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NOTE

Accurate Discretization of Gradients on Non-uniform Curvilinear Staggered Grids

1. INTRODUCTION

Keeping only the pressure term, the equations of incompressible flow are given by the following reduced form of the Navier–Stokes equations, choosing units such that the density $\rho \equiv 1$,

$$\partial \mathbf{u}/\partial t + \nabla p = 0 \tag{1.1}$$

$$\operatorname{div} \mathbf{u} = 0 \tag{1.2}$$

with ∇ the gradient operator. The equation

$$-\operatorname{div}(D \nabla p) = \sigma \tag{1.3}$$

plays an important role in the theory of flow in porous media and closely resembles the pressure equation in the IMPES (implicit pressure, explicit saturation) model in reservoir engineering. Often the domain contains interfaces across which D has large jumps. Therefore (1.3) is called the interface problem. For simplicity, the domain in which (1.1) or (1.2) is to be solved is assumed two-dimensional, but our considerations carry over to three dimensions.

When the domain has a complicated shape it is common to map it onto a rectangle by a boundary-fitted coordinate mapping. In the rectangle a uniform grid is chosen. Its image in the physical plane is a general (curvilinear, non-orthogonal, non-uniform) structured grid. Both in the classical staggered (marker-and-cell) discretization of the incompressible Navier–Stokes equations (proposed in [3] for Cartesian grids) and in so-called block-centered discretizations of (1.3) in reservoir engineering [1], the numerical approximation of p resides in the cell centers, whereas the normal component of $\mathbf{u}$ and ∇p (in the case of (1.1), (1.2)) and $D \nabla p$ are located in the centers of cell faces. In block-centered discretizations of (1.3) the cell-faces are usually placed along interfaces, so that D is not defined there, but $D \nabla p$ is smooth.

In [2] it is shown how in the context of (1.1) and (1.2) straightforward discretizations of ∇p may easily result in $O(1)$ errors on non-uniform grids, even when ∇p is constant, and numerical experiments are performed with four discretizations of ∇p, only one of which is found to be exact experimentally for ∇p constant. Our aim here is to provide a theoretical derivation of the best scheme in [2], providing an extension to (1.3) at the same time.

2. THE REDUCED FORM OF THE NAVIER–STOKES EQUATIONS

Let the boundary-fitted coordinate mapping be given by

$$\mathbf{x} = \mathbf{x}(\boldsymbol{\xi}) \tag{2.1}$$

with $\mathbf{x}$ Cartesian coordinates and $\boldsymbol{\xi}$ general coordinates. The covariant and contravariant base vectors are defined by, respectively,

$$\mathbf{a}_{(\alpha)} = \partial \mathbf{x}/\partial \xi^{\alpha}, \quad \mathbf{a}^{(\alpha)} = \nabla \xi^{\alpha} \tag{2.2}$$

and the Jacobian of the mapping is given by

$$\sqrt{g} = a^1_{(1)} a^2_{(2)} - a^2_{(1)} a^1_{(2)}. \tag{2.3}$$

Note that $\mathbf{a}_{(\alpha)}$ is easily computed from (2.2), whereas $\mathbf{a}^{(\alpha)}$ can be computed from

$$\mathbf{a}^{(\alpha)} \cdot \mathbf{a}_{(\beta)} = \delta^{\alpha}_{\beta}, \tag{2.4}$$

resulting in

$$\sqrt{g}\mathbf{a}^{(1)} = (a^2_{(2)}, -a^1_{(2)})^{\mathrm{T}}, \quad \sqrt{g}\mathbf{a}^{(2)} = (-a^2_{(1)}, a^1_{(1)})^{\mathrm{T}}. \tag{2.5}$$

Instead of using the normal component of $\mathbf{u}$ in cell face centers it is better to use normal mass flux components (as argued in [7, 4]). These are given by

$$V^{\alpha} = \sqrt{g}\mathbf{a}^{(\alpha)} \cdot \mathbf{u}. \tag{2.6}$$

Here $V^1\, d\xi^2$ is the mass flux normal to coordinate lines $\xi^1 =$ constant through a line element of length $|\partial x/\partial \xi^2|\, d\xi^2$, and similarly for $V^2\, d\xi^1$.

Taking the inner product of (1.1) with $\sqrt{g}\mathbf{a}^{(\alpha)}$ gives

$$\partial V^{\alpha}/\partial t + \sqrt{g}\mathbf{a}^{(\alpha)} \cdot \nabla p = 0. \tag{2.7}$$

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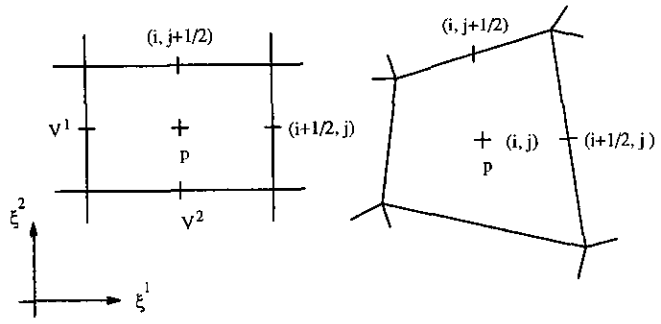

FIG. 2.1. Cell in computational domain G and its image in the physical domain Ω.

Figure 2.1 presents a cell of the staggered grid in physical space and in the computational rectangle.

The sides of the cell are straight in Fig. 2.1, which implies a piecewise bilinear coordinate mapping, but our considerations are independent of the way in which the coordinate mapping is defined in between cell vertices. On the staggered grid we have to compute, for example, $dV^1_{i+1/2,j}/dt$, and we have to discretize the pressure term in (2.7) in the grid point $(i + 1/2, j)$. We want to do this such that the result is exact for constant ∇p on arbitrary non-uniform grids. An elegant way to achieve this is as follows. We can write

$$p\big|_{ij}^{i+1,j} = \int_{ij}^{i+1,j} \nabla p \cdot d\mathbf{x} \cong \nabla p_{i+1/2,j} \cdot \tilde{\mathbf{a}}_{(1)}\, \Delta\xi^1 \tag{2.8}$$

with

$$\tilde{\mathbf{a}}_{(1)} \equiv \frac{1}{\Delta\xi^1} \mathbf{x}\big|_{ij}^{i+1,j}. \tag{2.9}$$

Note that (2.8) is exact for ∇p constant. A second equation expressing ∇p in differences of p is obtained by writing down an equation similar to (2.8), but with a different path-integral. For reasons of symmetry and, hence, low truncation error on smooth grids we choose the average of two paths as

$$\begin{aligned}\frac{1}{4}\{p\big|_{i,j-1}^{i,j+1} + p\big|_{i+1,j-1}^{i+1,j+1}\} &= \frac{1}{4}\left\{\int_{i,j-1}^{i,j+1} + \int_{i+1,j-1}^{i+1,j+1}\right\} \nabla p \cdot d\mathbf{x} \\ &\cong \nabla p_{i+1/2,j} \cdot \tilde{\mathbf{a}}_{(2)}\, \nabla\xi^2\end{aligned} \tag{2.10}$$

with

$$\tilde{\mathbf{a}}_{(2)} \equiv \frac{1}{4\,\Delta\xi^2}\{\mathbf{x}\big|_{i,j-1}^{i,j+1} + \mathbf{x}\big|_{i+1,j-1}^{i+1,j+1}\} \tag{2.11}$$

which is again exact for ∇p constant. Equations (2.8) and (2.10) can be solved for ∇p as follows. In analogy with (2.5) we define

$$\tilde{\mathbf{a}}^{(1)} \equiv (\tilde{a}^2_{(2)}, -\tilde{a}^1_{(2)})^{\mathrm{T}}/\sqrt{\tilde{g}}, \quad \tilde{\mathbf{a}}^{(2)} \equiv (-\tilde{a}^2_{(1)}, \tilde{a}^1_{(1)})^{\mathrm{T}}/\sqrt{\tilde{g}}, \tag{2.12}$$

$$\sqrt{\tilde{g}} \equiv \tilde{a}^1_{(1)}\tilde{a}^2_{(2)} - \tilde{a}^2_{(1)}\tilde{a}^1_{(2)} \tag{2.13}$$

so that $\tilde{\mathbf{a}}^{(\alpha)} \cdot \tilde{\mathbf{a}}_{(\beta)} = \delta^\alpha_\beta$. Inspection shows that the solution is given by

$$\nabla p_{i+1/2,j} \cong \frac{1}{\Delta\xi^1}\tilde{\mathbf{a}}^{(1)} p\big|_{ij}^{i+1,j} + \frac{1}{4\Delta\xi^2}\tilde{\mathbf{a}}^{(2)}\{p\big|_{i,j-1}^{i,j+1} + p\big|_{i+1,j-1}^{i+1,j+1}\}. \tag{2.14}$$

In a similar way an approximation of $\nabla p_{i,j+1/2}$ can be obtained. Substitution of (2.14) in (2.7) gives a discretization which is exact if ∇p = const, regardless of the smoothness of the grid.

Next, we have to determine how to approximate $\sqrt{g}\mathbf{a}^{(\alpha)}$ in (2.6) and (2.7). This follows from the treatment of (1.2). In order to ensure mass conservation, we discretize (1.2) by finite volume integration over a cell. By way of the Gauss divergence theorem we obtain a contour integral consisting of contributions such as

$$\int_{i+1/2,j-1/2}^{i+1/2,j+1/2} \mathbf{u} \cdot (dx^2, -dx^1)^{\mathrm{T}} \cong \{\mathbf{u} \cdot (x^2, -x^1)^{\mathrm{T}}\}\big|_{i+1/2,j-1/2}^{i+1/2,j+1/2} \tag{2.15}$$

which is exact for $\mathbf{u}$ constant (in space), corresponding to ∇p being constant. It is immediately obvious that we have to choose in (2.6) and (2.7)

$$(\sqrt{g}\mathbf{a}^{(1)})_{i+1/2,j} \equiv \sqrt{\hat{g}}\hat{\mathbf{a}}^{(1)} \equiv \frac{1}{\Delta\xi^2}(x^2, -x^1)^{\mathrm{T}}\big|_{i+1/2,j-1/2}^{i+1/2,j+1/2} \tag{2.16}$$

and, similarly,

$$(\sqrt{g}\mathbf{a}^{(2)})_{i,j+1/2} \equiv \sqrt{\hat{g}}\hat{\mathbf{a}}^{(2)} \equiv \frac{1}{\Delta\xi^1}(-x^2, x^1)^{\mathrm{T}}\big|_{i-1/2,j+1/2}^{i+1/2,j+1/2}, \tag{2.17}$$

where the hat symbol serves to distinguish this approximation of $\sqrt{g}\mathbf{a}^{(\alpha)}$ from that in (2.12). The following discretization of (1.2) is obtained:

$$\Delta\xi^2 V^1\big|_{i-1/2,j}^{i+1/2,j} + \Delta\xi^1 V^2\big|_{i,j-1/2}^{i,j+1/2} = 0 \tag{2.18}$$

and we reiterate that V^α is defined by (2.6) with $\sqrt{g}\mathbf{a}^{(\alpha)}$ approximated by (2.16) and (2.17).

In order to solve (1.2) and (2.7) simultaneously an implicit time discretization must be used, because p is in fact a Lagrange multiplier determined by the constraint (2.7) or by the constraint (2.18) in the discrete case. Employing the backward Euler method the discrete system becomes

$$V^{1,n+1}_{i+1/2,j} = V^{1,n}_{i+1/2,j} - \Delta t(\sqrt{g}\mathbf{a}^{(1)} \cdot \nabla p)_{i+1/2,j} \tag{2.16}$$

$$V^{2,n+1}_{i,j+1/2} = V^{2,n}_{i,j+1/2} - \Delta t(\sqrt{g}\mathbf{a}^{(2)} \cdot \nabla p)_{i,j+1/2} \tag{2.17}$$

$$\Delta\xi^2 V^{1,n+1}\big|_{i-1/2,j}^{i+1/2,j} + \Delta\xi^1 V^{2,n+1}\big|_{i,j-1/2}^{i,j+1/2} = 0. \tag{2.18}$$

We may regard $V^{\alpha,n+1}$ as the projection of $V^{\alpha,n}$ on the space of solenoidal vector fields, where solenoidal is defined in the discrete sense by (2.18). This is the point of view taken in [2], where four discretization methods to perform this projection are tested. Our discretization is identical to the discretization which is found to be best on the basis of numerical experiments in [2]. Thus we have given a theoretical justification of this method, proving that it is exact for ∇p constant on arbitrary grids.

The projection on the space of solenoidal vector fields (of which (2.16)–(2.18) is a superior numerical implementation [2]) is the basis of the pressure-correction method for solving the instationary incompressible Navier–Stokes equations. However, use of this method is not mandatory. An alternative is, for example, Vanka's method [5]. Also in this case the discretization of ∇p needs to be accurate, which is therefore a more fundamental issue than the accuracy of projection on the space of solenoidal vector fields. Generalization to three dimensions is straightforward.

3. THE INTERFACE PROBLEM

A similar approach may be taken to discretize the interface problem (1.3) on the block-centered grid of Fig. 2.1, such that the discretization is exact for $D\ \nabla p$ constant on arbitrary grids, if D is piecewise constant. Discontinuities of D are allowed only on interfaces.

Integration of (1.3) over a cell in a finite volume discretization procedure leads via the Gauss divergence theorem to integrals over cell faces, such as

$$\int_{i+1/2,j-1/2}^{i+1/2,j+1/2} D\ \nabla p \cdot d\mathbf{s} \cong (D\ \nabla p)_{i+1/2,j} \cdot \int_{i+1/2,j-1/2}^{i+1/2,j+1/2} d\mathbf{s} \tag{3.1}$$

where $d\mathbf{s}$ is normal to the face in the outward direction and has length equal to a line-increment along the face. The approximation in (3.1) is exact for $D\ \nabla p$ constant. We have

$$\int_{i+1/2,j-1/2}^{i+1/2,j+1/2} D\ \nabla p \cdot (dx^2, -dx^1)^{\mathrm{T}} \cong (D\ \nabla p)_{i+1/2,j} \cdot \sqrt{\hat{g}}\hat{\mathbf{a}}^{(1)}\,\Delta\xi^2 \tag{3.2}$$

(cf. (2.15) and (2.16)), which is exact for $D\ \nabla p$ constant. In order to approximate $D\ \nabla p$ in terms of grid values for p we follow a procedure quite similar to that for ∇p in Section 2 and write, exploiting the smoothness of $D\ \nabla p$,

$$p\big|_{ij}^{i+1,j} = \int_{ij}^{i+1,j} \frac{1}{D} D\ \nabla p \cdot d\mathbf{x} \cong (D\ \nabla p)_{i+1/2,j} \cdot \mathbf{b}_{(1)} \tag{3.3}$$

with

$$\mathbf{b}_{(1)} \equiv \int_{ij}^{i+1,j} \frac{1}{D}\, d\mathbf{x}. \tag{3.4}$$

This is exact for $D\ \nabla p$ constant. Assuming D to be constant in each cell we have exactly

$$\mathbf{b}_{(1)} = \{(\mathbf{a}_{(1)}^*/D)_{ij} + (\mathbf{a}_{(1)}^*/D)_{i+1,j}\}\,\Delta\xi^1/2 \tag{3.5}$$

and, assuming the mapping $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi})$ to be bilinear,

$$\mathbf{a}_{(1)ij}^* \equiv \frac{1}{2\,\Delta\xi^1}\{\mathbf{x}\big|_{i-1/2,j+1/2}^{i+1/2,j+1/2} + \mathbf{x}\big|_{i-1/2,j-1/2}^{i+1/2,j-1/2}\}. \tag{3.6}$$

In order to obtain a second equation for $(D\ \nabla p)_{i+1/2,j}$ we choose the average of the same two paths as for ∇p, for the same reasons, plus the fact that this gives us the standard discretization in the Cartesian case $\mathbf{x} = \boldsymbol{\xi}$. We write, omitting some details which should be clear from the foregoing,

$$p\big|_{i,j-1}^{i,j+1} + p\big|_{i+1,j-1}^{i+1,j+1} \cong (D\ \nabla p)_{i+1/2,j} \cdot \mathbf{b}_{(2)} \tag{3.7}$$

with

$$\begin{aligned}\mathbf{b}_{(2)} = {} & \frac{1}{D_{i,j-1}}\mathbf{x}\big|_{i,j-1}^{i,j-1/2} + \frac{1}{D_{ij}}\mathbf{x}\big|_{i,j-1/2}^{i,j+1/2} + \frac{1}{D_{i,j+1}}\mathbf{x}\big|_{i,j+1/2}^{i,j+1} \\ & + \frac{1}{D_{i+1,j-1}}\mathbf{x}\big|_{i+1,j-1}^{i+1,j-1/2} + \frac{1}{D_{i+1,j}}\mathbf{x}\big|_{i+1,j-1/2}^{i+1,j+1/2} \\ & + \frac{1}{D_{i+1,j+1}}\mathbf{x}\big|_{i+1,j+1/2}^{i+1,j+1}.\end{aligned} \tag{3.8}$$

Defining

$$\begin{aligned}&\mathbf{b}^{(1)} \equiv (b_{(2)}^2, -b_{(2)}^1)^{\mathrm{T}}/B, \quad \mathbf{b}^{(2)} \equiv (-b_{(1)}^2, b_{(1)}^1)^{\mathrm{T}}/B, \\ &B = b_{(1)}^1 b_{(2)}^2 - B_{(1)}^2 b_{(2)}^1,\end{aligned} \tag{3.9}$$

we have $\mathbf{b}^{(\alpha)} \cdot \mathbf{b}_{(\beta)} = \delta_\beta^\alpha$, and the solution of (3.3) and (3.7) is found to be

$$(D\ \nabla p)_{i+1/2,j} \cong \mathbf{b}^{(1)} p\big|_{ij}^{i+1,j} + \mathbf{b}^{(2)}\{p\big|_{i,j-1}^{i,j+1} + p\big|_{i+1,j-1}^{i+1,j+1}\}. \tag{3.10}$$

The treatment of $(D\ \nabla p)_{i,j+1/2}$ is similar. Extension to three dimensions is straightforward, but somewhat laborious. In the Cartesian case $\mathbf{x} = \boldsymbol{\xi}$ the well-known stencil is obtained,

$$\begin{bmatrix} & -w_{i,j+1/2} & \\ -w_{i-1/2,j} & \Sigma & -w_{i+1/2,j} \\ & -w_{i,j-1/2} & \end{bmatrix}, \tag{3.11}$$

where Σ is the negative sum of the surrounding coefficients and $w_{i+1/2,j}$ the harmonic average of the neighbouring diffusion coefficients:

$$w_{i+1/2,j} = 1 \Big/ \left(\frac{1}{2D_{ij}} + \frac{1}{2D_{i+1,j}} \right). \tag{3.12}$$

The formula for $w_{i,j+1/2}$ is analogous. A derivation of (3.12) from first principles may be found, for example, in [6, Section 3.3].

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