{3} \left(\sum_{i=1}^3 u_i^A + L^A Q_s \right) \quad (3.7)$$

The system (3.4) is inverted and (3.7) is used to obtain:

$$\begin{aligned} Q_i^A = & -\frac{\det(\mathbf{K})^A}{|A|} [\mathbf{r}_{jk}^T (\mathbf{K}^A)^{-1} \mathbf{r}_{jk} u_i^A \\ & + \mathbf{r}_{jk}^T (\mathbf{K}^A)^{-1} \mathbf{r}_{ki} u_j^A + \mathbf{r}_{jk}^T (\mathbf{K}^A)^{-1} \mathbf{r}_{ij} u_k^A] + \frac{Q_s^A}{3} \end{aligned} \quad (3.8)$$

The final system of equations is obtained using continuity properties of the flux and state variable, which yields

$$\begin{cases} Q_i^A + Q_i^B \\ u_i^A = u_i^B = u_i \end{cases} \quad (3.9)$$

and therefore, the discretized equation of system (1.1) and (1.2) is

$$\begin{aligned}
 & \frac{\det(\mathbf{K}^A)}{|A|} [\mathbf{r}_{jk}^T(\mathbf{K}^A)^{-1} \mathbf{r}_{jk} u_i^A \\
 & + \mathbf{r}_{jk}^T(\mathbf{K}^A)^{-1} \mathbf{r}_{ki} u_j^A + \mathbf{r}_{jk}^T(\mathbf{K}^A)^{-1} \mathbf{r}_{ij} u_k^A] \\
 & + \frac{\det(\mathbf{K}^B)}{|B|} [\mathbf{r}_{jk}^T(\mathbf{K}^B)^{-1} \mathbf{r}_{jk} u_i^B \\
 & + \mathbf{r}_{jk}^T(\mathbf{K}^B)^{-1} \mathbf{r}_{ki} u_j^B + \mathbf{r}_{jk}^T(\mathbf{K}^B)^{-1} \mathbf{r}_{ij} u_k^B] \\
 & = \frac{Q_s^A}{3} + \frac{Q_s^B}{3}
 \end{aligned} \tag{3.10}$$

This equation is slightly modified when the edge belongs to the domain boundary.

3.2 The corresponding re-formulation

The same development as for the case of a scalar parameter K is used (see equations (2.21) and (2.22)). The coefficients π_i^A , ξ_i^A and γ_i^A are

$$\begin{cases} \pi_i^A = \frac{\det(\mathbf{K}^A)}{4|A|^2} [\mathbf{r}_{ik}^T(\mathbf{K}^A)^{-1} \mathbf{r}_{jk}] [\mathbf{r}_{ij}^T(\mathbf{K}^A)^{-1} \mathbf{r}_{kj}] \\ \xi_i^A = -\frac{4|A|}{[\mathbf{r}_{ij}^T(\mathbf{K}^A)^{-1} \mathbf{r}_{ik}]} \\ \gamma_1^A = \gamma_2^A = \gamma_3^A = \frac{Q_s^A}{3} \end{cases} \tag{3.11}$$

Replacing this last relation in the balance equation for an element A surrounded by three elements B , C and D (Figure 2.2) leads to the equation

$$\begin{aligned}
 & \frac{\xi_i^A \xi_i^B}{\xi_i^A + \xi_i^B} (U^A - U^B) \\
 & + \frac{\xi_i^A \xi_i^C}{\xi_i^A + \xi_i^C} (U^A - U^C) + \frac{\xi_k^A \xi_k^D}{\xi_k^A + \xi_k^D} (U^A - U^D) \\
 & = Q_s^A - \left[\frac{\xi_i^B \gamma_i^A - \xi_i^A \gamma_i^B}{\xi_i^A + \xi_i^B} + \frac{\xi_i^C \gamma_i^A - \xi_i^A \gamma_i^C}{\xi_i^A + \xi_i^C} + \frac{\xi_i^D \gamma_i^A - \xi_i^A \gamma_i^D}{\xi_i^A + \xi_i^D} \right]
 \end{aligned} \tag{3.12}$$