Computational Fluid Dynamics

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1 Objective

2 Physics

The Navier-Stokes equations govern the motion of viscous fluids. These equations arise from applying conservation of mass, conservation of momentum, and conservation of energy to the motion of fluids and build upon the notion that fluids are a continuous medium rather than a set of discrete particles. The so-called convective form of the Navier-Stokes equations for an incompressible Newtonian fluid without the presence of body forces is:

Continuity equation:
$$\nabla \cdot \mathbf{u} = 0$$
 (2.1a)

Momentum equation:
$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u}$$
 (2.1b)

where ${\bf u}$ is the velocity field, t is the time, ρ is the density, p is the pressure field, and ν is the kinematic viscosity. A more tangible notation of these formidable equations is obtained by writing out the vector components and utilizing Einstein's summation convention:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2.2a}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_i^2}$$
 (2.2b)

Equations (2.2a) and (2.2b) are dimensional. That is, each parameter such as u_i , p, and ν is expressed in terms of a physical quantity. Non-dimensionalization can reduce the number of free parameters and can help to gain a greater insight into the relative size of the various terms present in the equations. The dimensionless parameters are defined as follows:

$$u_i^* \equiv \frac{u_i}{U} \tag{2.3a}$$

$$x_i^* \equiv \frac{x_i}{L} \tag{2.3b}$$

$$t^* \equiv t \frac{U}{L} \tag{2.3c}$$

$$p^* \equiv \frac{\overline{p}}{\rho U^2} \tag{2.3d}$$

$$Re \equiv \frac{\nu}{UL} \tag{2.3e}$$

where U is the velocity scale and L is the length scale of the flow. Multiplication of Equations (2.2a) and (2.2b) by $\frac{L}{U}$ and $\frac{L}{U^2}$, respectively, gives

$$\frac{L}{U}\frac{\partial u_i}{\partial x_i} = 0 \tag{2.4a}$$

$$\frac{L}{U^2}\frac{\partial u_i}{\partial t} + \frac{L}{U^2}u_j\frac{\partial u_i}{\partial x_j} = -\frac{L}{U^2}\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{L}{U^2}\nu\frac{\partial^2 u_i}{\partial x_i^2}$$
(2.4b)

Rearrangement yields

$$\frac{\partial \frac{u_i}{U}}{\partial \frac{x_i}{L}} = 0 \tag{2.5a}$$

$$\frac{\partial \frac{u_i}{U}}{\partial t \frac{U}{L}} + \frac{u_j}{U} \frac{\partial \frac{u_i}{U}}{\partial \frac{x_j}{L}} = -\frac{1}{\rho} \frac{\partial \frac{p}{U^2}}{\partial \frac{x_i}{L}} + \frac{\nu}{UL} \frac{\partial^2 \frac{u_i}{U}}{\partial \frac{x_j}{L} \partial \frac{x_j}{L}}$$
(2.5b)

Substituting Equations (2.3a)–(2.3e), we obtain

$$\frac{\partial u_i^*}{\partial x_i^*} = 0 \tag{2.6a}$$

$$\frac{\partial u_i^*}{\partial t^*} + u_j^* \frac{\partial u_i^*}{\partial x_j^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{\text{Re}} \frac{\partial^2 u_i^*}{\partial x_j^* \partial x_j^*}$$
(2.6b)

or $\nabla \cdot \mathbf{u}^* = 0 \tag{2.7a}$

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + (\mathbf{u}^* \cdot \nabla) \,\mathbf{u}^* = -\nabla p^* + \frac{1}{\text{Re}} \nabla^2 \mathbf{u}^*$$
 (2.7b)

Because it is now understood that the governing equations are dimensionless, the asterisk will be omitted in the remainder of this report.

$$\nabla \cdot \mathbf{u} = 0 \tag{2.8a}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{u}$$
 (2.8b)

For reasons that will be the subject of Chapter 3, it is convenient to rewrite the Navier-Stokes equations in terms of the divergence, curl, and gradient operator. Consider the following vector identities: if \mathbf{u} is a three-dimensional vector field, then

$$\nabla^2 \mathbf{u} = \nabla \left(\nabla \cdot \mathbf{u} \right) - \nabla \times \left(\nabla \times \mathbf{u} \right) \tag{2.9}$$

and

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \left(\frac{1}{2} \|\mathbf{u}\|^{2}\right) - \mathbf{u} \times (\nabla \times \mathbf{u})$$
(2.10)

Using these vector identities, Equation (2.8b) can be written as

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \left(\frac{1}{2} \|\mathbf{u}\|^{2}\right) - \mathbf{u} \times (\nabla \times \mathbf{u}) = -\nabla p + \frac{1}{\text{Re}} \left(\nabla \left(\nabla \cdot \mathbf{u}\right) - \nabla \times \left(\nabla \times \mathbf{u}\right)\right) \quad (2.11)$$

Recall that in a velocity field, the curl of the velocity is equal to the vorticity:

$$\xi = \nabla \times \mathbf{u} \tag{2.12}$$

Substituting Equation (2.12) into Equation (2.11), we have

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \left(\frac{1}{2} \|\mathbf{u}\|^{2}\right) - \mathbf{u} \times \xi = -\nabla p + \frac{1}{\text{Re}} \left(\nabla \left(\nabla \cdot \mathbf{u}\right) - \nabla \times \xi\right)$$

$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \times \xi + \nabla \left(p + \frac{1}{2} \| \mathbf{u} \|^2 \right) = \frac{1}{\text{Re}} \left(\nabla \left(\nabla \cdot \mathbf{u} \right) - \nabla \times \xi \right)$$
 (2.13)

In Equation (2.13), denote

$$P \equiv p + \frac{1}{2} \left\| \mathbf{u} \right\|^2 \tag{2.14}$$

and recognize that the continuity equation, $\nabla \cdot \mathbf{u} = 0$, appears in the right-hand side. Hence, Equation (2.13) is written as

$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \times \xi + \nabla P + \frac{1}{\text{Re}} \nabla \times \xi = 0 \tag{2.15}$$

Thus, the final system of equations is given by:

Continuity equation:
$$\nabla \cdot \mathbf{u} = 0$$
 (2.16a)

Velocity-vorticity relation:
$$\xi = \nabla \times \mathbf{u}$$
 (2.16b)

Momentum equation:
$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \times \xi + \nabla P + \frac{1}{\text{Re}} \nabla \times \xi = 0$$
 (2.16c)

3 Mathematics

In Chapter 2 we derived a system of dimensionless partial differential equations that govern the motion of viscous fluids. In this chapter, we cover some mathematical machinery to formulate the problem into a format understandable by a computer. Instead of using classical discretization methods like the finite difference method, we take a geometric approach using tools from discrete exterior calculus (DEC). A key ingredient in this geometric approach is the placement of physical quantities on the appropriate geometric structures. DEC is a vast mathematical field and a rigorous treatment is far beyond the scope of this assignment. The scope of this chapter is therefore limited to those particular concepts that are required to solve the lid-driven cavity flow problem.

3.1 Cells

Let us first introduce a discrete version of two-dimensional space. Two-dimensional space supports geometric structures with either zero, one, or two dimensions: points, lines, and planes. These k-dimensional geometric structures are formally called k-cells, denoted $\sigma^{(k)}$, where k represents the dimension of the cell. Three examples of k-cells are shown in Figure 3.1.

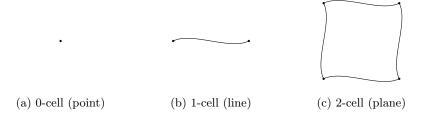


Figure 3.1: Examples of k-cells in two-dimensional space.

A point is a 0-cell, a line is a 1-cell, and a plane is a 2-cell. Just like a 1-cell is a line with a length but with no position, a 2-cell can be thought of as a plane with an area, but no position. Notice that k-cells are bounded by (k-1)-cells and that a cell's shape is arbitrary, as indicated by the wavy lines. (*Note:* The boundary of a point is empty by definition.)

We will be using points, lines, and planes as building blocks of our mesh. A mesh is a set of cells, called a cell-complex if the boundary of each cell is also part of the set. For example, the (rather primitive) mesh in Figure 3.1c is a cell-complex because the plane is bounded by lines and the lines are in turn bounded by points, all of which are part of the mesh.

3.2 Chains and Cochains

There are two additional concepts that require some elaboration: the notion of k-chains and the notion of k-cochains. A k-chain is essentially a set of k-cells. That is, nothing more and nothing less than a set of geometric structures of the same dimension. For instance, a set of lines or a set of planes. k-cochains build upon

chains; a k-cochain is essentially a set of k-cells tagged with a numerical value. k-cochains are in practice realized as a vector of single or double precision numbers and it may help to think of k-cochains as such.

Admittedly, these "definations" of chains and cochains are all but rigorous. However, there exists rigorous mathematical theory that supports these definitions that is omitted here for the sake of consiseness. For a rigorous treatment, see reference.

3.3 Orientation

In addition to dimension, k-cells have a property called orientation. A k-cell either has a positive or a negative orientation that can be freely per individual cell, as long as its orientation remains unchanged thereafter. However, in practice it may be a good idea to define an orientation that is consistent throughout all k-cells.

Figure 3.2 shows three k-cells in two-dimensional space with an intrinsic orientation that we call inner-oriented k-cells. Inner-oriented points for instance, can either represent sources or sinks and are arbitrarily chosen to be source-like (that it, an outflow is positive), as indicated by the outward pointing arrows in Figure 3.2a. Inner-oriented lines are chosen to be a positive when pointing to the right, as indicated by the arrow in Figure 3.2b. It is somewhat awkward to think of the orientation of a plane, but an inner-oriented plane is defined as positive when it is oriented counterclockwise, as indicated by the curled arrow in Figure 3.2c.

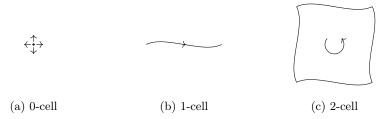


Figure 3.2: Inner-oriented k-cells in two-dimensional space.

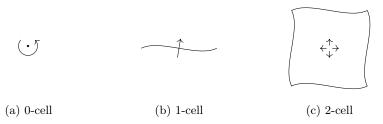


Figure 3.3: Outer-oriented k-cells in two-dimensional space.

Inner-oriented k-cells have outer-oriented counterparts with an circumcentric orientation, rather than an intrinsic orientation. For example, the orientation of an inner-oriented line is defined on that line whereas the orientation of an outer-oriented line is defined through that line. Figure 3.3 shows three outer-oriented k-cells in two-dimensional space.

The distinction between inner and outer-oriented k-cells makes sense from a physical point of view; certain physical quantities are naturally expressed in terms of inner-oriented cochains whereas other physical quantities are naturally expressed in terms of outer-oriented cochains.

3.4 The Exterior Derivative

The exterior derivative δ is used to compute derivatives, like gradients, divergences, or curls. The descrete exterior derivative is a linear map from a (k)-cochain to a (k+1)-cochain. It turns out that the standard treatment of vector calculus hides a number of important things that are applied implicitly. As shall be seen in the upcoming examples, all three of the multivariable derivatives in vector calculus (i.e. gradients, curls, and divergences) are actually one kind of derivative: the exterior derivative. The exterior derivative will be introduced by means of examples to simultaneously present the physical interpretations of some k-cochains.

3.4.1 Inner-Oriented Quantities

To capture the geometric structure of the governing equations, we define its physical quantities through integral values over the elements of the mesh. Depending on whether a given physical quantity is a point, line, or area density, its corresponding discrete representation "lives" at the associated zero, one, or two dimensional mesh elements.

We would eventually like to know the velocity field within the domain of our problem. We use circulation, i.e., the line integral of the velocity field, to encode velocity on the mesh elements. Let inner-oriented 1-cochains therefore represent circulation, defined as

$$u_{i,j} \equiv \int_{L} \mathbf{u} \cdot \hat{\mathbf{t}} \, dx \tag{3.1a}$$

and

$$v_{i,j} \equiv \int_{L} \mathbf{u} \cdot \hat{\mathbf{t}} \, dy \tag{3.1b}$$

where $\hat{\mathbf{t}}$ denotes the tangent vector along a line and where the notations u and v are reserved for horizontal and vertical lines, respectfully. It is crucial to note that this makes circulation an *integrated*, not pointwise, quantity. Thus, the physical quantity of circulation "lives" at the one-dimensional mesh elements (i.e., lines).

Figure 3.4 shows three examples of inner-oriented k-cochains (hence the numerical values) in two-dimensional space.

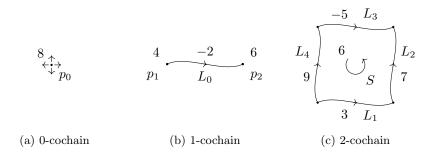


Figure 3.4: Examples of k-cochains in two-dimensional space.

Figure 3.4b shows a 0-cochain consisting of two points, p_1 and p_2 , and a 1-cochain composed of a line, L_0 . L_0 points from p_1 to p_2 , so p_1 acts as a source and p_2 acts as a sink. The recipe for applying δ is straightforward: simply add values at points that act as a source and subtract values at points that act as a sink. Because points are source-like by default, as indicated in Figure 3.4a, application of δ results in

$$u = \delta(L_0) = 4 - 6 = -2 \tag{3.2}$$

Assuming that points represent samples of a continuous scalar field, P, it is clearly seen that the application of δ on a 0-cochain is analogous to the *integrated* gradient operator:

$$4 - 6 = P(p_2) - P(p_1)$$

$$= \int_L \nabla \phi \cdot \mathbf{ds}$$
(3.3)

The physical interpretation of P is dimensionless total pressure $(P \equiv p + \frac{1}{2}||\mathbf{u}||^2)$.

Figure 3.4c shows a 1-cochain composed of four lines and a 2-cochain composed of a single plane, S. We apply the discrete exterior derivative by either adding or subtracting the line values; if the orientation of a line segment opposes the orientation of the plane, then its value must be subtracted. Thus, application of δ on S results in

$$\xi = \delta(S) = 3 + 7 - (-5) - 9 = 6 \tag{3.4}$$

Application of δ on a 1-cochain is analogous to the integrated curl operator because

$$3 + 7 - (-5) - 9 = u_1(L_1) + v_2(L_2) - u_2(L_3) - v_1(L_4)$$

$$= \int_{L_1} \mathbf{u} \cdot \mathbf{dl} + \int_{L_2} \mathbf{u} \cdot \mathbf{dl} - \int_{L_3} \mathbf{u} \cdot \mathbf{dl} - \int_{L_4} \mathbf{u} \cdot \mathbf{dl}$$

$$= \oint_{\partial S} \mathbf{u} \cdot \mathbf{dl}$$

$$= \iint_{S} (\nabla \times \mathbf{u}) \cdot dA$$

$$(3.5)$$

where $\partial S \equiv L_1 \cup L_2 \cup L_3 \cup L_4$. This is not the only insight to be gained here; recall that the circulation along a closed contour, denoted Γ , is defined as:

$$\Gamma \equiv \oint_C \mathbf{u} \cdot \mathbf{dl} \tag{3.6}$$

Comparing Equations (3.5) and (3.6), we conclude that $\delta(S)$ must represent the circulation around the edges of S. Circulation is related to vorticity; the circulation around a closed contour is equal to the integrated vorticity enclosed by that contour. From Stokes' theorem:

$$\Gamma \equiv \oint_C \mathbf{u} \cdot \mathbf{dl} = \iint_A (\nabla \times \mathbf{u}) \, dA = \iint_A \xi \, dA \tag{3.7}$$

Inner-oriented 2-cochains ξ can therefore be interpreted as vorticity.

Because 3-cochains are undefined in two-dimensional space, the application of δ on a 2-cochain results in the empty set by definition. In a similar vein, 0-cochains can only be the result of the application of δ on a real number.

3.4.2 Outer-Oriented Quantities

We use flux, i.e., the integral of the normal velocity along a line, as a representation of velocity on an outer-oriented mesh. Note again that this makes flux an integrated, not pointwise, quantity. Thus, let the outer-oriented 1-cochains represent flux, defined as

$$\tilde{u}_{i,j} \equiv \int_{L} \mathbf{u} \cdot \hat{\mathbf{n}} \, dy \tag{3.8a}$$

and

$$\tilde{v}_{i,j} \equiv \int_{I} \mathbf{u} \cdot \hat{\mathbf{n}} \, dx \tag{3.8b}$$

where $\hat{\mathbf{n}}$ denotes the normal vector along the line segment and where $u_{i,j}$ and $v_{i,j}$ are again reserved for horizontal and vertical lines, respectively. All outer-oriented

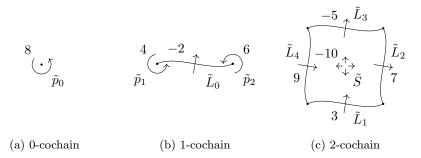


Figure 3.5: Examples of k-cochains in two-dimensional space.

geometric structures and quantities are marked with a tilde for easy recognition. Figure 3.5 shows three examples of outer-oriented k-cochains in two-dimensional space.

Figure 3.5b shows a 0-cochain composed of two points, \tilde{p}_1 and \tilde{p}_2 , and a 1-cochain composed of a line, \tilde{L}_0 . The recipe for applying δ is again straightforward: add values at points that share a common orientation with the line and subtract values whose orientation opposes the orientation of the line. The orientation of \tilde{p}_2 , for example, opposes the orientation of \tilde{L}_0 because the arrows point in opposite directions. Thus,

$$\tilde{u} = \delta(\tilde{L}_0) = 4 - 6 = -2 \tag{3.9}$$

This procedure is analogous to the integrated gradient operator because

$$4 - 6 = \tilde{\psi}(p_2) - \tilde{\psi}(p_1)$$

$$= \int_{L} \nabla \tilde{\psi} \cdot \mathbf{ds}$$
(3.10)

Let us consider the physical interpretation of 0-cochains, denoted $\tilde{\psi}$. If lines represent flux, then points must represent the stream function, $\tilde{\psi}$. Here is why: the numerical value of the stream function is defined such that the difference $\Delta \tilde{\psi}$ between two streamlines is equal to the mass flux between the two streamlines. This fact allows us to determine the stream function up to a constant.

Figure 3.5c shows an outer-oriented 1-cochain composed of four lines and an outer-oriented 2-cochain composed of a plane, \tilde{S} . The plane is source-like as indicated by the outward pointing arrows. We apply the discrete exterior derivative by adding inflows and subtracting outflows. Thus, application of δ yields

$$\tilde{\xi} = \delta(\tilde{S}) = -3 + 7 - 5 - 9 = -10 \tag{3.11}$$

The application of δ on a 1-cochain is analogous to the integrated curl operator because

$$-3 + 7 + (-5) - 9 = -\tilde{u}_{1}(\tilde{L}_{1}) + \tilde{v}_{2}(\tilde{L}_{2}) + \tilde{u}_{2}(\tilde{L}_{3}) - \tilde{v}_{1}(\tilde{L}_{4})$$

$$= -\int_{\tilde{L}_{1}} \mathbf{u} \cdot \mathbf{dl} + \int_{\tilde{L}_{2}} \mathbf{u} \cdot \mathbf{dl} + \int_{\tilde{L}_{3}} \mathbf{u} \cdot \mathbf{dl} - \int_{\tilde{L}_{4}} \mathbf{u} \cdot \mathbf{dl}$$

$$= \oint_{\partial \tilde{S}} \mathbf{u} \cdot \mathbf{dl}$$

$$= \iint_{\tilde{S}} (\nabla \times \mathbf{u}) \cdot dA$$

$$(3.12)$$

where $\partial \tilde{S} \equiv \tilde{L}_1 \cup \tilde{L}_2 \cup \tilde{L}_3 \cup \tilde{L}_4$.

What is the physical interpretation of $\tilde{\xi}$? The fluid is incompressible, so the velocity field must be divergence free (i.e., $\nabla \cdot \mathbf{u} = 0$). According to the generalized Stokes'

theorem the integral of the divergence over a plane equals the sum of the fluxes on all its four edges. In other words, everything that gets in must also get out. The 2-cochain $\tilde{\xi}$ therefore represents the rate of mass production in the plane at which it "lives". Thus, for the law of mass conservation to hold true, $\tilde{\xi}$ must be equal to zero at each and every plane.

3.4.3 DeRham Complex

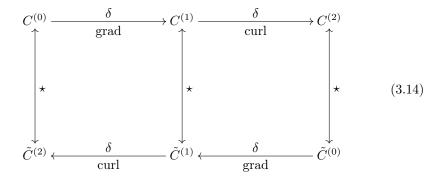
A major advantage of the discrete exterior derivative is that it satisfies the same rules and identities as its smooth counterpart. The discrete exterior derivative is mathematically exact because it acts on and produces integrated quantities. That is, application of δ does not introduce any error whatsoever. As we shall see, this property contributes to the strength of the geometric approach and it results in preservation of the physics implied in the smooth governing equations.

The results of this section can be summarized in a diagram called the DeRham complex:

3.5 The Hodge-⋆ Operator

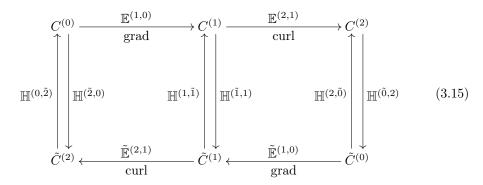
We have established that two-dimensional space supports points, lines, and planes. Let us briefly digress to three-dimensional space for the sake of familiarity; three-dimensional space supports points, lines, planes, and volumes. In three-dimensional space, we can have one linearly independent volume, three linearly independent planes, three linearly independent lines (just like vectors in \mathbb{R}^3), and again one linearly independent point. This 1–3–3–1 sequence suggests a pairing; there exists a vector space isomorphism between k-vectors and (n-k)-vectors. The Hodge- \star operator is a linear map between inner-oriented k-cochains and outer-oriented (n-k)-cochains or vice versa, where n denotes the dimension of the vector space. It simply scales the quantities stored on the mesh cells by the size of the corresponding k-cells.

We have introduced the δ operator to map (k)-cochains to (k+1)-cochains. However, the Navier-Stokes equations equate both inner and outer oriented cochains, which requires the Hodge- \star operator. The Hodge- \star operator links the DeRham complices for inner and outer oriented cochains. This linked structure is called the double DeRham complex:



In a discrete setting, cochains are stored in vectors, the δ operator is represented by incidence matrices, denoted \mathbb{E} , and the Hodge- \star operator is represented by Hodge

matrices, denoted \mathbb{H} . In such a framework, application of the δ or Hodge- \star operator becomes a matrix vector-multiplication. Hence, the double DeRham complex in Equation (3.14) becomes



3.6 Discretization of the Unit Square

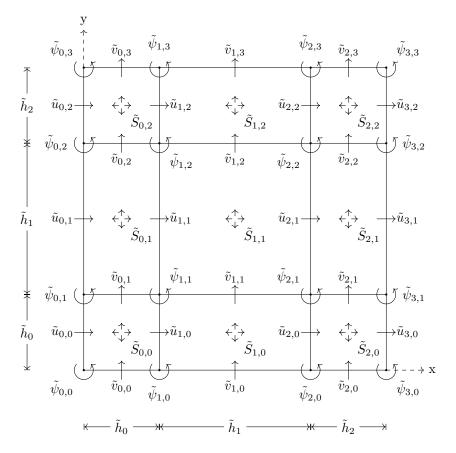


Figure 3.6: The outer-oriented grid.

It is impossible to derive the incidence and Hodge matrices without any a priori knowledge about the geometry of the grid or cell-complex. Let us therefore first discretize the unit square Ω into a grid composed of points, lines, and planes. The outer-oriented grid shown in Figure 3.6 was constructed for n=3, where n denotes the number of planes in the horizontal and vertical axis. The grid has an orthogonal structure, but is not uniform. The points are distributed via cosine spacing at equal angular increments because the smallest flow features are expected to emerge in the vicinity of the walls, which justifies this particular refinement of the grid. The inner-oriented grid associated with the outer-oriented grid is constructed such that the

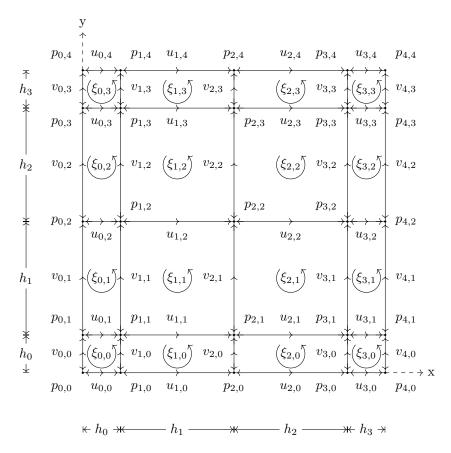


Figure 3.7: The inner-oriented grid.

inner-oriented points are located precisely in the center of the planes of the outeroriented grid, see Figure 3.7. The inner-oriented grid must be constructed in this manner for reasons that can be found in rigorous texts on DEC.

3.7 Physical Representation

We briefly digress here to summarize the physical interpretation of the k-cells that compose the inner and outer oriented grids. The orientation of the outer-oriented planes $\tilde{s}_{i,j}$ is source-like, as indicated by the outward pointing arrows. That is, an outflow is considered positive and an inflow is considered negative. The outeroriented line segments $\tilde{u}_{i,j}$ and $\tilde{v}_{i,j}$ represent flux in the form:

$$\tilde{u}_{i,j} = \int_{y_{i,j}}^{y_{i,j+1}} \mathbf{u} \cdot \hat{\mathbf{n}} \, dy \tag{3.16a}$$

and

$$\tilde{u}_{i,j} = \int_{y_{i,j}}^{y_{i,j+1}} \mathbf{u} \cdot \hat{\mathbf{n}} \, dy$$

$$\tilde{v}_{i,j} = \int_{x_{i,j}}^{x_{i+1,j}} \mathbf{u} \cdot \hat{\mathbf{n}} \, dx$$
(3.16a)

where $\hat{\mathbf{n}}$ denotes the normal vector along the line segment. (*Note:* it is important to remember that all physical quantities are still dimensionless.) A rightward and upward flux is considered positive, as indicated by the arrows through the line segments in Figure 3.6. If outer-oriented 1-cochains represent flux, then outer-oriented 0-cochains must represent samples of the the continuous stream function and outeroriented 2-cochains must represent the rate of mass production within the plane on which they are defined.

The inner-oriented line segments $u_{i,j}$ and $v_{i,j}$ represent circulation:

$$u_{i,j} = \int_{x_{i,j}}^{x_{i,j+1}} \mathbf{u} \cdot \hat{\mathbf{t}} \, dx \tag{3.17a}$$

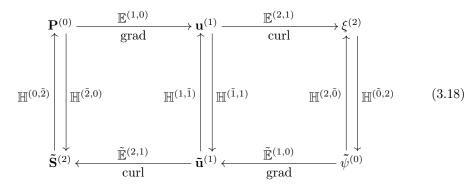
and

$$u_{i,j} = \int_{x_{i,j}}^{x_{i,j+1}} \mathbf{u} \cdot \hat{\mathbf{t}} dx$$

$$v_{i,j} = \int_{y_{i,j}}^{y_{i+1,j}} \mathbf{u} \cdot \hat{\mathbf{t}} dy$$
(3.17a)

where $\hat{\mathbf{t}}$ denotes the tangent vector along the line segment. As discussed in the preceding section, application of the integrated curl operator on a velocity field yields vorticity, assuming that the surfaces are infinitesimal. The inner-oriented 2-cochains $\xi_{(i,j)}$ do therefore represent vorticity and the inner-oriented 0-cochains $p_{i,j}$ represent total pressure. Notice that the orientation of the inner-oriented 0-cochains $p_{i,j}$ is sink-like, as indicated by the inward pointing arrows.

We have constructed the inner and outer oriented grid and we have established what the k-cells physically represent. The double DeRham complex can be updated incorporating the physical quantities:



3.8 Structure of the Navier-Stokes Equations

Recall the system of equations derived in Chapter 2:

Continuity equation:
$$\nabla \cdot \mathbf{u} = 0$$
 (3.19a)

Velocity-vorticity relation:
$$\xi = \nabla \times \mathbf{u}$$
 (3.19b)

Momentum equation:
$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \times \xi + \nabla P + \frac{1}{\text{Re}} \nabla \times \xi = 0$$
 (3.19c)

Let us first add superscripts to denote the dimensions of the k-cochains:

$$\nabla \cdot \mathbf{u}^{(1)} = 0 \tag{3.20a}$$

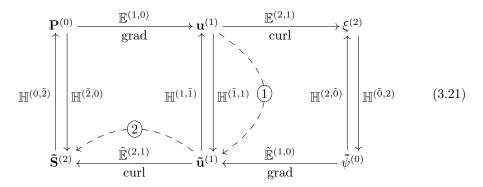
$$\xi^{(2)} = \nabla \times \mathbf{u}^{(1)} \tag{3.20b}$$

$$\frac{\partial \mathbf{u}^{(1)}}{\partial t} - \mathbf{u}^{(1)} \times \xi^{(2)} + \nabla P^{(0)} + \frac{1}{\text{Re}} \nabla \times \xi^{(2)} = 0$$
 (3.20c)

To make these equations consistent, all terms within an equation must be reduced to k-cells of the same dimension and orientation. For example, it is not allowed to equate 2-cochains and 1-cochains, let alone of different orientations.

3.8.1 Continuity Equation

The continuity equation, Equation (3.20a), involves the divergence operator. The divergence operator is equivalent to a (1) mapping of velocity to mass flow and a (2) subsequent application of the curl operator. These two operations are annotated in the double DeRham complex:



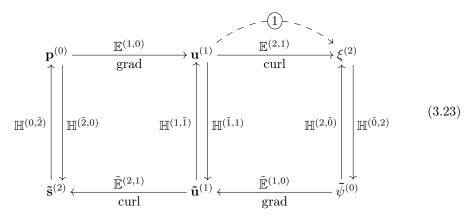
Thus, Equation (3.13a) is equivalent to

$$\tilde{\mathbb{E}}^{(2,1)}\mathbb{H}^{(\tilde{1},1)}\mathbf{u}^{(1)} = 0 \tag{3.22}$$

which is in turn equivalent to writing $\tilde{\mathbf{S}}^{(2)} = 0$. Recall that the physical interpretation of $\tilde{\mathbf{S}}$ is the rate of mass production within the planes that compose the mesh. Thus, $\tilde{\mathbf{S}}^{(2)} = 0$ implies that the net production of mass equals zero, which is precisely what the continuity equation tells us.

3.8.2 Velocity-Vorticity relation

The velocity-vorticity relation states that vorticity, ξ , is equal to the curl of velocity, \mathbf{u} . This represents a mapping from an inner-oriented 1-cochain to an inner-oriented 2-cochain. This operation is represented by a single jump in the double DeRham complex, denoted $\widehat{1}$ in the double DeRham complex:



Equation 3.20b can therefore be written as

$$\xi^{(2)} = \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} \tag{3.24}$$

3.8.3 Momentum Equation

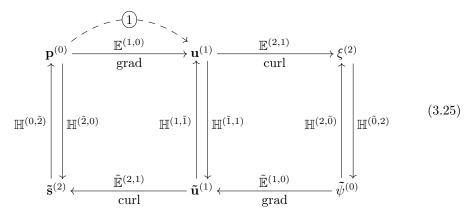
The momentum equation involves three terms that must be expressed in terms of incidence and Hodge matrices:

1.
$$\mathbf{u}^{(1)} \times \xi^{(2)}$$

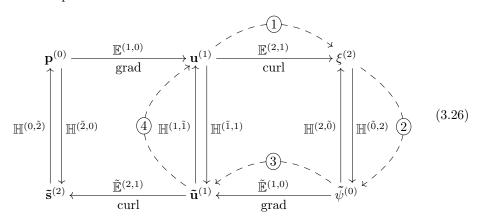
- 2. $\nabla P^{(0)}$
- 3. $\nabla \times \xi^{(2)}$

The cross product $\mathbf{u}^{(1)} \times \boldsymbol{\xi}^{(2)}$ represents the nonlinear convective term of the Navier-Stokes equations and is a bit of a special case. We will therefore replace the nonlinear term by a generic vector named "convective", to be derived at a later stage.

The pressure gradient, $\nabla P^{(0)}$, represents a mapping from an inner-oriented 0-cochain to an inner-oriented 1-cochain. This mapping is denoted $\widehat{1}$ in the double DeRham complex:



The third term, the curl of vorticity or the curl of the curl of velocity, is less straighforward. Both velocity and vorticity are vector fields. Within the realms of ordinary calculus, there would be no difference between the two. However, within the realms of discrete exterior calculus, there is an important distinction: velocity is an integral value associated with lines whereas vorticity is an integral value associated with surfaces. So the only way to apply the curl operator to velocity a second time is to take a slight detour accross the double DeRham complex. First, apply the curl operator to velocity as usual, denoted (1). Second, map vorticity to its outer oriented counterpart, the stream function, denoted (2). Third, apply the gradient operator (which is the transpose of the curl operator, $\mathbb{E}^{(2,1)}$, as we shall soon see) to obtain mass flow, denoted (3). Last but not least, map the mass flow to velocity, denoted (4), because we eventually want all quantities in the momentum equation to be expressed in terms of velocity. This chain of mappings is graphically depicted in the double DeRham complex:



Hence, Equation 3.20c can be written as

$$\frac{\partial \mathbf{u}^{(1)}}{\partial t} + \text{convective}^{(1)} - \mathbb{E}^{(1,0)} P^{(0)} + \frac{1}{\text{Re}} \mathbb{H}^{(1,\tilde{1})} \tilde{\mathbb{E}}^{(1,0)} \mathbb{H}^{(\tilde{0},2)} \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} = 0 \qquad (3.27)$$

3.8.4 Summary

The Navier-Stokes equations are rewritten in terms of incidence matrices and Hodge matrices, as follows:

$$\tilde{\mathbb{E}}^{(2,1)} \mathbb{H}^{(\tilde{1},1)} \mathbf{u}^{(1)} = 0 \tag{3.28a}$$

$$\xi^{(2)} = \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} \tag{3.28b}$$

$$\frac{\partial \mathbf{u}^{(1)}}{\partial t} + \text{convective}^{(1)} - \mathbb{E}^{(1,0)} P^{(0)} + \frac{1}{\text{Re}} \mathbb{H}^{(1,\tilde{1})} \tilde{\mathbb{E}}^{(1,0)} \mathbb{H}^{(\tilde{0},2)} \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} = 0 \quad (3.28c)$$

3.9 The Incidence Matrices and Hodge Matrices

The incidence matrices \mathbb{E} and the Hodge matrices \mathbb{H} are derived using the mesh introduced in the Section 3.6. The incidence and Hodge matrices derived in this section are exclusively valid for the mesh shown in Figure 3.6 and Figure 3.7. That is, the validity is limited to the rather coarse spacing of n=3. However, the format of those matrices belonging to denser grids can be correctly deduced by careful analysis of the matrix structure at n=3, which is of course what we are after.

3.9.1 $\tilde{\mathbb{E}}^{(2,1)}$

The application of the incidence matrix $\tilde{\mathbb{E}}^{(2,1)}$ to the 1-cochain that represent flux, $\tilde{\mathbf{u}}^{(1)}$, yields the rate of mass production in the plane enclosed by those line segments, $\tilde{\mathbf{S}}^{(2)}$. Let us construct a linear equation for each of the planes $\tilde{s}_{i,j}$ in the mesh:

$$\tilde{s}_{0,0} = -\tilde{u}_{0,0} + \tilde{u}_{1,0} - \tilde{v}_{0,0} + \tilde{v}_{0,1}
\tilde{s}_{1,0} = -\tilde{u}_{1,0} + \tilde{u}_{2,0} - \tilde{v}_{1,0} + \tilde{v}_{1,1}
\vdots
\tilde{s}_{2,2} = -\tilde{u}_{2,2} + \tilde{u}_{3,2} - \tilde{v}_{2,2} + \tilde{v}_{2,3}$$
(3.29)

Equation (3.29) expressed in matrix notation becomes

$$\tilde{\mathbf{s}}^{(2)} = \tilde{\mathbb{E}}^{(2,1)} \tilde{\mathbf{u}}^{(1)} \tag{3.30}$$

The mass flow rates $\tilde{u}_{i,j}$ and $\tilde{v}_{i,j}$ adjacent to the boundary of the unit square are known because the boundary conditions of the problem are known. The matrices in the right-hand side of Equation (3.30) can be split into a matrix of unknowns and into a matrix of knows. Splitting the matrix into two parts yields

$$\tilde{\mathbf{s}}^{(2)} = \tilde{\mathbb{E}}^{(2,1)} \tilde{\mathbf{u}}^{(1)} + \tilde{\mathbb{E}}_{known}^{(2,1)} \tilde{\mathbf{u}}_{known}^{(1)}$$
(3.31)

where

$$\tilde{\mathbb{E}}^{(2,1)} = \begin{bmatrix}
1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
-1 & 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & -1 & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & -1 & \cdot & \cdot & -1 & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & -1 & \cdot & \cdot & -1 & \cdot & 1 \\
\cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & -1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & -1
\end{bmatrix}$$
(3.32)

(*Note:* The zero elements are replaced by dots to make the non-zero elements stand out. This turns out to be useful because it makes it far easier to see the structure of the matrices in the blink of an eye.)

Notice that every column of $\tilde{\mathbb{E}}^{(2,1)}$ contains two non-zero elements. The number of non-zero elements (NNZ) in $\tilde{\mathbb{E}}^{(2,1)}$ therefore equals

$$NNZ(\tilde{\mathbb{E}}^{(2,1)}) = 2 \cdot 4n = 8n \tag{3.34}$$

Also notice that every column of $\tilde{\mathbb{E}}_{known}^{(2,1)}$ contains one non-zero element. Thus,

$$NNZ(\tilde{\mathbb{E}}_{known}^{(2,1)}) = 4n \tag{3.35}$$

It should be no surprise here that the extreme sparsity of these indicence matrices is a property worth exploiting.

3.9.2 $\mathbb{E}^{(1,0)}$

The incidence matrix $\mathbb{E}^{(1,0)}$ maps an inner-oriented 0-cochain to an inner-oriented 1-cochain. Let us create a linear equation for each of the line segments $u_{(i,j)}$ in the inner-oriented grid, considering that the points $P_{(i,j)}$ are sink-like. The equations are given by

$$u_{1,1} = -p_{1,1} + p_{2,1}$$

$$u_{2,1} = -p_{2,1} + p_{3,1}$$

$$\vdots$$

$$u_{2,3} = -p_{2,3} + p_{3,3}$$

$$v_{1,1} = -p_{1,1} + p_{1,2}$$

$$v_{2,1} = -p_{2,1} + p_{2,2}$$

$$\vdots$$

$$v_{3,2} = -p_{3,2} + p_{3,3}$$

$$(3.36)$$

Equation (3.36) can be written in matrix notation as

$$\mathbf{u}^{(1)} = \mathbb{E}^{(1,0)} \mathbf{p}^{(0)} \tag{3.37}$$

where

It is important to recognize that

$$\mathbb{E}^{(1,0)} = -\left(\tilde{\mathbb{E}}^{(2,1)}\right)^T \tag{3.39}$$

because this little shortcut will save us some computational effort.

3.9.3 $\mathbb{E}^{(2,1)}$

The incidence matrix $\mathbb{E}^{(2,1)}$ maps an inner-oriented 1-cochain to an inner-oriented 2-cochain. That is, it maps circulation along line segments to vorticity in the planes enclosed by those line segments. The derivation of $\mathbb{E}^{(2,1)}$ is straightforward: add the circulation along those line segments that share a common orientation with the plane and subtract the circulation along those line segments whose orientation opposes the orientation of the plane. Executing this procedure for all planes $\xi_{i,j}$, we have

$$\xi_{0,0} = u_{0,0} - u_{0,1} - v_{0,0} + v_{1,0}$$

$$\xi_{1,0} = u_{1,0} - u_{1,1} - v_{1,0} + v_{2,0}$$

$$\vdots$$

$$\xi_{3,3} = u_{3,3} - u_{3,4} - v_{3,3} + v_{4,3}$$
(3.40)

which is in accordance to the formula

$$\xi_{i,j} = u_{i,j} - u_{i,j+1} - v_{i,j} + v_{i+1,j} \tag{3.41}$$

Equation (3.40) written in matrix notation yields

$$\xi^{(2)} = \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} \tag{3.42}$$

The velocities adjacent to the boundary are again known because the boundary conditions of the problem are known. Splitting the incidence matrix $\mathbb{E}^{(2,1)}$ into a matrix of unknowns and into a matrix of knows yields

$$\xi^{(2)} = \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} + \mathbb{E}_{\text{known}}^{(2,1)} \mathbf{u}_{\text{known}}^{(1)}$$
(3.43)

where

and

The product $\mathbb{E}_{known}^{(2,1)}\mathbf{u}_{known}^{(1)}$ can be evaluated because both factors are known. Equation (3.43) reduces to

$$\xi^{(2)} = \mathbb{E}^{(2,1)} \mathbf{u}^{(1)} + \mathbf{u}_{\text{prescribed}}^{(1)}$$
 (3.46)

Note that each column of the matrix $\mathbb{E}^{(2,1)}$ contains two non-zero elements. Therefore, the total number of non-zero elements in $\mathbb{E}^{(2,1)}$ amounts to

$$NNZ(\mathbb{E}^{(2,1)}) = 2 \cdot 4 \cdot n = 8n \tag{3.47}$$

3.9.4 $\tilde{\mathbb{E}}^{(1,0)}$

The incidence matrix $\tilde{\mathbb{E}}^{(1,0)}$ maps an outer-oriented 0-cochain to an outer-oriented 1-cochain. That is, it maps values of the stream function located at the discrete points of the mesh to flux through the line segments. Deriving $\tilde{\mathbb{E}}^{(1,0)}$ is again straightforward; each of the line segments is bounded by two points. The flux through a line is equal to the sum of the values of the stream function at the bounding points. Add values at points whose orientation is equal to that of the line and subtract values at points whose orientation opposes the orientation of the line. Repeating this process for each of the line segments, we have

$$\tilde{u}_{1,0} = -\tilde{\psi}_{1,0} + \tilde{\psi}_{1,1}$$

$$\tilde{u}_{2,0} = -\tilde{\psi}_{3,0} + \tilde{\psi}_{2,1}$$

$$\vdots$$

$$\tilde{u}_{2,2} = -\tilde{\psi}_{2,2} + \tilde{\psi}_{2,3}$$

$$\tilde{v}_{0,1} = \tilde{\psi}_{0,1} - \tilde{\psi}_{1,1}$$

$$\tilde{v}_{1,1} = \tilde{\psi}_{1,1} - \tilde{\psi}_{2,1}$$

$$\vdots$$

$$\tilde{v}_{2,2} = \tilde{\psi}_{2,2} - \tilde{\psi}_{3,2}$$

$$(3.48)$$

Expressing Equation (3.48) in matrix notation yields

$$\tilde{\mathbf{u}} = \tilde{\mathbb{E}}^{(1,0)} \tilde{\psi} \tag{3.49}$$

where

Also take note that

$$\widetilde{\mathbb{E}}^{(1,0)} = \left(\mathbb{E}^{(2,1)}\right)^T \tag{3.51}$$

which will again save us some computational effort.

3.9.5 $\mathbb{H}^{(\tilde{1},1)}$ and $\mathbb{H}^{(1,\tilde{1})}$

The Hodge matrix $\mathbb{H}^{(\bar{1},1)}$ represents a linear map between between the flux through a line segment and the circulation along a line segment. Its inverse, $\mathbb{H}^{(1,\bar{1})}$, represents a linear map between the circulation along a line segment and the flux through a line segment. The circulation along a line segment is equal to the velocity along that line segment times the length of the line segment. Or, expressed as a function of flux:

ciculation along
$$L_a = \underbrace{\frac{\text{mass flow through } L_b}{\text{length of } L_b}}_{\text{velocity}} \cdot \underbrace{\text{length of } L_a}_{\text{length}}$$
 (3.52)

Let us look at a specific example. The circulation along the line segment $u_{1,1}$ in Figure 3.7 is given by

$$u_{2,1} = \frac{\tilde{u}_{2,0}}{\tilde{h}_0} h_2 = \frac{h_2}{\tilde{h}_0} \tilde{u}_{2,0} \tag{3.53}$$

In general, the circulation along the line segments $u_{i,j}$ and $v_{i,j}$ can be found in accordance to the formulas

$$u_{i,j} = \frac{h_i}{\tilde{h}_{j-1}} \tilde{u}_{i,j-1} \tag{3.54a}$$

and

$$v_{i,j} = \frac{h_j}{\tilde{h}_{i-1}} \tilde{v}_{i-1,j} \tag{3.54b}$$

Equations (3.54a) and (3.54b) expressed in matrix notation yield

$$\mathbf{u}^{(1)} = \mathbb{H}^{(1,\tilde{1})}\tilde{\mathbf{u}}^{(1)} \tag{3.55}$$

The matrix $\mathbb{H}^{(1,\tilde{1})}$ is a diagonal matrix since it represents a linear operation.

3.9.6 $\mathbb{H}^{(\tilde{0},2)}$ and $\mathbb{H}^{(2,\tilde{0})}$

The Hodge matrix $\mathbb{H}^{(\tilde{0},2)}$ maps the vorticity associated with an inner-oriented 2-cochain to the stream function associated with an outer-oriented 0-cochain. This amounts to simply deviding the inner-oriented 2-cochain by its area:

$$\tilde{\psi}_{i,j} = (h_i h_j)^{-1} \xi_{i,j} \tag{3.56}$$

Equation (3.56) written in matrix notation yields

$$\tilde{\psi}^{(0)} = \mathbb{H}^{(\tilde{0},2)} \xi^{(2)} \tag{3.57}$$

where $\mathbb{H}^{(\tilde{0},2)}$ is again a diagonal matrix. Its inverse, $\mathbb{H}^{(2,\tilde{0})}$, represents a linear map between an outer-oriented 0-cochain and an inner-oriented 2-cochain.

3.9.7 The Convective Term

The derivation of the convective term, $\mathbf{u}^{(1)} \times \xi^{(2)}$, is not quite straightforward. The convective term is an exterior product of a 1-cochain and a 2-cochain. If $\xi^{(2)}$ and $\mathbf{u}^{(1)}$ are given by

$$\xi^{(2)} = \xi \, dx \, dy \tag{3.58}$$

and

$$\mathbf{u}^{(1)} = u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \tag{3.59}$$

respectively, then the exterior product yields

$$\mathbf{u}^{(1)} \times \xi^{(2)} = u\xi \, dy - v\xi \, dx \tag{3.60}$$

As an example, let us compute the convection through the line segment $u_{1,1}$. Line segment $u_{1,1}$ is shown in Figure 3.8 along with the adjacent lines and planes that are involved in the computation.

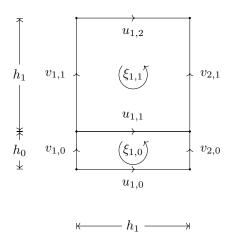


Figure 3.8: Convection through $u_{1,1}$.

Because $u_{1,1}$ is a strictly horizontal line segment, we do not need to consider the horizontal component of the convection through this line segment. Computing the mean vertical velocity in the plane below the line $u_{1,1}$ and multiplying it by $\tilde{\psi}_{1,0}$, we have

$$-\frac{1}{2} \left(\frac{v_{1,0}}{h_0} + \frac{v_{2,0}}{h_0} \right) \tilde{\psi}_{1,0} \tag{3.61}$$

For the plane above the line $u_{1,1}$, we have

$$-\frac{1}{2}\left(\frac{v_{1,1}}{h_1} + \frac{v_{2,1}}{h_1}\right)\tilde{\psi}_{1,1} \tag{3.62}$$

The average of Equations (3.61) and (3.62) multiplied by the length of $u_{1,1}$ yields the convection across $u_{1,1}$:

$$\frac{1}{2} \left[-\frac{1}{2} \left(\frac{v_{1,0}}{h_0} + \frac{v_{2,0}}{h_0} \right) \tilde{\psi}_{1,0} - \frac{1}{2} \left(\frac{v_{1,1}}{h_1} + \frac{v_{2,1}}{h_1} \right) \tilde{\psi}_{1,1} \right] h_1 \tag{3.63}$$

or

$$-\frac{h_1}{4h_0}\left(v_{1,0}+v_{2,0}\right)\tilde{\psi}_{1,0}-\frac{h_1}{4h_1}\left(v_{1,1}+v_{2,1}\right)\tilde{\psi}_{1,1}\tag{3.64}$$

The final multipliplication by h_1 , the length of the line segment $u_{1,1}$, is neseccary because the momentum equation is a 1-form equation. That is, all terms of the momentum equation must ultimately be expressed as inner-oriented 1-cochains. Repetition

of the above procedure for all line segments $u_{i,j}$ and $v_{i,j}$ yields

This representation of convection is all but exact. Each time you average quantities, you introduce a certain degree of error and this representation of the convective term involves not one, but *two* averages.

4 Code

5 Conclusion