Aye Aye Hlaing \* and Me Me Chit \*\*

#### Abstract

This paper starts control volume finite element methods which are locally conservative on each control volume. After that we consider potential- and flux-based upstream weighting strategies and the mixed finite element spaces on tetrahedra in three dimensions. Then various approaches such as linearization, implicit time approximation and explicit time approximation are studied. Finally, we discuss the application to one-phase flows and two-phase flows in porous media.

## **1 Control Volume Finite Element (CVFE) Methods 1.1 Basic CVFEs**

To see the idea of CVFE, we focus on linear triangular elements in two dimensions. We consider the stationary problem

$$-\nabla \cdot (\mathbf{K} \nabla \mathbf{P}) = \mathbf{f} \qquad \text{in } \Omega, \tag{1}$$

where  $\Omega$  is a bounded domain in the plane, **K** is a tensor and P is pressure.

Let  $V_i$  be a control volume. Replacing P by  $P_h \in V_h$ , the space of continuous piecewise linear functions on  $\overline{\Omega}$ , in (1) and integrating over  $V_i$ , we see that

$$-\int_{V_{i}} \nabla \cdot (\mathbf{K} \nabla P_{h}(x)) dx = \int_{V_{i}} f(x) dx$$

The divergence theorem implies

$$-\int_{\partial V_i} (\mathbf{K} \nabla P_h) \cdot \hat{\mathbf{n}} \, ds = \int_{V_i} f(x) \, dx, \qquad (2)$$

where  $\hat{\mathbf{n}}$  is the outward unit normal.

We note that  $\nabla P_h \cdot \hat{\mathbf{n}}$  is continuous across each segment of  $\partial V_i$ . Thus, if **K** is continuous across that segment, so is the flux  $(\mathbf{K} \nabla P_h) \cdot \hat{\mathbf{n}}$ . Therefore, the flux is continuous across the edges of the control volume  $V_i$ . Furthermore, (2) indicates that the CVFE method is locally conservative.

<sup>\*</sup> Lecturer, Dr., Department of Mathematics, Yadanabon University

<sup>\*\*</sup> Tutor, Dr., Department of Mathematics, Yadanabon University

Given a triangle T with vertices  $m_i, m_j$  and  $m_k$ , edge midpoints  $m_a, m_b$  and  $m_c$ , and centre  $m_g$ , it follows that the approximation  $P_h$  to P on T is given by

$$\mathbf{P}_{\mathbf{h}} = \mathbf{P}_{\mathbf{i}}\boldsymbol{\beta}_{\mathbf{i}} + \mathbf{P}_{\mathbf{j}}\boldsymbol{\beta}_{\mathbf{j}} + \mathbf{P}_{\mathbf{k}}\boldsymbol{\beta}_{\mathbf{k}},\tag{3}$$

where the local basis functions  $\beta_i = \beta_i(x)$  satisfy

$$\beta_{i}(m_{j}) = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases}$$

with

$$\beta_{i}(x) + \beta_{i}(x) + \beta_{k}(x) = 1, \quad x \in T.$$

$$(4)$$

These basis functions are called the **barycentric coordinates** of the triangle T.



Figure 1: Triangle T

Set

$$\begin{aligned} \mathbf{a}_{i} &= \mathbf{m}_{j,2} - \mathbf{m}_{k,2}, \\ \mathbf{b}_{i} &= -(\mathbf{m}_{j,1} - \mathbf{m}_{k,1}), \\ \mathbf{g}_{i} &= \mathbf{m}_{j,1} \, \mathbf{m}_{k,2} - \mathbf{m}_{j,2} \, \mathbf{m}_{k,1} \end{aligned}$$

where  $\mathbf{m}_i = [m_{i,1}, m_{i,2}]^T$  and (i, j, k) is cyclically permuted.

Then the local basis functions  $\beta_i, \beta_j$  and  $\beta_k$  are given by

$$\begin{bmatrix} \beta_{i} \\ \beta_{j} \\ \beta_{k} \end{bmatrix} = \frac{1}{2 \operatorname{meas}(T)} \begin{bmatrix} g_{i} & a_{i} & b_{i} \\ g_{j} & a_{j} & b_{j} \\ g_{k} & a_{k} & b_{k} \end{bmatrix} \begin{bmatrix} 1 \\ x_{1} \\ x_{2} \end{bmatrix},$$
(5)

where meas(T) is the area of the triangle T and  $x = (x_1, x_2) \in T$ . Consequently,

$$\frac{\partial \beta_{\ell}}{\partial x_1} = \frac{a_{\ell}}{2 \operatorname{meas}(T)}, \qquad \frac{\partial \beta_{\ell}}{\partial x_2} = \frac{b_{\ell}}{2 \operatorname{meas}(T)}, \quad \ell = i, j, k. \quad (6)$$

We consider the computation of the left-hand side of (2) on the triangle  $m_a m_g m_c$ ,

$$q_{i} = -\int_{m_{a}m_{g}} (\mathbf{K} \nabla P_{h}) \cdot \hat{\mathbf{n}} \, ds - \int_{m_{g}m_{c}} (\mathbf{K} \nabla P_{h}) \cdot \hat{\mathbf{n}} \, ds \,.$$
(7)

On the edge  $m_a m_g$ ,

$$\hat{\mathbf{n}} = \frac{[\mathbf{m}_{g,2} - \mathbf{m}_{a,2}, \mathbf{m}_{a,1} - \mathbf{m}_{g,1}]^{\mathrm{T}}}{|\mathbf{m}_{a}\mathbf{m}_{g}|}$$

and, on the edge  $m_g m_c$ ,

$$\hat{\mathbf{n}} = \frac{[\mathbf{m}_{c,2} - \mathbf{m}_{g,2}, \mathbf{m}_{g,1} - \mathbf{m}_{c,1}]^{\mathrm{T}}}{|\mathbf{m}_{g}\mathbf{m}_{c}|},$$

where  $|m_a m_g|$  and  $|m_g m_c|$  denote the lengths of edges  $m_a m_g$  and  $m_g m_c$ , respectively. Consequently, if **K** is constant on the triangle T, it follows from (3), (6)-(7), the definition of  $a_i$  and  $b_i$ , and simple algebraic calculations that

$$q_{i} = meas(T) \sum_{\ell=i}^{k} (\mathbf{K} \nabla \beta_{\ell}) \cdot (\mathbf{P}_{\ell} \nabla \beta_{i}), \qquad (8)$$

where  $P_{\ell}$  is the pressure at the vertices of triangles.

Equation in (8) can be recast in the finite difference form, by using (4), as

$$q_{i} = -T_{ij}(P_{j} - P_{i}) - T_{ik}(P_{k} - P_{i}),$$
(9)

where the **transmissibility coefficients**  $T_{ii}$  and  $T_{ik}$  are

 $T_{ij} = -\text{meas}(T)(\mathbf{K}\nabla\beta_j)\cdot\nabla\beta_i, \quad T_{ik} = -\text{meas}(T)(\mathbf{K}\nabla\beta_k)\cdot\nabla\beta_i.$ 

We now consider the assembly of the global transmissibility matrix. Each connection between any two adjacent nodes  $m_i$  and  $m_j$  includes the contributions from two triangles  $T^{(1)}$  and  $T^{(2)}$  that share the common edge with endpoints  $m_i$  and  $m_j$ . The transmissibility between  $m_i$  and  $m_j$ , where at least one of them is not on the external boundary, is

$$\mathbf{T}_{ij} = -\sum_{\ell=1}^{2} \left[ \operatorname{meas}(\mathbf{T}) (\mathbf{K} \nabla \beta_{j}) \cdot \nabla \beta_{i} \right]_{\mathbf{T}^{(\ell)}}.$$
 (10)

Applying (2) and (9), we obtain the linear system on the control volume  $V_i$  in terms of pressure values at the vertices of triangles as

$$-\sum_{j\in N_{i}} T_{ij}(P_{j} - P_{i}) = F_{i}, \qquad (11)$$

where N<sub>i</sub> is the set of all neighbouring nodes of  $m_i$  and  $F_i = \int_{V_i} f(x) dx$ .

If  $\partial V_i$  contains part of the Neumann boundary, then the flux on that part must be given. If it contains part of the Dirichlet boundary, then the pressure on the corresponding part must be given. The third boundary condition can be also incorporated.

#### **1.2 Positive transmissibilities**

The transmissibility coefficient  $T_{ij}$  defined in (10) must be positive. Positive transmissibilities always yield a direction of the discrete flux in the physical direction. Negative transmissibilities are not physically meaningful and generate unsatisfactory solutions.

For simplicity, consider a homogeneous anisotropic medium with  $\mathbf{K} = \text{diag}(a_{11}, a_{22})$ , where  $a_{11}$  and  $a_{22}$  are positive constants. In this case, using (6) and (10),  $T_{ii}$  restricted to each triangle T is

$$T_{ij} = -\frac{a_{11}a_ja_i + a_{22}b_jb_i}{4 \,\text{meas}(T)}$$

Let us introduce a coordinate transform:

$$\mathbf{x}'_1 = \frac{\mathbf{x}_1}{\sqrt{a_{11}}}, \qquad \mathbf{x}'_2 = \frac{\mathbf{x}_2}{\sqrt{a_{22}}}.$$

Under this transform, the area of the transformed triangle T' is

$$\operatorname{meas}(\mathbf{T}') = \frac{\operatorname{meas}(\mathbf{T})}{\sqrt{a_{11}a_{22}}}.$$

Consequently, T<sub>ij</sub> becomes

$$T_{ij} = \sqrt{a_{11}a_{22}} \frac{|m_{k'}m_{j'}| |m_{k'}m_{i'}| \cos \theta_{k'}}{4 \operatorname{meas}(T')} = \sqrt{a_{11}a_{22}} \frac{\cot \theta_{k'}}{2},$$

where  $\theta_{k'}$  is the angle of the triangle T' at node  $m_{k'}$  in the transformed plane. Because each global transmissibility consists of the contributions from two adjacent triangles, the global  $T_{ij}$  between nodes  $m_i$  and  $m_j$  is

$$T_{ij} = \sqrt{a_{11}a_{22}} \ \frac{\cot\theta_{k_1'} + \cot\theta_{k_2'}}{2}, \qquad (12)$$

where  $\theta_{k'_1}$  and  $\theta_{k'_2}$  are the opposite angles of the two triangles. Thus the requirement  $T_{ij} > 0$  is equivalent to

$$\theta_{k_1'} + \theta_{k_2'} < \pi \,. \tag{13}$$

For an edge on the external boundary, the requirement for the angle opposite this edge is

$$\theta_{\mathbf{k}'} < \frac{\pi}{2}.\tag{14}$$

We note that all these angles are measured in the  $(x'_1, x'_2)$ -coordinate plane.

#### **1.3 Upstream weighted CVFEs**

The basic idea of upstream weighting is to choose the value of a property coefficient according to the upstream direction of a flux. The same idea has been used in the upwind finite difference methods. In this section, we consider two upstream weighting strategies for (11).

## (i) Potential-based upstream weighting schemes

Suppose that (1) is of the form

$$-\nabla \cdot (\lambda \mathbf{K} \nabla \mathbf{P}) = \mathbf{f} \qquad \text{in } \Omega, \tag{15}$$

where **K** and  $\lambda$  can be a permeability tensor and a mobility coefficient, respectively. For this problem, a CVFE method analogous to (11) can be derived. If **K** is a scalar a and is different on the two sides of an edge, across that edge it should be approximated by the **harmonic average** 

$$a_{har}(x) = \frac{1}{\frac{1}{2} \left( \frac{1}{a^{+}(x)} + \frac{1}{a^{-}(x)} \right)}$$
$$= \frac{2a^{+}(x)a^{-}(x)}{a^{+}(x) + a^{-}(x)},$$

where  $a^+$  and  $a^-$  indicate the respective values from the two sides. The reason for using a harmonic average is that for an inactive node (i.e., the node where a = 0), this average gives the correct value, in contrast with the arithmetic average. If **K** is a tensor, this harmonic average is used for each component of **K**, and the result is denoted by **K**<sub>har</sub>. For the mobility coefficient  $\lambda$ , in practice, upstream weighting must be used to maintain stability for the CVFE methods. As a result of these two observations, the transmissibility between nodes  $m_i$  and  $m_j$  restricted to each triangle T becomes

$$\mathbf{T}_{ij} = -\operatorname{meas}(\mathbf{T}) \ \tilde{\lambda}_{ij} \ \mathbf{a}_{har} \nabla \beta_i \cdot \nabla \beta_j, \tag{16}$$

where the potential-based upstream weighting scheme is defined by

$$\tilde{\lambda}_{ij} = \begin{cases} \lambda(m_i) & \text{if } P_i > P_j, \\ \\ \lambda(m_j) & \text{if } P_i < P_j. \end{cases}$$
(17)

In fact, it is a pressure-based approach in the current context. The name potential-based is due to the fact that potentials are usually used in place of P in reservoir simulation.

This potential-based upstream weighting scheme is easy to implement. However, it violates the important flux continuity property

across the interfaces between control volumes. To see this, consider the case  $\mathbf{K} = \text{diag}(a_{11}, a_{22})$ , where  $\mathbf{K}$  is a constant diagonal tensor on the triangle T. Applying (6) and (16), the flux on edge  $m_a m_g$  is

$$\begin{split} \mathbf{q}_{i,m_{a}m_{g}} &= -\tilde{\lambda}_{ij} \Bigg( \mathbf{a}_{11}(m_{g,2} - m_{a,2}) \frac{\partial \beta_{j}}{\partial x_{1}} + \mathbf{a}_{22}(m_{a,1} - m_{g,1}) \frac{\partial \beta_{j}}{\partial x_{2}} \Bigg) (\mathbf{P}_{j} - \mathbf{P}_{i}) \\ &- \tilde{\lambda}_{ik} \Bigg( \mathbf{a}_{11}(m_{g,2} - m_{a,2}) \frac{\partial \beta_{k}}{\partial x_{1}} + \mathbf{a}_{22}(m_{a,1} - m_{g,1}) \frac{\partial \beta_{k}}{\partial x_{2}} \Bigg) (\mathbf{P}_{k} - \mathbf{P}_{i}), \end{split}$$

and on edge  $m_g m_c$ 

$$\begin{aligned} \mathbf{q}_{i,\mathbf{m}_{g}\mathbf{m}_{c}} &= -\tilde{\lambda}_{ij} \Bigg( \mathbf{a}_{11}(\mathbf{m}_{c,2} - \mathbf{m}_{g,2}) \frac{\partial \beta_{j}}{\partial x_{1}} + \mathbf{a}_{22}(\mathbf{m}_{g,1} - \mathbf{m}_{c,1}) \frac{\partial \beta_{j}}{\partial x_{2}} \Bigg) (\mathbf{P}_{j} - \mathbf{P}_{i}) \\ &- \tilde{\lambda}_{ik} \Bigg( \mathbf{a}_{11}(\mathbf{m}_{c,2} - \mathbf{m}_{g,2}) \frac{\partial \beta_{k}}{\partial x_{1}} + \mathbf{a}_{22}(\mathbf{m}_{g,1} - \mathbf{m}_{c,1}) \frac{\partial \beta_{k}}{\partial x_{2}} \Bigg) (\mathbf{P}_{k} - \mathbf{P}_{i}). \end{aligned}$$

Similarly, the fluxes on edges  $m_b m_g$  and  $m_g m_a$  at node  $m_j$  are, respectively,

$$q_{j,m_bm_g} = -\tilde{\lambda}_{jk} \left( a_{11}(m_{g,2} - m_{b,2}) \frac{\partial \beta_k}{\partial x_1} + a_{22}(m_{b,1} - m_{g,1}) \frac{\partial \beta_k}{\partial x_2} \right) (P_k - P_j)$$
$$-\tilde{\lambda}_{ji} \left( a_{11}(m_{g,2} - m_{b,2}) \frac{\partial \beta_i}{\partial x_1} + a_{22}(m_{b,1} - m_{g,1}) \frac{\partial \beta_i}{\partial x_2} \right) (P_i - P_j)$$

and

$$\begin{split} \mathbf{q}_{j,\mathbf{m}_{g}\mathbf{m}_{a}} &= -\tilde{\lambda}_{jk} \left( a_{11}(\mathbf{m}_{a,2} - \mathbf{m}_{g,2}) \frac{\partial \beta_{k}}{\partial x_{1}} + a_{22}(\mathbf{m}_{g,1} - \mathbf{m}_{a,1}) \frac{\partial \beta_{k}}{\partial x_{2}} \right) (\mathbf{P}_{k} - \mathbf{P}_{j}) \\ &- \tilde{\lambda}_{ji} \left( a_{11}(\mathbf{m}_{a,2} - \mathbf{m}_{g,2}) \frac{\partial \beta_{i}}{\partial x_{1}} + a_{22}(\mathbf{m}_{g,1} - \mathbf{m}_{a,1}) \frac{\partial \beta_{i}}{\partial x_{2}} \right) (\mathbf{P}_{i} - \mathbf{P}_{j}). \end{split}$$

And the fluxes on edges  $m_c m_g$  and  $m_g m_b$  at node  $m_k$  are, respectively,

$$q_{k,m_{c}m_{g}} = -\tilde{\lambda}_{ki} \left( a_{11}(m_{g,2} - m_{c,2}) \frac{\partial \beta_{i}}{\partial x_{1}} + a_{22}(m_{c,1} - m_{g,1}) \frac{\partial \beta_{i}}{\partial x_{2}} \right) (P_{i} - P_{k})$$
$$-\tilde{\lambda}_{kj} \left( a_{11}(m_{g,2} - m_{c,2}) \frac{\partial \beta_{j}}{\partial x_{1}} + a_{22}(m_{c,1} - m_{g,1}) \frac{\partial \beta_{j}}{\partial x_{2}} \right) (P_{j} - P_{k})$$

and

$$\begin{aligned} q_{k,m_gm_b} &= -\tilde{\lambda}_{ki} \Biggl( a_{11}(m_{b,2} - m_{g,2}) \frac{\partial \beta_i}{\partial x_1} + a_{22}(m_{g,1} - m_{b,1}) \frac{\partial \beta_i}{\partial x_2} \Biggr) (P_i - P_k) \\ &- \tilde{\lambda}_{kj} \Biggl( a_{11}(m_{b,2} - m_{g,2}) \frac{\partial \beta_j}{\partial x_1} + a_{22}(m_{g,1} - m_{b,1}) \frac{\partial \beta_j}{\partial x_2} \Biggr) (P_j - P_k). \end{aligned}$$

For the flux to be continuous across edge  $m_am_g,$  it is required that  $q_{i,m_am_g}+q_{j,m_gm_a}=0\,;\,i.e.,$ 

$$\begin{split} &-\tilde{\lambda}_{ij} \Bigg( a_{11}(m_{g,2}-m_{a,2}) \frac{\partial \beta_j}{\partial x_1} + a_{22}(m_{a,1}-m_{g,1}) \frac{\partial \beta_j}{\partial x_2} \Bigg) (P_j - P_i) \\ &-\tilde{\lambda}_{ik} \Bigg( a_{11}(m_{g,2}-m_{a,2}) \frac{\partial \beta_k}{\partial x_1} + a_{22}(m_{a,1}-m_{g,1}) \frac{\partial \beta_k}{\partial x_2} \Bigg) (P_k - P_i) \\ &-\tilde{\lambda}_{jk} \Bigg( a_{11}(m_{a,2}-m_{g,2}) \frac{\partial \beta_k}{\partial x_1} + a_{22}(m_{g,1}-m_{a,1}) \frac{\partial \beta_k}{\partial x_2} \Bigg) (P_k - P_j) \\ &-\tilde{\lambda}_{ji} \Bigg( a_{11}(m_{a,2}-m_{g,2}) \frac{\partial \beta_i}{\partial x_1} + a_{22}(m_{g,1}-m_{a,1}) \frac{\partial \beta_i}{\partial x_2} \Bigg) (P_i - P_j) = 0 \,. \end{split}$$

Because it must be satisfied for all choices of K, this equation reduces to

$$\begin{split} a_{11}(m_{a,2} - m_{g,2}) \Bigg[ \tilde{\lambda}_{ij} \frac{\partial \beta_j}{\partial x_1} (P_j - P_i) + \tilde{\lambda}_{ji} \frac{\partial \beta_i}{\partial x_1} (P_j - P_i) \\ &+ \tilde{\lambda}_{ik} \frac{\partial \beta_k}{\partial x_1} (P_k - P_i) + \tilde{\lambda}_{jk} \frac{\partial \beta_k}{\partial x_1} (P_j - P_k) \Bigg] = 0 \end{split}$$

and

$$\begin{split} a_{22}(m_{g,l} - m_{a,l}) \Bigg[ \tilde{\lambda}_{ij} \frac{\partial \beta_j}{\partial x_2} (P_j - P_i) + \tilde{\lambda}_{ji} \frac{\partial \beta_i}{\partial x_2} (P_j - P_i) \\ &+ \tilde{\lambda}_{ik} \frac{\partial \beta_k}{\partial x_2} (P_k - P_i) + \tilde{\lambda}_{jk} \frac{\partial \beta_k}{\partial x_2} (P_j - P_k) \Bigg] = 0. \end{split}$$

For these two equations to hold simultaneously for any type of triangle, the only possibility is

$$P_k \ge P_i = P_i$$

In the same manner, we can prove

$$P_i \ge P_j = P_k$$
 and  $P_j \ge P_i = P_k$ .

Hence, for the flux to be continuous across the edges,  $P_i = P_j = P_k$ . That is, the flux is continuous across the edges if and only if the approximate solution  $P_h$  has the same value at all vertices, which is generally not true. Therefore, in general, the potential-based upstream weighted CVFE method generates a discontinuous flux across the edges. On the other hand, the above argument leads to another upstream weighting strategy.

#### (ii) Flux-based upstream weighting schemes

For the flux-based approach, the upstream direction is determined by the sign of a flux. It follows from (7) and (16) that the flux on edge  $m_a m_{\sigma}$  at node  $m_i$  is

$$\mathbf{q}_{i,m_{a}m_{g}} = -\sum_{\ell=i}^{k} \tilde{\lambda} \mathbf{K}_{har} \nabla \lambda_{\ell} \cdot [\mathbf{m}_{g,2} - \mathbf{m}_{a,2}, \mathbf{m}_{a,1} - \mathbf{m}_{g,1}]^{\mathrm{T}} \mathbf{P}_{\ell}$$

and, at node m<sub>i</sub>,

$$q_{j,m_gm_a} = -\sum_{\ell=i}^{k} \tilde{\lambda} \mathbf{K}_{har} \nabla \lambda_{\ell} \cdot [m_{a,2} - m_{g,2}, m_{g,1} - m_{a,1}]^{T} P_{\ell},$$

where the upstream weighting is now defined by

$$\tilde{\lambda} = \begin{cases} \lambda(m_i) & \text{if } q_{i,m_a m_g} > 0, \\ \lambda(m_j) & \text{if } q_{i,m_a m_g} < 0. \end{cases}$$
(18)

From this definition it follows that

$$q_{i,m_am_g} + q_{j,m_gm_a} = 0.$$
 (19)

The fluxes on other edges can be defined in the same fashion. It is evident from (19) that the flux-based upstream weighted CVFE method has a continuous flux across the edges.

# 2 Mixed Finite Element Methods2.1 Finite element spaces on tetrahedra

Let  $T_h$  be a partition of  $\Omega \subset \Box^3$  into tetrahedra such that adjacent elements completely share their common face. In three dimensions,  $P_k$  is now the space of polynomials of degree k in three variables  $x_1, x_2$  and  $x_3$ .



Figure 2: Tetrahedron T<sub>h</sub>

## (i) Raviart-Thomas-Nédélec (RTN) spaces on tetrahedra

These spaces are the three-dimensional analogues of the Raviart-Thomas(RT) spaces on triangles and they are defined for each  $k \ge 0$  by

 $V_{h}(T) = (P_{k}(T))^{3} \oplus ((x_{1}, x_{2}, x_{3})P_{k}(T)), \qquad W_{h}(T) = P_{k}(T),$ where  $(x_{1}, x_{2}, x_{3})P_{k}(T) = (x_{1}P_{k}(T), x_{2}P_{k}(T), x_{3}P_{k}(T)).$  As in

dimensions, for k = 0,  $V_h$  is

 $V_h(T) = \{v \mid v = (a_T + d_T x_1, b_T + d_T x_2, c_T + d_T x_3), a_T, b_T, c_T, d_T \in \Box \}$ , and its dimension is four. The degrees of freedom are the values of normal components of functions at the centroid of each face T.

In general, for  $k \ge 0$ , the dimensions of  $V_h(T)$  and  $W_h(T)$  are

$$\begin{split} & \dim(V_h(T)) \;\; = \;\; \frac{(k+1)(k+2)(k+4)}{2} \,, \\ & \dim(W_h(T)) \;\; = \;\; \frac{(k+1)(k+2)(k+3)}{6} \,. \end{split}$$

two

#### (ii) Brezzi-Douglas-Durán-Fortin(BDDF) spaces on tetrahedra

The BDDF spaces are an extension of the Brezzi-Douglas-Marini(BDM) spaces on triangles to tetrahedra, and they are given for each  $k \ge 1$  by

$$V_h(T) = (P_k(T))^3, \quad W_h(T) = P_{k-1}(T).$$

The dimensions of  $V_h(T)$  and  $W_h(T)$  are

$$\dim(V_{h}(T)) = \frac{(k+1)(k+2)(k+3)}{2},$$
  
$$\dim(W_{h}(T)) = \frac{k(k+1)(k+2)}{6}.$$

## **3** Characteristic Finite Element Methods

In this section, we consider an application of finite element methods to the reaction-diffusion-advection problem:

$$\frac{\partial(\mathbf{\phi}\mathbf{P})}{\partial \mathbf{t}} + \nabla \cdot (\mathbf{P}\mathbf{b} - \mathbf{A}\nabla\mathbf{P}) + \mathbf{R}\mathbf{P} = \mathbf{f}, \qquad (20)$$

for the unknown solution P, where  $\phi$ , **b**, **A**,R and f are given functions. We note that (20) involves advection **b**, diffusion **A**, and reaction R. Many equations arise in this form, e.g., saturation and concentration equations for multiphase, multicomponent flows in porous media.

The modified method of characteristics (MMOC) was independently developed by Douglas and Russel (1982) and Pironneau (1982). It is based on a nondivergence form of (20). In the engineering literature the name Eulerian-Lagrangian method is often used.

#### **3.1** A one-dimensional model problem

For the purpose of introduction, we consider a one-dimensional model problem on the whole real line:

$$\phi(\mathbf{x})\frac{\partial \mathbf{P}}{\partial t} + b(\mathbf{x})\frac{\partial \mathbf{P}}{\partial \mathbf{x}} - \frac{\partial}{\partial \mathbf{x}} \left( \mathbf{a}(\mathbf{x}, t)\frac{\partial \mathbf{P}}{\partial \mathbf{x}} \right) + \mathbf{R}(\mathbf{x}, t)\mathbf{P} = \mathbf{f}(\mathbf{x}, t), \quad \mathbf{x} \in \Box, \ t > 0, \quad (21)$$

$$P(x,0) = P_0(x), \quad x \in \Box$$
 (22)

Set

$$\psi(\mathbf{x}) = \left[ (\phi(\mathbf{x}))^2 + (b(\mathbf{x}))^2 \right]^{\frac{1}{2}}.$$

Assume that

$$\phi(\mathbf{x}) > 0, \quad \mathbf{x} \in \Box \; ,$$

so that  $\psi(x) > 0$ ,  $x \in \Box$ . Let the characteristic direction,  $\phi \frac{\partial P}{\partial t} + b \frac{\partial P}{\partial x}$ ,

associated with the hyperbolic part of (21) be denoted by y, so that

$$\frac{\partial}{\partial y} = \frac{\phi(x)}{\psi(x)} \frac{\partial}{\partial t} + \frac{b(x)}{\psi(x)} \frac{\partial}{\partial x}.$$

Then (21) can be rewritten as

$$\psi(x)\frac{\partial P}{\partial y} - \frac{\partial}{\partial x} \left( a(x,t)\frac{\partial P}{\partial x} \right) + R(x,t)P = f(x,t), \quad x \in \Box, \ t > 0.$$
(23)

We assume that the coefficients a, b, R and  $\phi$  are bounded and satisfy

$$\left| \frac{\mathbf{b}(\mathbf{x})}{\mathbf{\phi}(\mathbf{x})} \right| + \left| \frac{\mathbf{d}}{\mathbf{dx}} \frac{\mathbf{b}(\mathbf{x})}{\mathbf{\phi}(\mathbf{x})} \right| \le \mathbf{C}, \qquad \mathbf{x} \in \Box,$$

where C is a positive constant. We introduce the linear space

$$\mathbf{V} = \mathbf{H}^1(\Box).$$

We recall the scalar product

$$\langle \mathbf{v}, \mathbf{w} \rangle = \int_{\Box} \mathbf{v}(\mathbf{x}) \, \mathbf{w}(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

in  $L^2(\Box)$ . Now, multiplying (23) by any  $v \in V$  and applying integration by parts in space, (23) can be written in the equivalent variational form

$$\left\langle \psi \frac{\partial P}{\partial y}, v \right\rangle + \left\langle a \frac{\partial P}{\partial x}, \frac{dv}{dx} \right\rangle + \left\langle RP, v \right\rangle = \left\langle f, v \right\rangle, \quad v \in V, t > 0, \tag{24}$$

Let  $0 = t^0 < t^1 < \cdots < t^n < \cdots$  be a partition in time, with  $\Delta t^n = t^n - t^{n-1}$ . For a generic function v of time, set  $v^n = v(\cdot, t^n)$ . The characteristic derivative is approximated in the following way. Let

$$\hat{x}^{n} = x - \frac{\Delta t^{n}}{\phi(x)} b(x).$$
(25)

We note that, at  $t = t^n$ ,

$$\psi \frac{\partial P}{\partial y} \approx \psi(x) \frac{P(x,t^{n}) - P(\hat{x}^{n},t^{n-1})}{\left[ (x - \hat{x}^{n})^{2} + (\Delta t^{n})^{2} \right]^{\frac{1}{2}}}$$
$$= \phi(x) \frac{P(x,t^{n}) - P(\hat{x}^{n},t^{n-1})}{\Delta t^{n}}.$$
(26)

That is, a backtracking algorithm is used to approximate the characteristic derivative.  $\hat{x}^n$  is the foot at level  $t^{n-1}$  of the characteristic corresponding to x at the head, at level  $t^n$ .

Let  $V_h$  be a finite element subspace of  $V \cap W^{1,\infty}(\Box)$ . Because we are considering the whole line,  $V_h$  is necessarily infinite-dimensional. In practice, we can assume that the support of  $P_0$  is compact, the portion of the line on which we need to know P is bounded, and P is very small outside that set. Then  $V_h$  can be taken to be finite-dimensional.

The MMOC for (21) is defined as follows:

For  $n = 1, 2, ..., find P_h^n \in V_h$  such that

$$\left\langle \phi \frac{P_{h}^{n} - P_{h}^{n-1}}{\Delta t^{n}}, v \right\rangle + \left\langle a^{n} \frac{dP_{h}^{n}}{dx}, \frac{dv}{dx} \right\rangle + \left\langle R^{n} P_{h}^{n}, v \right\rangle = \left\langle f^{n}, v \right\rangle \text{ for all } v \in V_{h}, \quad (27)$$

where

$$P_{h}^{n-1} = P_{h}(\hat{x}^{n}, t^{n-1}) = P_{h}\left\langle x - \frac{\Delta t^{n}}{\phi(x)}b(x), t^{n-1}\right\rangle.$$
 (28)

The initial approximation  $P_h^0$  can be defined as the interpolant of  $P_0$  in  $V_h$ .

Equation in (27) determines  $\{P_h^n\}$  uniquely in terms of the data  $P_0$ and f. This can be seen as follows. Since (27) is a finite-dimensional system, it suffices to show uniqueness of the solution. Let  $f = P_0 = 0$ , and take  $v = P_h^n$  in (27) to see that

$$\left\langle \phi \frac{\mathbf{P}_{h}^{n} - \mathbf{P}_{h}^{n-1}}{\Delta t^{n}}, \mathbf{P}_{h}^{n} \right\rangle + \left\langle a^{n} \frac{d\mathbf{P}_{h}^{n}}{dx}, \frac{d\mathbf{P}_{h}^{n}}{dx} \right\rangle + \left\langle \mathbf{R}^{n} \mathbf{P}_{h}^{n}, \mathbf{P}_{h}^{n} \right\rangle = 0,$$

with an assumption that  $P_h^{n-1} = 0$ , this equation implies  $P_h^n = 0$ .

It is obvious that the linear system arising from (27) is symmetric positive definite, even in the presence of the advection term.

We end with a remark on a convergence result for (27). Let  $V_h \subset V$  be a finite element space with the following approximation property:

$$\inf_{\mathbf{v}_{h}\in\mathbf{V}_{h}}\left\{ \|\mathbf{v}-\mathbf{v}_{h}\|_{L^{2}(\Box)} + h\|\mathbf{v}-\mathbf{v}_{h}\|_{H^{1}(\Box)} \right\} \leq Ch^{k+1} \|\mathbf{v}\|_{H^{k+1}(\Box)}, \qquad (29)$$

where the constant C > 0 is independent of h, and k > 0 is an integer. Then, under appropriate assumptions on the smoothness of the solution P and a suitable choice of  $P_h^0$  it can be shown that

$$\max_{1 \le n \le N} \left\{ \| P^{n} - P_{h}^{n} \|_{L^{2}(\Box)} + h \| P^{n} - P_{h}^{n} \|_{H^{1}(\Box)} \right\} \le C(P)(h^{k+1} + \Delta t), \quad (30)$$

where N is an integer such that  $t^N = T < \infty$  and [0,T] is the time interval of interest.

#### **3.2 Periodic boundary conditions**

In the previous subsection, (21) was considered on the whole line. For an interval (0,1), the MMOC has a difficulty in handling general boundary conditions. In this case, it is normally developed for periodic boundary conditions

$$P(0,t) = P(1,t), \quad \frac{\partial P}{\partial x}(0,t) = \frac{\partial P}{\partial x}(1,t). \quad (31)$$

In the periodic case, assume that all functions in (21) are spatially (0,1)-periodic. Accordingly, the linear space V is modified to

 $V = \{v \in H^1(0,1) \mid v \text{ is } (0,1) \text{-periodic} \}.$ 

With this modification, the developments in (24) and (27) remain unchanged.

## 3.3 Extension to two- and three-dimensional problems

We now extend the MMOC to (20) defined on a higher-dimensional domain. Let  $\Omega \subset \Box^{d}$  (d = 2 or 3) be a rectangle (respectively, a rectangular parallelepiped), and assume that all functions in (20) are spatially  $\Omega$ -periodic. We write (20) in nondivergence form:

$$\phi(\mathbf{x})\frac{\partial \mathbf{P}}{\partial t} + \mathbf{b}(\mathbf{x},t)\cdot\nabla\mathbf{P} - \nabla\cdot(\mathbf{A}(\mathbf{x},t)\nabla\mathbf{P}) + \mathbf{R}(\mathbf{x},t)\mathbf{P} = \mathbf{f}(\mathbf{x},t), \ \mathbf{x} \in \Omega, \ t > 0, (32)$$
$$\mathbf{P}(\mathbf{x},0) = \mathbf{P}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega.$$
(33)

Set

$$\psi(\mathbf{x},t) = \left[ (\phi(\mathbf{x}))^2 + |\mathbf{b}(\mathbf{x},t)|^2 \right]^{\frac{1}{2}}$$

Assume that

$$\phi(x) > 0, \quad x \in \Omega.$$

Now, if the characteristic direction,  $\oint \frac{\partial \mathbf{P}}{\partial t} + \mathbf{b} \cdot \nabla \mathbf{P}$ , corresponding to the hyperbolic part of (32) is y, then

$$\frac{\partial}{\partial y} = \frac{\phi(x)}{\psi(x,t)} \frac{\partial}{\partial t} + \frac{1}{\psi(x,t)} \mathbf{b}(x,t) \cdot \nabla \mathbf{b$$

With this definition, (32) becomes

$$\psi(x,t)\frac{\partial P}{\partial y} - \nabla \cdot \left(\mathbf{A}(x,t)\nabla P\right) + R(x,t)P = f(x,t), \quad x \in \Omega, \ t > 0, \ (34)$$

We define the linear space

$$V = \{v \in H^1(\Omega) \mid v \text{ is } \Omega \text{-periodic} \}.$$

Recall the notations

$$\langle \mathbf{v}, \mathbf{w} \rangle_{\mathbf{S}} = \int_{\mathbf{S}} \mathbf{v}(\mathbf{x}) \mathbf{w}(\mathbf{x}) d\mathbf{x},$$
  
 $\langle \nabla \mathbf{v}, \nabla \mathbf{w} \rangle_{\mathbf{S}} = \int_{\mathbf{S}} \nabla \mathbf{v}(\mathbf{x}) \cdot \nabla \mathbf{w}(\mathbf{x}) d\mathbf{x}$ 

If  $S = \Omega$ , we omit it in this notation. Now, applying Green's formula in space and the periodic boundary conditions, (34) can be written in the equivalent variational form:

$$\left\langle \psi \frac{\partial \mathbf{P}}{\partial y}, \mathbf{v} \right\rangle + \left\langle \mathbf{A} \nabla \mathbf{P}, \nabla \mathbf{v} \right\rangle + \left\langle \mathbf{R} \mathbf{P}, \mathbf{v} \right\rangle = \left\langle \mathbf{f}, \mathbf{v} \right\rangle, \text{ for all } \mathbf{v} \in \mathbf{V}, \ \mathbf{t} > 0.$$
 (35)

The characteristic is approximated by

$$\hat{\mathbf{x}}^{n} = \mathbf{x} - \frac{\Delta t^{n}}{\phi(x)} \mathbf{b}(x, t^{n}), \qquad (36)$$

where  $\mathbf{x} = (x_1, \dots, x_d)$  and  $\mathbf{x} = [x_1, \dots, x_d]^T$ . Furthermore, we see that, at  $t = t^n$ ,

$$\psi \frac{\partial \mathbf{P}}{\partial \mathbf{y}} \approx \psi(\mathbf{x}, \mathbf{t}^{n}) \frac{\mathbf{P}(\mathbf{x}, \mathbf{t}^{n}) - \mathbf{P}(\hat{\mathbf{x}}^{n}, \mathbf{t}^{n-1})}{\left[ |\mathbf{x} - \hat{\mathbf{x}}^{n}|^{2} + (\Delta \mathbf{t}^{n})^{2} \right]^{\frac{1}{2}}}$$
$$= \phi(\mathbf{x}) \frac{\mathbf{P}(\mathbf{x}, \mathbf{t}^{n}) - \mathbf{P}(\hat{\mathbf{x}}^{n}, \mathbf{t}^{n-1})}{\Delta \mathbf{t}^{n}}.$$
(37)

A backtracking algorithm similar to that employed in one dimension is used to approximate the characteristic derivative.

Let  $V_h \subset V$  be a finite element space associated with a partition  $T_h$  of  $\Omega$ . The MMOC for (32) is given as follows:

For n = 1, 2, ..., find 
$$P_h^n \in V_h$$
 such that  
 $\left\langle \phi \frac{P_h^n - P_h^{n-1}}{\Delta t^n}, v \right\rangle + \left\langle \mathbf{A}^n \nabla P_h^n, \nabla v \right\rangle + \left\langle \mathbf{R}^n P_h^n, v \right\rangle = \left\langle f^n, v \right\rangle$  for all  $v \in V_h$ , (38)

where

$$P_h^{n-1} = P_h(\hat{x}^n, t^{n-1}).$$
 (39)

Existence and uniqueness of a solution for A and R can be shown, and the error estimate (30) under appropriate assumptions on P also holds for (38) provided that an approximation property similar to (24) holds for  $V_h$  in the multiple dimensions.

## **4** Finite Element Methods for One-Phase Flows

We now turn to the three-dimensional one-phase flow equation. We write it in a more general form:

$$c(P)\frac{\partial P}{\partial t} - \nabla \cdot (\mathbf{K}(P)\nabla P) = f(P) \qquad \text{in } \Omega \times (0,T), \qquad (40)$$

$$(\mathbf{K}(\mathbf{P})\nabla\mathbf{P})\cdot\hat{\mathbf{n}} = 0$$
 on  $\Gamma \times (0,T)$ , (41)

$$P(\cdot, 0) = P_0 \qquad \text{in } \Omega, \qquad (42)$$

where P is the pressure, **K** is the absolute permeability tensor,  $\hat{\mathbf{n}}$  is the outward unit normal to the boundary  $\Gamma$  of  $\Omega$ , the function P<sub>0</sub> is given and (0,T) is the time interval of interest.

We assume that (40)-(42) admits a unique solution. Furthermore, we assume that the coefficients c, **K** and f are Lipschitz continuous P.

With  $V = H^{1}(\Omega)$ , (40)-(41) can be written in the variational form:

Find  $P: (0, T) \rightarrow V$  such that

$$\langle \mathbf{c}(\mathbf{P})\frac{\partial \mathbf{P}}{\partial t}, \mathbf{v} \rangle + \langle \mathbf{K}(\mathbf{P})\nabla \mathbf{P}, \nabla \mathbf{v} \rangle = \langle \mathbf{f}(\mathbf{P}), \mathbf{v} \rangle \text{ for all } \mathbf{v} \in \mathbf{V}, \mathbf{t} \in (0, \mathbf{T}).$$
(43)

Let  $V_h$  be a finite element subspace of V. The finite element version of (43) and (42) is as follows:

Find  $P_h: (0,T) \to V_h$  such that

After the introduction of basis functions in  $V_h$ , (44)-(45) can be stated in matrix form as

$$\mathbf{C}(\mathbf{P}) \ \frac{d\mathbf{P}}{dt} + \mathbf{K}(\mathbf{P}) \ \mathbf{P} = \mathbf{f}(\mathbf{P}), \qquad t \in (0, T), \quad (46)$$

$$\mathbf{BP}(0) = \mathbf{P}_0. \tag{47}$$

Under the assumption that the coefficient c(P) is bounded below by a positive constant, this nonlinear system of ordinary differential equations possesses a unique solution. In fact, because of the assumption on c, **A** and f, the solution **P**(t) exists for all t.

#### 4.1 Linearization approaches

Let  $0 = t^0 < t^1 < t^2 < \dots < t^N = T$  be a partition of (0,T), and set  $\Delta t^n = t^n - t^{n-1}$ , or  $n = 1, 2, \dots, N$ . The nonlinear system in (46)-(47) can be

linearized by allowing the nonlinearities to lag one time step behind. Thus the modified backward Euler method for (40)-(42) takes the form:

Find  $P_h^n \in V_h$ , n = 1, 2, ..., N, such that

$$\left\langle c(P_{h}^{n-1}) \frac{P_{h}^{n} - P_{h}^{n-1}}{\Delta t^{n}}, v_{h} \right\rangle + \left\langle \mathbf{K}(P_{h}^{n-1}) \nabla P_{h}^{n}, \nabla v_{h} \right\rangle = \left\langle f(P_{h}^{n-1}), v_{h} \right\rangle$$
 for all  $v_{h} \in V_{h}$ , (48)

$$\left\langle \mathbf{P}_{h}^{0}, \mathbf{v}_{h} \right\rangle = \left\langle \mathbf{P}_{0}, \mathbf{v}_{h} \right\rangle \quad \text{for all } \mathbf{v}_{h} \in \mathbf{V}_{h}.$$
 (49)

In matrix form it is given by

$$\mathbf{C}(\mathbf{P}^{n-1}) \frac{\mathbf{P}^n - \mathbf{P}^{n-1}}{\Delta t} + \mathbf{K}(\mathbf{P}^{n-1}) \mathbf{P}^n = \mathbf{f}(\mathbf{P}^{n-1}),$$
(50)

$$\mathbf{BP}(0) = \mathbf{P}_0. \tag{51}$$

We note that (50)-(51) is a system of linear equations in  $\mathbf{P}^n$ , which can be solved by using iterative algorithms.We may use the Crank-Nicholson discretization method in (48). However, the linearization decreases the order of the time discretization error to  $O(\Delta t)$ . This is true for any higher order time discretization method with the present linearization technique. This drawback can be overcome by using extrapolation techniques in the linearization of the coefficients c, **K** and f. Combined with an appropriate extrapolation, the Crank-Nicholson method can be shown to produce an error of order  $O((\Delta t)^2)$  in time.

#### **4.2 Implicit time approximations**

We now consider a fully implicit time approximation method for (40)-(42):

Find 
$$P_h^n \in V_h$$
,  $n = 1, 2, ..., N$ , such that  
 $\left\langle c(P_h^n) \frac{P_h^n - P_h^{n-1}}{\Delta t^n}, v_h \right\rangle + \left\langle \mathbf{K}(P_h^n) \nabla P_h^n, \nabla v_h \right\rangle = \left\langle f(P_h^n), v_h \right\rangle$ 
for all  $v_h \in V_h$ , (52)

with (49). Its matrix form is

$$\mathbf{C}(\mathbf{P}^{n})\frac{\mathbf{P}^{n}-\mathbf{P}^{n-1}}{\Delta t^{n}}+\mathbf{K}(\mathbf{P}^{n})\mathbf{P}^{n} = \mathbf{f}(\mathbf{P}^{n}).$$
(53)

Now, (53) is a system of nonlinear equations in  $\mathbf{P}^n$ , which must be solved at each time step via an iteration method.

#### **4.3 Explicit time approximations**

We conclude with a remark about the application of a forward explicit time approximation method to (40)-(42):

Find  $P_h^n \in V_h$ , n = 1, 2, ..., N, such that

$$\left\langle c(\mathbf{P}_{h}^{n}) \frac{\mathbf{P}_{h}^{n} - \mathbf{P}_{h}^{n-1}}{\Delta t^{n}}, \mathbf{v}_{h} \right\rangle + \left\langle \mathbf{K}(\mathbf{P}_{h}^{n-1}) \nabla \mathbf{P}_{h}^{n-1}, \nabla \mathbf{v}_{h} \right\rangle = \left\langle f(\mathbf{P}_{h}^{n-1}), \mathbf{v}_{h} \right\rangle$$
 for all  $\mathbf{v}_{h} \in \mathbf{V}_{h}$ , (54)

with (49). In matrix form it is written as

$$\mathbf{C}(\mathbf{P}^{n}) \frac{\mathbf{P}^{n} - \mathbf{P}^{n-1}}{\Delta t} + \mathbf{K}(\mathbf{P}^{n-1}) \mathbf{P}^{n-1} = \mathbf{f}(\mathbf{P}^{n-1}).$$
(55)

We note that the nonlinearity is only in **C**.

For the explicit method in (54) to be stable, a stability condition of the following type must be satisfied:

$$\Delta t^{n} \leq Ch^{2}, \qquad n = 1, 2, \dots, N, \tag{56}$$

where C now depends on c and  $\mathbf{K}$ . Unfortunately, this condition on the time steps is very restrictive for long-time integration.

## **5** Finite Element Methods for Two-Phase Flows

The various discretization methods are now applied to the solution of the differential equations

$$\frac{\partial}{\partial t} (\phi \rho_{w} \mathbf{S}_{w}) = -\nabla \cdot (\rho_{w} \mathbf{u}_{w}) + q_{w}, 
\frac{\partial}{\partial t} (\phi \rho_{o} \mathbf{S}_{o}) = -\nabla \cdot (\rho_{o} \mathbf{u}_{o}) + q_{o},$$
(57)

where  $\phi$  is the porosity of the porous medium;  $S_w$ ,  $\rho_w$ ,  $\mathbf{u}_w$  and  $q_w$  are saturation, density, Darcy's velocity and mass flow rate for wetting phase;  $S_o$ ,  $\rho_o$ ,  $\mathbf{u}_o$  and  $q_o$  are saturation, density, Darcy's velocity and mass flow rate for nonwetting phase;

$$\mathbf{u}_{w} = -\frac{m_{w}}{\mu_{w}} \mathbf{K} (\nabla P_{w} - \rho_{w} g \nabla z),$$

$$\mathbf{u}_{0} = -\frac{m_{o}}{\mu_{o}} \mathbf{K} (\nabla P_{o} - \rho_{o} g \nabla z),$$
(58)

where **K** is the absolute permeability tensor of the porous medium;  $m_w, P_w$ and  $\mu_w$  are the relative permeability, pressure and viscosity for wetting phase;  $m_o, P_o$  and  $\mu_o$  are the relative permeability, pressure and viscosity for nonwetting phase; g is the magnitude of the gravitational acceleration; and z is the depth. Here

$$\mathbf{S}_{\mathrm{w}} + \mathbf{S}_{\mathrm{o}} = 1, \tag{59}$$

$$\mathbf{P}_{\mathrm{c}}(\mathbf{S}_{\mathrm{w}}) = \mathbf{P}_{\mathrm{o}} - \mathbf{P}_{\mathrm{w}},\tag{60}$$

where  $P_c$  is the capillary pressure governing two-phase flows in a porous medium  $\Omega \subset \Box^3$ . The standard finite element methods for one-phase flows can be extended to the present case. Here we discuss the application of the mixed, control volume and characteristic finite element methods to (57)-(60). The first two methods are good choices for the pressure equation.

## 5.1 Mixed finite element methods for two-phase flows

As an example, we present mixed finite element methods for the global formulation. Recall that the pressure equation consists of

$$\nabla \cdot \mathbf{u} = \tilde{q} \tag{61}$$

and

$$\mathbf{u} = -\mathbf{K}(\lambda(\mathbf{S})\nabla \mathbf{P} - (\lambda_{w}\,\rho_{w} + \lambda_{o}\,\rho_{o})\,\mathbf{g}\,\nabla \mathbf{z}),\tag{62}$$

where  $\mathbf{u}$  is the total velocity, in this formulation. The model is completed by specifying boundary and initial conditions. For simplicity, a no-flow boundary conditions used for the pressure equation

$$\mathbf{u}(\mathbf{x},t)\cdot\hat{\mathbf{n}}(\mathbf{x},t) = 0, \qquad \mathbf{x}\in\Gamma, \ t>0.$$
(63)

It follows from (61) and (63) that compatibility of the fluids requires

$$\int\limits_\Omega \widetilde{q}\,dx=0,\qquad t\ge 0\;.$$

Set

$$\begin{split} \mathrm{H}(\mathrm{div},\,\Omega) &= \, \{ \mathbf{v} \in (\mathrm{H}^{1}(\Omega))^{3} \,|\, \mathrm{div}\,\mathbf{v} = 0 \ \mathrm{in} \ \Omega \}, \\ \mathbf{V} &= \, \{ \mathbf{v} \in \mathrm{H}(\mathrm{div},\Omega) \,|\, \mathbf{v} \cdot \hat{\mathbf{n}} = 0 \ \mathrm{on} \ \Gamma \}, \\ \mathrm{W} &= \, L^{2}(\Omega) \,. \end{split}$$

For simplicity, let  $\Omega$  be a convex polygonal domain. For 0 < h < l, let  $T_h$  be a regular partition of  $\Omega$  into elements, say, tetrahedra, with maximum mesh size h. Associated with the partition  $T_h$ , let  $V_h \times W_h \subset V \times W$  represent the mixed finite element spaces. Now, the mixed method for (61)-(62) is as follows:

For 
$$0 \le n \le N$$
, find  $\mathbf{u}_{h}^{n} \in \mathbf{V}_{h}$  and  $P_{h}^{n} \in W_{h}$  such that  
 $\left\langle \nabla \cdot \mathbf{u}_{h}^{n}, \mathbf{w}_{h} \right\rangle = \left\langle \tilde{q}(P_{h}^{n}, S_{h}^{n}), \mathbf{w}_{h} \right\rangle$  for all  $\mathbf{w}_{h} \in W_{h}$ , (64)

$$\left\langle \mathbf{K}\,\lambda(\mathbf{S}_{h}^{n})^{-1}\,\mathbf{u}_{h}^{n},\mathbf{v}_{h}\right\rangle - \left\langle \mathbf{P}_{h}^{n},\nabla\cdot\mathbf{v}_{h}\right\rangle = \left\langle \gamma(\mathbf{S}_{h}^{n}),\mathbf{v}_{h}\right\rangle \text{for all }\mathbf{v}_{h}\in\mathbf{V}_{h},\tag{65}$$

where  $S_h^n$  is an approximation to  $S^n$  and

$$\gamma(\mathbf{S}) = \left( \mathbf{f}_{w}(\mathbf{S}) \, \boldsymbol{\rho}_{w} + \mathbf{f}_{o}(\mathbf{S}) \, \boldsymbol{\rho}_{o} \right) \, \mathbf{g} \, \nabla \mathbf{z}. \tag{66}$$

We note that system in (64)-(65) is nonlinear. The various approaches developed in the preceding section for the standard finite element methods can be applied to it in the same fashion.

## 5.2 CVFE methods

Assume that a partition  $\,T_{h}\,$  of  $\Omega$  consists of a set of control volumes  $V_{i}\!:$ 

$$\overline{\Omega} = \bigcup_{i} \overline{V}_{i}, \quad V_{i} \cap V_{j} = \emptyset, \ i \neq j.$$

On each  $V_i$ , integration of (61) over  $V_i$  and application of the divergence theorem gives

$$\int_{\partial V_i} \mathbf{u} \cdot \hat{\mathbf{n}} \, ds = \int_{V_i} \tilde{q} \, dx \; . \tag{67}$$

Substituting (62) into this equation yields

$$-\int_{\partial V_{i}} \lambda(S) (\mathbf{K} \nabla P) \cdot \hat{\mathbf{n}} \, ds = \int_{V_{i}} \tilde{q} \, dx - \int_{V_{i}} (\lambda_{w}(S) \rho_{w} + \lambda_{o}(S) \rho_{o}) g(\mathbf{K} \nabla z) \cdot \hat{\mathbf{n}} \, ds.$$
(68)

Let  $V_h \subset H^1(\Omega)$  be a finite element space associated with the CVFE partition  $T_h$ . Then the CVFE method for the pressure equation reads:

For 
$$0 \le n \le N$$
, find  $p_h^n \in V_h$  such that  

$$-\int_{\partial V_i} \lambda(S_h^n) (\mathbf{K} \nabla P_h^n) \cdot \hat{\mathbf{n}} \, ds = \int_{V_i} \tilde{q}(P_h^n, S_h^n) \, dx - \int_{V_i} \left( \lambda_w(S_h^n) \, \rho_w + \lambda_o(S_h^n) \, \rho_o \right) g(\mathbf{K} \nabla z) \cdot \hat{\mathbf{n}} \, ds.$$
(69)

The upstream weighting techniques introduced in Subsection 1.3 can be applied to (69).

## **5.3** Characteristic finite element methods

As an example, we present the MMOC described in Section 3 for the saturation. Introduce

$$\tilde{q}_1(\mathbf{P},\mathbf{S}) = \tilde{q}_w(\mathbf{P},\mathbf{S}) - \tilde{q}(\mathbf{P},\mathbf{S})f_w(\mathbf{S}) + \nabla \cdot \big(\mathbf{K} f_w(\mathbf{S}) \lambda_o(\mathbf{S})(\rho_o - \rho_w)g\nabla z\big).$$

Using (61) and

$$\phi \frac{\partial \mathbf{S}}{\partial t} + \nabla \cdot \left( \mathbf{K} f_{w}(\mathbf{S}) \lambda_{o}(\mathbf{S}) \left( \frac{d\mathbf{P}_{c}}{d\mathbf{S}} \nabla \mathbf{S} + (\rho_{o} - \rho_{w}) g \nabla z \right) + f_{w}(\mathbf{S}) \mathbf{u} \right) = \tilde{q}_{w}(\mathbf{P}, \mathbf{S}),$$

the saturation equation becomes

$$\phi \frac{\partial S}{\partial t} + \frac{df_w}{dS} \mathbf{u} \cdot \nabla S + \nabla \cdot \left( \mathbf{K} f_w(S) \lambda_o(S) \frac{dP_c}{dS} \nabla S \right) = q_1(P, S).$$
(70)

Let

$$\mathbf{b}(\mathbf{x}, \mathbf{t}) = \frac{\mathrm{d}\mathbf{f}_{w}}{\mathrm{d}\mathbf{S}} \mathbf{u},$$
  
$$\psi(\mathbf{x}, \mathbf{t}) = \left[ (\phi(\mathbf{x}))^{2} + |\mathbf{b}(\mathbf{x}, \mathbf{t})|^{2} \right]^{\frac{1}{2}},$$

and let the characteristic direction associated with the operator  $\oint \frac{\partial}{\partial t} + \mathbf{b} \cdot \nabla$ 

be denoted by y(x, t), so that

$$\frac{\partial}{\partial y} = \frac{\phi(x)}{\psi(x,t)} \frac{\partial}{\partial t} + \frac{\mathbf{b}(x,t)}{\psi(x,t)} \cdot \nabla.$$

Then (70) reduces to

$$\psi \frac{\partial S}{\partial y} + \nabla \cdot \left( K f_w(S) \lambda_o(S) \frac{dP_c}{dS} \nabla S \right) = q_1(P,S).$$
(71)

We note that the characteristic direction y depends on the velocity **u**. Because the saturation step  $t^{n-1,m}$  relates to pressure steps by  $t^{n-1} < t^{n-1,m} \le t^n$ , we need a velocity approximation for (71) based on  $\mathbf{u}_h^{n-1}$  and earlier values. For this, we utilize a linear extrapolation approach:

If  $n \ge 2$ , take the linear extrapolation of  $\mathbf{u}_h^{n-2}$  and  $\mathbf{u}_h^{n-1}$  determined by

$$\mathbf{E}(\mathbf{u}_{h}^{n-1,m}) = \left(1 + \frac{t^{n-1,m} - t^{n-1}}{t^{n-1} - t^{n-2}}\right) \mathbf{u}_{h}^{n-1} - \frac{t^{n-1,m} - t^{n-1}}{t^{n-1} - t^{n-2}} \mathbf{u}_{h}^{n-2}.$$

For n = 1, define

$$\mathbf{E}(\mathbf{u}_{h}^{0,m})=\mathbf{u}_{h}^{0}.$$

 $\mathbf{E}(\mathbf{u}_{h}^{n-1,m})$  is first order accurate in time in the first pressure step and second order accurate in the later steps.

The MMOC is defined with periodic boundary conditions. For this reason, we assume that  $\Omega$  is a rectangular domain, and all functions in (71) are spatially  $\Omega$ -periodic. Let  $V_h \subset H^1(\Omega)$  be any finite element space. Then an MMOC procedure for (71) is as follows:

For each 
$$0 \le n \le N$$
 and  $1 \le m \le M^{(n)}$ , find  $S_h^{n,m} \in V_h$  such that  
 $\left\langle \phi \frac{S_h^{n,m} - \hat{S}_h^{n,m-1}}{t^{n,m} - t^{n,m-1}}, w_h \right\rangle + \left\langle \mathbf{A}(S_h^{n,m-1}) \nabla s_h^{n,m}, \nabla w_h \right\rangle = \left\langle \tilde{q}_1(P_h^n, S_h^{n,m-1}), w_h \right\rangle,$   
 $w_h \in V_h,$  (72)

where

$$\begin{split} \mathbf{A}(\mathbf{S}) &= -\mathbf{K} \, \mathbf{f}_{w}(\mathbf{S}) \, \lambda_{o}(\mathbf{S}) \, \frac{d\mathbf{P}_{c}}{d\mathbf{S}}, \\ \hat{\mathbf{S}}_{h}^{n,m-1} &= \left. \mathbf{S}_{h}^{n,m-1} \left\langle \mathbf{x} - \frac{d\mathbf{f}_{w}}{d\mathbf{S}} (\mathbf{S}_{h}^{n,m-1}) \frac{\mathbf{E}(\mathbf{u}_{h}^{n,m})}{\phi(\mathbf{x})} \Delta t^{n,m}, t^{n,m-1} \right\rangle, \end{split}$$

with  $\Delta t^{n,m} = t^{n,m} - t^{n,m-1}$ . The initial approximate solution  $S_h^0$  can be defined as any appropriate projection of  $S_0$  in  $V_h$ . For the improved approach, the term  $\left\langle \mathbf{A}(\mathbf{S}_h^{n,m-1}) \nabla \mathbf{S}_h^{n,m}, \nabla \mathbf{w}_h \right\rangle$  in (72) is replaced by  $\left\langle \mathbf{A}(\mathbf{S}_h^{n,m-1}) \nabla \mathbf{S}_h^{n,m-1}, \nabla \mathbf{w}_h \right\rangle$ .

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