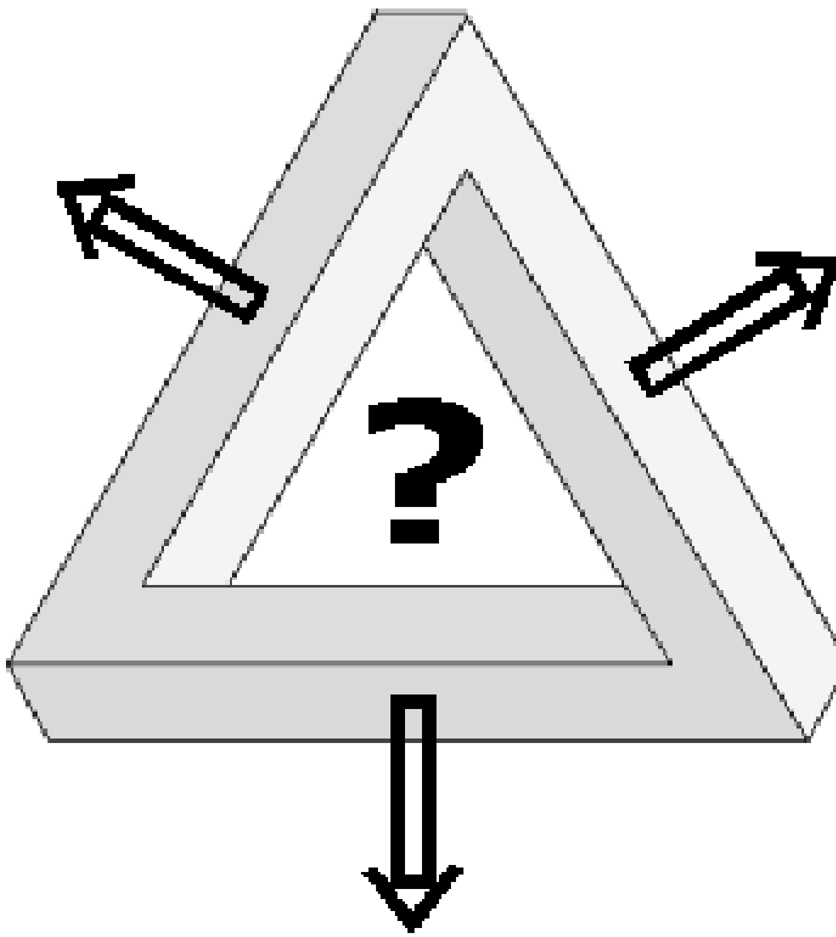
Cell shapes suitable for the shift transformation method

Freek van der Blij



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Abstract

Hicken *et al.* introduced the use of shift transformations to obtain a fully conservative method on an unstructured Cartesian mesh. In this work, this method is investigated on its possibilities to implement on other unstructured grids, with a main focus on the triangulated mesh. By means of a Taylor series development of the error, a matrix is constituted, which rank is related to the possibility of constructing a second order accurate shift transformation, assuming the underlying velocity field is incompressible. An analysis of the linear dependencies between the rows of this matrix yields the proof of the main theorem of this report. This theorem states that one cannot find such a second order accurate shift transformation on triangles while using its circumcenter as the center of the cell. Furthermore, it is proven that of all the quadrilaterals, only the rectangles are appropriate cell shapes in combination with the circumcenter.

Explanation of the cover

The main goal of this work is to examine whether some kind of averaging of the vectors on the faces of a shape can be constructed on a triangle, so as to determine a sufficiently accurate value at the circumcenter. This turns out to be impossible; just as the Penrose triangle is not (fysically) possible.

Master's Thesis

Cell shapes suitable for the shift transformation method

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Chapter 1

Introduction

Many studies on the simulation of the famous equations of Claude Navier (1822) and George Stokes (1845)

$$\partial_t u + (u \cdot \nabla)u - \frac{1}{Re}\nabla \cdot \nabla u + \nabla p = 0 \tag{1.1}$$

$$\nabla \cdot u = 0 \tag{1.2}$$

focus on the balance between the conserving properties and the accuracy of the discretization of these equations. The challenge to combine both resulted in different methods: for example the spectral methods, accurate and fast, but limited to simple geometries, and the methods where the local truncation error is minimized, at the same time causing a loss of the conservation properties on nonuniform grids, which are present in the continuous formulation (see [1]). This lack of conservation means also a lack of stability, unless artificial dissipation is added. But the hereby disturbed balance between convective transport and physical dissipation, especially at the smallest scales of motion, strains the possibility of simulating turbulence. This motivates the study to conservative discretizations on nonuniform grids.

The variables on those grids can be arranged in different ways. The most common variants are the staggered mesh scheme, dating originally from Harlow and Welch [2], and the collocated scheme; the difference lies in the positioning of the velocity. The staggered scheme places the velocities halfway along the faces in the direction of the normals, whereas the collocated scheme situates them in the pressure-center (see Figure 1). Observe that in the collocated scheme still variables are defined on the faces, namely the fluxes. Those are used to enforce mass conservation and should actually not be considered as solution variables, but rather as coupled to the pressure-centered velocity field through an interpolation (see [3] and [4]).

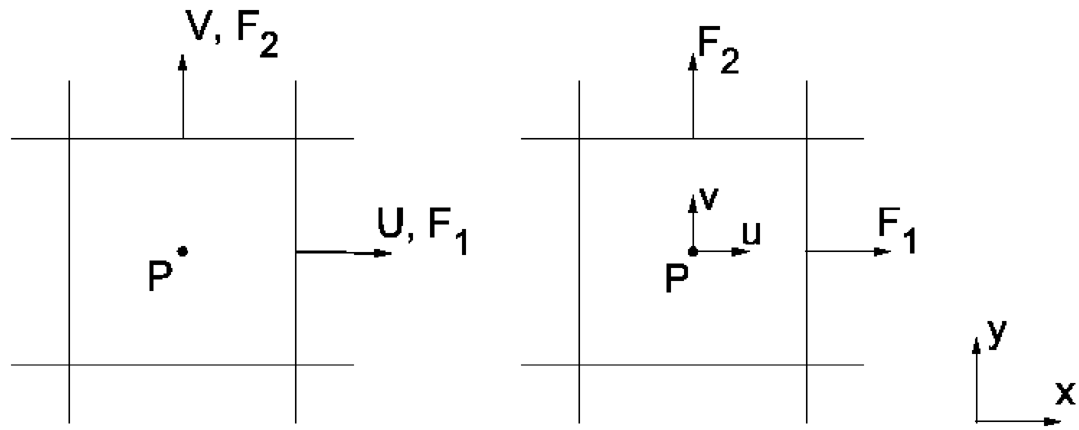

Figure 1.1: Staggered (l) and collocated (r) scheme

Both schemes have advantages and disadvantages. When using a collocated scheme, one can easily construct conserving convective and diffusive operators. However, the energy conservation requires a relation between the gradient and the divergence operator (see [3]), which implies a decoupling of the pressure-field (also known as the checkerboard problem). The staggered scheme at its turn does not experience these decoupling difficulties; the problem here is to define a conservative convective and diffusive operator. These properties are summed up in the tabular below (where, of course, the minus means a difficult discretizable operator and a plus, a straightforward discretizable operator).

	Staggered scheme	Collocated scheme
Convection	-	+
Diffusion	-	+
Pressure gradient	+	-
Conservation of mass	+	-

In this work, we will look at staggered grids, following Hicken *et al.* [3], and generalize towards the investigation of a scheme for unstructured staggered grids, and amongst them, especially, the triangulated one.
For staggered, structured Cartesian grids, schemes were obtained which conserve total mass, momentum and, if the physical dissipation is turned off, kinetic energy. Perot [5] treats the conservation of momentum, kinetic energy and circulation of two discretization schemes on unstructured staggered meshes.
Verstappen and Veldman [1] introduced the notion of mimicking crucial properties of the differential operators. They provide a discretization on a structured Cartesian grid, which not only conserves the above mentioned physical properties (total mass, momentum and kinetic energy), but also inherits a preservation of the symmetry of the differential operators. The skew-symmetric convective and symmetric diffusive difference operator ensure a unconditionally stable and conservative discretization.
Hicken *et al.* [3] succeeded to generalize the ideas of Verstappen & Veldman and Perot. They

used transformations to shift the staggered variables into collocated ones and vice versa, which enabled them to use collocated operators for both the convective and the diffusive term of the Navier-Stokes equations. By using symmetric collocated operators and shift transformations which satisfy certain constraints, the combination of those operators and transformations yielded a symmetry-preserving discretization.

In their article, Hicken *et al.* [3] elaborated their idea about the shift transformation for an unstructured, time-adaptive Cartesian mesh; the question remains whether it also works on general unstructured meshes. For example, a very current mesh is a triangulated one, which approximates curves a lot better than a rectangular mesh. The main objective of this work will thereby be to investigate the possibility of developing a fully conservative, symmetry-preserving discretization on a triangulated mesh, using the technique of shift transformations. This will be done in 2D, using a Cartesian coordinate system.

Having investigated the triangulated case, the logical consecutive question arising is of a more general nature: to which cell shapes does the technique of shift transformations apply? As this is a very broad subject, it will only be partially treated in this article; the rest is left for further research.

Chapter 2

Overview of the shift transformation method

Before we get to the principal part of this article - the answer to the questions addressed at the end of the previous chapter - a brief overview of the shift transformation method introduced by Hicken *et al.* [3] will be given. Although the rest of the article will focus on the 2D problem, this overview will treat a 3D method, in accordance with the article of Hicken *et al.* [3].

2.1 Discretization

The matrix-vector notation of the spatial discretization of the Navier-Stokes equations ((1.1) and (1.2)) on a staggered mesh is given by

$$\Omega \frac{\mathrm{d}\mathbf{u}_s}{\mathrm{d}t} + C(u)\mathbf{u}_s + D\mathbf{u}_s + \Omega G \mathbf{p}_c = \mathbf{0}_s \tag{2.1}$$

$$M\mathbf{u}_s = \mathbf{0}_c \tag{2.2}$$

In this equation, Ω stands for the matrix consisting of the volumes of the cells and $\mathbf{u}_s$ is the vector of staggered velocities. $C(u)$ and D are respectively the convective and the diffusive operators, where $C(u)$ depends on u emphasizing its non-linearity. Furthermore, G is the gradient operator and the pressures constitute the vector $\mathbf{p}_c$. Finally, M is the divergence operator.
Before treating the shift transformations, which will get the collocated operators to be applicable on a staggered scheme, we will consider the collocated operators themselves.

First, the collocated convective operator $C_c(u)$ acting on a collocated variable ϕ_c at some cell k, is defined as

$$[C_c(u)\phi_c]_k = \sum_{f \in F(k)} \frac{(\phi_k + \phi_j)}{2} A_f U_f \tag{2.3}$$

where f stands for a face in the set $F(k)$ of all faces bordering the pressure-cell k, and A_f is the area of this face. Furthermore, U_f is defined as $\mathbf{u}_f \cdot \mathbf{n}_f$, so it represents the discrete face normal velocity. Finally, ϕ_k is the collocated variable in cell k and ϕ_j is the collocated variable in the other cell bordering f, with the convention that the normal vector always points from cell k to cell j (see Figure 2.1).

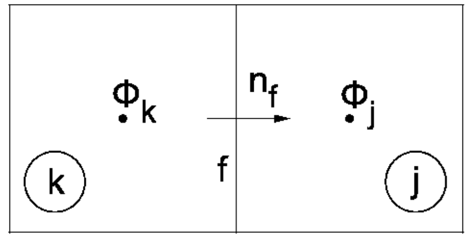

Figure 2.1: The cells k and j with the normal vector

Because the velocity vector (on which $C(u)$ eventually will act) consists in each collocated cell of 3 Cartesian components (and say all the collocated velocities are sorted in a vector starting with all the x-components, followed by the y-components and finally the z-components), a matrix is needed to let the collocated convective operator act on the velocities

$$C_u(u) = \begin{pmatrix} C_c(u) & 0 & 0 \\ 0 & C_c(u) & 0 \\ 0 & 0 & C_c(u) \end{pmatrix} \tag{2.4}$$

Next, consider the collocated diffusive operator, which will lead us to a staggered equivalent. It reads

$$[D_c \phi_c]_k = \frac{1}{Re} \sum_{f \in F(k)} \frac{(\phi_j - \phi_k) A_f}{\delta n_f} \tag{2.5}$$

This is the same diffusive operator as the one used by Hicken *et al.* [3], where $\delta n_f = \Delta V_f / A_f$ is an approximation of the distance between the centers of the cells c_1 and c_2. As in the convective case, a matrix is build to cope with the 3 Cartesian velocity components, resulting in the diffusive collocated operator

$$D_u = \begin{pmatrix} D_c & 0 & 0 \\ 0 & D_c & 0 \\ 0 & 0 & D_c \end{pmatrix} \tag{2.6}$$

2.2 Shift transformation from staggered to collocated variables

In order to (indirectly) use the defined collocated operators to discretize convection and diffusion on a staggered mesh, a shift transformation from the staggered to the collocated variables is needed. There are several possibilities, but to keep it simple, we restrict ourselves to shift transformations involving only immediate faces of a cell. Naturally, neighbouring cells can be taken into consideration, but this imposes a lot of difficulties on unstructured meshes.

When such a shift transformation Γ is applied, the staggered variables are shifted to the centers of the cells, which enables the use of the collocated operator. The last step is to shift the cell-centered values back to the faces, i.e. to the staggered positions. For example, if the procedure is followed for a random collocated operator K_c, we obtain

$$K_s = \Pi K_c \Gamma$$

where K_s is the staggered equivalent of K_c and Π the shift transformation back from the cell-centers to the faces. Hicken *et al.* [3] showed that the desired energy conservation yields the skew-symmetry of the staggered convective operator $C(u)$, which at his turn imposes a constraint on the shift transformation(s):

$$C(u) = \Pi C_u(u)\Gamma \text{ which should equal } \Gamma^* C_u(u)\Pi^* = -\Gamma^* C_u(u^*)\Pi^* = -C^*(u)$$

which can be satisfied by using the transpose of Γ for the shift transformation back Π. In general, it is even possible to define a staggered operator by means of more shift transformations

$$K_s = \frac{1}{N}\sum_{i=1}^{N} \Gamma_i^* K_c \Gamma_i$$

which still ensures energy conservation. Actually, Hicken *et al.* [3] proposed a pair of shift transformations for unstructured Cartesian meshes

$$[\Gamma_1 \mathbf{u}_s]_{ik} = \frac{\sum_{f\in F(k)} A_f U_f \ \max(n_{f,i}, 0)}{\sum_{f\in F(k)} A_f \ \max(n_{f,i}, 0)} \tag{2.7a}$$

$$[\Gamma_2 \mathbf{u}_s]_{ik} = \frac{\sum_{f\in F(k)} A_f U_f \ \min(n_{f,i}, 0)}{\sum_{f\in F(k)} A_f \ \max(-n_{f,i}, 0)} \tag{2.7b}$$

where $n_{f,i}$ is the ith component of the outward face normal $\mathbf{n}_f$. These two shift transformations split the collection of faces in two parts: one with the normals directed in the positive i-direction and another one with the normals directed in the negative i-direction (the reason for this splitting is explained in [3]).

When also global momentum conservation is taken into consideration, another condition for the shift transformation is added

$$\Gamma_i \mathbf{1}_s = \mathbf{1}_{3c} \tag{2.8}$$

where $\mathbf{1}_{3c}$ is a $3n$-vector, because all n collocated elements consist of 3 components each, namely the 3 Cartesian directions. Put differently, this means that the transformations should keep constant vectors constant.

2.3 Conservation properties

With the help of the shift transformation the staggered operators can be formed

$$C(u) = \Gamma^* C_u(u)\Gamma \tag{2.9}$$

$$D = \Gamma^* D_u \Gamma \tag{2.10}$$

The main question at this moment reads: is this discretization still conserving total mass, momentum, kinetic energy and are the symmetric properties of the differential operators preserved in the difference operators? The answer is yes, because the collocated operator is the same as in Hicken *et al.* [3], where it is proven to be skew-symmetric, and the transformation does not affect this property; thereby energy is conserved. Furthermore, the shift transformation satisfies the constraint $\Gamma \mathbf{1}_s = \mathbf{1}_{3c}$, so as shown by Hicken *et al.* [3] also momentum is conserved.

2.4 Pressure gradient and mass conservation

As we are working on a staggered mesh, the pressure gradient G and the divergence operator M can be defined straightforward. A suitable discretization for the mass conservation is given by

$$[M\mathbf{u}_s]_k = \sum_{f \in F(k)} U_f A_f = 0 \tag{2.11}$$

This is the same discretization as for the Cartesian mesh; no adaptations are needed. Energy conservation insists on a relationship between the integrated pressure gradient operator ΩG and the negative conjugate transpose of M (see for example [1] and [3]), hence the first follows from the latter

$$[\Omega G \mathbf{p}_c]_f = [-M^* \mathbf{p}_c]_f = (p_j - p_k) A_f \tag{2.12}$$

where the face normal is pointing from cell k to cell j.

Chapter 3

General formula for the shift transformation

Now the overall method has been cleared up, we can take a closer look at the actual shift transformation. Hicken *et al.* [3] chose (2.7) to be their shift transformation on an unstructured Cartesian mesh; we will start with a formulation as general as possible to keep all the options open.

Recall that the only information present is the discrete face normal velocities U_f and the normals $\mathbf{n}_f$ and that the objective is to determine an average velocity vector $\mathbf{u}^0$ in the center of the cell. This has to be done by means of a linear operator, since it is to be put in matrix-form. The general formula is thereby stated as

$$\sum_{f\in F(k)} C_f U_f n_{f,i} \tag{3.1}$$

where C_f are the (still to be determined) face-depending constants which should make this weighted average as accurate as possible.

Moreover, (2.8) demands that the shift transformation should leave an unity vector $\mathbf{1}$ unaffected (not taking into account the vector size). Now such an unity $\mathbf{u}_f$ determines U_f

$$\mathbf{u}_f = \mathbf{1} \Rightarrow U_f = \mathbf{u}_f \cdot \mathbf{n}_f = \sum_j n_{f,j}$$

where j stands for the spatial directions (in our 2D case x and y). If this is substituted in (3.1), it returns

$$\sum_{f\in F(k)} C_f (\sum_j n_{f,j}) n_{f,i}$$

which thus has to be $\mathbf{1}$ again. Normalizing (3.1) with this term looks after that and makes the general formula satisfy (2.8). Consequently, the general formula is of the form

$$[\Gamma \mathbf{u}_s]_{ik} = \frac{\sum_{f\in F(k)} C_f U_f n_{f,i}}{\sum_{f\in F(k)} C_f (\sum_j n_{f,j}) n_{f,i}} \tag{3.2}$$

where f are the faces of the cell and i the directions.

This general formula looks at first glance a bit devious from the pair used by Hicken *et al.*

[3] ((2.7a) and (2.7b)). But if their particular cellshape -in 2D a non-rotated rectangle- is taken into account, the formulas turn out to give equal results. First of all, Hicken *et al.* [3] chose the constants C_f to equal the face area A_f (in 2D the length of the face). This choice is justified at the end of Chapter 5. Next, observe that the counters in (2.7a) and (2.7b) combine towards the counter of (3.2) with A_f substituted for C_f. Finally, on a non-rotated rectangle the normals are

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 \\ -1 \end{pmatrix} \tag{3.3}$$

so the denominator of (3.2) becomes

$$\sum_{f \in F(k)} C_f (\sum_j n_{f,j}) n_{f,i} = \sum_{f \in F(k)} C_f |n_{f,i}|$$

which is the same as the (combination of) denominators in (2.7a) and (2.7b), with A_f instead of C_f.

The general formula for the shift transformation now satisfies the conditions it needs to and the remaining challenge will be to find the best constants C_f, i.e. those which are leading to the most accurate average. After trying several methods (see also Chapter 10) without the desired results, an approach with the well-known Taylor series did lead to results, as is shown in the following chapters.

Chapter 4

Taylor series approach

Consider an arbitrary convex cell with center (x_c, y_c), face f and the middle (x_f, y_f) of this face f (see Figure 4.1)

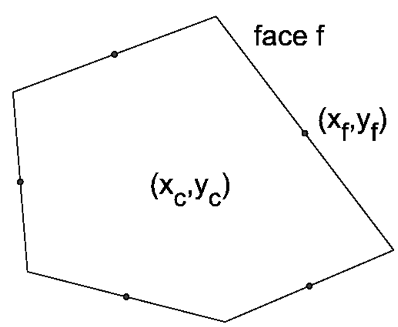

Figure 4.1: Arbitrary cell

Then Δx_f and Δy_f can respectively be defined as the (not necessarily positive) differences in the x- and the y-direction between the center and the middle of the considered side f, i.e.

$$\Delta x_f = x_c - x_f$$
$$\Delta y_f = y_c - y_f$$

By means of a Taylor series development of the general formula (3.2) on such a random cell, an attempt to determine the constants C_f can be made. This construction will trivially be based on minimalizing the error made by replacing $[\Gamma \mathbf{u}_s]_{ik}$ by its truncated Taylor approximation. The variable U_f (or actually $\mathbf{u_f}$) will be developed and expressed in terms of $\mathbf{u}^0$ (the value of $\mathbf{u}$ in the center) and its derivatives, using the abovementioned Δx_f and Δy_f. The derivation is done in 2D; a 3D approach might result in different conclusions. This problem however is not addressed here and is left for further research, as discussed in Chapter 10.

The Taylor series development now becomes

$$
\begin{aligned}
U_f &= \mathbf{u}_f \cdot \mathbf{n}_f \\
&= (\mathbf{u}^0 + \mathbf{u}^0_x \Delta x_f + \mathbf{u}^0_y \Delta y_f + \frac{1}{2}\mathbf{u}^0_{xx}(\Delta x_f)^2 + \mathbf{u}^0_{xy}\Delta x_f \Delta y_f + \frac{1}{2}\mathbf{u}^0_{yy}(\Delta y_f)^2) \cdot \mathbf{n}_f \\
&\quad + \mathcal{O}(\Delta x_f^3, \Delta y_f^3) \\
&= (\mathbf{u}^0 \cdot \mathbf{n}_f) + (\mathbf{u}^0_x \cdot \mathbf{n}_f)\Delta x_f + (\mathbf{u}^0_y \cdot \mathbf{n}_f)\Delta y_f + \frac{1}{2}(\mathbf{u}^0_{xx} \cdot \mathbf{n}_f)(\Delta x_f)^2 \\
&\quad + (\mathbf{u}^0_{xy} \cdot \mathbf{n}_f)\Delta x_f \Delta y_f + \frac{1}{2}(\mathbf{u}^0_{yy} \cdot \mathbf{n}_f)(\Delta y_f)^2 + \mathcal{O}(\Delta x_f^3, \Delta y_f^3)
\end{aligned}
$$

where $\mathbf{u}^0$ with subscript(s) stands for the value of the derivative of $\mathbf{u}$ in the direction(s) indicated by the subscript, calculated at the center of the examined cell. To avoid to much confusing notation, a subscript indicating the cell under examination (cell k) is omitted; this will not cause ambiguity, as we consider only one particular cell during the derivation.

Inserting this elaboration in the original general formula (3.2) and splitting the division in parts of equal order (with respect to the derivatives of the velocity field) we obtain

$$[\Gamma \mathbf{u}_s]_i = [T_0 \mathbf{u}_s]_i + [T_1 \mathbf{u}_s]_i + [T_2 \mathbf{u}_s]_i + \mathcal{O}(\Delta x_f^3, \Delta y_f^3)$$

with

$$[T_0 \mathbf{u}_s]_i = \frac{\sum_{f \in F(k)} C_f (\mathbf{u}^0 \cdot \mathbf{n}_f) n_{f,i}}{\sum_{f \in F(k)} C_f (\sum_j n_{f,j}) n_{f,i}} \tag{4.1}$$

$$[T_1 \mathbf{u}_s]_i = \frac{\sum_{f \in F(k)} C_f ((\mathbf{u}^0_x \cdot \mathbf{n}_f)\Delta x_f + (\mathbf{u}^0_y \cdot \mathbf{n}_f)\Delta y_f) n_{f,i}}{\sum_{f \in F(k)} C_f (\sum_j n_{f,j}) n_{f,i}} \tag{4.2}$$

$$[T_2 \mathbf{u}_s]_i = \frac{\sum_{f \in F(k)} C_f (\frac{1}{2}(\mathbf{u}^0_{xx} \cdot \mathbf{n}_f)(\Delta x_f)^2 + (\mathbf{u}^0_{xy} \cdot \mathbf{n}_f)\Delta x_f \Delta y_f + \frac{1}{2}(\mathbf{u}^0_{yy} \cdot \mathbf{n}_f)(\Delta y_f)^2) n_{f,i}}{\sum_{f \in F(k)} C_f (\sum_j n_{f,j}) n_{f,i}} \tag{4.3}$$

With the notation $\mathbf{u}^0 = (u^0, v^0)$ (remember we work in 2D), (4.1) can be rewritten as

$$[T_0 \mathbf{u}_s]_i = \frac{\sum_{f \in F(k)} C_f (\mathbf{u}^0 \cdot \mathbf{n}_f) n_{f,i}}{\sum_{f \in F(k)} C_f (\sum_j n_{f,j}) n_{f,i}} = \frac{\sum_{f \in F(k)} C_f (u^0 n_{f,x} n_{f,i} + v^0 n_{f,y} n_{f,i})}{\sum_{f \in F(k)} C_f (n_{f,i}^2 + n_{f,x} n_{f,y})}$$

For the x- and the y-direction the derivation continues slightly different. First look at the x-direction

$$\begin{aligned}
[T_0\mathbf{u}_s]_x &= \frac{\sum_{f\in F(k)} C_f(u^0 n_{f,x}^2 + v^0 n_{f,y}n_{f,x})}{\sum_{f\in F(k)} C_f(n_{f,x}^2 + n_{f,x}n_{f,y})} \\
&= \frac{\sum_{f\in F(k)} C_f(u^0(n_{f,x}^2 + n_{f,x}n_{f,y}) + (v^0 - u^0)n_{f,y}n_{f,x})}{\sum_{f\in F(k)} C_f(n_{f,x}^2 + n_{f,x}n_{f,y})} \\
&= \frac{\sum_{f\in F(k)} C_f u^0(n_{f,x}^2 + n_{f,x}n_{f,y})}{\sum_{f\in F(k)} C_f(n_{f,x}^2 + n_{f,x}n_{f,y})} + \frac{\sum_{f\in F(k)} C_f(v^0 - u^0)n_{f,y}n_{f,x})}{\sum_{f\in F(k)} C_f(n_{f,x}^2 + n_{f,x}n_{f,y})} \\
&= u^0 + (v^0 - u^0)\frac{\sum_{f\in F(k)} C_f n_{f,y}n_{f,x}}{\sum_{f\in F(k)} C_f(n_{f,x}^2 + n_{f,x}n_{f,y})}
\end{aligned}$$

For the y-direction a similar procedure can be followed, producing

$$[T_0\mathbf{u}_s]_y = v^0 + (u^0 - v^0)\frac{\sum_{f\in F(k)} C_f n_{f,y}n_{f,x}}{\sum_{f\in F(k)} C_f(n_{f,y}^2 + n_{f,x}n_{f,y})} \tag{4.4}$$

So when the direction is not specified

$$[T_0\mathbf{u}_s]_i = [\mathbf{u}^0]_i + (-1)^z(u^0 - v^0)\frac{\sum_{f\in F(k)} C_f \prod_j n_{f,j}}{\sum_{f\in F(k)} C_f(n_{f,i}^2 + \prod_j n_{f,j})} \tag{4.5}$$

where $[\mathbf{u}^0]_i$ refers to the i-th component of $\mathbf{u}^0$ (the brackets serve to distinguish it from a derivative) and z is defined as

$$z = \begin{cases} 1 & \text{if} \quad i = x \\ 0 & \text{if} \quad i = y \end{cases}$$

Realize the operator $[\Gamma u_s]_i$ is meant to approximate the value $[\mathbf{u}^0]_i$ out of the values U_f, so the error in the i-direction made while applying this operator can be stated as

$$\begin{aligned}
\text{Error}_i &= [\Gamma u_s]_i - [\mathbf{u}^0]_i \\
&= [T_0\mathbf{u}_s]_i + [T_1\mathbf{u}_s]_i + [T_2\mathbf{u}_s]_i - [\mathbf{u}^0]_i + \mathcal{O}(\Delta x_f^3, \Delta y_f^3) \\
&= (-1)^z(u^0 - v^0)\frac{\sum_{f\in F(k)} C_f \prod_j n_{f,j}}{\sum_{f\in F(k)} C_f(n_{f,i}^2 + \prod_j n_{f,j})} \\
&\quad + [T_1\mathbf{u}_s]_i + [T_2\mathbf{u}_s]_i + \mathcal{O}(\Delta x_f^3, \Delta y_f^3)
\end{aligned} \tag{4.6}$$

It would be preferable to obtain results using this formula, which is valid for all types of shapes and centers. This will be tried in Chapter 6 and 7, but it will turn out to be very tough. By choosing a center and inserting the characteristics of a specific shape, the general error formula can be simplified. An example of this will be given in the next chapter, by computing suitable constants C_f on a parallelogram. The substitution of a specific center will also be used to prove a theorem about triangles and one about quadrilaterals (see Chapter 8).

Chapter 5

An example: C_f on a parallelogram

To elucidate the general error formula (4.6) derived in the previous chapter, it will be used to calculate the second order accurate face-depending constants on a parallelogram, again in two dimensions. No assumptions are made about the size, rotation or exact position with respect to the origin. To calculate these C_f, first the characteristics of the particular shape are considered. As the general error formula (4.6) shows, the error is determined by the normals $\mathbf{n}_f$ of the faces and the values of Δx_f and Δy_f. In the parallelogram case, the normals are pairwise related to each other, namely

$$\mathbf{n}_1 = -\mathbf{n}_3$$
$$\mathbf{n}_2 = -\mathbf{n}_4$$

visualized in Figure 5.1.

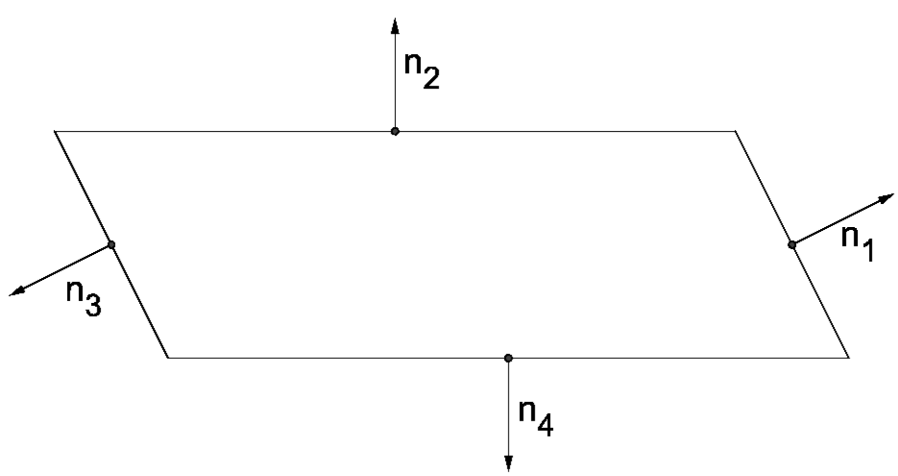

Figure 5.1: Parallelogram with its normals

This combined with the fact that we are working in two dimensions gives

$$\prod_j n_{1,j} = \prod_j (-n_{3,j}) = (-1)^2 \prod_j n_{3,j} = \prod_j n_{3,j}$$
$$\prod_j n_{2,j} = \prod_j (-n_{4,j}) = (-1)^2 \prod_j n_{4,j} = \prod_j n_{4,j}$$

From a symmetric point of view, a very logical choice of the center would be the intersection of the two diagonals (see Figure 5.2).

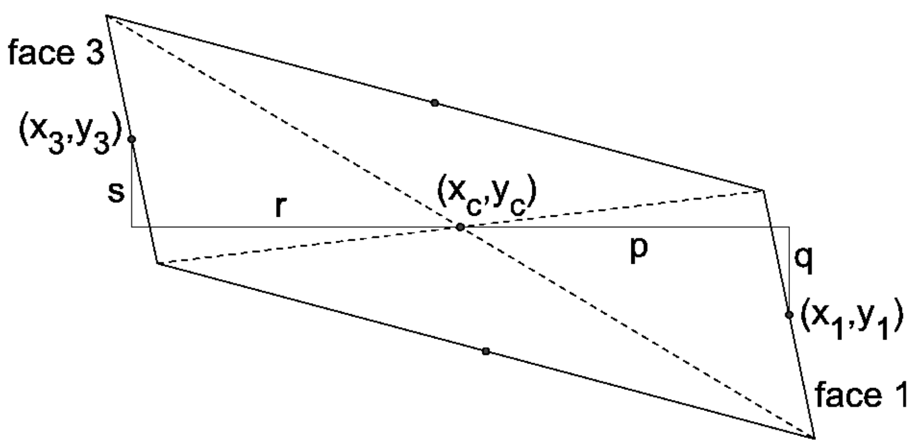

Figure 5.2: Parallelogram with chosen center

In this figure, the Euclidian distance p is defined as $|x_1 - x_c| = x_1 - x_c$ and the Euclidian distance r as $|x_3 - x_c| = x_c - x_3$. In parallelograms with the specified center these p and r are of equal length, and therefore $x_1 - x_c = x_c - x_3$. Note that q and s are similarly related. Now recall the definition of Δx_f and Δy_f to obtain

$$\Delta x_1 = -\Delta x_3$$
$$\Delta x_2 = -\Delta x_4$$
$$\Delta y_1 = -\Delta y_3$$
$$\Delta y_2 = -\Delta y_4$$

This results into a simplified error formula

$$
\begin{aligned}
&[\Gamma u_s]_i - [\mathbf{u}^0]_i \\
&= (-1)^z(u^0 - v^0)\frac{(C_1+C_3)\prod_j n_{1,j} + (C_2+C_4)\prod_j n_{2,j}}{(C_1+C_3)(n_{1,i}^2 + \prod_j n_{1,j}) + (C_2+C_4)(n_{2,i}^2 + \prod_j n_{2,j})} \\
&+\frac{(C_1-C_3)((\mathbf{u}_x^0\cdot n_1)n_{1,i}\Delta x_1 + (\mathbf{u}_y^0\cdot n_1)n_{1,i}\Delta y_1)}{(C_1+C_3)(n_{1,i}^2 + \prod_j n_{1,j}) + (C_2+C_4)(n_{2,i}^2 + \prod_j n_{2,j})} \\
&+\frac{(C_2-C_4)((\mathbf{u}_x^0\cdot n_2)n_{2,i}\Delta x_2 + (\mathbf{u}_y^0\cdot n_2)n_{2,i}\Delta y_2)}{(C_1+C_3)(n_{1,i}^2 + \prod_j n_{1,j}) + (C_2+C_4)(n_{2,i}^2 + \prod_j n_{2,j})} \\
&+\frac{(C_1+C_3)((\frac{1}{2}\mathbf{u}_{xx}^0\cdot n_1)n_{1,i}(\Delta x_1)^2 + (\mathbf{u}_{xy}^0\cdot n_1)n_{1,i}\Delta x_1\Delta y_1 + \frac{1}{2}(\mathbf{u}_{yy}^0\cdot n_1)n_{1,i}(\Delta y_1)^2)}{(C_1+C_3)(n_{1,i}^2 + \prod_j n_{1,j}) + (C_2+C_4)(n_{2,i}^2 + \prod_j n_{2,j})} \\
&+\frac{(C_2+C_4)((\frac{1}{2}\mathbf{u}_{xx}^0\cdot n_2)n_{2,i}(\Delta x_2)^2 + (\mathbf{u}_{xy}^0\cdot n_2)n_{2,i}\Delta x_2\Delta y_2 + \frac{1}{2}(\mathbf{u}_{yy}^0\cdot n_2)n_{2,i}(\Delta y_2)^2)}{(C_1+C_3)(n_{1,i}^2 + \prod_j n_{1,j}) + (C_2+C_4)(n_{2,i}^2 + \prod_j n_{2,j})} \\
&+\mathcal{O}(\Delta x_f^3, \Delta y_f^3)
\end{aligned}
$$

In a general velocity field, the term $(u^0 - v^0)$ will not vanish. So, in order to get rid of the zeroth order term, the equation

$$(C_1+C_3)\prod_j n_{1,j} + (C_2+C_4)\prod_j n_{2,j} = 0 \tag{5.1}$$

needs to be solved. A solution of this equation is

$$\frac{C_1+C_3}{C_2+C_4} = \frac{-\prod_j n_{2,j}}{\prod_j n_{1,j}}$$

Furthermore, for a second order accurate shift transformation, the first order term must also vanish. This can easily be achieved by choosing

$$C_1 = C_3 \text{ and } C_2 = C_4 \tag{5.2}$$

Consequently, (5.1) reduces to

$$\frac{C_1}{C_2} = \frac{-\prod_j n_{2,j}}{\prod_j n_{1,j}} \tag{5.3}$$

Now there still seems to be one degree of freedom left. However, since the constants -while plugged into Γ- can be simultaneously multiplied by a random factor (this factor will disappear due to the normalization), the second order accurate constants for a parallelogram are sufficiently defined by the equations (5.2) and (5.3) and read

$$[C_1\ C_2\ C_3\ C_4] = [-\prod_j n_{2,j}\quad \prod_j n_{1,j}\quad -\prod_j n_{2,j}\quad \prod_j n_{1,j}] \tag{5.4}$$

In Chapter 3 we promised to justify the choice for the constants C_f made by Hicken *et al.* [3]. As mentioned, they chose the face areas A_f to be their constants. To see whether or not

this is in alignment with (5.4), first of all it should be stressed that their formula was meant to be applied on an unstructured Cartesian mesh with refinement. This might entail multiple neighbouring cells adjacent to one face, something we did not consider in the deduction of (5.4). Thereby we will only treat the comparison of the formula of Hicken *et al.* [3] with (5.4) on Cartesian meshes with only one value of U_f per face (so four in total).
Note that on this Cartesian mesh the normals $\mathbf{n}_1$ and $\mathbf{n}_2$ are perpendicular. Expressed using a rotation matrix

$$\mathbf{n}_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{n}_1$$

which results in

$$\prod_j n_{2,j} = (0 \cdot n_{1,x} - 1 \cdot n_{1,y})(1 \cdot n_{1,x} + 0 \cdot n_{1,y}) = -n_{1,y}n_{1,x} = -\prod_j n_{1,j}$$

implying a vector (5.4) with equal elements. This, however, contradicts with $C_f = A_f$, because on the rectangles used in a Cartesian mesh the A_f's are only pairwise equal. Nevertheless the choice of Hicken *et al.* [3] is correct, as they only considered non-rotated rectangles, which induces normals as in (3.3). Thereby (5.1) is always satisfied, regardless of the choice of the C_f. For the first order term of the error $[T_1\mathbf{u}_s]_i$ to vanish, the pairwise equality of the A_f's will suffice, alike (5.2). This proofs the second order accuracy of the formula of Hicken *et al.* [3]
However, chosing A_f does restrict the cells to non-rotatable rectangles and rotatable squares (on a square all the A_f's are equal anyway). That advocates a different choice, namely constants which are all equal to each other, in accordance to (5.4). This would make the rectangle rotatable and thus better applicable. However, the choice of Hicken *et al.* [3] is justified by the applicability on refined meshes, something we do not treat in this work.

Chapter 6

Conditions for the existence of a second order accurate operator

The main goal of our research was to find a second order accurate operator on a triangle, which means, to construct the three constants of the general formula (3.2) necessary to fulfil this demand. Likewise the parallelogram case, one's primary idea would be to analyze the characteristics of the triangle and substitute them in the general error formula (4.6). However, a triangle, even a equilateral one, does not possess the same simplifying charateristics as a parallelogram. The condition to let the operator be of first order can still be derived quite easily, but the problem of finding a second order accurate shift transformation turns out to be a lot harder to solve.
Having observed this problem, a more general question arises: what are the restrictions on the shape of a cell for finding an operator with the desired second order accuracy? So far, we did not assume anything regarding the (unknown) velocityfield $\mathbf{u}$. However, in order to obtain useful results, we are forced to make such assumptions; a very common one to impose on the velocity field is that it is incompressible, which we also will assume throughout the rest of this work. In this chapter an effort is made to derive the restrictions on cell shapes on such velocity fields. These restrictions enable us to investigate cell shapes in general and triangles in particular. This will be done by imposing another condition on the velocity field, namely that it is induced by a potential. This assumption will simplify the problem, and from the solutions of the simplified problem the solutions of the original problem will be extracted.

Consider a velocity field $\mathbf{u} = (u, v)$. Now the counter of the first order term of the general error formula (4.2) can be written as

$$[T_1\mathbf{u}_s]_i = \sum_f C_f((\begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial x} \end{pmatrix} \cdot \mathbf{n}_f)\Delta x_f + (\begin{pmatrix} \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial y} \end{pmatrix} \cdot \mathbf{n}_f)\Delta y_f)n_{f,i} \tag{6.1}$$

Further, the normals on the sides are expressed in their angles θ_f with respect to the positive x-axis (see also Figure 6.1)

$$\mathbf{n}_f = \begin{pmatrix} \cos\theta_f \\ \sin\theta_f \end{pmatrix}$$

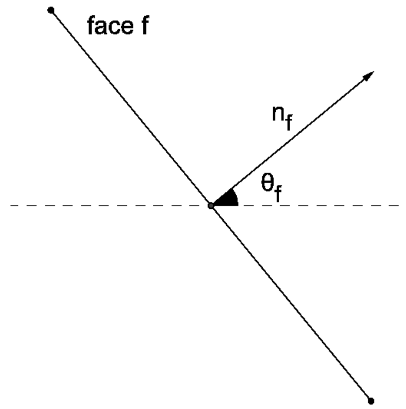

Figure 6.1: Normal expressed in θ

Hence, elaborating the dot product in (6.1) results in

$$[T_1\mathbf{u}_s]_i = \sum_f C_f((\frac{\partial u}{\partial x}\cos\theta_f + \frac{\partial v}{\partial x}\sin\theta_f)\Delta x_f + (\frac{\partial u}{\partial y}\cos\theta_f + \frac{\partial v}{\partial y}\sin\theta_f)\Delta y_f)n_{f,i}$$

As said, the common assumption of imcompressibility will be folllowed, constraining the velocity field by

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{6.2}$$

Using (6.2) gives

$$[T_1\mathbf{u}_s]_i = \sum_f C_f(\frac{\partial u}{\partial x}(\cos\theta_f\Delta x_f - \sin\theta_f\Delta y_f) + \frac{\partial u}{\partial y}\sin\theta_f\Delta x_f + \frac{\partial v}{\partial x}\cos\theta_f\Delta y_f)n_{f,i} \tag{6.3}$$

In a general velocity field the three derivatives of $\mathbf{u}$ in (6.3) are independent of each other. So if (6.3) is to equal zero in both the x- and the y-direction (ensuring a zero-valued first order term of the general error formula (4.2)), it yields 6 equations:

$$\sum_f C_f\frac{\partial u}{\partial x}(\cos\theta_f\Delta x_f - \sin\theta_f\Delta y_f)\cos\theta_f = 0 \tag{6.4a}$$

$$\sum_f C_f\frac{\partial u}{\partial x}(\cos\theta_f\Delta x_f - \sin\theta_f\Delta y_f)\sin\theta_f = 0 \tag{6.4b}$$

$$\sum_f C_f\frac{\partial u}{\partial y}\sin\theta_f\cos\theta_f\Delta x_f = 0 \tag{6.4c}$$

$$\sum_f C_f\frac{\partial u}{\partial y}\sin^2\theta_f\Delta x_f = 0 \tag{6.4d}$$

$$\sum_f C_f\frac{\partial v}{\partial x}\cos^2\theta_f\Delta y_f = 0 \tag{6.4e}$$

$$\sum_f C_f\frac{\partial v}{\partial x}\sin\theta_f\cos\theta_f\Delta y_f = 0 \tag{6.4f}$$

We could continue solving these equations. However, we can simplify our problem by what at start might sound a bit counterintuitive: introducing an extra assumption on the incompressible velocity field (from here on called VF_I). As one will see at the end of this chapter, the solution of this simplified, but at the same time more specific problem will be used to draw conclusions with respect to the original problem using VF_I.
The mentioned assumption states that the incompressible velocity field is induced by a potential Q. This field will be referred to as VF_{IP} and can be described as $VF_{IP} = (\frac{\partial Q}{\partial x}, \frac{\partial Q}{\partial y})$, implying

$$\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} = 0 \tag{6.5}$$

This simplifies (6.3) to

$$[T_1 \mathbf{u}_s]_i = \sum_f C_f (\frac{\partial u}{\partial x}(\cos\theta_f \Delta x_f - \sin\theta_f \Delta y_f) + \frac{\partial u}{\partial y}(\sin\theta_f \Delta x_f + \cos\theta_f \Delta y_f)) n_{f,i} \tag{6.6}$$

If we then assume that the two remaining derivatives of $\mathbf{u}$ are again independent of each other, the 6 equations (6.4) reduce to only 4 equations:

$$\sum_f C_f \frac{\partial u}{\partial x}(\cos\theta_f \Delta x_f - \sin\theta_f \Delta y_f)\cos\theta_f = 0 \tag{6.7a}$$

$$\sum_f C_f \frac{\partial u}{\partial x}(\cos\theta_f \Delta x_f - \sin\theta_f \Delta y_f)\sin\theta_f = 0 \tag{6.7b}$$

$$\sum_f C_f \frac{\partial u}{\partial y}(\sin\theta_f \Delta x_f + \cos\theta_f \Delta y_f)\cos\theta_f = 0 \tag{6.7c}$$

$$\sum_f C_f \frac{\partial u}{\partial y}(\sin\theta_f \Delta x_f + \cos\theta_f \Delta y_f)\sin\theta_f = 0 \tag{6.7d}$$

Next to a zero T_1 (4.2), it is also desired to let the zeroth order term T_0 (4.1) vanish, as we are looking for a second order accurate shift transformation. We again assume $(u^0 - v^0)$ not to equal zero, so we are left with

$$\sum_f C_f \cos\theta_f \sin\theta_f = 0 \tag{6.8}$$

(where again the normals are expressed in terms of θ_f). With the derivatives of $\mathbf{u}$ taken away in (6.7) (since they do not depend on f), this total of 5 equations can be put in matrix-vector form

$$M^T \mathbf{v} = \mathbf{0} \tag{6.9}$$

where $\mathbf{v}$ is the vector with the constants C_f

$$\mathbf{v} = (C_1 \cdots C_{\#f})$$

and M a matrix depending on θ_f, Δx_f and Δy_f

$$M = \begin{pmatrix} (-)_1 \cos\theta_1 & (-)_1 \sin\theta_1 & (+)_1 \cos\theta_1 & (+)_1 \sin\theta_1 & \cos\theta_1 \sin\theta_1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (-)_{\#f} \cos\theta_{\#f} & (-)_{\#f} \sin\theta_{\#f} & (+)_{\#f} \cos\theta_{\#f} & (+)_{\#f} \sin\theta_{\#f} & \cos\theta_{\#f} \sin\theta_{\#f} \end{pmatrix} \tag{6.10}$$

using the notation

$$\begin{aligned}(-)_i &= \cos\theta_i \Delta x_i - \sin\theta_i \Delta y_i \\ (+)_i &= \sin\theta_i \Delta x_i + \cos\theta_i \Delta y_i\end{aligned}$$

and with $\#f$ representing the amount of faces of the cell. Now the following Theorem about M and a second order accurate shift transformation can be proven

Theorem 6.1 *On an incompressible velocity field induced by a potential, an at least second order accurate shift transformation can be found if and only if* $rank(M) < \#f$

Proof Recall that we are looking for a $\mathbf{v}$ which satisfies the linear equation (6.9) and thereby supplies the constants C_f for a second order accurate shift transformation. However, not only this specific vector then should result in a second order accurate formula, but also any multiple of this vector; this multiple will vanish by the (mandatory) normalization in the general formula (3.2). In terms of linear algebra this means we are looking for a generating vector $\mathbf{v} \in V$ which spans (a part of) the null space of M, and a second order accurate shift transformation will exist if and only if this $\mathbf{v}$ can be found. To ensure the existence of such a $\mathbf{v}$ spanning (a part of) $ker(M)$, $dim(ker(M)$ should be larger than zero. If that is the case, $\mathbf{v}$ (and thus the constants C_f) can be computed by solving equation (6.9).
Now apply the well-known rank-nullity theorem, which reads

$$dim(V) = dim(ker(M)) + rank(M)$$

so in this case

$$\#f = dim(ker(M)) + rank(M)$$

Recall that the C_f could be traced if and only if $dim(ker(M) > 0$, so if and only if

$$rank(M) = \#f - dim(ker(M)) < \#f \tag{6.11}$$

Thereby Theorem 6.1 has been proven. ∎

Corollary 6.2 *It is impossible to find a vector of constants* $\mathbf{v}$ *and thus a second order accurate formula on an incompressible velocity field induced by a potential, if* $rank(M) = \#f$.

Proof This follows directly from Theorem 6.1. ∎

This result rephrases the existence of a second order accurate shift transformation to the investigation of the rank of M, which will be done in the next chapter. However, it only treats specific velocity fields, namely incompressible fields *induced by a potential*. Nevertheless, despite the at first glance unnessecarily particularizing, we can draw conclusions which are valid for incompressible velocity fields in general. To do so, realize that if a $\mathbf{v}$ solves simultaneously (6.4c) and (6.4e), it will also solve (6.7c) (recall that the derivatives of $\mathbf{u}$ can be taken away). In the same manner, if a $\mathbf{v}$ solves simultaneously (6.4d) and (6.4f), it will also solve (6.7d). Since (6.4a) equals (6.7a) and (6.4b) equals (6.7b), a $\mathbf{v}$ solving (6.4) will also solve (6.7). This means that all the solutions of the VF_I problem are included in the set of solutions of the problem dealing with VF_{IP}. This reasoning combined with Corollary 6.2 results in the following Theorem

Theorem 6.3 *It is impossible to find a vector of constants* $\mathbf{v}$ *and thus a second order accurate formula on an incompressible velocity field, if* $rank(M) = \#f$.

Proof The abovementioned reasoning combined with Corollary 6.2 proofs the theorem. ∎

An equivalent of Theorem 6.1 can be stated if a matrix $\tilde{M}$ is formed out of (6.4) and (6.8). This $\tilde{M}$ can be used to make an analysis of the case of VF_I, similar to the case of potential-based field treated in the upcoming chapters. However, if the cell shapes have to satisfy certain conditions to lead to solutions in the case of VF_{IP}, Theorem 6.3 tells us the cell shapes in the case of VF_I at least need to satisfy the same conditions to lead to solutions. In fact, it is not even sure if the cell shapes which do satisfy these conditions, will lead to solutions. Consequently, if we want to determine appropiate cell shapes on VF_I, it suffices to take the appropiate cell shapes on VF_{IP} and then test their applicability on VF_I.

Chapter 7

The rank of M

The preceding chapter showed that the rank of M determines the existence of a second order shift transformation. The next step will thereby trivially be to investigate the rank of M.

While the rank of a matrix is the same as the row rank of a matrix, it is enough to consider only this row rank. If all the rows of M are linearly independent, the row rank equals $\#f$. This number is reduced if and only if a row is a linear combination of other rows.

7.1 Dependency of one row on one other row

To start, we look if a row can be linearly dependent on 1 other row and prove the following Lemma

Lemma 7.1 *None of the rows of M is a multiple of another row of M*

This can also be stated as: the elementwise division of two rows cannot be a constant vector.

Proof We will proof this by contradiction. Take the elementwise division of row p and q

$$\left[\frac{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\cos\theta_p}{(\cos\theta_q\Delta x_q - \sin\theta_q\Delta x_q)\cos\theta_q} \; \frac{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\sin\theta_p}{(\cos\theta_q\Delta x_q - \sin\theta_q\Delta x_q)\sin\theta_q} \; \frac{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\cos\theta_p}{(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\cos\theta_q} \right.$$
$$\left. \frac{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\sin\theta_p}{(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\sin\theta_q} \; \frac{\sin\theta_p\cos\theta_p}{\sin\theta_q\cos\theta_q}\right] \tag{7.1}$$

We will assume this vector to be constant, which will lead to a contradiction. Hence, amongst others the first element must equal the second, which gives

$$\frac{\cos\theta_p}{\cos\theta_q} = \frac{\sin\theta_p}{\sin\theta_q} \text{ or } \frac{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)}{(\cos\theta_q\Delta x_q - \sin\theta_q\Delta x_q)} = 0$$

and also the third should equal the fourth, resulting in

$$\frac{\cos\theta_p}{\cos\theta_q} = \frac{\sin\theta_p}{\sin\theta_q} \text{ or } \frac{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)}{(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)} = 0$$

To satisfy this equations, the first possibility is that

$$\frac{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)}{(\cos\theta_q\Delta x_q - \sin\theta_q\Delta x_q)} = 0 \text{ and } \frac{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)}{(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)} = 0 \tag{7.2}$$

holds. If it does not, the only other option is that

$$\frac{\cos\theta_p}{\cos\theta_q} = \frac{\sin\theta_p}{\sin\theta_q} \tag{7.3}$$

Starting with the first, it demands

$$\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p = 0 \text{ and } \sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p = 0 \tag{7.4}$$

so

$$\cos\theta_p\Delta x_p = \sin\theta_p\Delta y_p \text{ and } \sin\theta_p\Delta x_p = -\cos\theta_p\Delta y_p$$

and thereby

$$\frac{\cos\theta_p}{\sin\theta_p} = \frac{\Delta y_p}{\Delta x_p} \text{ and } \frac{\cos\theta_p}{\sin\theta_p} = -\frac{\Delta x_p}{\Delta y_p}$$

which are only satisfied when

$$\frac{\Delta y_p}{\Delta x_p} = -\frac{\Delta x_p}{\Delta y_p} \Rightarrow \Delta x_p^2 = -\Delta y_p^2 \Rightarrow \Delta x_p = \Delta y_p = 0$$

Of course shapes with a zero distance from the center to the middle of a face are not allowed, so (7.2) is not possible. Trivially, this means (7.4) is not possible too; a result to which will be reffered to in upcoming proofs as well. Thereby it will be put as a remark

Remark For each face f, the expressions $\cos\theta_f\Delta x_f - \sin\theta_f\Delta y_f$ and $\sin\theta_f\Delta x_f + \cos\theta_f\Delta y_f$ cannot simultaneously equal zero.

So we are left with the only other option:

$$\frac{\cos\theta_p}{\cos\theta_q} = \frac{\sin\theta_p}{\sin\theta_q}$$

Realizing that the left division stands for the factor between the x-components of the normals $\mathbf{n}_p$ and $\mathbf{n}_q$ and at the same time the right fraction is equivalent to the factor between the y-components, this means that those two factors are the same, or consequently, that $\mathbf{n}_p$ is a multiple of $\mathbf{n}_q$. As all normals are by definition of length 1, it results in $\mathbf{n}_p = \pm\mathbf{n}_q$. But assuming a convex cell, the normals of different sides cannot be exactly the same, thus

$$\mathbf{n}_p = -\mathbf{n}_q \tag{7.5}$$

So when the normals of two sides differ by a factor -1, that is, the sides are parallel in the convex cell, the first term in the vector of the division of the two rows (7.1) equals the second, and the third equals the fourth. To see if this is not only a necessary, but also sufficient condition, i.e. if there are no more necessary conditions, substitute

$$\mathbf{n}_p = -\mathbf{n}_q \Rightarrow \cos\theta_p = -\cos\theta_q \text{ and } \sin\theta_p = -\sin\theta_q$$

in the vector of the two divided rows (7.1)

$$\left[\frac{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\cos\theta_p}{(-\cos\theta_p\Delta x_q + \sin\theta_p\Delta x_q)(-\cos\theta_p)} \quad \frac{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\sin\theta_p}{(-\cos\theta_p\Delta x_q + \sin\theta_p\Delta x_q)(-\sin\theta_p)}\right.$$

$$\left. \frac{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\cos\theta_p}{(-\sin\theta_p\Delta x_q - \cos\theta_p\Delta y_q)(-\cos\theta_p)} \quad \frac{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\sin\theta_p}{(-\sin\theta_p\Delta x_q - \cos\theta_p\Delta y_q)(-\sin\theta_p)} \quad \frac{\sin\theta_p\cos\theta_p}{-\sin\theta_p(-\cos\theta_p)}\right]$$

which simplifies to

$$\left[\frac{\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p}{\cos\theta_p\Delta x_q - \sin\theta_p\Delta y_q} \quad \frac{\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p}{\cos\theta_p\Delta x_q - \sin\theta_p\Delta y_q} \quad \frac{\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p}{\sin\theta_p\Delta x_q + \cos\theta_p\Delta y_q} \quad \frac{\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p}{\sin\theta_p\Delta x_q + \cos\theta_p\Delta y_q} \quad 1\right]$$

Recall this vector was assumed constant, leading to

$$\frac{\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p}{\cos\theta_p\Delta x_q - \sin\theta_p\Delta y_q} = \frac{\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p}{\sin\theta_p\Delta x_q + \cos\theta_p\Delta y_q} = 1 \tag{7.6}$$

yielding

$$\left\{\begin{array}{rcl} \cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p & = & \cos\theta_p\Delta x_q - \sin\theta_p\Delta y_q \\ \sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p & = & \sin\theta_p\Delta x_q + \cos\theta_p\Delta y_q \end{array}\right.$$

$$\Rightarrow \left\{\begin{array}{rcl} \cos\theta_p(\Delta x_p - \Delta x_q) & = & \sin\theta_p(\Delta y_p - \Delta y_q) \\ \cos\theta_p(\Delta y_p - \Delta y_q) & = & \sin\theta_p(-(\Delta x_p - \Delta x_q)) \end{array}\right.$$

$$\Rightarrow \left\{\begin{array}{rcl} \dfrac{\cos\theta_p}{\sin\theta_p} & = & \dfrac{\Delta y_p - \Delta y_q}{\Delta x_p - \Delta x_q} \\ \dfrac{\cos\theta_p}{\sin\theta_p} & = & \dfrac{-(\Delta x_p - \Delta x_q)}{\Delta y_p - \Delta y_q} \end{array}\right.$$

This gives

$$\frac{\Delta y_p - \Delta y_q}{\Delta x_p - \Delta x_q} = \frac{-(\Delta x_p - \Delta x_q)}{\Delta y_p - \Delta y_q} \Rightarrow -(\Delta x_p - \Delta x_q)^2 = (\Delta y_p - \Delta y_q)^2$$

Because the left side of this equation is smaller or equal to zero and the right side larger or equal to zero, both sides must be zero:

$$\Rightarrow \left\{\begin{array}{rcl} \Delta x_p - \Delta x_q & = & 0 \\ \Delta y_p - \Delta y_q & = & 0 \end{array}\right. \Rightarrow \left\{\begin{array}{rcl} \Delta x_p & = & \Delta x_q \\ \Delta y_p & = & \Delta y_q \end{array}\right. \tag{7.7}$$

This condition demands that the middles of the sides p and q are situated at the same point, which is impossible for all cell shapes. Now we have arrived at a contradiction: both (7.2) and (7.3) are not possible. So our primary assumption must have been wrong: the elementwise division of two rows of M cannot produce a constant vector. Thus can be concluded that a one-to-one linear dependency of rows in M is never possible and hence Lemma 7.1 has been proven. ∎

7.2 Dependency of one row on two other rows

A row which can be formed out of two other rows is another indicator of linear dependency. To see under which conditions this can take place, consider the three rows **p**, **q**, and **r**. If they are linear dependent, there exist a, b such that

$$a\mathbf{p} + b\mathbf{q} = \mathbf{r}$$

To see when this is solvable, write it as

$$\begin{pmatrix} (\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\cos\theta_p & (\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\cos\theta_q \\ (\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\sin\theta_p & (\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\sin\theta_q \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$= \begin{pmatrix} (\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\cos\theta_r \\ (\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\sin\theta_r \end{pmatrix}$$

$$\begin{pmatrix} (\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\cos\theta_p & (\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\cos\theta_q \\ (\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\sin\theta_p & (\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\sin\theta_q \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$= \begin{pmatrix} (\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\cos\theta_r \\ (\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\sin\theta_r \end{pmatrix}$$

$$a\sin\theta_p\cos\theta_p + b\sin\theta_q\cos\theta_q = \sin\theta_r\cos\theta_r$$

and solve the first two matrix-vector equations

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\sin(\theta_q-\theta_r)}{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\sin(\theta_q-\theta_p)} \\ \frac{(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\sin(\theta_r-\theta_p)}{(\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\sin(\theta_q-\theta_p)} \end{pmatrix} \tag{7.8}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\sin(\theta_q-\theta_r)}{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\sin(\theta_q-\theta_p)} \\ \frac{(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\sin(\theta_r-\theta_p)}{(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\sin(\theta_q-\theta_p)} \end{pmatrix} \tag{7.9}$$

Equal them to each other

$$\frac{\sin(\theta_q-\theta_r)}{\sin(\theta_q-\theta_p)}\left(\frac{\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r}{\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p} - \frac{\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r}{\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p}\right) = 0 \tag{7.10}$$

$$\frac{\sin(\theta_r-\theta_p)}{\sin(\theta_q-\theta_p)}\left(\frac{\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r}{\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q} - \frac{\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r}{\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q}\right) = 0 \tag{7.11}$$

We will first prove that the parts outside the parentheses

$$\frac{\sin(\theta_q-\theta_r)}{\sin(\theta_q-\theta_p)} \quad \text{and} \quad \frac{\sin(\theta_r-\theta_p)}{\sin(\theta_q-\theta_p)} \tag{7.12}$$

cannot equal zero, to finally conclude that the parts inside do have to equal zero in order to solve these equations.

First assume that one of the abovementioned parts (7.12) is zero and the other one non-zero. This would yield a zero last part of the fractions in the expressions for either a or b. That would imply a completely zero a or b and consequently a dependency from one row on one other row (recall that $a\mathbf{p}+b\mathbf{q}=\mathbf{r}$) - which has been proven to be impossible-, unless the first parts of the fractions expressing a or b could become infinite and the final outcome of the complete fraction could differ from zero. However, it is impossible that the two first parts of the fractions in the two expressions for either a or b

$$\frac{(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)}{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta x_p)} \text{ and } \frac{(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)}{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)}$$

both become infinity at the same time (see the Remark in the proof of Lemma 7.1 applied to the denominators of these fractions).

If the parts outside the parentheses (7.12) would simultaneously equal zero, we would even obtain a zero-valued row $\mathbf{r}$. A quick look at the matrix M shows this is not possible: the fifth column demands in this case a zero $\sin\theta_r$ or $\cos\theta_r$ (and thus respectively a $\cos\theta_r$ or $\sin\theta_r$ valued 1). For $\sin\theta_r = 0$ and $\cos\theta_r = 1$ the vector $\mathbf{r}$ then equals

$$[\Delta x_r \;\; 0 \;\; \Delta y_r \;\; 0 \;\; 0]$$

and for $\cos\theta_r = 0$ and $\sin\theta_r = 1$ it is equal to

$$[0 \;\; -\Delta y_r \;\; 0 \;\; \Delta x_r \;\; 0]$$

So $\mathbf{r}$ can only become completely zero by the impossible condition $\Delta x_r = \Delta y_r = 0$.
Now the parts outside the parentheses in (7.10) and (7.11) cannot equal zero, the parts inside must be zero in order to solve those equations. Hence we are left with

$$\frac{\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r}{\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p} = \frac{\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r}{\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p} \tag{7.13}$$

$$\frac{\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r}{\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q} = \frac{\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r}{\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q} \tag{7.14}$$

Unfortunately it is not really evident to see whether these equations lead to the conclusion that the rows of M cannot be constructed out of two other rows or otherwise motivate constraints on either the θ_f (the directions of the normals) or the Δx_f and Δy_f (the location of the center). The fifth equation (6.8), which has not been taken into consideration in the abovementioned derivation, can add even more constraints. However, if we lose a bit of generality and make a choice for a specific center, there can be drawn conclusions, as is shown in Chapter 8.

7.3 Dependency of one row on three other rows

It is to be expected that other general formulas considering the linear dependency of a row on three or more rows will be even more complicated and will also not lead to clear constraints for the shape or the center of a cell. Despite of this, a general condition for the linear dependency of three rows will be derived, so that it can serve as a starting point in the case that a choice for a specific center has been made.
Assume a row $\mathbf{s}$ can be expressed in three other rows $\mathbf{p}, \mathbf{q}$ and $\mathbf{r}$

$$a\mathbf{p} + b\mathbf{q} + c\mathbf{r} = \mathbf{s}$$

In order to avoid huge formulas imposed by resolving a 3×3 linear system, we chose to use the same method as in the case of dependency on two rows. This results in a slightly peculiar way to derive conditions that make this equation solvable. Rewrite the first four equations to

$$\begin{pmatrix} (\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\cos\theta_p & (\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\cos\theta_q \\ (\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\sin\theta_p & (\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\sin\theta_q \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$= \begin{pmatrix} (\cos\theta_s\Delta x_s - \sin\theta_s\Delta y_s)\cos\theta_s - c(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\cos\theta_r \\ (\cos\theta_s\Delta x_s - \sin\theta_s\Delta y_s)\sin\theta_s - c(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\sin\theta_r \end{pmatrix} \tag{7.15}$$

$$\begin{pmatrix} (\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\cos\theta_p & (\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\cos\theta_q \\ (\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\sin\theta_p & (\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\sin\theta_q \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$= \begin{pmatrix} (\sin\theta_s\Delta x_s + \cos\theta_s\Delta y_s)\cos\theta_s - c(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\cos\theta_r \\ (\sin\theta_s\Delta x_s + \cos\theta_s\Delta y_s)\sin\theta_s - c(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\sin\theta_r \end{pmatrix} \tag{7.16}$$

and solve these two matrix-vector equations for a and b

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{(\cos\theta_s\Delta x_s - \sin\theta_s\Delta y_s)\sin(\theta_q-\theta_s) + c(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\sin(\theta_r-\theta_q)}{(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)\sin(\theta_q-\theta_p)} \\ \frac{(\cos\theta_s\Delta x_s - \sin\theta_s\Delta y_s)\sin(\theta_s-\theta_p) + c(\cos\theta_r\Delta x_r - \sin\theta_r\Delta y_r)\sin(\theta_p-\theta_r)}{(\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\sin(\theta_q-\theta_p)} \end{pmatrix} \tag{7.17}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{(\sin\theta_s\Delta x_s + \cos\theta_s\Delta y_s)\sin(\theta_q-\theta_s) + c(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\sin(\theta_r-\theta_q)}{(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)\sin(\theta_q-\theta_p)} \\ \frac{(\sin\theta_s\Delta x_s + \cos\theta_s\Delta y_s)\sin(\theta_s-\theta_p) + c(\sin\theta_r\Delta x_r + \cos\theta_r\Delta y_r)\sin(\theta_p-\theta_r)}{(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\sin(\theta_q-\theta_p)} \end{pmatrix} \tag{7.18}$$

Again, equal them to each other and solve for c

$$c = \frac{\sin(\theta_q-\theta_s)(\sin(\theta_s-\theta_p)(\Delta x_p\Delta x_s + \Delta y_p\Delta y_s) + \cos(\theta_s-\theta_p)(\Delta x_p\Delta y_s - \Delta y_p\Delta x_s))}{\sin(\theta_r-\theta_q)(\sin(\theta_p-\theta_r)(\Delta x_r\Delta x_p + \Delta y_r\Delta y_p) + \cos(\theta_p-\theta_r)(\Delta x_r\Delta y_p - \Delta y_r\Delta x_p))} \tag{7.19}$$

$$c = \frac{\sin(\theta_s-\theta_p)(\sin(\theta_s-\theta_q)(\Delta x_q\Delta x_s + \Delta y_q\Delta y_s) + \cos(\theta_s-\theta_q)(\Delta x_q\Delta y_s - \Delta y_q\Delta x_s))}{\sin(\theta_p-\theta_r)(\sin(\theta_q-\theta_r)(\Delta x_r\Delta x_q + \Delta y_r\Delta y_q) + \cos(\theta_q-\theta_r)(\Delta x_r\Delta y_q - \Delta y_r\Delta x_q))} \tag{7.20}$$

A condition for linear dependency of one row on three others is that these two expressions for c are equal. This is not enough to ensure the linear dependency, as also the fifth equation (6.8) needs to be considered, but it does exclude various possibilities, which will be showed in Chapter 8.

An important remark regarding the preceding derivation is that silently the assumption of non-zero determinants of the matrices in the matrix-vector equations (7.15) and (7.16) has been made, in order to solve them and obtain conditions for the shape of the cell. This was necessary due to our devious solution method. If it turns out the determinants do equal zero, either no vector at all or the span of a vector solves the equation, depending on the right hand side. However, before even investigating these possible outcomes, it suffices to take a look at the two determinants

$$(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p)(\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q)\sin(\theta_q-\theta_p)$$

$$(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p)(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q)\sin(\theta_q-\theta_p)$$

and observe that in any shape, there always exist two faces f and g which are not parallel, so for which $\sin(\theta_g - \theta_f) \neq 0$. Without loss of generality those two sides can be chosen p and q, and the remaining options for (one of) the determinants to become 0 are

$$(\cos\theta_p\Delta x_p - \sin\theta_p\Delta y_p) = 0 \tag{7.21a}$$

$$(\cos\theta_q\Delta x_q - \sin\theta_q\Delta y_q) = 0 \tag{7.21b}$$

$$(\sin\theta_p\Delta x_p + \cos\theta_p\Delta y_p) = 0 \tag{7.21c}$$

$$(\sin\theta_q\Delta x_q + \cos\theta_q\Delta y_q) = 0 \tag{7.21d}$$

However, these equations do not impose constraints on the relationships between the faces, but on the orientation of the faces on their own. This could result in problems while rotating the cell, because that changes the orientation. While designing the grid, one does not want to take into account the actual orientation of the axes. One should be able to rotate a cell without causing it to be invalid; from here on we shall call these valid cell shapes *rotatable shapes*.
Because of this rotatability condition, it is unlikely that the possibility of the determinant equalling zero (and the corresponding constraints) lead to a new category of allowed shapes, but nevertheless this will be investigated in further detail when a choice for the center is made.

Chapter 8

Shapes with a circumcenter

The equations derived in the previous chapter were too general to produce restrictions on cell shapes. Hence a choice for the specific center of the cell is made. In our work, we will mainly focus on the circumcenter. This choice is based on the article of Perot [5], where also the circumcenter is used. A secondary motivation was given by the fact that it implies a more accurate implementation of the divergence operator, since the distance δn_f between the centers of two neighbouring cells (used in the definition of D_c, see (2.5)) is in that case simply the sum of the the distances of the centers of the individual cells to the middle of the shared face.

$$\delta n_f = W_f^k + W_f^j \tag{8.1}$$

where W_f^k stands for the distance of the face f to the center of the cell k (see Figures 8.1 and 8.2).

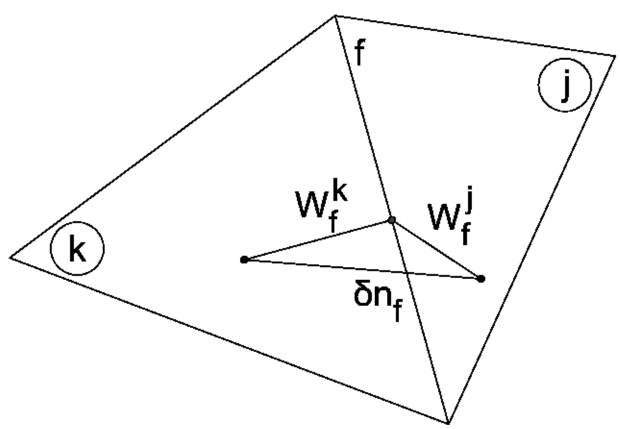

Figure 8.1: δn_f in a cell with a random center

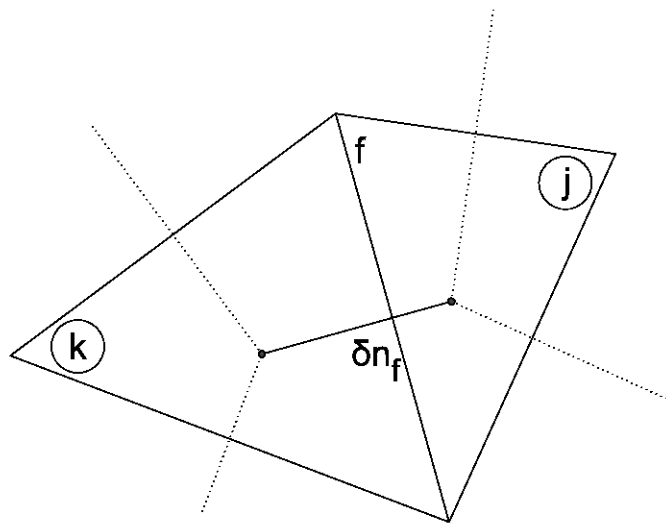

Figure 8.2: δn_f in a cell with a circumcenter

The equation (8.1) holds, because the line through the circumcenter of cell k and perpendicular on a face f bisects this face by definition. As this is also valid for cell j and face f, the both circumcenters must be situated on the same line. The length of this line is of course the distance between the both circumcenters, but by the perpendicularity to the face f, it is also the sum of the distances of the circumcenters to the face. When other definitions of cell centres are used, the equal sign in (8.1) disappears and it will become an estimate, which emphasizes the advantage of the choice for the circumcenter.
This choice does include some restrictions for the allowed triangles in the triangulated grid though. When obtuse triangles are used, the circumcenters would be situated outside the cells. This causes problems when their positions happen to coincide: the distance between the circumcenters δn_f returns zero, so the diffusive operator will break down. Right triangles might also be problematic, since their circumcenters are located on the hypotenuse. When two of those triangles share their hypotenuse, the circumcenters again coincide. This makes a grid with acute triangles necessary. Nevertheless, this leaves us enough freedom to construct grids and is worth to be investigated more thoroughly, considering the advantages of the triangulated grids while treating curved areas.

Using the circumcenter, the distances Δx_f and Δy_f can be expressed in the angle θ_f of the normal n_f with the positive x-axis

$$\Delta x_f = R_f \cos\theta_f \tag{8.2a}$$

$$\Delta y_f = R_f \sin\theta_f \tag{8.2b}$$

where R_f is the Euclidian distance from the middle of the cell to the circumcenters. This is visualized in the Figure 8.3

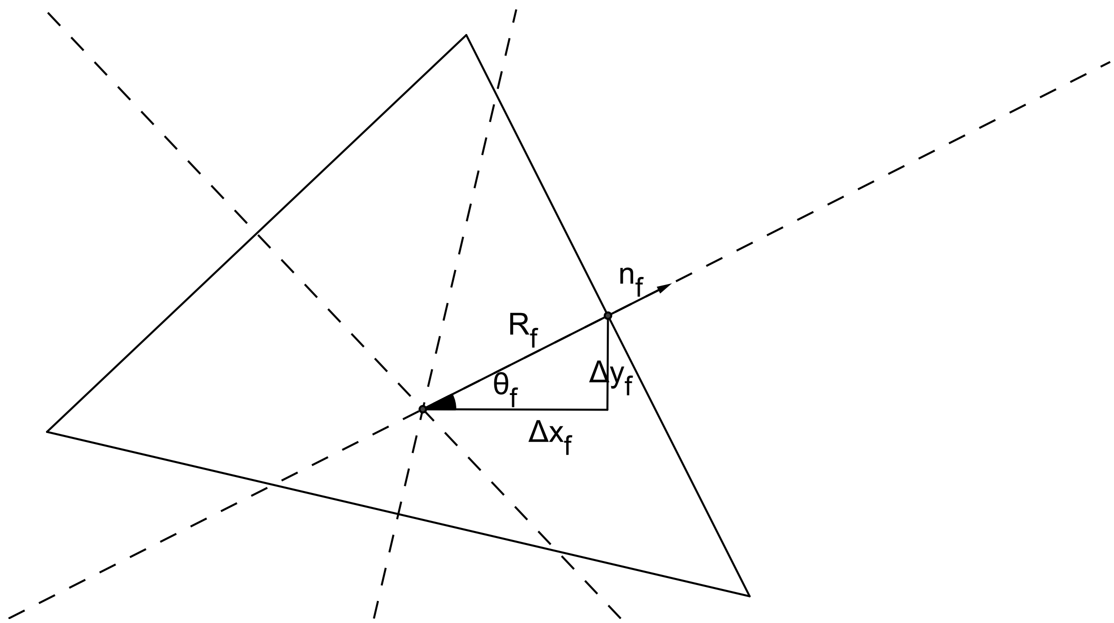

Figure 8.3: Δx_f and Δy_f expressed in θ_f

In other words, the vector from the center to the middle of any face points in the same direction as the normal on that face. In general, shapes with four or more sides do not possess a circumcenter - obviously only if their nodes are collocated on a circle - but triangles always do. Actually, we are only interested in the shapes with an *interior* circumcenter, but this extra constraint is superfluous in the triangle case, as we are about to proof a theorem valid for all sorts of triangles. In fact, it gives the answer to the main topic posed in the introduction of this work: is it possible to develop a fully conservative, symmetry-preserving discretization on a triangulated mesh using the technique of shift transformations? The fairly surprising answer to this question is *no, at least not a sufficiently accurate one*, stated in the following theorem

Theorem 8.1 *Using the circumcenter as the center of the cell, it is impossible to construct a second order accurate shift transformation on any triangle.*

Before we proof this, we will first proof the next Lemma.

Lemma 8.2 *Using the circumcenter as the center of the cell, a row of M cannot be a linear combination of two other rows.*

Proof When the characteristics of a circumcenter (8.2) are substituted in the equations for linear dependency on two other rows ((7.13) and (7.14) from Chapter 7), they simplify to

$$\begin{cases} \dfrac{R_r(\cos^2\theta_r - \sin^2\theta_r)}{R_p(\cos^2\theta_p - \sin^2\theta_p)} = \dfrac{R_r(2\sin\theta_r\cos\theta_r)}{R_p(2\sin\theta_p\cos\theta_p)} \\ \dfrac{R_r(\cos^2\theta_r - \sin^2\theta_r)}{R_q(\cos^2\theta_q - \sin^2\theta_q)} = \dfrac{R_r(2\sin\theta_r\cos\theta_r)}{R_q(2\sin\theta_q\cos\theta_q)} \end{cases}$$

so, using trigonometric formulas and the fact that $R_f \neq 0 \,\forall f$,

$$\begin{cases} \dfrac{\cos(2\theta_r)}{\cos(2\theta_p)} & = & \dfrac{\sin(2\theta_r)}{\sin(2\theta_p)} \\ \dfrac{\cos(2\theta_r)}{\cos(2\theta_q)} & = & \dfrac{\sin(2\theta_r)}{\sin(2\theta_q)} \end{cases} \Rightarrow \begin{cases} \tan(2\theta_r) & = & \tan(2\theta_p) \\ \tan(2\theta_r) & = & \tan(2\theta_q) \end{cases} \Rightarrow \begin{cases} 2\theta_r & = & 2\theta_p \bmod 180^\circ \\ 2\theta_r & = & 2\theta_q \bmod 180^\circ \end{cases}$$

and finally leading to the condition necessary for linear dependency of one row on two others

$$\theta_r = \theta_p \bmod 90^\circ = \theta_q \bmod 90^\circ \tag{8.3}$$

This result already excludes triangles as shapes with a linear dependency of one row on two others, for as it says that each angle between the three sides p, q and r should be a multiple of 90° (i.e. the three sides form an 'open square') to ensure this linear dependency. Hence it is strong enough to use in the proof of Theorem 8.1, but in order to be able to draw future conclusions regarding quadrilaterals, we will continue the proof of Lemma 8.2.
Recall the expressions (7.8) and (7.9) for a and b, applied on shapes with a circumcenter

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{R_r \cos(2\theta_r)\sin(\theta_q-\theta_r)}{R_p \cos(2\theta_p)\sin(\theta_q-\theta_p)} \\ \frac{R_r \cos(2\theta_r)\sin(\theta_r-\theta_p)}{R_q \cos(2\theta_q)\sin(\theta_q-\theta_p)} \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{R_r \sin(2\theta_r)\sin(\theta_q-\theta_r)}{R_p \sin(2\theta_p)\sin(\theta_q-\theta_p)} \\ \frac{R_r \sin(2\theta_r)\sin(\theta_r-\theta_p)}{R_q \sin(2\theta_q)\sin(\theta_q-\theta_p)} \end{pmatrix}$$

Now look again at the just derived condition (8.3) for linear dependency on two rows, which implies

$$\cos(2\theta_r) = \pm\cos(2\theta_p) \ \text{ and } \ \cos(2\theta_r) = \pm\cos(2\theta_q)$$

which turns the expressions for a and b into

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \pm\frac{R_r \sin(\theta_q-\theta_r)}{R_p \sin(\theta_q-\theta_p)} \\ \pm\frac{R_r \sin(\theta_r-\theta_p)}{R_q \sin(\theta_q-\theta_p)} \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \pm\frac{R_r \sin(\theta_q-\theta_r)}{R_p \sin(\theta_q-\theta_p)} \\ \pm\frac{R_r \sin(\theta_r-\theta_p)}{R_q \sin(\theta_q-\theta_p)} \end{pmatrix}$$

Moreover, note that sines of the pairwise differences between the angles θ_p, θ_q and θ_r appear: $\sin(\theta_q - \theta_r)$, $\sin(\theta_q - \theta_p)$ and $\sin(\theta_r - \theta_p)$. Keep in mind that in a cell the angles θ of two faces cannot be the same (that would imply two coinciding faces) and that a face can have at most one other parallel face. If these sines are now to satisfy (8.3) -which states that the angles between the faces are a multiple of 90°- two of the sines result in ± 1 (the ones in which the θ's differ 90° and 270°) and one returns zero (in which the θ's differ 180°). Put differently: two of the three sides form a pair of parallel sides, the other side is perpendicular. If $\sin(\theta_q - \theta_r)$ or $\sin(\theta_r - \theta_p)$ would be zero, a or respectively b would also become zero, leading to an impossible dependency of one row on one other row. However, $\sin(\theta_q - \theta_p) = 0$ brings about an infinite a and b, which is also not allowed. Consequently, there exists no shape with a circumcenter which can satisfy the conditions for one row being a linear combination of two other rows (8.3). Thereby Lemma 8.2 has been proven. ∎

With this observation, we arrive at proving the main theorem of this work, Theorem 8.1.

Proof of Theorem 8.1 As a triangle only consists of three faces, the matrix M also has only three rows. Theorem 6.3 tells us that the rank of M needs to be reduced in order to ensure a second order accurate shift transformation. The rank of a matrix is the same as the row rank of a matrix, so at least one of the rows should be linear dependent to reduce it. However, Lemma 7.1 and Lemma 8.2 show that a row can never be a multiple of one single other row and neither a combination of two other rows, so there are no linear dependent rows. Thereby Theorem 8.1 has been proven. ∎

Now the primary question of our research has been answered, we can carry on with our investigation by considering shapes with more sides. The proof of Theorem 8.1 is unfortunately not sufficient yet to conclude anything regarding these shapes in combination with a circumcenter, because it passes by on the possibility of a row depending linearly on three or more other rows. It turns out that this extra opportunity to reduce the row rank of M (induced by the use of at least four sides) does lead to possible cellshapes. This was to be expected, as the original formula of Hicken *et al.* [3] works on a square. In fact,

Lemma 8.3 *Using the circumcenter as the center of the cell, every shape consisting of (at least) two pairs of parallel sides is suitable for constructing a second order accurate shift transformation, assuming the velocity field is incompressible and induced by a potential.*

Proof According to Theorem 6.1 is suffices to check whether a shape with two pairs of parallel sides combined with a circumcenter really makes a row of M linearly dependent on other rows and thus decreases the rank of M. It was already proven that a row could not be linearly dependent on one or two other rows (see Lemma 7.1 and Lemma 8.2), but we will see that this specific shape with two pairs of parallel sides does make a row dependent on three others. Therefore, we assume $(\mathbf{p}, \mathbf{r})$ and $(\mathbf{q}, \mathbf{s})$ are the parallel pairs, so their angles relate as $\theta_p = \theta_r + 180°$ and $\theta_q = \theta_s + 180°$. Substitute these θ_f's and the characteristics of the circumcenter (8.2) in the matrix M and note that these two pairs of parallel sides are related to each other with similar constants as used for the parallelogram (see Chapter 5)

$$a\mathbf{p} + b\mathbf{q} + c\mathbf{r} = d\mathbf{s}$$

with

$$[a\ b\ c\ d] = [-R_r(R_q + R_s)\sin\theta_q\cos\theta_q \qquad R_s(R_p + R_r)\sin\theta_p\cos\theta_p$$
$$-R_p(R_q + R_s)\sin\theta_q\cos\theta_q \qquad R_q(R_p + R_r)\sin\theta_p\cos\theta_p]$$

This can be easily verified by substituting $\mathbf{p}, \mathbf{r}, \mathbf{q}$ and $\mathbf{s}$ and elaborating the equation. Thereby Lemma 8.3 has been proven. ∎

Moreover, consisting of at least two pairs of parallel sides is not only sufficient for a shape to be able to define a second order accurate shift transformation on it, the following Lemma proves it is also necessary.

Lemma 8.4 *Using the circumcenter as the center of the cell, the only possible rotatable shape that makes a row of M linearly dependent on three other rows, is one with two pairs of parallel sides.*

Proof To verify whether a shape with two pairs of parallel sides is the only possible shape, we will use the derivation of Chapter 7 and consequently the assumption that side p and q are not parallel (which can be done, as argued, without loss of generality). Likewise the proof of Lemma 8.2, start with substituting the characteristics of a circumcenter (8.2) in the equations for linear dependency on three other rows (7.19) and (7.20). The first equation yields

$$\begin{aligned}
\text{counter } c &= \sin(\theta_q-\theta_s)(\sin(\theta_s-\theta_p)R_pR_s(\cos\theta_p\cos\theta_s+\sin\theta_p\sin\theta_s)\\
&\quad+\cos(\theta_s-\theta_p)R_pR_s(\cos\theta_p\sin\theta_s-\sin\theta_p\cos\theta_s))\\
\text{denominator } c &= \sin(\theta_r-\theta_q)(\sin(\theta_p-\theta_r)R_rR_p(\cos\theta_r\cos\theta_p+\sin\theta_r\sin\theta_p)\\
&\quad+\cos(\theta_p-\theta_r)R_rR_p(\cos\theta_r\sin\theta_p-\sin\theta_r\cos\theta_p))
\end{aligned}$$

and the second one

$$\begin{aligned}
\text{counter } c &= \sin(\theta_s-\theta_p)(\sin(\theta_s-\theta_q)R_qR_s(\cos\theta_q\cos\theta_s+\sin\theta_q\sin\theta_s)\\
&\quad+\cos(\theta_s-\theta_q)R_qR_s(\cos\theta_q\sin\theta_s-\sin\theta_q\cos\theta_s))\\
\text{denominator } c &= \sin(\theta_p-\theta_r)(\sin(\theta_q-\theta_r)R_rR_q(\cos\theta_r\cos\theta_q+\sin\theta_r\sin\theta_q)\\
&\quad+\cos(\theta_q-\theta_r)R_rR_q(\cos\theta_r\sin\theta_q-\sin\theta_r\cos\theta_q))
\end{aligned}$$

Use the trigonometric addition formulas:

$$c=\frac{R_s\sin(\theta_q-\theta_s)(\sin(\theta_s-\theta_p)\cos(\theta_s-\theta_p)+\cos(\theta_s-\theta_p)\sin(\theta_s-\theta_p))}{R_r\sin(\theta_r-\theta_q)(\sin(\theta_p-\theta_r)\cos(\theta_p-\theta_r)+\cos(\theta_p-\theta_r)\sin(\theta_p-\theta_r))} \tag{8.4}$$

$$c=\frac{R_s\sin(\theta_s-\theta_p)(\sin(\theta_s-\theta_q)\cos(\theta_s-\theta_q)+\cos(\theta_s-\theta_q)\sin(\theta_s-\theta_q))}{R_r\sin(\theta_p-\theta_r)(\sin(\theta_q-\theta_r)\cos(\theta_q-\theta_r)+\cos(\theta_q-\theta_r)\sin(\theta_q-\theta_r))} \tag{8.5}$$

Equalling them to each other gives (again use $R_f \neq 0\ \forall f$)

$$\frac{2\sin(\theta_q-\theta_s)\sin(\theta_s-\theta_p)\cos(\theta_s-\theta_p)}{2\sin(\theta_r-\theta_q)\sin(\theta_p-\theta_r)\cos(\theta_p-\theta_r)}=\frac{2\sin(\theta_s-\theta_p)\sin(\theta_s-\theta_q)\cos(\theta_s-\theta_q)}{2\sin(\theta_p-\theta_r)\sin(\theta_q-\theta_r)\cos(\theta_q-\theta_r)}$$

So

$$\frac{\sin(\theta_q-\theta_s)\sin(\theta_s-\theta_p)}{\sin(\theta_p-\theta_r)\sin(\theta_r-\theta_q)}\left(\frac{\cos(\theta_s-\theta_p)}{\cos(\theta_p-\theta_r)}-\frac{\cos(\theta_s-\theta_q)}{\cos(\theta_q-\theta_r)}\right)=0$$

Trigonometric addition formulas rewrite the part between the brackets and the total becomes

$$\frac{\sin(\theta_q-\theta_s)\sin(\theta_s-\theta_p)\sin(\theta_q-\theta_p)\sin(\theta_r-\theta_s)}{\sin(\theta_p-\theta_r)\sin(\theta_r-\theta_q)\cos(\theta_p-\theta_r)\cos(\theta_r-\theta_q)}=0$$

The solutions to this equation are $\sin(\theta_q-\theta_s)=0$, $\sin(\theta_s-\theta_p)=0$, $\sin(\theta_r-\theta_s)=0$ and $\sin(\theta_q-\theta_p)=0$, where the last one is not valid due to the assumption about the non-parallel sides p and q. So

$$\theta_q=\theta_s+180^\circ \tag{8.6a}$$

$$\theta_s=\theta_p+180^\circ \tag{8.6b}$$

$$\theta_r=\theta_s+180^\circ \tag{8.6c}$$

(recall that two angles θ cannot be the same in a convex cell).
Considering the first two possibilities, at first glance this would imply $c=0$ in (8.4) and (8.5)

and so an impossible dependency of one row on two others. But if the denominator of c will also become zero (of course in both expressions for c, for as they are to equal each other), c can have another value. This happens in (8.4) if $\sin(\theta_r - \theta_q) = 0$ or $\sin(2(\theta_p - \theta_r)) = 0$ and in (8.5) if $\sin(\theta_p - \theta_r) = 0$ or $\sin(2(\theta_q - \theta_r)) = 0$, so if at least one condition out of each of the following two lists holds (where the first column refers to the conditions induced by (8.4) and the second to the conditions induced by (8.5))

$$\begin{array}{rlcrl} \theta_r = & \theta_q + 180^\circ & \quad & \theta_r = & \theta_p + 180^\circ \\ \theta_r = & \theta_p + 90^\circ & & \theta_r = & \theta_q + 90^\circ \\ \theta_r = & \theta_p + 180^\circ & & \theta_r = & \theta_q + 180^\circ \\ \theta_r = & \theta_p + 270^\circ & & \theta_r = & \theta_q + 270^\circ \end{array}$$

By analyzing this together with (8.6) we can find all the valid combinations (without overlapping θ's). For example, start with (8.6a), i.e. $\theta_q = \theta_s + 180^\circ$. Now we cannot choose $\theta_r = \theta_q + 180^\circ$ from the left list anymore, because in that case $\theta_r = \theta_q + 180^\circ = \theta_s + 180^\circ + 180^\circ = \theta_s$, which comes down to overlapping θ's. Proceed to the next option from the left list, $\theta_r = \theta_p + 90^\circ$. This one appears to be possible to choose and we are now only to select one from the list on the right. The first one is impossible, as we already chose $\theta_r = \theta_p + 90^\circ$. The second one fails too, because the combination $\theta_r = \theta_p + 90^\circ$ and $\theta_r = \theta_q + 90^\circ$ would imply $\theta_p = \theta_q$. The third option has to be dropped due to the same reasons as the first item from the left list, and the fourth and last one $\theta_r = \theta_q + 270^\circ$ combines with $\theta_r = \theta_p + 90^\circ$ (our current choice from the left list) into $\theta_p = \theta_q + 180^\circ$. This does not get along with our inicial equation, i.e. $\theta_q = \theta_s + 180^\circ$, because it causes overlapping θ_p and θ_s. Thus can be concluded that the second item on the left list is also not a valid combination with (8.6a). A similar argument applies to the fourth item on the left list, whereas the third one, $\theta_r = \theta_p + 180^\circ$ appears in both lists and serves as the only correct choice. This, together with an analysis of (8.6b) executed in the same manner, results in

$$\theta_q = \theta_s + 180^\circ \text{ and } \theta_r = \theta_p + 180^\circ \tag{8.7a}$$

$$\theta_s = \theta_p + 180^\circ \text{ and } \theta_r = \theta_q + 180^\circ \tag{8.7b}$$

The third possibility (8.6c) substituted in the equations for c (8.4) and (8.5) gives $c = -R_s/R_r$. Now recall (7.17) and (7.18), adapted to the use of a circumcenter

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{R_s \cos(2\theta_s)\sin(\theta_q - \theta_s) + cR_r \cos(2\theta_r)\sin(\theta_r - \theta_q)}{R_p \cos(2\theta_p)\sin(\theta_q - \theta_p)} \\ \frac{R_s \cos(2\theta_s)\sin(\theta_s - \theta_p) + cR_r \cos(2\theta_r)\sin(\theta_p - \theta_r)}{R_q \cos(2\theta_q)\sin(\theta_q - \theta_p)} \end{pmatrix} \tag{8.8}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{R_s \sin(2\theta_s)\sin(\theta_q - \theta_s) + cR_r \sin(2\theta_r)\sin(\theta_r - \theta_q)}{R_p \sin(2\theta_p)\sin(\theta_q - \theta_p)} \\ \frac{R_s \sin(2\theta_s)\sin(\theta_s - \theta_p) + cR_r \sin(2\theta_r)\sin(\theta_p - \theta_r)}{R_q \sin(2\theta_q)\sin(\theta_q - \theta_p)} \end{pmatrix} \tag{8.9}$$

Substitute $c = R_s/R_r$ and combine this with $\theta_r = \theta_s + 180^\circ$ to obtain zero-valued counters of a and b. This means an impossible one-to-one dependency of rows, unless the denominator of a and b also becomes zero, in both (8.8) as in (8.9). Observe that $R_f \neq 0\ \forall f$ and moreover $\sin(2\theta_f)$ and $\cos(2\theta_f)$ cannot simultaneously become zero, so the only remaining option would be $\sin(\theta_q - \theta_p) = 0$. However, this is also rejected, because p and q were assumed not to be parallel. So finally, the only shapes possible to make a row of M linearly dependent on 3 other rows, are those who satisfy (8.7), which means that the shape must consist of (at least) 2 pairs of parallel sides.

As mentioned before, the determinant of the system becomes zero if one of the four equations (7.21) is satisfied. These simplify in the case of a circumcenter to

$$\begin{aligned} \cos 2\theta_p &= 0 \\ \cos 2\theta_q &= 0 \\ \sin 2\theta_p &= 0 \\ \sin 2\theta_q &= 0 \end{aligned}$$

and thus to $\theta_p = 0 \bmod 90°$ or $\theta_q = 0 \bmod 90°$. But as this restricts the rotatability, it is not yielding any new possibilities for rotatable shapes and hence there is no need for further investigation. Thereby Lemma 8.4 has been proven. $\blacksquare$

It should be noted that Lemma 8.4 does not imply that a shape has to exist of at least two parallel pairs to reduce the rank of M and thereby create the possibility of a second order accurate shift transformation; this because it only treats dependency of one row on three others, and not on more than three. If there are only four rows in M -i.e. if we are considering quadrilaterals- Lemma 8.4 does have consequences though, expressed in the following Corollary.

Corollary 8.5 *Using the circumcenter as the center of the cell, the only rotatable quadrilaterals on which a second order accurate shift transformation can be defined, are the rectangles.*

Proof In case of a four-sided cell, Lemma 8.4 tells it has to be a parallelogram. In using the circumcenter, we implicitly assumed it exists. However, in general parallelograms do not possess circumcenter, which is conceived easily considering Figure 8.4

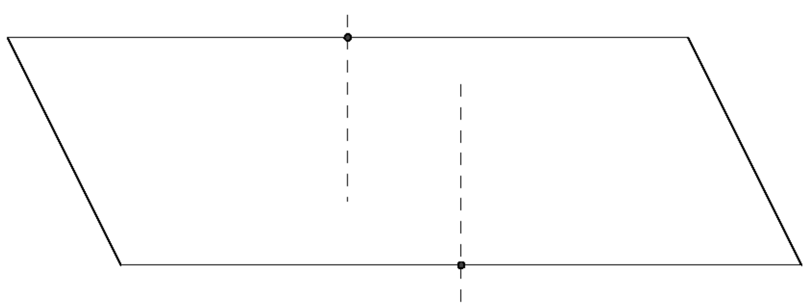

Figure 8.4: Parallelogram with lines indicating equal distance to pairs of cornerpoints

In this figure, the two dashed vertical lines indicate the points with equal distance to respectively the upper two and the lower two cornerpoints of the parallelogram. Realizing that the circumcenter is defined as having the same distance towards all the cornerpoints, it should be situated on the intersection of the vertical lines. But this intersection trivially does not exist, unless these two lines completely coincide. This only happens in a parallelogram with two perpendicular pairs of parallel sides, i.e. rectangles. However, so far this still only has been proven on VF_{IP}, because the proof is based on M. To determine the appropriate shapes on VF_I, we consider the appropriate shapes on VF_{IP} and test whether they remain valid without the potential field assumption (as argued at the end of Chapter 6). In this case it is easy, as we already figured at the end of Chapter 5 that a rectangle is a rotatable shape on any velocity field while using equal C_f's. Hence Corollary 8.5 has now also been proven on incompressible velocity fields in general. ∎

One might have noticed that Lemma 8.3 is only valid on VF_{IP}. However, Corollary 8.5 already treats the quadrilateral case on VF_I. Moreover,pentagons do not have to be considered, because one cannot construct a pentagon with two pairs of parallel sides. So there are no suitable pentagons on VF_{IP} which can be tested upon their applicability on VF_I. Finally, Lemma 8.3 is superfluous regarding hexagons and shapes with even more sides -this will be explained in the next chapter- and thereby it is no good trying to extend Lemma 8.3 to VF_I.

Chapter 9

Other centers and more faces

So far, triangles and quadrilaterals in combination with a circumcenter were treated. Of course, other choices for a center are possible and the investigation can be extended to shapes with more than four faces.

Triangles. It was shown in Theorem 8.1 that our favourite choice for the center, the circumcenter, cannot provide a second order accurate shift transformation on any triangle. One might expect other centers could do the job, but as on a equilateral triangle all the logical centers (circumcenter, incenter, orthocenter and centroid) coincide, and the circumcenter does not work on an equilateral triangle, the other centers cannot work as well on this specific triangle. Although it is not a formal proof, it raises doubt about the fitness of those other centers for other triangles than equilateral ones. Moreover, since equilateral triangles are considered to be the most regular triangles, it would be quite counterintuitive if a shift transformation would exist for all triangles but equilateral ones. But yet again, this is not a formal proof and should be investigated more thoroughly.

Quadrilaterals. Regarding quadrilaterals, there cannot be made such a strong statement as for triangles (yet). Corrolary 8.5 tells that while using the circumcenter, the only useful (because rotatable) shapes are rectangles. This means that, as opposed to triangles, a shift transformation can be found on the most regular quadrilateral, the square. This clears the way for the presumption that other choices of centers may lead to new appropriate shapes, especially when you bear in mind that only a specific class of quadrilaterals posseses a circumcenter and other centers thus come with other shapes. For example, as seen in Chapter 5, the parallelogram is a shape which can be used for a second order accurate shift transformation, assuming the center is defined by the intersection of the diagonals. It still has to be examined whether other quadrilaterals are suitable with this or other centers; this could probably be executed by means of similar calculations as in the previous chapter and is left as a subject for further research.

Pentagons. On the subject of pentagons, no research was done. Following the previously elaborated method it would demand at least an exploration of the linear dependency of one row on four others, which is to be expected more complicated than the one-on-three or one-on-two dependencies. This is also left as a subject for further research.

Hexagons and shapes with more sides. As hexagons have six sides, the matrix M will exist of six rows. But the amount of columns remains unaffected, i.e. five. Hence, the matrixrank will be at most five, which is less than the amount of faces of the cell $\#f$. Applying Theorem 6.1 gives that an at least second order accurate shift transformation can be found on incompressible velocity fields induced by a potential. This proof is of course also valid for shapes with seven or more sides. Unfortunately, we cannot conclude straight away the same about the applicability when the potential field assumption is omitted; a analysis of $\tilde{M}$ is necessary. As the matrix $\tilde{M}$ consists of seven columns, we need at least eight sides to unconditionally validate all possible shapes.

It should be emphasized that the considered shapes are only tested on their fitness for constructing a second order accurate shift transformation and not on their usefulness while designing grids.

Chapter 10

Concluding remarks and more ideas for further research

The main result proven in this work is the non-existence of second order accurate shift transformations on any triangle using the circumcenter as the center of the cell. Thereby we fullfilled the primary objective of this work: to investigate the possibility of developing a fully conservative, symmetry-preserving discretization on a triangulated mesh, using the technique of shift transformations. It might sound a bit counterintuitive that such a shift transformation cannot be found: why is one not capable of averaging three values to obtain a sufficiently accurate estimation in the center, whereas this is possible for a rectangle? The absence of two parallel sides being the reason of the failure on triangles, was inicially not that obvious at all. The primary focus of this research was to actually find the shift transformation, already supposing it would exist. But during various attempts with different approaches -one with Green's function, one dividing the triangle in smaller triangles and one in which the outcomes of a computer algorithm searching for the optimal values of C_f were analyzed- the idea of the absence of a solution made its appearance and started to grow stronger and stronger. Finally the use of the famous Taylor series development gave the assuring answer on all the fruitless attempts: no matter what method used, the triangles with circumcenter cannot be caught in a second order accurate shift transformation.

As discussed in the previous chapter, other centres in triangles can be chosen, but they supposedly will not alter the situation. A less trivial alternative: not choosing the center of a triangle, but defining it by the demand to result in a second order accurate shift transformation. There is no guarantee this will work, but it might be worth a try. Other ideas for further research: extend the proof to three dimensions to see if it still holds, or try to construct an average which uses not only the faces of the particular cell, but also those of its neighbours.

As opposed to the triangles, there does exist a suitable shape in combination with a circumcenter on the realm of quadrilaterals, namely the rectangle. But unfortunately this shape is not very accurate while applied on curved domains. Regarding pentagons nothing can be concluded yet, and for hexagons and shapes consisting of even more sides one can always find a second order accurate shift transformation on incompressible velocity fields induced by a potential. Unfortunately, to state the same on general incompressible velocity fields, at least shapes with eight sides are needed.

A more general extension of this research would be to try to reverse the problem and define a shift transformation from collocated to staggered variables. In that way, also a fully conservative symmetry-preserving for collocated schemes is obtained, using the convective and diffusive difference operators of the original collocated scheme and, in combination with the transformation, the pressure gradient and mass conservation of a staggered scheme.

Summing up, the method of Hicken *et al.* [3] using shift transformations is not to be applied to triangulated grids combined with a circumcenter, as it cannot provide a second order accurate approximation. As argued, this makes one doubt whether it should be used on triangulated grids at all. Moreover, of all the quadrilaterals combined with a circumcenter, only the rectangles are suitable. However, there are still a lot of uninvestigated shapes left for further research, as well as a three-dimensional point of view and other approaches using a shift transformation, so it is very well possible that the shift transformation method does work on implementable grids that approximate curves better than the unstructured, Cartesian grid examined in [3].

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