ASPECTS OF NON-SMOOTHNESS IN FLOW COMPUTATIONS

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We discuss some numerical consequences of non-smoothness of the pressure gradient in the incompressible Navier-Stokes equations in general coordinates, and non-smoothness of grid and diffusion coefficient for interface problems.

DISCRETIZATION OF GRADIENTS ON NON-SMOOTH BOUNDARY-FITTED GRIDS

An example where non-smoothness requires special measures in flow computations is the following. Suppose one wishes to solve the incompressible Navier-Stokes equations in general curvilinear boundary-fitted coordinates on a staggered grid, generalizing the classical "marker and cell" method [7] from Cartesian to general coordinates. Let $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi})$ be the coordinate mapping, with $\mathbf{x}$ Cartesian coordinates in the two-dimensional domain Ω and $\boldsymbol{\xi} \in G = (0, 1) \times (0, 1)$. G is divided uniformly into cells. The mapping is generated numerically; $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi})$ is given in cell vertices and extended by bilinear interpolation. The situation is sketched in figure 1.

Figure 1: Cell in computational domain G and its image in the physical domain Ω

The discrete unknowns are the pressure p , located in cell centers, and the normal mass fluxes V^1, V^2 located in cell face centers. In order to obtain a discretization, in general coordinates, the tensor formulation of the Navier-Stokes equations may be discretized on the grid in G . This is done in [11], [21], [13], [23], [16], [15], [14], [12] for example. Here we will consider the discretization of the pressure gradient. Omitting all other terms, the momentum equation in general coordinates becomes, using the summation convention,

$$\frac{\partial V^\alpha}{\partial t} + \frac{\partial \sqrt{g} g^{\alpha\beta} p}{\partial \xi^\beta} + \sqrt{g} \{ \begin{smallmatrix} \alpha \\ \beta\gamma \end{smallmatrix} \} g^{\beta\gamma} p = 0 \quad (1)$$

where

$$\begin{aligned} V^\alpha &= \sqrt{g} \mathbf{a}^{(\alpha)} \cdot \mathbf{u}, & g^{\alpha\beta} &= \mathbf{a}^{(\alpha)} \cdot \mathbf{a}^{(\beta)}, & \sqrt{g} &= a_{(1)}^1 a_{(2)}^2 - a_{(1)}^2 a_{(2)}^1, \\ \{ \begin{smallmatrix} \alpha \\ \beta\gamma \end{smallmatrix} \} &= \mathbf{a}^{(\alpha)} \cdot \frac{\partial \mathbf{a}_{(\beta)}}{\partial \xi^\gamma} \end{aligned} \quad (2)$$

and

$$\mathbf{a}^{(\alpha)} = \nabla \xi^\alpha, \quad \mathbf{a}_{(\alpha)} = \partial \mathbf{x} / \partial \xi^\alpha \quad (3)$$

A straightforward way to discretise (1) is to compute $\alpha_{(\alpha)}$ by finite differences, $\mathbf{a}^{(\alpha)}$ from $\mathbf{a}^{(\alpha)} \cdot \mathbf{a}_{(\beta)} = \delta_\beta^\alpha$ and taking finite differences in (1). However, the resulting discretization is not exact if the gradient $\nabla p = 0$. The underlying reason is discontinuities in the quantities defined in (2) across cell boundaries. As a result large errors may result on non-uniform grids, as in the case of the isobar pattern shown in figure 2(b).

A systematic way to obtain a coordinate-invariant discretization which is exact for $\nabla p = 0$ on arbitrary (structured) grids is as follows. In vector notation we have

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla p = 0 \quad (4)$$

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

$$\frac{\partial V^\alpha}{\partial t} + \sqrt{g} \mathbf{a}^{(\alpha)} \cdot \nabla p = 0 \quad (5)$$

Instead of writing this in a tensor form such as (1) we proceed as follows. On the staggered grid of figure 1 we have to compute, for example, $dV_{i+1/2,j}^1/dt$. We have

$$\sqrt{g} \mathbf{a}^{(1)} = (a_{(2)}^2, -a_{(2)}^1)^T \quad (6)$$

which can be evaluated exactly in $(i + 1/2, j)$. Furthermore, we may write

$$p|_{ij}^{i+1,j} = \int_{ij}^{i+1,j} \nabla p \cdot d\mathbf{x} \cong \nabla p_{i+1/2,j} \cdot \tilde{\mathbf{a}}_{(1)} \Delta \xi^1 \quad (7)$$

Figure 2: Poiseuille flow; (a): the grid; (b): wrong isobars; (c): correct isobars.

$$\frac{1}{4} \{p|_{i,j-1}^{i,j+1} + p|_{i+1,j-1}^{i+1,j+1}\} = \frac{1}{4} \left\{ \int_{i,j-1}^{i,j+1} + \int_{i+1,j-1}^{i+1,j+1} \right\} \Delta p \cdot d\mathbf{x} \cong \nabla p_{i+1/2,j} \cdot \tilde{\mathbf{a}}_{(2)} \Delta \xi^2 \quad (8)$$

where

$$\tilde{\mathbf{a}}_{(1)} \equiv \mathbf{a}_{(1)i+1/2,j} \equiv \frac{1}{\Delta \xi^1} \mathbf{x}|_{ij}^{i+1,j} \quad (9)$$

$$\tilde{\mathbf{a}}_{(2)} \equiv \mathbf{a}_{(2)i+1/2,j} \equiv \frac{1}{4\Delta \xi^2} \{ \mathbf{x}|_{i,j-1}^{i,j+1} + \mathbf{x}|_{i+1,j-1}^{i+1,j+1} \} \quad (10)$$

Note that (7) and (8) are exact for ∇p constant. We can solve for ∇p from (7) and (8) as follows. Define

$$\tilde{\mathbf{a}}^{(1)} \equiv \mathbf{a}_{i+1/2,j}^{(1)} \equiv (\tilde{a}_{(2)}^2, -\tilde{a}_{(2)}^1)^T / \sqrt{\tilde{g}} \quad (11)$$

$$\tilde{\mathbf{a}}^{(2)} \equiv \mathbf{a}_{i+1/2,j}^{(2)} \equiv (-\tilde{a}_{(1)}^2, \tilde{a}_{(1)}^1)^T / \sqrt{\tilde{g}} \quad (12)$$

$$\sqrt{\tilde{g}} \equiv \sqrt{g}_{i+1/2,j} \equiv \tilde{a}_{(1)}^1 \tilde{a}_{(2)}^2 - \tilde{a}_{(1)}^2 \tilde{a}_{(2)}^1 \quad (13)$$

Then $\tilde{\mathbf{a}}^{(\alpha)} \cdot \tilde{\mathbf{a}}_{(\beta)} = \delta_{\beta}^{\alpha}$, and the solution of (7), (8) can be written as

$$\nabla p_{i+1/2,j} \cong \frac{1}{\Delta \xi^1} \tilde{\mathbf{a}}^{(1)} p|_{ij}^{i+1,j} + \frac{1}{4\Delta \xi^2} \tilde{\mathbf{a}}^{(2)} \{p|_{i,j-1}^{i,j+1} + p|_{i+1,j-1}^{i+1,j+1}\} \quad (14)$$

In a similar way an approximation to $\nabla p_{i,j+1/2}$ can be obtained. Substitution of (6) and (14) in (5) gives a spatial discretization which is exact if $\nabla p = \text{constant}$, regardless of the smoothness of the grid, and which results in the correct isobars of

figure 2. Generalization to three dimensions is straightforward.

DISCRETIZATION OF AN INTERFACE PROBLEM

Consider the following equation:

$$- \operatorname{div} (D \nabla \varphi) = \sigma \quad (15)$$

This equation 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. When this is the case we call (15) an interface problem.

Suppose the domain has a complicated shape, and (15) is solved with a boundary-fitted grid, such as shown in figure 1. We assume that φ is located in cell-centers, and that interfaces consist only of cell-faces. Integration of (15) over a cell in a finite volume discretization procedure leads to integrals over cell faces, such as

$$\int_{i+1/2, j-1/2}^{i+1/2, j+1/2} D \nabla \varphi ds \cong (D \nabla \varphi) \cdot (\sqrt{g} \mathbf{a}^{(1)})_{i+1/2, j} \Delta \xi^2 \quad (16)$$

with $\sqrt{g} \mathbf{a}^{(1)}$ given by (6). This is exact for $D \nabla \varphi = \text{constant}$. Everything hinges on the approximation of $(D \nabla \varphi)_{i+1/2, j}$. The fact that D may be discontinuous at $(i + 1/2, j)$ has to be taken into account, and we would like to obtain zero error for $D \nabla \varphi$ constant on non-smooth grids. This may be achieved in a way quite similar to what we just did for the pressure term in the Navier-Stokes equations.

Assuming D to be constant in each cell, we may write

$$\varphi|_{ij}^{i+1, j} = \int_{ij}^{i+1, j} \nabla \varphi \cdot d\mathbf{x} \cong (D \nabla \varphi)_{i+1/2, j} \cdot \int_{ij}^{i+1, j} \frac{1}{D} d\mathbf{x} \quad (17)$$

which is obviously exact for $D \nabla \varphi$ constant. We have, exactly for D piecewise constant and the mapping $\mathbf{x} = \mathbf{x}(\xi)$ piecewise bilinear,

$$\mathbf{b}_{(1)} \equiv \int_{ij}^{i+1, j} \frac{1}{D} d\mathbf{x} = \{ \mathbf{a}_{(1)}/D \}_{ij} + \{ \mathbf{a}_{(1)}/D \}_{i+1, j} \frac{\Delta \xi^1}{2} \quad (18)$$

Next, we choose the following two integration paths:

$$\begin{aligned} C1 : & (i+1, j-1) \rightarrow (i+1, j) \rightarrow (i-1, j) \rightarrow (i-1, j+1) \\ C2 : & (i-1, j-1) \rightarrow (i-1, j) \rightarrow (i+1, j) \rightarrow (i+1, j+1) \end{aligned} \quad (19)$$

Adding the integrals of $\nabla\varphi$ over C_1 and C_2 gives

$$\frac{1}{4}\{\varphi|_{i,j-1}^{i,j+1} + \varphi|_{i+1,j-1}^{i+1,j+1}\} \cong (D\nabla\varphi)_{i+1/2,j} \cdot \mathbf{b}_{(2)} \quad (20)$$

with

$$\mathbf{b}_{(2)} = \frac{1}{4}\left\{\int_{C_1} + \int_{C_2}\right\} \frac{1}{D} d\mathbf{x} \quad (21)$$

We have for piecewise constant D

$$\begin{aligned} \mathbf{b}_{(2)} &= \frac{1}{D_{i,j-1}}(\mathbf{x}_{i,j-1/2} - \mathbf{x}_{i,j-1}) + \frac{1}{D_{ij}}(\mathbf{x}_{i,j+1/2} - \mathbf{x}_{i,j-1/2}) \\ &+ \frac{1}{D_{i,j+1}}(\mathbf{x}_{i,j+1} - \mathbf{x}_{i,j-1/2}) + \frac{1}{D_{i+1,j-1}}(\mathbf{x}_{i+1,j-1/2} - \mathbf{x}_{i+1,j-1}) \\ &+ \frac{1}{D_{i+1,j}}(\mathbf{x}_{i+1,j+1/2} - \mathbf{x}_{i+1,j-1/2}) + \frac{1}{D_{i+1,j+1}}(\mathbf{x}_{i+1,j+1} - \mathbf{x}_{i+1,j-1/2}) \end{aligned} \quad (22)$$

Defining

$$\begin{aligned} \mathbf{b}^{(1)} &\equiv (b_{(2)}^2, -b_{(2)}^1)^T / B, \quad \mathbf{b}^2 \equiv (-b_{(1)}^2, b_{(1)}^1)^T / B \\ B &\equiv b_{(1)}^1 b_{(2)}^2 - b_{(1)}^2 b_{(2)}^1 \end{aligned} \quad (23)$$

we find the solution of (17) and (21) to be

$$(D\nabla\varphi)_{i+1/2,j} = \mathbf{b}^{(1)}\varphi|_{ij}^{i+1,j} + \mathbf{b}^{(2)}\{\varphi|_{i,j-1}^{i,j+1} + \varphi|_{i+1,j-1}^{i+1,j+1}\} \quad (24)$$

The treatment of $(D\nabla\varphi)_{i,j+1/2}$ is similar. Extension to three dimensions is straightforward, but somewhat laborious.

MULTIGRID FOR INTERFACE PROBLEMS

Next, we consider the solution of the discrete system obtained by discretization of the interface problem by multigrid methods. Because only this case has been considered in the literature, and because the principles involved can also be discussed in the context of this case, we consider the Cartesian case only, i.e. $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi})$. The remaining non-smoothness is that of D ; this has consequences for the application of multigrid, which we will discuss.

Let us consider finite volume discretization on the fine grid of figure 3. The grid is uniform with mesh-size h in both directions. The resulting finite volume discretization is called cell-centered or block-centered. Domain boundaries are located at cell faces. The discretization discussed before leads to the following stencil for the discretization matrix A :

$$[A] = \begin{bmatrix} & -w_{i,j+1/2} & \\ -w_{i-1/2,j} & \Sigma & -w_{i+1/2,j} \\ & -w_{i,j-1/2} & \end{bmatrix} \quad (25)$$

Figure 3: Fine and coarse grid for cell-centered multigrid

where

$$w_{i+1/2,j} = 1 / \left(\frac{1}{2D_{ij}} + \frac{1}{2D_{i+1,j}} \right) \quad (26)$$

and a similar formula for $w_{i,j+1/2}$; Σ is the negative sum of the surrounding coefficients. A derivation of (26) from first principles may be found, for example, in [22].

When using multigrid to efficiently solve the resulting system of equations, it is natural to use cell centered multigrid, in which coarse grids are constructed by taking unions of fine grid cells, as illustrated in figure 3. The alternative, more widely used, is vertex-centered multigrid, in which coarse grids are constructed by deleting grid points where the numerical approximation is defined. This is more natural than cell-centered multigrid for vertex-centered discretizations, and is illustrated in figure 4. For interface problems, there is a huge difference between cell-centered and vertex-centered multigrid. In the cell-centered case, standard multigrid works with the usual interpolatory transfer operators between the grids. Some theoretical backing of this is given in [20]; details and numerical experiments may be found in [19], [9] and [10]. In the vertex-centered case, however, standard multigrid does not work. As explained in [1] and [8], the transfer operators have to be chosen in a more complicated way, in dependence on $[A]$, at a price of extra computing time and memory. This approach has been further developed in [6], [2], [3], [4] and [5]. The cell-centered approach has been further developed in [17] and [18]. Both approaches can be made to work efficiently with $O(N)$ complexity.

The reason why standard vertex-centered multigrid does not work for interface problems is that $\text{grad } \varphi$ is discontinuous where D is discontinuous, so that prolongation by linear interpolation is inaccurate. In the cell-centered case prolongation may be done by piecewise constant interpolation, which does not suffer from discontinuities

Figure 4: Fine and coarse grid for vertex-centered multigrid

in $\text{grad } \varphi$.

References

- [1] R.E. Alcouffe, A. Brandt, J.E. Dendy Jr., and J.W. Painter. The multigrid method for diffusion equations with strongly discontinuous coefficients. *SIAM J. Sci. Stat. Comp.*, 2:430-454, 1981.
- [2] J.E. Dendy Jr. Black box multigrid. *J. Comp. Phys.*, 48:366-386, 1982.
- [3] J.E. Dendy Jr. Black box multigrid for nonsymmetric problems. *Appl. Math. Comp.*, 13:261-284, 1983.
- [4] J.E. Dendy Jr. Black box multigrid for systems. *Appl. Math. Comp.*, 19:57-74, 1986.
- [5] J.E. Dendy Jr. Two multigrid methods for three-dimensional problems with discontinuous and anisotropic coefficients. *SIAM J. Sci. Stat. Comp.*, 8:673-685, 1987.
- [6] J.E. Dendy, Jr. and J.M. Hyman. Multi-grid and ICCG for problems with interfaces. In M.H. Schultz, editor, *Elliptic problem solvers*, pages 247-253, New York, 1981. Academic Press.
- [7] F.H. Harlow and J.E. Welch. Numerical calculation of time-dependent viscous incompressible flow of fluid with a free surface. *The Physics of Fluids*, 8:2182-2189, 1965.

- [8] R. Kettler and J.A. Meijerink. A multigrid method and a combined multigrid-conjugate gradient method for elliptic problems with strongly discontinuous coefficients in general domains. Technical Report Shell Publ. 604, KSEPL, Rijswijk, The Netherlands, 1981.
- [9] M. Khalil. *Analysis of Linear Multigrid Methods for Elliptic Differential Equations with Discontinuous and Anisotropic Coefficients*. PhD thesis, Delft University of Technology, Delft, The Netherlands, 1989.
- [10] M. Khalil and P. Wesseling. Vertex-centered and cell-centered multigrid for interface problems. *J. Comp. Phys.*, 98:1–10, 1992.
- [11] A.E. Mynett, P. Wesseling, A. Segal, and C.G.M. Kassels. The ISNaS incompressible Navier-Stokes solver: invariant discretization. *Applied Scientific Research*, 48:175–191, 1991.
- [12] C.W. Oosterlee. *Robust multigrid methods for the steady and unsteady incompressible Navier-Stokes equations in general coordinates*. PhD thesis, Delft University of Technology, The Netherlands, 1993.
- [13] C.W. Oosterlee and P. Wesseling. A multigrid method for an invariant formulation of the incompressible Navier-Stokes equations in general co-ordinates. *Communications in Applied Numerical Methods*, 8:721–734, 1992.
- [14] C.W. Oosterlee and P. Wesseling. A robust multigrid method for a discretization of the incompressible Navier-Stokes equations in general coordinates. *Impact Comp. Science Engng.*, 5:128–151, 1993.
- [15] C.W. Oosterlee, P. Wesseling, A. Segal, and E. Brakkee. Benchmark solutions for the incompressible Navier-Stokes equations in general co-ordinates on staggered grids. *Int. J. Num. Meth. Fluids*, 17:301–321, 1993.
- [16] A. Segal, P. Wesseling, J. Van Kan, C.W. Oosterlee, and C.G.M. Kassels. Invariant discretization of the incompressible Navier-Stokes equations in boundary fitted co-ordinates. *Int. J. Num. Meth. Fluids*, 15:411–426, 1992.
- [17] G.J. Shaw and P.I. Crumpton. Discretization and multigrid solution of elliptic equations with strongly discontinuous coefficients. Report 92/16, Oxford University Computing Laboratory, 1992.
- [18] R. Teigland and B.G. Ersland. Comparison of two cell-centered multigrid schemes for problems with discontinuous coefficients. IBM Report 91/6, Bergen Scientific Centre, 1991. ISBN 82-415-0081-5.
- [19] P. Wesseling. Cell-centered multigrid for interface problems. *J. Comp. Phys.*, 79:85–91, 1988.

- [20] P. Wesseling. Two remarks on multigrid methods. In W. Hackbusch, editor, *Robust multi-grid methods*, pages 209–216, Braunschweig, 1988. Vieweg. Notes on Numerical Fluid Mechanics 23.
- [21] P. Wesseling. Large scale modeling in computational fluid dynamics. In E.F. Deprettere and A.-J. van der Veen, editors, *Algorithms and parallel VLSI architectures, Volume A: Tutorials*, pages 277–308, Amsterdam, 1991. Elsevier.
- [22] P. Wesseling. *An introduction to multigrid methods*. John Wiley & Sons, Chichester, 1992.
- [23] P. Wesseling, A. Segal, J.J.I.M. van Kan, C.W. Oosterlee, and C.G.M. Kassels. Finite volume discretization of the incompressible Navier-Stokes equations in general coordinates on staggered grids. *Comp. Fluid Dynamics Journal*, 1:27–33, 1992.