OpenFOAM

The Open Source CFD Toolbox

Programmer's Guide

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Contents

Chapter 1

Tensor mathematics

This Chapter describes tensors and their algebraic operations and how they are represented in mathematical text in this book. It then explains how tensors and tensor algebra are programmed in OpenFOAM.

1.1 Coordinate system

OpenFOAM is primarily designed to solve problems in continuum mechanics, *i.e.* the branch of mechanics concerned with the stresses in solids, liquids and gases and the deformation or flow of these materials. OpenFOAM is therefore based in 3 dimensional space and time and deals with physical entities described by tensors. The coordinate system used by OpenFOAM is the right-handed rectangular Cartesian axes as shown in Figure 1.1. This system of axes is constructed by defining an origin O from which three lines are drawn at right angles to each other, termed the Ox, Oy, Oz axes. A right-handed set of axes is defined such that to an observer looking down the Oz axis (with O nearest them), the arc from a point on the Ox axis to a point on the Oy axis is in a clockwise sense.

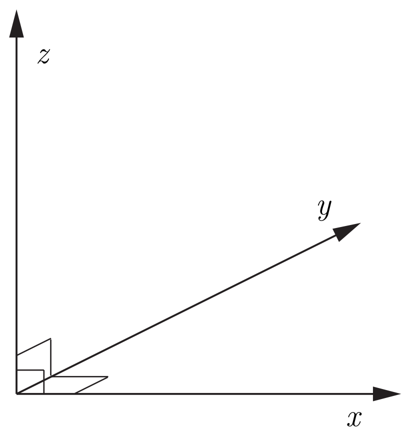

Figure 1.1: Right handed axes

1.2 Tensors

The term tensor describes an entity that belongs to a particular space and obeys certain mathematical rules. Briefly, tensors are represented by a set of *component values* relating to a set of unit base vectors; in OpenFOAM the unit base vectors $\mathbf{i}_x$, $\mathbf{i}_y$ and $\mathbf{i}_z$ are aligned with the right-handed rectangular Cartesian axes x, y and z respectively. The base vectors are therefore orthogonal, *i.e.* at right-angles to one another. Every tensor has the following attributes:

Dimension d of the particular space to which they belong, *i.e.* $d = 3$ in OpenFOAM;

Rank An integer $r \geq 0$, such that the number of component values $= d^r$.

While OpenFOAM 1.x is set to 3 dimensions, it offers tensors of ranks 0 to 3 as standard while being written in such a way to allow this basic set of ranks to be extended indefinitely. Tensors of rank 0 and 1, better known as scalars and vectors, should be familiar to readers; tensors of rank 2 and 3 may not be so familiar. For completeness all ranks of tensor offered as standard in OpenFOAM 1.x are reviewed below.

Rank 0 'scalar' Any property which can be represented by a single real number, denoted by characters in italics, *e.g.* mass m, volume V, pressure p and viscosity μ.

Rank 1 'vector' An entity which can be represented physically by both magnitude and direction. In component form, the vector $\mathbf{a} = (a_1, a_2, a_3)$ relates to a set of Cartesian axes x, y, z respectively. The *index notation* presents the same vector as a_i, $i = 1, 2, 3$, although the list of indices $i = 1, 2, 3$ will be omitted in this book, as it is intuitive since we are always dealing with 3 dimensions.

Rank 2 'tensor' or second rank tensor, $\mathbf{T}$ has 9 components which can be expressed in array notation as:

$$\mathbf{T} = T_{ij} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \tag{1.1}$$

The components T_{ij} are now represented using 2 indices since $r = 2$ and the list of indices $i, j = 1, 2, 3$ is omitted as before. The components for which $i = j$ are referred to as the diagonal components, and those for which $i \neq j$ are referred to as the off-diagonal components. The *transpose* of $\mathbf{T}$ is produced by exchanging components across the diagonal such that

$$\mathbf{T}^{\mathrm{T}} = T_{ji} = \begin{pmatrix} T_{11} & T_{21} & T_{31} \\ T_{12} & T_{22} & T_{32} \\ T_{13} & T_{23} & T_{33} \end{pmatrix} \tag{1.2}$$

Note: a rank 2 tensor is often colloquially termed 'tensor' since the occurrence of higher order tensors is fairly rare.

Symmetric rank 2 The term 'symmetric' refers to components being symmetric about the diagonal, *i.e.* $T_{ij} = T_{ji}$. In this case, there are only 6 independent components since $T_{12} = T_{21}$, $T_{13} = T_{31}$ and $T_{23} = T_{32}$. OpenFOAM distinguishes between symmetric and non-symmetric tensors to save memory by storing 6 components rather than 9 if the tensor is symmetric. Most tensors encountered in continuum mechanics are symmetric.

Rank 3 has 27 components and is represented in index notation as P_{ijk} which is too long to represent in array notation as in Equation 1.1.

Symmetric rank 3 Symmetry of a rank 3 tensor is defined in OpenFOAM to mean that $P_{ijk} = P_{ikj} = P_{jik} = P_{jki} = P_{kij} = P_{kji}$ and therefore has 10 independent components. More specifically, it is formed by the outer product of 3 identical vectors, where the outer product operation is described in Section 1.3.4.

1.2.1 Tensor notation

This is a book on computational continuum mechanics that deals with problems involving complex PDEs in 3 spatial dimensions and in time. It is vital from the beginning to adopt a notation for the equations which is compact yet unambiguous. To make the equations easy to follow, we must use a notation that encapsulates the idea of a tensor as an entity in the own right, rather than a list of scalar components. Additionally, any tensor operation should be perceived as an operation on the entire tensor entity rather than a series of operations on its components.

Consequently, in this book the *tensor notation* is preferred in which any tensor of rank 1 and above, *i.e.* all tensors other than scalars, are represented by letters in bold face, *e.g.* **a**. This actively promotes the concept of a tensor as a entity in its own right since it is denoted by a single symbol, and it is also extremely compact. The potential drawback is that the rank of a bold face symbol is not immediately apparent, although it is clearly not zero. However, in practice this presents no real problem since we are aware of the property each symbol represents and therefore intuitively know its rank, *e.g.* we know velocity **U** is a tensor of rank 1.

A further, more fundamental idea regarding the choice of notation is that the mathematical representation of a tensor should not change depending on our coordinate system, *i.e.* the vector **a**is the same vector irrespective of where we view it from. The tensor notation supports this concept as it implies nothing about the coordinate system. However, other notations, *e.g.* a_i, expose the individual components of the tensor which naturally implies the choice of coordinate system. The unsatisfactory consequence of this is that the tensor is then represented by a set of values which are not unique — they depend on the coordinate system.

That said, the index notation, introduced in Section 1.2, is adopted from time to time in this book mainly to expand tensor operations into the constituent components. When using the index notation, we adopt the *summation convention* which states that whenever the same letter subscript occurs twice in a term, the that subscript is to be given all values, *i.e.* 1, 2, 3, and the results added together, *e.g.*

$$a_i b_i = \sum_{i=1}^{3} a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3 \tag{1.3}$$

In the remainder of the book the symbol $\sum$ is omitted since the repeated subscript indicates the summation.

1.3 Algebraic tensor operations

This section describes all the algebraic operations for tensors that are available in OpenFOAM. Let us first review the most simple tensor operations: addition, subtraction, and scalar multiplication and division. Addition and subtraction are both commutative and associative and are only valid between tensors of the same rank. The operations are performed by addition/subtraction of respective components of the tensors, *e.g.* the subtraction of two vectors **a** and **b** is

$$\mathbf{a} - \mathbf{b} = a_i - b_i = (a_1 - b_1, a_2 - b_2, a_3 - b_3) \tag{1.4}$$

Multiplication of any tensor **a** by a scalar s is also commutative and associative and is performed by multiplying all the tensor components by the scalar. For example,

$$s\mathbf{a} = s a_i = (s a_1, s a_2, s a_3) \tag{1.5}$$

Division between a tensor $\mathbf{a}$ and a scalar is only relevant when the scalar is the second argument of the operation, *i.e.*

$$\mathbf{a}/s = a_i/s = (a_1/s, a_2/s, a_3/s) \tag{1.6}$$

Following these operations are a set of more complex products between tensors of rank 1 and above, described in the following Sections.

1.3.1 The inner product

The inner product operates on any two tensors of rank r_1 and r_2 such that the rank of the result $r = r_1 + r_2 - 2$. Inner product operations with tensors up to rank 3 are described below:

- The inner product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is commutative and produces a scalar $s = \mathbf{a} \bullet \mathbf{b}$ where

$$s = a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3 \tag{1.7}$$

- The inner product of a tensor $\mathbf{T}$ and vector $\mathbf{a}$ produces a vector $\mathbf{b} = \mathbf{T} \bullet \mathbf{a}$, represented below as a column array for convenience

$$b_i = T_{ij} a_j = \begin{pmatrix} T_{11}a_1 + T_{12}a_2 + T_{13}a_3 \\ T_{21}a_1 + T_{22}a_2 + T_{23}a_3 \\ T_{31}a_1 + T_{32}a_2 + T_{33}a_3 \end{pmatrix} \tag{1.8}$$

  It is non-commutative if $\mathbf{T}$ is non-symmetric such that $\mathbf{b} = \mathbf{a} \bullet \mathbf{T} = \mathbf{T}^{\mathrm{T}} \bullet \mathbf{a}$ is

$$b_i = a_j T_{ji} = \begin{pmatrix} a_1 T_{11} + a_2 T_{21} + a_3 T_{31} \\ a_1 T_{12} + a_2 T_{22} + a_3 T_{32} \\ a_1 T_{13} + a_2 T_{23} + a_3 T_{33} \end{pmatrix} \tag{1.9}$$

- The inner product of two tensors $\mathbf{T}$ and $\mathbf{S}$ produces a tensor $\mathbf{P} = \mathbf{T} \bullet \mathbf{S}$ whose components are evaluated as:

$$P_{ij} = T_{ik} S_{kj} \tag{1.10}$$

  It is non-commutative such that $\mathbf{T} \bullet \mathbf{S} = \left(\mathbf{S}^{\mathrm{T}} \bullet \mathbf{T}^{\mathrm{T}}\right)^{\mathrm{T}}$

- The inner product of a vector $\mathbf{a}$ and third rank tensor $\mathbf{P}$ produces a second rank tensor $\mathbf{T} = \mathbf{a} \bullet \mathbf{P}$ whose components are

$$T_{ij} = a_k P_{kij} \tag{1.11}$$

  Again this is non-commutative so that $\mathbf{T} = \mathbf{P} \bullet \mathbf{a}$ is

$$T_{ij} = P_{ijk} a_k \tag{1.12}$$

- The inner product of a second rank tensor $\mathbf{T}$ and third rank tensor $\mathbf{P}$ produces a third rank tensor $\mathbf{Q} = \mathbf{T} \bullet \mathbf{P}$ whose components are

$$Q_{ijk} = T_{il} P_{ljk} \tag{1.13}$$

  Again this is non-commutative so that $\mathbf{Q} = \mathbf{P} \bullet \mathbf{T}$ is

$$Q_{ijk} = P_{ijl} T_{lk} \tag{1.14}$$

1.3.2 The double inner product of two tensors

The double inner product of two second-rank tensors **T** and **S** produces a scalar $s = \mathbf{T} \mathbin{:} \mathbf{S}$ which can be evaluated as the sum of the 9 products of the tensor components

$$\begin{aligned} s = T_{ij} S_{ij} = \; & T_{11} S_{11} + T_{12} S_{12} + T_{13} S_{13} + \\ & T_{21} S_{21} + T_{22} S_{22} + T_{23} S_{23} + \\ & T_{31} S_{31} + T_{32} S_{32} + T_{33} S_{33} \end{aligned} \tag{1.15}$$

The double inner product between a second rank tensor **T** and third rank tensor **P** produces a vector $\mathbf{a} = \mathbf{T} \mathbin{:} \mathbf{P}$ with components

$$a_i = T_{jk} P_{jki} \tag{1.16}$$

This is non-commutative so that $\mathbf{a} = \mathbf{P} \mathbin{:} \mathbf{T}$ is

$$a_i = P_{ijk} T_{jk} \tag{1.17}$$

1.3.3 The triple inner product of two third rank tensors

The triple inner product of two third rank tensors **P** and **Q** produces a scalar $s = \mathbf{P} \overset{3}{\vdots} \mathbf{Q}$ which can be evaluated as the sum of the 27 products of the tensor components

$$s = P_{ijk} Q_{ijk} \tag{1.18}$$

1.3.4 The outer product

The outer product operates between vectors and tensors as follows:

- The outer product of two vectors **a** and **b** is non-commutative and produces a tensor $\mathbf{T} = \mathbf{ab} = (\mathbf{ba})^{\mathrm{T}}$ whose components are evaluated as:

$$T_{ij} = a_i b_j = \begin{pmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{pmatrix} \tag{1.19}$$

- An outer product of a vector **a** and second rank tensor **T** produces a third rank tensor $\mathbf{P} = \mathbf{aT}$ whose components are

$$P_{ijk} = a_i T_{jk} \tag{1.20}$$

  This is non-commutative so that $\mathbf{P} = \mathbf{T}\,\mathbf{a}$ produces

$$P_{ijk} = T_{ij} a_k \tag{1.21}$$

1.3.5 The cross product of two vectors

The cross product operation is exclusive to vectors only. For two vectors **a** with **b**, it produces a vector $\mathbf{c} = \mathbf{a} \times \mathbf{b}$ whose components are

$$c_i = e_{ijk} a_j b_k = (a_2 b_3 - a_3 b_2, a_3 b_1 - a_1 b_3, a_1 b_2 - a_2 b_1) \tag{1.22}$$

where the *permutation symbol* is defined by

$$e_{ijk} = \begin{cases} 0 & \text{when any two indices are equal} \\ +1 & \text{when } i,j,k \text{ are an even permutation of 1,2,3} \\ -1 & \text{when } i,j,k \text{ are an odd permutation of 1,2,3} \end{cases} \tag{1.23}$$

in which the even permutations are 123, 231 and 312 and the odd permutations are 132, 213 and 321.

1.3.6 Other general tensor operations

Some less common tensor operations and terminology used by OpenFOAM are described below.

Square of a tensor is defined as the outer product of the tensor with itself, *e.g.* for a vector $\mathbf{a}$, the square $\mathbf{a}^2 = \mathbf{aa}$.

n**th power** of a tensor is evaluated by n outer products of the tensor, *e.g.* for a vector $\mathbf{a}$, the 3rd power $\mathbf{a}^3 = \mathbf{aaa}$.

Magnitude squared of a tensor is the rth inner product of the tensor of rank r with itself, to produce a scalar. For example, for a second rank tensor $\mathbf{T}$, $|\mathbf{T}|^2 = \mathbf{T} \mathbin{\mathbf{:}} \mathbf{T}$.

Magnitude is the square root of the magnitude squared, *e.g.* for a tensor $\mathbf{T}$, $|\mathbf{T}| = \sqrt{\mathbf{T} \mathbin{\mathbf{:}} \mathbf{T}}$. Vectors of unit magnitude are referred to as *unit vectors*.

Component maximum is the component of the tensor with greatest value, inclusive of sign, *i.e.* not the largest magnitude.

Component minimum is the component of the tensor with smallest value.

Component average is the mean of all components of a tensor.

Scale As the name suggests, the scale function is a tool for scaling the components of one tensor by the components of another tensor of the same rank. It is evaluated as the product of corresponding components of 2 tensors, *e.g.*, scaling vector $\mathbf{a}$ by vector $\mathbf{b}$ would produce vector $\mathbf{c}$ whose components are

$$c_i = \text{scale}(\mathbf{a}, \mathbf{b}) = (a_1 b_1, a_2 b_2, a_3 b_3) \tag{1.24}$$

1.3.7 Geometric transformation and the identity tensor

A second rank tensor $\mathbf{T}$ is strictly defined as a linear vector function, i.e. it is a function which associates an argument vector $\mathbf{a}$ to another vector $\mathbf{b}$ by the inner product $\mathbf{b} = \mathbf{T} \bullet \mathbf{a}$. The components of $\mathbf{T}$ can be chosen to perform a specific geometric transformation of a tensor from the x, y, z coordinate system to a new coordinate system x^*, y^*, z^*; $\mathbf{T}$ is then referred to as the *transformation tensor*. While a scalar remains unchanged under a transformation, the vector $\mathbf{a}$ is transformed to $\mathbf{a}^*$ by

$$\mathbf{a}^* = \mathbf{T} \bullet \mathbf{a} \tag{1.25}$$

A second rank tensor $\mathbf{S}$ is transformed to $\mathbf{S}^*$ according to

$$\mathbf{S}^* = \mathbf{T} \bullet \mathbf{S} \bullet \mathbf{T}^{\mathrm{T}} \tag{1.26}$$

The *identity tensor* $\mathbf{I}$ is defined by the requirement that it transforms another tensor onto itself. For all vectors $\mathbf{a}$

$$\mathbf{a} = \mathbf{I} \bullet \mathbf{a} \tag{1.27}$$

and therefore

$$\mathbf{I} = \delta_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.28}$$

where δ_{ij} is known as the *Kronecker delta* symbol.

1.3.8 Useful tensor identities

Several identities are listed below which can be verified by under the assumption that all the relevant derivatives exist and are continuous. The identities are expressed for scalar s and vector $\mathbf{a}$.

$$
\begin{aligned}
&\nabla \bullet (\nabla \times \mathbf{a}) \equiv 0 \\
&\nabla \times (\nabla s) \equiv \mathbf{0} \\
&\nabla \bullet (s\mathbf{a}) \equiv s\nabla \bullet \mathbf{a} + \mathbf{a} \bullet \nabla s \\
&\nabla \times (s\mathbf{a}) \equiv s\nabla \times \mathbf{a} + \nabla s \times \mathbf{a} \\
&\nabla(\mathbf{a} \bullet \mathbf{b}) \equiv \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a}) + (\mathbf{a} \bullet \nabla)\mathbf{b} + (\mathbf{b} \bullet \nabla)\mathbf{a} \\
&\nabla \bullet (\mathbf{a} \times \mathbf{b}) \equiv \mathbf{b} \bullet (\nabla \times \mathbf{a}) - \mathbf{a} \bullet (\nabla \times \mathbf{b}) \\
&\nabla \times (\mathbf{a} \times \mathbf{b}) \equiv \mathbf{a}(\nabla \bullet \mathbf{b}) - \mathbf{b}(\nabla \bullet \mathbf{a}) + (\mathbf{b} \bullet \nabla)\mathbf{a} - (\mathbf{a} \bullet \nabla)\mathbf{b} \\
&\nabla \times (\nabla \times \mathbf{a}) \equiv \nabla(\nabla \bullet \mathbf{a}) - \nabla^2 \mathbf{a} \\
&(\nabla \times \mathbf{a}) \times \mathbf{a} \equiv \mathbf{a} \bullet (\nabla \mathbf{a}) - \nabla(\mathbf{a} \bullet \mathbf{a})
\end{aligned}
\tag{1.29}
$$

It is sometimes useful to know the $e - \delta$ identity to help to manipulate equations in index notation:

$$
e_{ijk} e_{irs} = \delta_{jr}\delta_{ks} - \delta_{js}\delta_{kr} \tag{1.30}
$$

1.3.9 Operations exclusive to tensors of rank 2

There are several operations that manipulate the components of tensors of rank 2 that are listed below:

Transpose of a tensor $\mathbf{T} = T_{ij}$ is $\mathbf{T}^{\mathrm{T}} = T_{ji}$ as described in Equation 1.2.

Symmetric and skew (antisymmetric) tensors As discussed in section 1.2, a tensor is said to be symmetric if its components are symmetric about the diagonal, i.e. $\mathbf{T} = \mathbf{T}^{\mathrm{T}}$. A skew or antisymmetric tensor has $\mathbf{T} = -\mathbf{T}^{\mathrm{T}}$ which intuitively implies that $T_{11} = T_{22} = T_{33} = 0$. Every second order tensor can be decomposed into symmetric and skew parts by

$$
\mathbf{T} = \underbrace{\frac{1}{2}(\mathbf{T} + \mathbf{T}^{\mathrm{T}})}_{symmetric} + \underbrace{\frac{1}{2}(\mathbf{T} - \mathbf{T}^{\mathrm{T}})}_{skew} = \operatorname{symm}\mathbf{T} + \operatorname{skew}\mathbf{T} \tag{1.31}
$$

Trace The trace of a tensor $\mathbf{T}$ is a scalar, evaluated by summing the diagonal components

$$
\operatorname{tr}\mathbf{T} = T_{11} + T_{22} + T_{33} \tag{1.32}
$$

Diagonal returns a vector whose components are the diagonal components of the second rank tensor $\mathbf{T}$

$$
\operatorname{diag}\mathbf{T} = (T_{11}, T_{22}, T_{33}) \tag{1.33}
$$

Deviatoric and hydrostatic tensors Every second rank tensor $\mathbf{T}$ can be decomposed into a deviatoric component, for which $\operatorname{tr}\mathbf{T} = 0$ and a hydrostatic component of the form $\mathbf{T} = s\mathbf{I}$ where s is a scalar. Every second rank tensor can be decomposed into deviatoric and hydrostatic parts as follows:

$$
\mathbf{T} = \underbrace{\mathbf{T} - \frac{1}{3}(\operatorname{tr}\mathbf{T})\,\mathbf{I}}_{deviatoric} + \underbrace{\frac{1}{3}(\operatorname{tr}\mathbf{T})\,\mathbf{I}}_{hydrostatic} = \operatorname{dev}\mathbf{T} + \operatorname{hyd}\mathbf{T} \tag{1.34}
$$

Determinant The determinant of a second rank tensor is evaluated by

$$\det \mathbf{T} = \begin{vmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{vmatrix} = \begin{array}{l} T_{11}(T_{22}T_{33} - T_{23}T_{32}) - \\ T_{12}(T_{21}T_{33} - T_{23}T_{31}) + \\ T_{13}(T_{21}T_{32} - T_{22}T_{31}) \end{array}$$
$$= \frac{1}{6} e_{ijk} e_{pqr} T_{ip} T_{jq} T_{kr} \tag{1.35}$$

Cofactors The *minors* of a tensor are evaluated for each component by deleting the row and column in which the component is situated and evaluating the resulting entries as a 2×2 *determinant*. For example, the minor of T_{12} is

$$\begin{vmatrix} \cancel{T_{11}} & \cancel{T_{12}} & \cancel{T_{13}} \\ T_{21} & \cancel{T_{22}} & T_{23} \\ T_{31} & \cancel{T_{32}} & T_{33} \end{vmatrix} = \begin{vmatrix} T_{21} & T_{23} \\ T_{31} & T_{33} \end{vmatrix} = T_{21}T_{33} - T_{23}T_{31} \tag{1.36}$$

The cofactors are *signed minors* where each minor is component is given a sign based on the rule

$$\begin{array}{l} +\text{ve if } i + j \text{ is even} \\ -\text{ve if } i + j \text{ is odd} \end{array} \tag{1.37}$$

The cofactors of $\mathbf{T}$ can be evaluated as

$$\operatorname{cof} \mathbf{T} = \frac{1}{2} e_{jkr} e_{ist} T_{sk} T_{tr} \tag{1.38}$$

Inverse The inverse of a tensor can be evaluated as

$$\operatorname{inv} \mathbf{T} = \frac{\operatorname{cof} \mathbf{T}^{\mathrm{T}}}{\det \mathbf{T}} \tag{1.39}$$

Hodge dual of a tensor is a vector whose components are

$$* \mathbf{T} = (T_{23}, -T_{13}, T_{12}) \tag{1.40}$$

1.3.10 Operations exclusive to scalars

OpenFOAM supports most of the well known functions that operate on scalars, *e.g.* square root, exponential, logarithm, sine, cosine *etc.*., a list of which can be found in Table 1.2. There are 3 additional functions defined within OpenFOAM that are described below:

Sign of a scalar s is

$$\operatorname{sgn}(s) = \begin{cases} 1 & \text{if } s \geq 0, \\ -1 & \text{if } s < 0. \end{cases} \tag{1.41}$$

Positive of a scalar s is

$$\operatorname{pos}(s) = \begin{cases} 1 & \text{if } s \geq 0, \\ 0 & \text{if } s < 0. \end{cases} \tag{1.42}$$

Limit of a scalar s by the scalar n

$$\operatorname{limit}(s, n) = \begin{cases} s & \text{if } s < n, \\ 0 & \text{if } s \geq n. \end{cases} \tag{1.43}$$

1.4 OpenFOAM tensor classes

OpenFOAM contains a C++ class library primitive that contains the classes for the tensor mathematics described so far. The basic tensor classes that are available as standard in OpenFOAM are listed in Table 1.1. The Table also lists the functions that allow the user to access individual components of a tensor, known as access functions.

Rank	Common name	Basic class	Access functions
0	Scalar	scalar	
1	Vector	vector	`x()`, `y()`, `z()`
2	Tensor	tensor	`xx()`, `xy()`, `xz()`...

Table 1.1: Basic tensor classes in OpenFOAM

We can declare the tensor

$$\mathbf{T} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \tag{1.44}$$

in OpenFOAM by the line:

```
tensor T(1, 2, 3, 4, 5, 6, 7, 8, 9);
```

We can then access the component T_{13}, or T_{xz} using the `xz()` access function. For instance the code

```
Info << ‘‘Txz = ’’ << T.xz() << endl;
```

outputs to the screen:

```
Txz = 3
```

1.4.1 Algebraic tensor operations in OpenFOAM

The algebraic operations described in Section 1.3 are all available to the OpenFOAM tensor classes using syntax which closely mimics the notation used in written mathematics. Some functions are represented solely by descriptive functions, *e.g.*`symm()`, but others can also be executed using symbolic operators, *e.g.*`*`. All functions are listed in Table 1.2.

Operation	Comment	Mathematical Description	Description in OpenFOAM
Addition		$\mathbf{a}+\mathbf{b}$	`a + b`
Subtraction		$\mathbf{a}-\mathbf{b}$	`a - b`
Scalar multiplication		$s\mathbf{a}$	`s * a`
Scalar division		$\mathbf{a}/s$	`a / s`
Outer product	rank $\mathbf{a},\mathbf{b} >= 1$	$\mathbf{ab}$	`a * b`
Inner product	rank $\mathbf{a},\mathbf{b} >= 1$	$\mathbf{a}\bullet\mathbf{b}$	`a & b`
Double inner product	rank $\mathbf{a},\mathbf{b} >= 2$	$\mathbf{a}:\mathbf{b}$	`a && b`
Cross product	rank $\mathbf{a},\mathbf{b} = 1$	$\mathbf{a}\times\mathbf{b}$	`a ^ b`
Square		$\mathbf{a}^2$	`sqr(a)`

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Operation	Comment	Mathematical Description	Description in OpenFOAM
Magnitude squared		$\lvert\mathbf{a}\rvert^2$	`magSqr(a)`
Magnitude		$\lvert\mathbf{a}\rvert$	`mag(a)`
Power	$n = 0, 1, ..., 4$	$\mathbf{a}^n$	`pow(a,n)`
Component average	$i = 1, ..., N$	$\overline{a_i}$	`cmptAv(a)`
Component maximum	$i = 1, ..., N$	$\max(a_i)$	`max(a)`
Component minimum	$i = 1, ..., N$	$\min(a_i)$	`min(a)`
Scale		$\mathrm{scale}(\mathbf{a},\mathbf{b})$	`scale(a,b)`
Geometric transformation	transforms $\mathbf{a}$ using tensor $\mathbf{T}$		`transform(T,a)`
Operations exclusive to tensors of rank 2			
Transpose		$\mathbf{T}^{\mathrm{T}}$	`T.T()`
Diagonal		$\mathrm{diag}\,\mathbf{T}$	`diag(T)`
Trace		$\mathrm{tr}\,\mathbf{T}$	`tr(T)`
Deviatoric component		$\mathrm{dev}\,\mathbf{T}$	`dev(T)`
Symmetric component		$\mathrm{symm}\,\mathbf{T}$	`symm(T)`
Skew-symmetric component		$\mathrm{skew}\,\mathbf{T}$	`skew(T)`
Determinant		$\det\mathbf{T}$	`det(T)`
Cofactors		$\mathrm{cof}\,\mathbf{T}$	`cof(T)`
Inverse		$\mathrm{inv}\,\mathbf{T}$	`inv(T)`
Hodge dual		$*\,\mathbf{T}$	`*T`
Operations exclusive to scalars			
Sign (boolean)		$\mathrm{sgn}(s)$	`sign(s)`
Positive (boolean)		$s >= 0$	`pos(s)`
Negative (boolean)		$s < 0$	`neg(s)`
Limit	n scalar	$\mathrm{limit}(s, n)$	`limit(s,n)`
Square root		$\sqrt{s}$	`sqrt(s)`
Exponential		$\exp s$	`exp(s)`
Natural logarithm		$\ln s$	`log(s)`
Base 10 logarithm		$\log_{10} s$	`log10(s)`
Sine		$\sin s$	`sin(s)`
Cosine		$\cos s$	`cos(s)`
Tangent		$\tan s$	`tan(s)`
Arc sine		$\mathrm{asin}\, s$	`asin(s)`
Arc cosine		$\mathrm{acos}\, s$	`acos(s)`
Arc tangent		$\mathrm{atan}\, s$	`atan(s)`
Hyperbolic sine		$\sinh s$	`sinh(s)`
Hyperbolic cosine		$\cosh s$	`cosh(s)`
Hyperbolic tangent		$\tanh s$	`tanh(s)`
Hyperbolic arc sine		$\mathrm{asinh}\, s$	`asinh(s)`
Hyperbolic arc cosine		$\mathrm{acosh}\, s$	`acosh(s)`
Hyperbolic arc tangent		$\mathrm{atanh}\, s$	`atanh(s)`
Error function		$\mathrm{erf}\, s$	`erf(s)`
Complement error function		$\mathrm{erfc}\, s$	`erfc(s)`
Logarithm gamma function		$\ln\Gamma s$	`lgamma(s)`
Type 1 Bessel function of order 0		$\mathrm{J}_0\, s$	`j0(s)`
Type 1 Bessel function of order 1		$\mathrm{J}_1\, s$	`j1(s)`

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Operation	Comment	Mathematical Description	Description in OpenFOAM
Type 2 Bessel function of order 0		$Y_0\, s$	`y0(s)`
Type 2 Bessel function of order 1		$Y_1\, s$	`y1(s)`

$\mathbf{a}, \mathbf{b}$ are tensors of arbitrary rank unless otherwise stated
s is a scalar, N is the number of tensor components

Table 1.2: Algebraic tensor operations in OpenFOAM

1.5 Dimensional units

In continuum mechanics, properties are represented in some chosen units, *e.g.* mass in kilograms (kg), volume in cubic metres (m^3), pressure in Pascals ($\mathrm{kg\,m\,s^{-2}}$). Algebraic operations must be performed on these properties using consistent units of measurement; in particular, addition, subtraction and equality are only physically meaningful for properties of the same dimensional units. As a safeguard against implementing a meaningless operation, OpenFOAM encourages the user to attach dimensional units to any tensor and will then perform dimension checking of any tensor operation.

Units are defined using the dimensionSet class, *e.g.*

```
dimensionSet pressureDims(1, -1, -2, 0, 0, 0, 0);
```

No.	Property	Unit	Symbol
1	Mass	kilogram	k
2	Length	metre	m
3	Time	second	s
4	Temperature	Kelvin	K
5	Quantity	moles	mol
6	Current	ampere	A
7	Luminous intensity	candela	cd

Table 1.3: S.I. base units of measurement

where each of the values corresponds to the power of each of the S.I. base units of measurement listed in Table 1.3. The line of code declares `pressureDims` to be the dimensionSet for pressure $\mathrm{kg\,m\,s^{-2}}$ since the first entry in the `pressureDims` array, 1, corresponds to k^1, the second entry, -1, corresponds to m^{-1} *etc.*. A tensor with units is defined using the dimensioned<Type> template class, the <Type> being scalar, vector, tensor, *etc.*. The dimensioned<Type> stores a variable name of class word,the value <Type> and a dimensionSet

```
dimensionedTensor sigma
    (
        "sigma",
        dimensionSet(1, -1, -2, 0, 0, 0, 0),
        tensor(1e6,0,0,0,1e6,0,0,0,1e6),
    );
```

creates a tensor with correct dimensions of pressure, or stress

$$\boldsymbol{\sigma} = \begin{pmatrix} 10^6 & 0 & 0 \\ 0 & 10^6 & 0 \\ 0 & 0 & 10^6 \end{pmatrix} \tag{1.45}$$

Chapter 2

Discretisation procedures

So far we have dealt with algebra of tensors at a point. The PDEs we wish to solve involve derivatives of tensors with respect to time and space. We therefore need to extend our description to a *tensor field*, *i.e.* a tensor that varies across time and spatial domains. In this Chapter we will first present a mathematical description of all the differential operators we may encounter. We will then show how a tensor field is constructed in OpenFOAM and how the derivatives of these fields are discretised into a set of algebraic equations.

2.1 Differential operators

Before defining the spatial derivatives we first introduce the nabla *vector operator* ∇, represented in index notation as ∂_i:

$$\nabla \equiv \partial_i \equiv \frac{\partial}{\partial x_i} \equiv \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right) \tag{2.1}$$

The nabla operator is a useful notation that obeys the following rules:

- it operates on the tensors to its right and the conventional rules of a derivative of a product, *e.g.* $\partial_i ab = (\partial_i a)\, b + a\, (\partial_i b)$;
- otherwise the nabla operator behaves like any other vector in an algebraic operation.

2.1.1 Gradient

If a scalar field s is defined and continuously differentiable then the gradient of s, ∇s is a vector field

$$\nabla s = \partial_i s = \left(\frac{\partial s}{\partial x_1}, \frac{\partial s}{\partial x_2}, \frac{\partial s}{\partial x_3} \right) \tag{2.2}$$

The gradient can operate on any tensor field to produce a tensor field that is one rank higher. For example, the gradient of a vector field $\mathbf{a}$ is a second rank tensor field

$$\nabla \mathbf{a} = \partial_i a_j = \begin{pmatrix} \partial a_1/\partial x_1 & \partial a_2/\partial x_1 & \partial a_3/\partial x_1 \\ \partial a_1/\partial x_2 & \partial a_2/\partial x_2 & \partial a_3/\partial x_2 \\ \partial a_1/\partial x_3 & \partial a_2/\partial x_3 & \partial a_3/\partial x_3 \end{pmatrix} \tag{2.3}$$

2.1.2 Divergence

If a vector field $\mathbf{a}$ is defined and continuously differentiable then the divergence of $\mathbf{a}$ is a scalar field

$$\nabla \bullet \mathbf{a} = \partial_i a_i = \frac{\partial a_1}{\partial x_1} + \frac{\partial a_2}{\partial x_2} + \frac{\partial a_3}{\partial x_3} \tag{2.4}$$

The divergence can operate on any tensor field of rank 1 and above to produce a tensor that is one rank lower. For example the divergence of a second rank tensor field $\mathbf{T}$ is a vector field (expanding the vector as a column array for convenience)

$$\nabla \bullet \mathbf{T} = \partial_i T_{ij} = \begin{pmatrix} \partial T_{11}/\partial x_1 + \partial T_{12}/\partial x_1 + \partial T_{13}/\partial x_1 \\ \partial T_{21}/\partial x_2 + \partial T_{22}/\partial x_2 + \partial T_{23}/\partial x_2 \\ \partial T_{31}/\partial x_3 + \partial T_{32}/\partial x_3 + \partial T_{33}/\partial x_3 \end{pmatrix} \tag{2.5}$$

2.1.3 Curl

If a vector field $\mathbf{a}$ is defined and continuously differentiable then the curl of $\mathbf{a}$, $\nabla \times \mathbf{a}$ is a vector field

$$\nabla \times \mathbf{a} = e_{ijk}\partial_j a_k = \left(\frac{\partial a_3}{\partial x_2} - \frac{\partial a_2}{\partial x_3}, \frac{\partial a_1}{\partial x_3} - \frac{\partial a_3}{\partial x_1}, \frac{\partial a_2}{\partial x_1} - \frac{\partial a_1}{\partial x_2} \right) \tag{2.6}$$

The curl is related to the gradient by

$$\nabla \times \mathbf{a} = 2\,(* \operatorname{skew} \nabla \mathbf{a}) \tag{2.7}$$

2.1.4 Laplacian

The Laplacian is an operation that can be defined mathematically by a combination of the divergence and gradient operators by $\nabla^2 \equiv \nabla \bullet \nabla$. However, the Laplacian should be considered as a single operation that transforms a tensor field into another tensor field of the same rank, rather than a combination of two operations, one which raises the rank by 1 and one which reduces the rank by 1.

In fact, the Laplacian is best defined as a *scalar operator*, just as we defined nabla as a vector operator, by

$$\nabla^2 \equiv \partial^2 \equiv \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \tag{2.8}$$

For example, the Laplacian of a scalar field s is the scalar field

$$\nabla^2 s = \partial^2 s = \frac{\partial^2 s}{\partial x_1^2} + \frac{\partial^2 s}{\partial x_2^2} + \frac{\partial^2 s}{\partial x_3^2} \tag{2.9}$$

2.1.5 Temporal derivative

There is more than one definition of temporal, or time, derivative of a tensor. To describe the temporal derivatives we must first recall that the tensor relates to a property of a volume of material that may be moving. If we track an infinitesimally small volume of material, or particle, as it moves and observe the change in the tensorial property ϕ in time, we have the *total*, or *material* time derivative denoted by

$$\frac{D\phi}{Dt} = \lim_{\Delta t \to 0} \frac{\Delta \phi}{\Delta t} \tag{2.10}$$

However in continuum mechanics, particularly fluid mechanics, we often observe the change of a ϕ in time at a fixed point in space as different particles move across that point. This change at a point in space is termed the *spatial* time derivative which is denoted by $\partial/\partial t$ and is related to the material derivative by:

$$\frac{D\phi}{Dt} = \frac{\partial\phi}{\partial t} + \mathbf{U} \bullet \nabla\phi \tag{2.11}$$

where $\mathbf{U}$ is the velocity field of property ϕ. The second term on the right is known as the convective rate of change of ϕ.

2.2 Overview of discretisation

The term discretisation means *approximation of a problem into discrete quantities*. The FV method and others, such as the finite element and finite difference methods, all discretise the problem as follows:

Spatial discretisation Defining the solution domain by a set of points that fill and bound a region of space when connected;

Temporal discretisation (For transient problems) dividing the time domain into into a finite number of time intervals, or steps;

Equation discretisation Generating a system of algebraic equations in terms of discrete quantities defined at specific locations in the domain, from the PDEs that characterise the problem.

2.2.1 OpenFOAM lists and fields

OpenFOAM frequently needs to store sets of data and perform functions, such as mathematical operations, on the data. OpenFOAM therefore provides an array template class List<Type>, making it possible to create a list of any object of class Type that inherits the functions of the Type. For example a List of vector is List<vector>.

Lists of the tensor classes are defined as standard in OpenFOAM by the template class Field<Type>. For better code legibility, all instances of Field<Type>, *e.g.*Field<vector>, are renamed using `typedef` declarations as scalarField, vectorField, tensorField, symmTensorField, tensorThirdField and symmTensorThirdField. Algebraic operations can be performed between Fields subject to obvious restrictions such as the fields having the same number of elements. OpenFOAM also supports operations between a field and single tensor, *e.g.* all values of a Field `U` can be multiplied by the scalar 2 with the operation `U = 2.0 * U`.

2.3 Discretisation of the solution domain

Discretisation of the solution domain is shown in Figure 2.1. The space domain is discretised into computational mesh on which the PDEs are subsequently discretised. Discretisation of time, if required, is simple: it is broken into a set of time steps Δt that may change during a numerical simulation, perhaps depending on some condition calculated during the simulation.

On a more detailed level, discretisation of space requires the subdivision of the domain into a number of cells, or control volumes. The cells are contiguous, *i.e.* they do not overlap one another and completely fill the domain. A typical cell is shown in Figure 2.2.

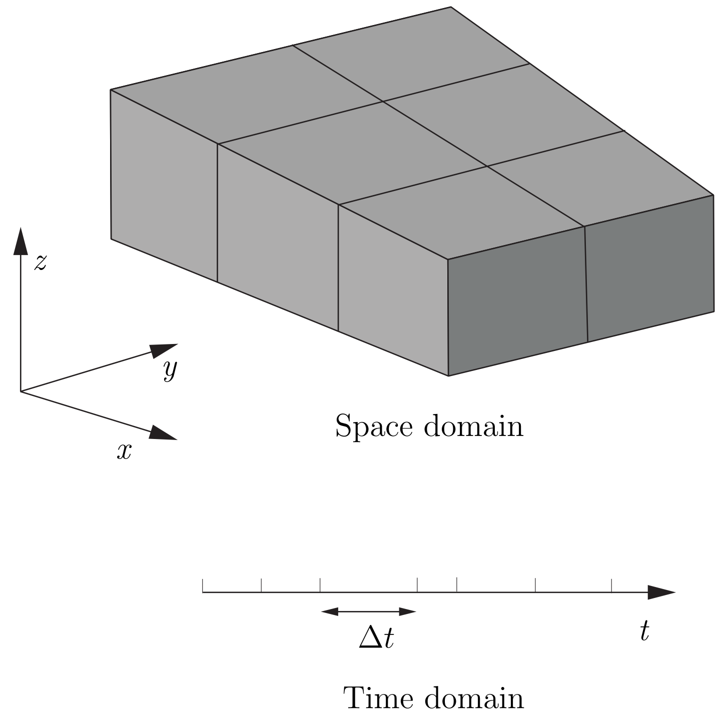


Figure 2.1: Discretisation of the solution domain

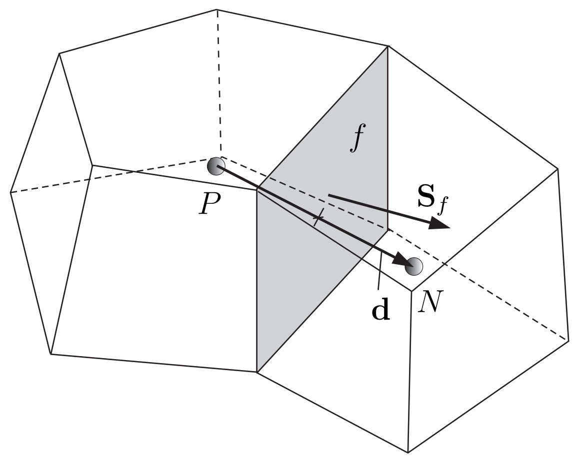


Figure 2.2: Parameters in finite volume discretisation

Dependent variables and other properties are principally stored at the cell centroid P although they may be stored on faces or vertices. The cell is bounded by a set of flat faces, given the generic label f. In OpenFOAM there is no limitation on the number of faces bounding each cell, nor any restriction on the alignment of each face. This kind of mesh is often referred to as "arbitrarily unstructured" to differentiate it from meshes in which the cell faces have a prescribed alignment, typically with the coordinate axes. Codes with arbitrarily unstructured meshes offer greater freedom in mesh generation and manipulation in particular when the geometry of the domain is complex or changes over time.

Whilst most properties are defined at the cell centroids, some are defined at cell faces. There are two types of cell face.

Internal faces Those faces that connect two cells (and it can never be more than two). For each internal face, OpenFOAM designates one adjoining cell to be the face *owner* and the other to be the *neighbour*;

Boundary faces Those belonging to one cell since they coincide with the boundary of the domain. These faces simply have an owner cell.

2.3.1 Defining a mesh in OpenFOAM

There are different levels of mesh description in OpenFOAM, beginning with the most basic mesh class, named polyMesh since it is based on polyhedra. A polyMesh is constructed using the minimum information required to define the mesh geometry described below and presented in Figure 2.3:

Points A list of cell vertex point coordinate vectors, *i.e.* a vectorField, that is renamed pointField using a `typedef` declaration;

Faces A list of cell faces List<face>, or faceList, where the face class is defined by a list of vertex numbers, corresponding to the pointField;

Cells a list of cells List<cell>, or cellList, where the cell class is defined by a list of face numbers, corresponding to the faceList described previously.

Boundary a polyBoundaryMesh decomposed into a list of patches, polyPatchList representing different regions of the boundary. The boundary is subdivided in this manner to allow different boundary conditions to be specified on different patches during a solution. All the faces of any polyPatch are stored as a single block of the faceList, so that its faces can be easily accessed using the slice class which stores references to the first and last face of the block. Each polyPatch is then constructed from

- a slice;
- a word to assign it a name.

FV discretisation uses specific data that is derived from the mesh geometry stored in polyMesh. OpenFOAM therefore extends the polyMesh class to fvMesh which stores the additional data needed for FV discretisation. fvMesh is constructed from polyMesh and stores the data in Table 2.1 which can be updated during runtime in cases where the mesh moves, is refined *etc.*.

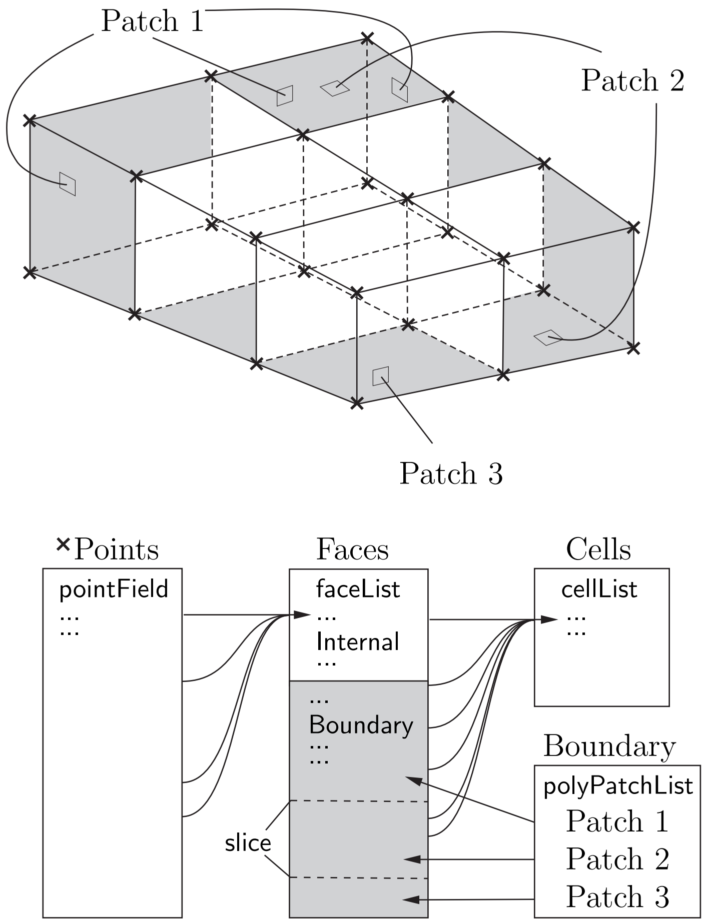


Figure 2.3: Schematic of the basic mesh description used in OpenFOAM

2.3.2 Defining a geometricField in OpenFOAM

So far we can define a field, *i.e.* a list of tensors, and a mesh. These can be combined to define a tensor field relating to discrete points in our domain, specified in OpenFOAM by the template class geometricField<Type>. The Field values are separated into those defined within the internal region of the domain, *e.g.* at the cell centres, and those defined on the domain boundary, *e.g.* on the boundary faces. The geometricField<Type> stores the following information:

Internal field This is simply a Field<Type>, described in Section 2.2.1;

BoundaryField This is a GeometricBoundaryField, in which a Field is defined for the faces of each patch and a Field is defined for the patches of the boundary. This is then a field of fields, stored within an object of the FieldField<Type> class. A reference to the fvBoundaryMesh is also stored [**].

Mesh A reference to an fvMesh, with some additional detail as to the whether the field is defined at cell centres, faces, *etc.*.

Dimensions A dimensionSet, described in Section 4.2.6.

Old values Discretisation of time derivatives requires field data from previous time steps. The geometricField<Type> will store references to stored fields from the previous, or old, time step and its previous, or old-old, time step where necessary.

Class	Description	Symbol	Access function
volScalarField	Cell volumes	V	`V()`
surfaceVectorField	Face area vectors	$\mathbf{S}_f$	`Sf()`
surfaceScalarField	Face area magnitudes	$\|\mathbf{S}_f\|$	`magSf()`
volVectorField	Cell centres	$\mathbf{C}$	`C()`
surfaceVectorField	Face centres	$\mathbf{C}_f$	`Cf()`
surfaceScalarField	Face motion fluxes **	ϕ_g	`phi()`

Table 2.1: fvMesh stored data.

Previous iteration values The iterative solution procedures can use under-relaxation which requires access to data from the previous iteration. Again, if required, geometricField<Type> stores a reference to the data from the previous iteration.

As discussed in Section 2.3, we principally define a property at the cell centres but quite often it is stored at the cell faces and on occasion it is defined on cell vertices. The geometricField<Type> is renamed using `typedef` declarations to indicate where the field variable is defined as follows:

volField<Type> A field defined at cell centres;

surfaceField<Type> A field defined on cell faces;

pointField<Type> A field defined on cell vertices.

These `typedef` field classes of geometricField<Type>are illustrated in Figure 2.4. A geometricField<Type> inherits all the tensor algebra of Field<Type> and has all operations subjected to dimension checking using the dimensionSet. It can also be subjected to the FV discretisation procedures described in the following Section. The class structure used to build geometricField<Type> is shown in Figure 2.5[1].

2.4 Equation discretisation

Equation discretisation converts the PDEs into a set of algebraic equations that are commonly expressed in matrix form as:

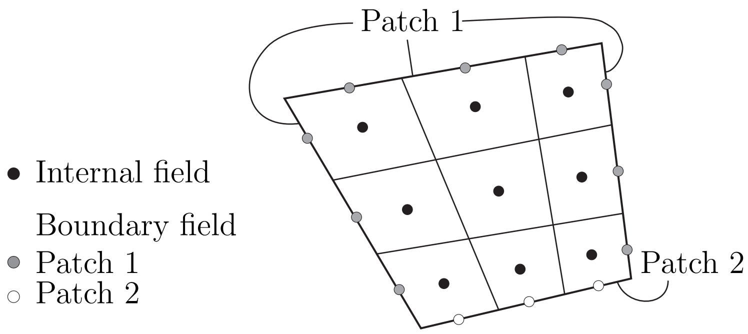
$$[A]\,[x] = [b] \tag{2.12}$$

where $[A]$ is a square matrix, $[x]$ is the column vector of dependent variable and $[b]$ is the source vector. The description of $[x]$ and $[b]$ as 'vectors' comes from matrix terminology rather than being a precise description of what they truly are: a list of values defined at locations in the geometry, *i.e.* a geometricField<Type>, or more specifically a volField<Type> when using FV discretisation.

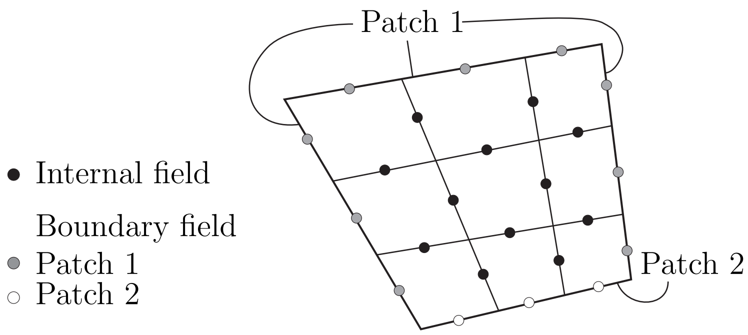
$[A]$ is a list of coefficients of a set of algebraic equations, and cannot be described as a geometricField<Type>. It is therefore given a class of its own: fvMatrix. fvMatrix<Type> is created through discretisation of a geometric<Type>Field and therefore inherits the <Type>. It supports many of the standard algebraic matrix operations of addition `+`, subtraction `-` and multiplication `*`.

Each term in a PDE is represented individually in OpenFOAM code using the classes of static functions finiteVolumeMethod and finiteVolumeCalculus, abbreviated by a `typedef`

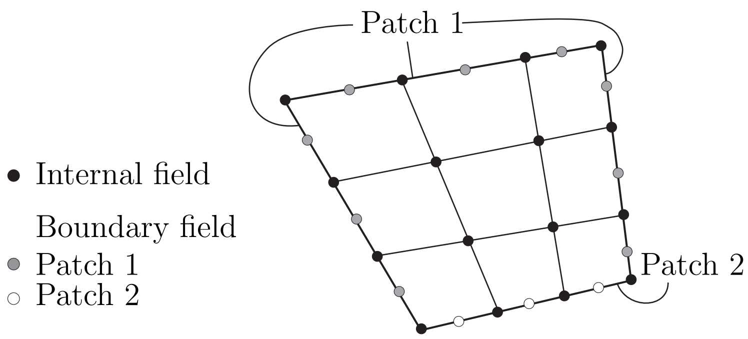
[1]The diagram is not an exact description of the class hierarchy, rather a representation of the general structure leading from some primitive classes to geometric<Type>Field.



(a) A volField<Type>



(b) A surfaceField<Type>



(c) A pointField<Type>

Figure 2.4: Types of geometricField<Type> defined on a mesh with 2 boundary patches (in 2 dimensions for simplicity)

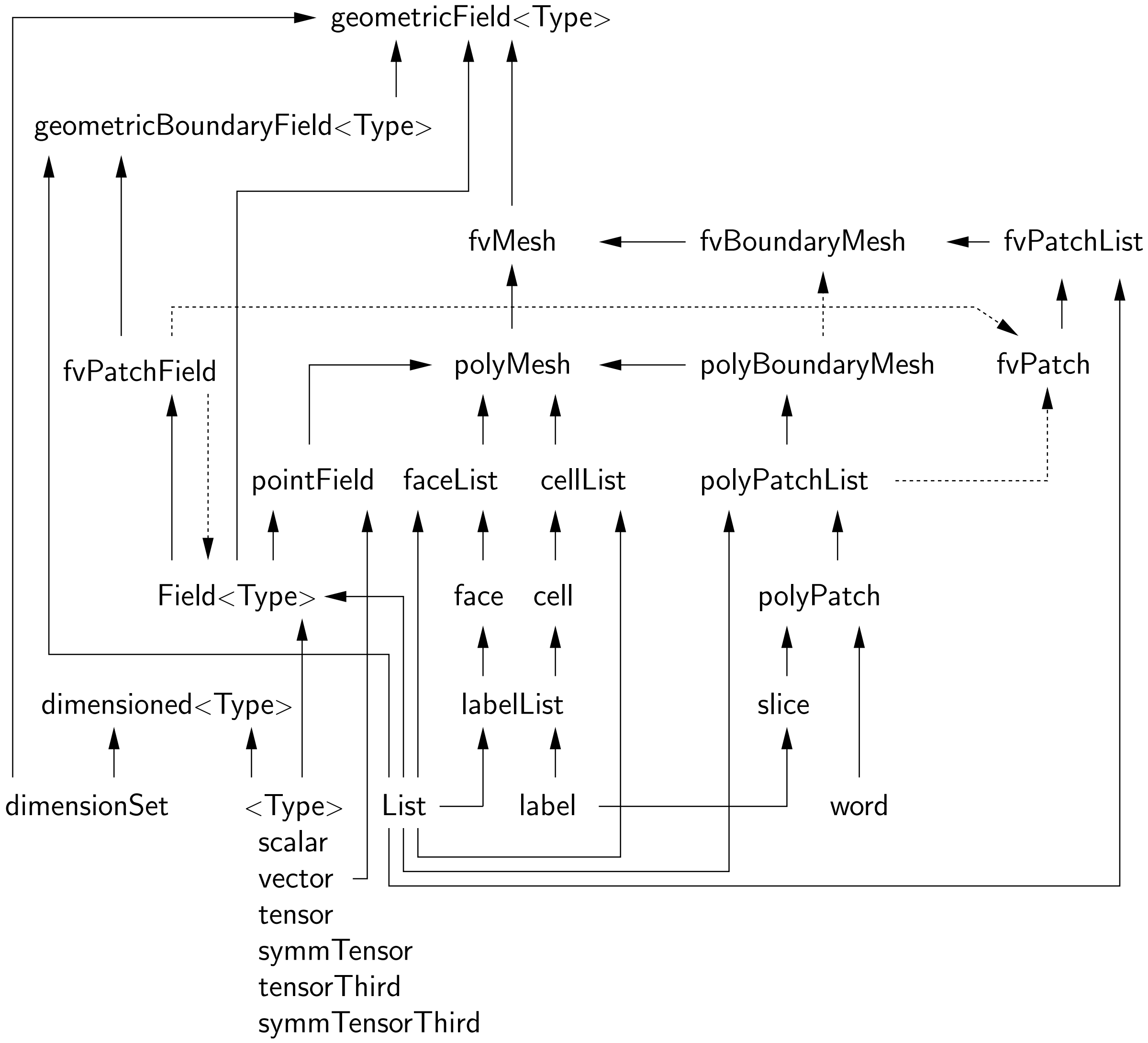


Figure 2.5: Basic class structure leading to geometricField<Type>

to fvm and fvc respectively. fvm and fvc contain static functions, representing differential operators, *e.g.* ∇^2, $\nabla\bullet$ and $\partial/\partial t$, that discretise geometricField<Type>s. The purpose of defining these functions within two classes, fvm and fvc, rather than one, is to distinguish:

- functions of fvm that calculate implicit derivatives of and return an fvMatrix<Type>
- some functions of fvc that calculate explicit derivatives and other explicit calculations, returning a geometricField<Type>.

Figure 2.6 shows a geometricField<Type> defined on a mesh with 2 boundary patches and illustrates the explicit operations merely transform one field to another and drawn in 2D for simplicity.

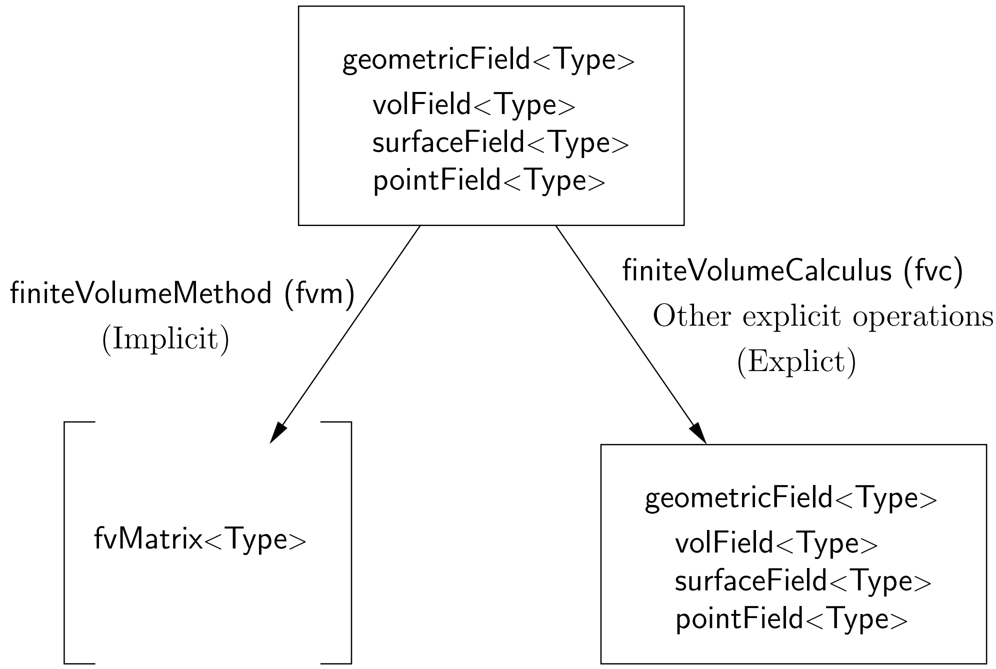


Figure 2.6: A geometricField<Type> and its operators

Table 2.2 lists the main functions that are available in fvm and fvc to discretise terms that may be found in a PDE. FV discretisation of each term is formulated by first integrating the term over a cell volume V. Most spatial derivative terms are then converted to integrals over the cell surface S bounding the volume using Gauss's theorem

$$\int_V \nabla \star \phi \; dV = \int_S d\mathbf{S} \star \phi \tag{2.13}$$

where $\mathbf{S}$ is the surface area vector, ϕ can represent any tensor field and the star notation $\star$ is used to represent any tensor product, *i.e.* inner, outer and cross and the respective derivatives: divergence $\nabla\bullet\phi$, gradient $\nabla\phi$ and $\nabla\times\phi$. Volume and surface integrals are then linearised using appropriate schemes which are described for each term in the following Sections. Some terms are always discretised using one scheme, a selection of schemes is offered in OpenFOAM for the discretisation of other terms. The choice of scheme is either made by a direct specification within the code or it can be read from an input file at job run-time and stored within an fvSchemes class object.

Term description	Implicit / Explicit	Text expression	fvm::/fvc:: functions
Laplacian	Imp/Exp	$\nabla^2\phi$ $\nabla \bullet \Gamma\nabla\phi$	`laplacian(phi)` `laplacian(Gamma, phi)`
Time derivative	Imp/Exp	$\dfrac{\partial\phi}{\partial t}$ $\dfrac{\partial\rho\phi}{\partial t}$	`ddt(phi)` `ddt(rho,phi)`
Second time derivative	Imp/Exp	$\dfrac{\partial}{\partial t}\left(\rho\dfrac{\partial\phi}{\partial t}\right)$	`d2dt2(rho, phi)`
Convection	Imp/Exp	$\nabla \bullet (\psi)$ $\nabla \bullet (\psi\phi)$	`div(psi,scheme)`* `div(psi, phi, word)`* `div(psi, phi)`
Divergence	Exp	$\nabla \bullet \chi$	`div(chi)`

Gradient	Exp	$\nabla\chi$
		$\nabla\phi$
			`grad(chi)`
			`gGrad(phi)`
			`lsGrad(phi)`
			`snGrad(phi)`
			`snGradCorrection(phi)`

Grad-grad squared	Exp	$\lvert\nabla\nabla\phi\rvert^2$	`sqrGradGrad(phi)`
Curl	Exp	$\nabla \times \phi$	`curl(phi)`
Source	Imp Imp/Exp†	$\rho\phi$	`Sp(rho,phi)` `SuSp(rho,phi)`

†`fvm::SuSp` source is discretised implicit or explicit depending on the sign of `rho`.
†An explicit source can be introduced simply as a vol<Type>Field, *e.g.*`rho*phi`.
Function arguments can be of the following classes:
`phi`: vol<Type>Field
`Gamma`: scalar volScalarField, surfaceScalarField, volTensorField, surfaceTensorField.
`rho`: scalar, volScalarField
`psi`: surfaceScalarField.
`chi`: surface<Type>Field, vol<Type>Field.

Table 2.2: Discretisation of PDE terms in OpenFOAM

2.4.1 The Laplacian term

The Laplacian term is integrated over a control volume and linearised as follows:

$$\int_V \nabla \bullet (\Gamma \nabla \phi)\, dV = \int_S d\mathbf{S} \bullet (\Gamma \nabla \phi) = \sum_f \Gamma_f \mathbf{S}_f \bullet (\nabla \phi)_f \tag{2.14}$$

The face gradient discretisation is implicit when the length vector **d** between the centre of the cell of interest P and the centre of a neighbouring cell N is orthogonal to the face plane, *i.e.* parallel to $\mathbf{S}_f$:

$$\mathbf{S}_f \bullet (\nabla \phi)_f = |S_f| \frac{\phi_N - \phi_P}{|\mathbf{d}|} \tag{2.15}$$

In the case of non-orthogonal meshes, an additional explicit term is introduced which is evaluated by interpolating cell centre gradients, themselves calculated by central differencing cell centre values.

2.4.2 The convection term

The convection term is integrated over a control volume and linearised as follows:

$$\int_V \nabla \bullet (\rho \mathbf{U} \phi)\, dV = \int_S d\mathbf{S} \bullet (\rho \mathbf{U} \phi) = \sum_f \mathbf{S}_f \bullet (\rho \mathbf{U})_f \phi_f = \sum_f F \phi_f \tag{2.16}$$

The face field ϕ_f can be evaluated using a variety of schemes:

Central differencing (CD) is second-order accurate but unbounded

$$\phi_f = f_x \phi_P + (1 - f_x)\phi_N \tag{2.17}$$

where $f_x \equiv \overline{fN}/\overline{PN}$ where $\overline{fN}$ is the distance between f and cell centre N and $\overline{PN}$ is the distance between cell centres P and N.

Upwind differencing (UD) determines ϕ_f from the direction of flow and is bounded at the expense of accuracy

$$\phi_f = \begin{cases} \phi_P & \text{for } F \geq 0 \\ \phi_N & \text{for } F < 0 \end{cases} \tag{2.18}$$

Blended differencing (BD) schemes combine UD and CD in an attempt to preserve boundedness with reasonable accuracy,

$$\phi_f = (1 - \gamma)\,(\phi_f)_{UD} + \gamma\,(\phi_f)_{CD} \tag{2.19}$$

OpenFOAM has several implementations of the Gamma differencing scheme to select the blending coefficient γ but it offers other well-known schemes such as van Leer, SUPERBEE, MINMOD *etc.*.

2.4.3 First time derivative

The first time derivative $\partial/\partial t$ is integrated over a control volume as follows:

$$\frac{\partial}{\partial t}\int_V \rho\phi \; dV \tag{2.20}$$

The term is discretised by simple differencing in time using:

new values $\phi^n \equiv \phi(t + \Delta t)$ at the time step we are solving for;

old values $\phi^o \equiv \phi(t)$ that were stored from the previous time step;

old-old values $\phi^{oo} \equiv \phi(t - \Delta t)$ stored from a time step previous to the last.

One of two discretisation schemes can be declared using the `timeScheme` keyword in the appropriate input file, described in detail in section 4.4 of the User Guide.

Euler implicit scheme, `timeScheme EulerImplicit`, that is first order accurate in time:

$$\frac{\partial}{\partial t}\int_V \rho\phi \; dV = \frac{(\rho_P\phi_P V)^n - (\rho_P\phi_P V)^o}{\Delta t} \tag{2.21}$$

Backward differencing scheme, `timeScheme BackwardDifferencing`, that is second order accurate in time by storing the old-old values and therefore with a larger overhead in data storage than `EulerImplicit`:

$$\frac{\partial}{\partial t}\int_V \rho\phi \; dV = \frac{3\,(\rho_P\phi_P V)^n - 4\,(\rho_P\phi_P V)^o + (\rho_P\phi_P V)^{oo}}{2\Delta t} \tag{2.22}$$

2.4.4 Second time derivative

The second time derivative is integrated over a control volume and linearised as follows:

$$\frac{\partial}{\partial t}\int_V \rho\frac{\partial\phi}{\partial t} \; dV = \frac{(\rho_P\phi_P V)^n - 2\,(\rho_P\phi_P V)^o + (\rho_P\phi_P V)^{oo}}{\Delta t^2} \tag{2.23}$$

It is first order accurate in time.

2.4.5 Divergence

The divergence term described in this Section is strictly an explicit term that is distinguished from the convection term of Section 2.4.2, *i.e.* in that it is not the divergence of the product of a velocity and dependent variable. The term is integrated over a control volume and linearised as follows:

$$\int_V \nabla \bullet \phi \; dV = \int_S d\mathbf{S} \bullet \phi = \sum_f \mathbf{S}_f \bullet \phi_f \tag{2.24}$$

The `fvc::div` function can take as its argument either a surface<Type>Field, in which case ϕ_f is specified directly, or a vol<Type>Field which is interpolated to the face by central differencing as described in Section 2.4.10:

2.4.6 Gradient

The gradient term is an explicit term that can be evaluated in a variety of ways. The scheme can be evaluated either by selecting the particular grad function relevant to the discretisation scheme, *e.g.*`fvc::gGrad`, `fvc::lsGrad` *etc.*, or by using the `fvc::grad` function combined with the appropriate `timeScheme` keyword in an input file

Gauss integration is invoked using the `fvc::grad` function with `timeScheme Gauss` or directly using the `fvc::gGrad` function. The discretisation is performed using the standard method of applying Gauss's theorem to the volume integral:

$$\int_V \nabla\phi \, dV = \int_S d\mathbf{S}\,\phi = \sum_f \mathbf{S}_f \phi_f \tag{2.25}$$

As with the `fvc::div` function, the Gaussian integration `fvc::grad` function can take either a surfaceField<Type> or a volField<Type> as an argument.

Least squares method is based on the following idea:

1. a value at point P can be extrapolated to neighbouring point N using the gradient at P;
2. the extrapolated value at N can be compared to the actual value at N, the difference being the error;
3. if we now minimise the sum of the square of weighted errors at all neighbours of P with the respect to the gradient, then the gradient should be a good approximation.

Least squares is invoked using the `fvc::grad` function with `timeScheme leastSquares` or directly using the `fvc::lsGrad` function. The discretisation is performed as by first calculating the tensor $\mathbf{G}$ at every point P by summing over neighbours N:

$$\mathbf{G} = \sum_N w_N^2 \mathbf{dd} \tag{2.26}$$

where $\mathbf{d}$ is the vector from P to N and the weighting function $w_N = 1/|\mathbf{d}|$. The gradient is then evaluated as:

$$(\nabla\phi)_P = \sum_N w_N^2 \mathbf{G}^{-1} \bullet \mathbf{d}\,(\phi_N - \phi_P) \tag{2.27}$$

Surface normal gradient The gradient normal to a surface $\mathbf{n}_f \bullet (\nabla\phi)_f$ can be evaluated at cell faces using the scheme

$$(\nabla\phi)_f = \frac{\phi_N - \phi_P}{|\mathbf{d}|} \tag{2.28}$$

This gradient is called by the function `fvc::snGrad` and returns a surfaceField<Type>. The scheme is directly analogous to that evaluated for the Laplacian discretisation scheme in Section 2.4.1, and in the same manner, a correction can be introduced to improve the accuracy of this face gradient in the case of non-orthogonal meshes. This correction is called using the function `fvc::snGradCorrection` [Check**].

2.4.7 Grad-grad squared

The grad-grad squared term is evaluated by: taking the gradient of the field; taking the gradient of the resulting gradient field; and then calculating the magnitude squared of the result. The mathematical expression for grad-grad squared of ϕ is $|\nabla(\nabla\phi)|^2$.

2.4.8 Curl

The curl is evaluated from the gradient term described in Section 2.4.6. First, the gradient is discretised and then the curl is evaluated using the relationship from Equation 2.7, repeated here for convenience

$$\nabla \times \phi = 2 \, {}^*(\text{skew}\, \nabla\phi)$$

2.4.9 Source terms

Source terms can be specified in 3 ways

Explicit Every explicit term is a volField<Type>. Hence, an explicit source term can be incorporated into an equation simply as a field of values. For example if we wished to solve Poisson's equation $\nabla^2\phi = f$, we would define `phi` and `f` as volScalarField and then do

```
solve(fvm::laplacian(phi) == f)
```

Implicit An implicit source term is integrated over a control volume and linearised by

$$\int_V \rho\phi \, dV = \rho_P V_P \phi_P \tag{2.29}$$

Implicit/Explicit The implicit source term changes the coefficient of the diagonal of the matrix. Depending on the sign of the coefficient and matrix terms, this will either increase or decrease diagonal dominance of the matrix. Decreasing the diagonal dominance could cause instability during iterative solution of the matrix equation. Therefore OpenFOAM provides a mixed source discretisation procedure that is implicit when the coefficients that are greater than zero, and explicit for the coefficients less than zero. In mathematical terms the matrix coefficient for node P is $V_P \max(\rho_P, 0)$ and the source term is $V_P \phi_P \min(\rho_P, 0)$.

2.4.10 Other explicit discretisation schemes

There are some other discretisation procedures that convert volField<Type>s into surface<Type>Fields and visa versa.

Surface integral `fvc::surfaceIntegrate` performs a summation of surface<Type>Field face values bounding each cell and dividing by the cell volume, *i.e.* $(\sum_f \phi_f)/V_P$. It returns a volField<Type>.

Surface sum `fvc::surfaceSum` performs a summation of surface<Type>Field face values bounding each cell, *i.e.* $\sum_f \phi_f$ returning a volField<Type>.

Average `fvc::average` produces an area weighted average of surface<Type>Field face values, *i.e.* $(\sum_f S_f \phi_f)/\sum_f S_f$, and returns a volField<Type>.

Reconstruct

Face interpolate The geometric<Type>Field function `faceInterpolate()` interpolates volField<Type> cell centre values to cell faces using central differencing, returning a surface<Type>Field.

2.5 Temporal discretisation

Although we have described the discretisation of temporal derivatives in Sections 2.4.3 and 2.4.4, we need to consider how to treat the spatial derivatives in a transient problem. If we denote all the spatial terms as $\mathcal{A}\phi$ where $\mathcal{A}$ is any spatial operator, *e.g.* Laplacian, then we can express a transient PDE in integral form as

$$\int_t^{t+\Delta t} \left[\frac{\partial}{\partial t} \int_V \rho\phi \, dV + \int_V \mathcal{A}\phi \, dV \right] dt = 0 \tag{2.30}$$

Using the Euler implicit method of Equation 2.21, the first term can be expressed as

$$\begin{aligned} \int_t^{t+\Delta t} \left[\frac{\partial}{\partial t} \int_V \rho\phi \, dV \right] dt &= \int_t^{t+\Delta t} \frac{(\rho_P\phi_P V)^n - (\rho_P\phi_P V)^o}{\Delta t} \, dt \\ &= \frac{(\rho_P\phi_P V)^n - (\rho_P\phi_P V)^o}{\Delta t} \Delta t \end{aligned} \tag{2.31}$$

The second term can be expressed as

$$\int_t^{t+\Delta t} \left[\int_V \mathcal{A}\phi \, dV \right] dt = \int_t^{t+\Delta t} \mathcal{A}^*\phi \, dt \tag{2.32}$$

where $\mathcal{A}^*$ represents the spatial discretisation of $\mathcal{A}$. The time integral can be discretised in three ways:

Euler implicit uses implicit discretisation of the spatial terms, thereby taking current values ϕ^n.

$$\int_t^{t+\Delta t} \mathcal{A}^*\phi \, dt = \mathcal{A}^*\phi^n \Delta t \tag{2.33}$$

It is first order accurate in time, guarantees boundedness and is unconditionally stable.

Explicit uses explicit discretisation of the spatial terms, thereby taking old values ϕ^o.

$$\int_t^{t+\Delta t} \mathcal{A}^*\phi \, dt = \mathcal{A}^*\phi^o \Delta t \tag{2.34}$$

It is first order accurate in time and is unstable if the Courant number Co is greater than 1. The Courant number is defined as

$$Co = \frac{\mathbf{U}_f \bullet \mathbf{d}}{|\mathbf{d}|^2 \Delta t} \tag{2.35}$$

where $\mathbf{U}_f$ is a characteristic velocity, *e.g.* velocity of a wave front, velocity of flow.

Crank Nicholson uses the trapezoid rule to discretise the spatial terms, thereby taking a mean of current values ϕ^n and old values ϕ^o.

$$\int_t^{t+\Delta t} \mathcal{A}^*\phi \, dt = \mathcal{A}^* \left(\frac{\phi^n + \phi^o}{2} \right) \Delta t \tag{2.36}$$

It is second order accurate in time, is unconditionally stable but does not guarantee boundedness.

2.5.1 Treatment of temporal discretisation in OpenFOAM

At present the treatment of the temporal discretisation is controlled by the implementation of the spatial derivatives in the PDE we wish to solve. For example, let us say we wish to solve a transient diffusion equation

$$\frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi \tag{2.37}$$

An Euler implicit implementation of this would read

```
solve(fvm::ddt(phi) == kappa*fvm::laplacian(phi))
```

where we use the `fvm` class to discretise the `Laplacian` term implicitly. An explicit implementation would read

```
solve(fvm::ddt(phi) == kappa*fvc::laplacian(phi))
```

where we now use the `fvc` class to discretise the `Laplacian` term explicitly. The Crank Nicholson scheme can be implemented by the mean of implicit and explicit terms:

```
solve
    (
    fvm::ddt(phi)
    ==
    kappa*0.5*(fvm::laplacian(phi) + fvc::laplacian(phi))
    )
```

2.6 Boundary Conditions

Boundary conditions are required to complete the problem we wish to solve. We therefore need to specify boundary conditions on all our boundary faces. Boundary conditions can be divided into 2 types:

Dirichlet prescribes the value of the dependent variable on the boundary and is therefore termed 'fixed value' in this guide;

Neumann prescribes the gradient of the variable normal to the boundary and is therefore termed 'fixed gradient' in this guide.

When we perform discretisation of terms that include the sum over faces $\sum_f$, we need to consider what happens when one of the faces is a boundary face.

Fixed value We specify a fixed value at the boundary ϕ_b

- We can simply substitute ϕ_b in cases where the discretisation requires the value on a boundary face ϕ_f, *e.g.* in the convection term in Equation 2.16.
- In terms where the face gradient $(\nabla\phi)_f$ is required, *e.g.* Laplacian, it is calculated using the boundary face value and cell centre value,

$$\mathbf{S}_f \bullet (\nabla\phi)_f = |S_f| \frac{\phi_b - \phi_P}{|\mathbf{d}|} \tag{2.38}$$

Fixed gradient The fixed gradient boundary condition g_b is a specification on inner product of the gradient and unit normal to the boundary, or

$$g_b = \left(\frac{\mathbf{S}}{|\mathbf{S}|} \bullet \nabla \phi \right)_f \tag{2.39}$$

- When discretisation requires the value on a boundary face ϕ_f we must interpolate the cell centre value to the boundary by

$$\begin{aligned} \phi_f &= \phi_P + \mathbf{d} \bullet (\nabla \phi)_f \\ &= \phi_P + |\mathbf{d}|\, g_b \end{aligned} \tag{2.40}$$

- ϕ_b can be directly substituted in cases where the discretisation requires the face gradient to be evaluated,

$$\mathbf{S}_f \bullet (\nabla \phi)_f = |S_f|\, g_b \tag{2.41}$$

2.6.1 Physical boundary conditions

The specification of boundary conditions is usually an engineer's interpretation of the true behaviour. Real boundary conditions are generally defined by some physical attributes rather than the numerical description as described of the previous Section. In incompressible fluid flow there are the following physical boundaries

Inlet The velocity field at the inlet is supplied and, for consistency, the boundary condition on pressure is zero gradient.

Outlet The pressure field at the outlet is supplied and a zero gradient boundary condition on velocity is specified.

No-slip impermeable wall The velocity of the fluid is equal to that of the wall itself, *i.e.* a fixed value condition can be specified. The pressure is specified zero gradient since the flux through the wall is zero.

In a problem whose solution domain and boundary conditions are symmetric about a plane, we only need to model half the domain to one side of the symmetry plane. The boundary condition on the plane must be specified according to

Symmetry plane The symmetry plane condition specifies the component of the gradient normal to the plane should be zero. [Check**]

Chapter 3

Examples of the use of OpenFOAM

In this section we shall describe several test cases supplied with the OpenFOAM distribution. The intention is to provide example cases, including those in the tutorials in chapter 2 of the User Guide, for every standard solver. The examples are designed to introduce certain tools and features of OpenFOAM, *e.g.* within pre-/post-processing, numerical schemes, algorithms. They also provide a means for validation of solvers although that is not their principal function.

Each example contains a description of the problem: the geometry, initial and boundary conditions, a brief description of the equations being solved, models used, and physical properties required. The solution domain is selected which may be a portion of the original geometry, *e.g.* if we introduce symmetry planes. The method of meshing, usually blockMesh, is specified; of course the user can simply view the mesh since every example is distributed with the *polyMesh* directory containing the data files that describe the mesh.

The examples coexist with the tutorials in the *tutorials* subdirectory of the OpenFOAM installation. They are organised into a set of subdirectories by solver, *e.g.* all the icoFoam cases are stored within a subdirectory *icoFoam*. Before running a particular example, the user is urged to copy it into their user account. We recommend that the user stores all OpenFOAM cases in a directory we recommend that the tutorials are copied into a directory *$FOAM_RUN*. If this directory structure has not yet been created in the user's account, it can be created with

```
mkdir -p $FOAM_RUN
```

The tutorials can then be copied into this directory with

```
cp -r $FOAM_TUTORIALS/* $FOAM_RUN
```

3.1 Flow around a cylinder

In this example we shall investigate potential flow around a cylinder using potentialFoam. This example introduces the following OpenFOAM features:

- non-orthogonal meshes;
- generating an analytical solution to a problem in OpenFOAM.

3.1.1 Problem specification

The problem is defined as follows:

Solution domain The domain is 2 dimensional and consists of a square domain with a cylinder collocated with the centre of the square as shown in Figure 3.1.

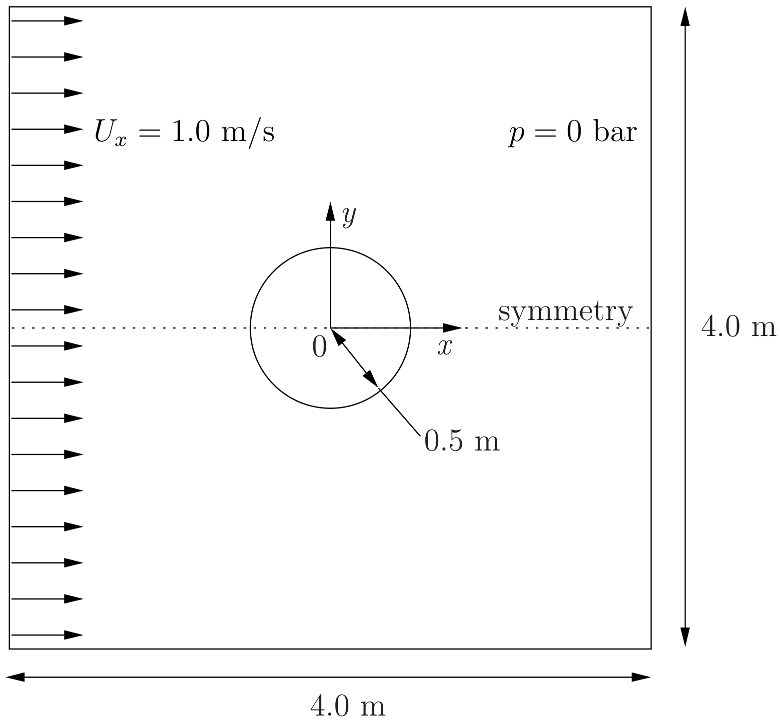


Figure 3.1: Geometry of flow round a cylinder

Governing equations

- Mass continuity for an incompressible fluid

$$\nabla \bullet \mathbf{U} = 0 \tag{3.1}$$

- Pressure equation for an incompressible, irrotational fluid assuming steady-state conditions

$$\nabla^2 p = 0 \tag{3.2}$$

Boundary conditions

- Inlet (left) with fixed velocity $\mathbf{U} = (1, 0, 0)$ m/s.
- Outlet (right) with a fixed pressure $p = 0$ Pa.
- No-slip wall (bottom);
- Symmetry plane (top).

Initial conditions $U = 0$ m/s, $p = 0$ Pa — required in OpenFOAM input files but not necessary for the solution since the problem is steady-state.

Solver name potentialFoam: a potential flow code, *i.e.* assumes the flow is incompressible, steady, irrotational, inviscid and it ignores gravity.

Case name *cylinder* case located in the *$FOAM_TUTORIALS/potentialFoam* directory.

3.1.2 Note on potentialFoam

potentialFoam is a useful solver to validate OpenFOAM since the assumptions of potential flow are such that an analytical solution exists for cases whose geometries are relatively simple. In this example of flow around a cylinder an analytical solution exists with which we can compare our numerical solution. potentialFoam can also be run more like a utility to provide a (reasonably) conservative initial **U** field for a problem. When running certain cases, this can useful for avoiding instabilities due to the initial field being unstable. In short, potentialFoam creates a conservative field from a non-conservative initial field supplied by the user.

3.1.3 Mesh generation

Mesh generation using blockMesh has been described in tutorials in the User Guide. In this case, the mesh consists of 10 blocks as shown in Figure 3.2. Remember that all

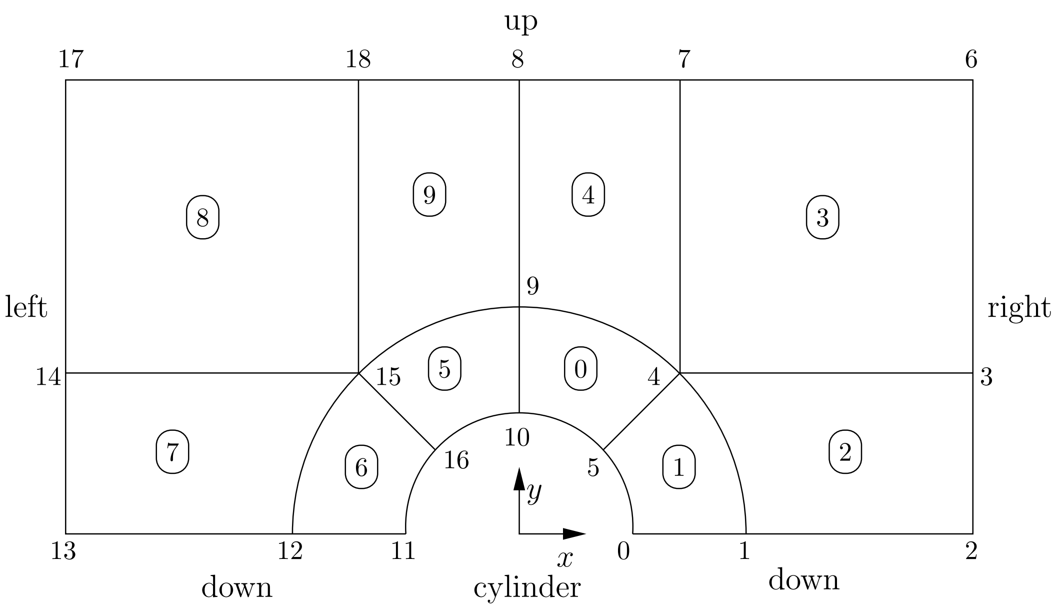


Figure 3.2: Blocks in cylinder geometry

meshes are treated as 3 dimensional in OpenFOAM. If we wish to solve a 2 dimensional problem, we must describe a 3 dimensional mesh that is only one cell thick in the third direction that is not solved. In Figure 3.2 we show only the back plane of the geometry, along $z = -0.5$, in which the vertex numbers are numbered 0-18. The other 19 vertices in the front plane, $z = +0.5$, are numbered in the same order as the back plane, as shown in the mesh description file below:

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      blockMeshDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

convertToMeters 1;
```

```

vertices #codeStream
{
    codeInclude
    #{
        #include "pointField.H"
    #};

    code
    #{
        pointField points(19);
        points[0]  = point(0.5, 0, -0.5);
        points[1]  = point(1, 0, -0.5);
        points[2]  = point(2, 0, -0.5);
        points[3]  = point(2, 0.707107, -0.5);
        points[4]  = point(0.707107, 0.707107, -0.5);
        points[5]  = point(0.353553, 0.353553, -0.5);
        points[6]  = point(2, 2, -0.5);
        points[7]  = point(0.707107, 2, -0.5);
        points[8]  = point(0, 2, -0.5);
        points[9]  = point(0, 1, -0.5);
        points[10] = point(0, 0.5, -0.5);
        points[11] = point(-0.5, 0, -0.5);
        points[12] = point(-1, 0, -0.5);
        points[13] = point(-2, 0, -0.5);
        points[14] = point(-2, 0.707107, -0.5);
        points[15] = point(-0.707107, 0.707107, -0.5);
        points[16] = point(-0.353553, 0.353553, -0.5);
        points[17] = point(-2, 2, -0.5);
        points[18] = point(-0.707107, 2, -0.5);

        // Duplicate z points
        label sz = points.size();
        points.setSize(2*sz);
        for (label i = 0; i < sz; i++)
        {
            const point& pt = points[i];
            points[i+sz] = point(pt.x(), pt.y(), -pt.z());
        }

        os  << points;
    #};
};


blocks
(
    hex (5 4 9 10 24 23 28 29) (10 10 1) simpleGrading (1 1 1)
    hex (0 1 4 5 19 20 23 24) (10 10 1) simpleGrading (1 1 1)
    hex (1 2 3 4 20 21 22 23) (20 10 1) simpleGrading (1 1 1)
    hex (4 3 6 7 23 22 25 26) (20 20 1) simpleGrading (1 1 1)
    hex (9 4 7 8 28 23 26 27) (10 20 1) simpleGrading (1 1 1)
    hex (15 16 10 9 34 35 29 28) (10 10 1) simpleGrading (1 1 1)
    hex (12 11 16 15 31 30 35 34) (10 10 1) simpleGrading (1 1 1)
    hex (13 12 15 14 32 31 34 33) (20 10 1) simpleGrading (1 1 1)
    hex (14 15 18 17 33 34 37 36) (20 20 1) simpleGrading (1 1 1)
    hex (15 9 8 18 34 28 27 37) (10 20 1) simpleGrading (1 1 1)
);

edges
(
    arc 0 5 (0.469846 0.17101 -0.5)
    arc 5 10 (0.17101 0.469846 -0.5)
    arc 1 4 (0.939693 0.34202 -0.5)
    arc 4 9 (0.34202 0.939693 -0.5)
    arc 19 24 (0.469846 0.17101 0.5)
    arc 24 29 (0.17101 0.469846 0.5)
    arc 20 23 (0.939693 0.34202 0.5)
    arc 23 28 (0.34202 0.939693 0.5)
    arc 11 16 (-0.469846 0.17101 -0.5)
    arc 16 10 (-0.17101 0.469846 -0.5)
    arc 12 15 (-0.939693 0.34202 -0.5)
    arc 15 9 (-0.34202 0.939693 -0.5)
    arc 30 35 (-0.469846 0.17101 0.5)
    arc 35 29 (-0.17101 0.469846 0.5)
    arc 31 34 (-0.939693 0.34202 0.5)
    arc 34 28 (-0.34202 0.939693 0.5)
);

```

```
boundary
(
    down
    {
        type symmetryPlane;
        faces
        (
            (0 1 20 19)
            (1 2 21 20)
            (12 11 30 31)
            (13 12 31 32)
        );
    }
    right
    {
        type patch;
        faces
        (
            (2 3 22 21)
            (3 6 25 22)
        );
    }
    up
    {
        type symmetryPlane;
        faces
        (
            (7 8 27 26)
            (6 7 26 25)
            (8 18 37 27)
            (18 17 36 37)
        );
    }
    left
    {
        type patch;
        faces
        (
            (14 13 32 33)
            (17 14 33 36)
        );
    }
    cylinder
    {
        type symmetryPlane;
        faces
        (
            (10 5 24 29)
            (5 0 19 24)
            (16 10 29 35)
            (11 16 35 30)
        );
    }
);

mergePatchPairs
(
);

// ************************************************************************* //
```

3.1.4 Boundary conditions and initial fields

Using FoamX or editing case files by hand, set the boundary conditions in accordance with the problem description in Figure 3.1, *i.e.* the left boundary should be an Inlet, the right boundary should be an Outlet and the down and cylinder boundaries should be symmetryPlane. The top boundary conditions is chosen so that we can make the most genuine comparison with our analytical solution which uses the assumption that the domain is infinite in the y direction. The result is that the normal gradient of $\mathbf{U}$ is small along a plane coinciding with our boundary. We therefore impose the condition that the normal component is zero, *i.e.* specify the boundary as a symmetryPlane, thereby ensuring that the comparison with the analytical is reasonable.

3.1.5 Running the case

No fluid properties need be specified in this problem since the flow is assumed to be incompressible and inviscid. In the *system* subdirectory, the *controlDict* specifies the control parameters for the run. Note that since we assume steady flow, we only run for 1 time step:

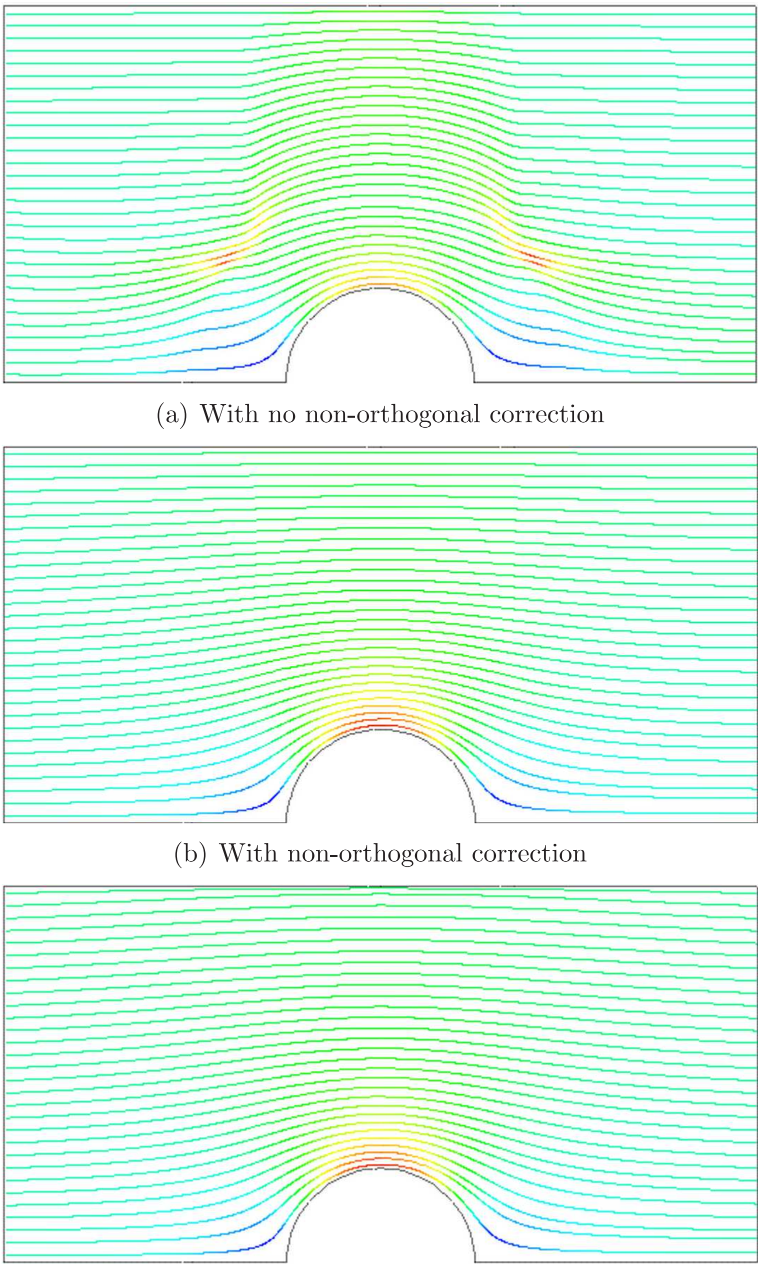
```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "system";
    object      controlDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

application     potentialFoam;

startFrom       startTime;

startTime       0;

stopAt          endTime;

endTime         1;

deltaT          1;

writeControl    timeStep;

writeInterval   1;

purgeWrite      0;

writeFormat     ascii;

writePrecision  6;

writeCompression off;

timeFormat      general;

timePrecision   6;

runTimeModifiable true;

functions
{
    difference
    {
        // Load the library containing the 'coded' functionObject
        functionObjectLibs ("libutilityFunctionObjects.so");
        type coded;
        // Name of on-the-fly generated functionObject
        redirectType error;
        code
        #{
            // Lookup U
            Info<< "Looking up field U\n" << endl;
            const volVectorField& U = mesh().lookupObject<volVectorField>("U");

            Info<< "Reading inlet velocity  uInfX\n" << endl;

            dimensionedScalar uInfX
            (
                "uInfx",
                dimensionSet(0, 1, -1, 0, 0),
                U.boundaryField()[3][0].x()
            );
            Info << "U at inlet = " << uInfX.value() << " m/s" << endl;

            dimensionedScalar radius
            (
                "radius",
```

```
                    dimensionSet(0, 1, 0, 0, 0),
                    mag(U.mesh().boundary()[4].Cf()[0])
                );

                Info << "Cylinder radius = " << radius.value() << " m" << endl;

                volVectorField UA
                (
                    IOobject
                    (
                        "UA",
                        mesh().time().timeName(),
                        U.mesh(),
                        IOobject::NO_READ,
                        IOobject::AUTO_WRITE
                    ),
                    U
                );

                Info<< "\nEvaluating analytical solution" << endl;

                const volVectorField& centres = UA.mesh().C();
                volScalarField magCentres(mag(centres));
                volScalarField theta(acos((centres & vector(1,0,0))/magCentres));

                volVectorField cs2theta
                (
                    cos(2*theta)*vector(1,0,0)
                  + sin(2*theta)*vector(0,1,0)
                );

                UA = uInfX*(dimensionedVector(vector(1,0,0))
                  - pow((radius/magCentres),2)*cs2theta);

                // Force writing of UA (since time has not changed)
                UA.write();

                volScalarField error("error", mag(U-UA)/mag(UA));

                Info<<"Writing relative error in U to " << error.objectPath()
                    << endl;

                error.write();
            #};
        }
    }


    // ************************************************************************* //
```

potentialFoam executes an iterative loop around the pressure equation which it solves in order that explicit terms relating to non-orthogonal correction in the Laplacian term may be updated in successive iterations. The number of iterations around the pressure equation is controlled by the `nNonOrthogonalCorrectors` keyword in *controlDict*. In the first instance we can set `nNonOrthogonalCorrectors` to 0 so that no loops are performed, *i.e.* the pressure equation is solved once, and there is no non-orthogonal correction. The solution is shown in Figure 3.3(a) (at $t = 1$, when the steady-state simulation is complete). We expect the solution to show smooth streamlines passing across the domain as in the analytical solution in Figure 3.3(c), yet there is clearly some error in the regions where there is high non-orthogonality in the mesh, *e.g.* at the join of blocks 0, 1 and 3. The case can be run a second time with some non-orthogonal correction by setting `nNonOrthogonalCorrectors` to 3. The solution shows smooth streamlines with no significant error due to non-orthogonality as shown in Figure 3.3(b).

3.2 Steady turbulent flow over a backward-facing step

In this example we shall investigate steady turbulent flow over a backward-facing step. The problem description is taken from one used by Pitz and Daily in an experimental investigation [**] against which the computed solution can be compared. This example introduces the following OpenFOAM features for the first time:



(a) With no non-orthogonal correction

(b) With non-orthogonal correction

(c) Analytical solution

Figure 3.3: Streamlines of potential flow

- generation of a mesh using blockMesh using full mesh grading capability;
- steady turbulent flow.

3.2.1 Problem specification

The problem is defined as follows:

Solution domain The domain is 2 dimensional, consisting of a short inlet, a backward-facing step and converging nozzle at outlet as shown in Figure 3.4.

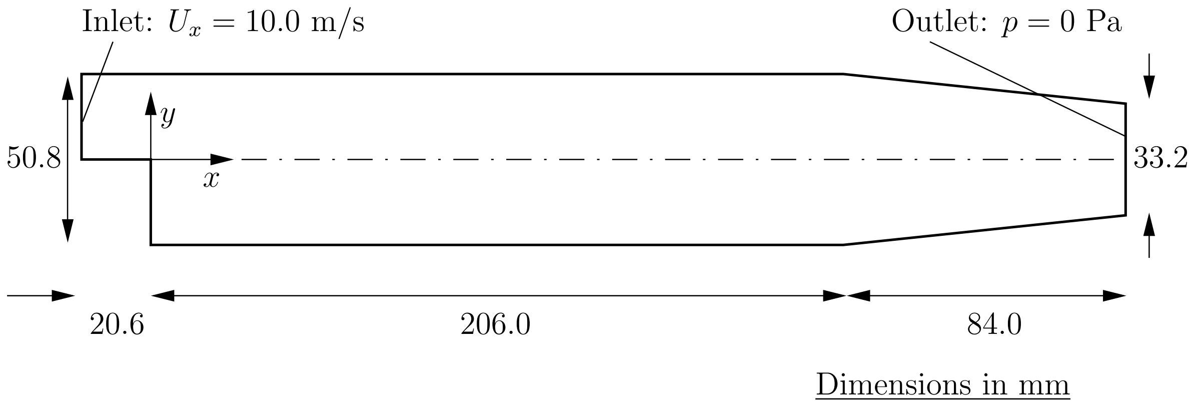


Figure 3.4: Geometry of backward-facing step

Governing equations

- Mass continuity for incompressible flow

$$\nabla \bullet \mathbf{U} = 0 \tag{3.3}$$

- Steady flow momentum equation

$$\nabla \bullet (\mathbf{U}\mathbf{U}) + \nabla \bullet \mathbf{R} = -\nabla p \tag{3.4}$$

where p is kinematic pressure and (in slightly over-simplistic terms) $\mathbf{R} = \nu_{eff} \nabla \mathbf{U}$ is the viscous stress term with an effective kinematic viscosity ν_{eff}, calculated from selected transport and turbulence models.

Initial conditions $U = 0$ m/s, $p = 0$ Pa — required in OpenFOAM input files but not necessary for the solution since the problem is steady-state.

Boundary conditions

- Inlet (left) with fixed velocity $\mathbf{U} = (10, 0, 0)$ m/s;
- Outlet (right) with fixed pressure $p = 0$ Pa;
- No-slip walls on other boundaries.

Transport properties

- Kinematic viscosity of air $\nu = \mu/\rho = 18.1 \times 10^{-6}/1.293 = 14.0\ \mu\mathrm{m}^2/\mathrm{s}$

Turbulence model

- Standard $k - \epsilon$;
- Coefficients: $C_\mu = 0.09; C_1 = 1.44; C_2 = 1.92; \alpha_k = 1; \alpha_\epsilon = 0.76923$.

Solver name simpleFoam: an implementation for steady incompressible flow.

Case name *pitzDaily*, located in the *$FOAM_TUTORIALS/simpleFoam* directory.

The problem is solved using simpleFoam, so-called as it is an implementation for steady flow using the SIMPLE algorithm [**]. The solver has full access to all the turbulence models in the incompressibleTurbulenceModels library and the non-Newtonian models incompressibleTransportModels library of the standard OpenFOAM release.

3.2.2 Mesh generation

We expect that the flow in this problem is reasonably complex and an optimum solution will require grading of the mesh. In general, the regions of highest shear are particularly critical, requiring a finer mesh than in the regions of low shear. We can anticipate where high shear will occur by considering what the solution might be in advance of any calculation. At the inlet we have strong uniform flow in the x direction and, as it passes over the step, it generates shear on the fluid below, generating a vortex in the bottom half of the domain. The regions of high shear will therefore be close to the centreline of the domain and close to the walls.

The domain is subdivided into 12 blocks as shown in Figure 3.5.

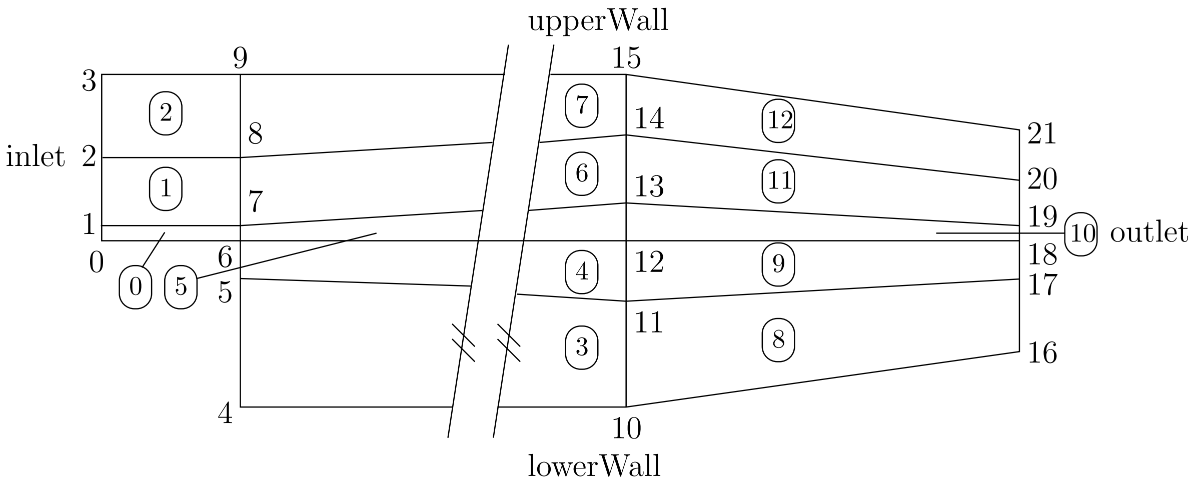


Figure 3.5: Blocks in backward-facing step

The mesh is 3 dimensional, as always in OpenFOAM, so in Figure 3.5 we are viewing the back plane along $z = -0.5$. The full set of vertices and blocks are given in the mesh description file below:

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      blockMeshDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
```

```
convertToMeters 0.001;

vertices
(
    (-20.6 0 -0.5)
    (-20.6 3 -0.5)
    (-20.6 12.7 -0.5)
    (-20.6 25.4 -0.5)
    (0 -25.4 -0.5)
    (0 -5 -0.5)
    (0 0 -0.5)
    (0 3 -0.5)
    (0 12.7 -0.5)
    (0 25.4 -0.5)
    (206 -25.4 -0.5)
    (206 -8.5 -0.5)
    (206 0 -0.5)
    (206 6.5 -0.5)
    (206 17 -0.5)
    (206 25.4 -0.5)
    (290 -16.6 -0.5)
    (290 -6.3 -0.5)
    (290 0 -0.5)
    (290 4.5 -0.5)
    (290 11 -0.5)
    (290 16.6 -0.5)
    (-20.6 0 0.5)
    (-20.6 3 0.5)
    (-20.6 12.7 0.5)
    (-20.6 25.4 0.5)
    (0 -25.4 0.5)
    (0 -5 0.5)
    (0 0 0.5)
    (0 3 0.5)
    (0 12.7 0.5)
    (0 25.4 0.5)
    (206 -25.4 0.5)
    (206 -8.5 0.5)
    (206 0 0.5)
    (206 6.5 0.5)
    (206 17 0.5)
    (206 25.4 0.5)
    (290 -16.6 0.5)
    (290 -6.3 0.5)
    (290 0 0.5)
    (290 4.5 0.5)
    (290 11 0.5)
    (290 16.6 0.5)
);

blocks
(
    hex (0 6 7 1 22 28 29 23) (18 7 1) simpleGrading (0.5 1.8 1)
    hex (1 7 8 2 23 29 30 24) (18 10 1) simpleGrading (0.5 4 1)
    hex (2 8 9 3 24 30 31 25) (18 13 1) simpleGrading (0.5 0.25 1)
    hex (4 10 11 5 26 32 33 27) (180 18 1) simpleGrading (4 1 1)
    hex (5 11 12 6 27 33 34 28) (180 9 1) edgeGrading (4 4 4 4 0.5 1 1 0.5 1 1 1 1)
    hex (6 12 13 7 28 34 35 29) (180 7 1) edgeGrading (4 4 4 4 1.8 1 1 1.8 1 1 1 1)
    hex (7 13 14 8 29 35 36 30) (180 10 1) edgeGrading (4 4 4 4 4 1 1 4 1 1 1 1)
    hex (8 14 15 9 30 36 37 31) (180 13 1) simpleGrading (4 0.25 1)
    hex (10 16 17 11 32 38 39 33) (25 18 1) simpleGrading (2.5 1 1)
    hex (11 17 18 12 33 39 40 34) (25 9 1) simpleGrading (2.5 1 1)
    hex (12 18 19 13 34 40 41 35) (25 7 1) simpleGrading (2.5 1 1)
    hex (13 19 20 14 35 41 42 36) (25 10 1) simpleGrading (2.5 1 1)
    hex (14 20 21 15 36 42 43 37) (25 13 1) simpleGrading (2.5 0.25 1)
);

edges
(
);

boundary
(
    inlet
    {
        type patch;
        faces
        (
            (0 22 23 1)
            (1 23 24 2)
            (2 24 25 3)
        );
```

```
    }
    outlet
    {
        type patch;
        faces
        (
            (16 17 39 38)
            (17 18 40 39)
            (18 19 41 40)
            (19 20 42 41)
            (20 21 43 42)
        );
    }
    upperWall
    {
        type wall;
        faces
        (
            (3 25 31 9)
            (9 31 37 15)
            (15 37 43 21)
        );
    }
    lowerWall
    {
        type wall;
        faces
        (
            (0 6 28 22)
            (6 5 27 28)
            (5 4 26 27)
            (4 10 32 26)
            (10 16 38 32)
        );
    }
    frontAndBack
    {
        type empty;
        faces
        (
            (22 28 29 23)
            (23 29 30 24)
            (24 30 31 25)
            (26 32 33 27)
            (27 33 34 28)
            (28 34 35 29)
            (29 35 36 30)
            (30 36 37 31)
            (32 38 39 33)
            (33 39 40 34)
            (34 40 41 35)
            (35 41 42 36)
            (36 42 43 37)
            (0 1 7 6)
            (1 2 8 7)
            (2 3 9 8)
            (4 5 11 10)
            (5 6 12 11)
            (6 7 13 12)
            (7 8 14 13)
            (8 9 15 14)
            (10 11 17 16)
            (11 12 18 17)
            (12 13 19 18)
            (13 14 20 19)
            (14 15 21 20)
        );
    }
);

mergePatchPairs
(
);

// ************************************************************************* //
```

A major feature of this problem is the use of the full mesh grading capability of blockMesh that is described in section 5.3.1 of the User Guide. The user can see that blocks 4,5 and 6 use the full list of 12 expansion ratios. The expansion ratios correspond to each edge of the block, the first 4 to the edges aligned in the local x_1 direction, the second 4 to the edges in the local x_2 direction and the last 4 to the edges in the local x_3 direction. In blocks 4, 5, and 6, the ratios are equal for all edges in the local x_1 and x_3

directions but not for the edges in the x_2 direction that corresponds in all blocks to the global y. If we consider the ratios used in relation to the block definition in section 5.3.1 of the User Guide, we realize that different gradings have been prescribed along the left and right edges in blocks 4,5 and 6 in Figure 3.5. The purpose of this differential grading is to generate a fine mesh close to the most critical region of flow, the corner of the step, and allow it to expand into the rest of the domain.

The mesh can be generated using blockMesh from the command line or from within FoamX and viewed as described in previous examples.

3.2.3 Boundary conditions and initial fields

The case files can be viewed, or edited from within FoamX or by hand. In this case, we are required to set the initial and boundary fields for velocity $\mathbf{U}$, pressure p, turbulent kinetic energy k and dissipation rate ε. The boundary conditions can be specified by setting the physical patch types in FoamX: the upper and lower walls are set to `Wall`, the left patch to `Inlet` and the right patch to `Outlet`. These physical boundary conditions require us to specify a fixedValue at the inlet on $\mathbf{U}$, k and ε. $\mathbf{U}$ is given in the problem specification, but the values of k and ϵ must be chosen by the user in a similar manner to that described in section 2.1.8.1 of the User Guide. We assume that the inlet turbulence is isotropic and estimate the fluctuations to be 5% of $\mathbf{U}$ at the inlet. We have

$$U'_x = U'_y = U'_z = \frac{5}{100} 10 = 0.5 \text{ m/s} \tag{3.5}$$

and

$$k = \frac{3}{2}(0.5)^2 = 0.375 \text{ m}^2/\text{s}^2 \tag{3.6}$$

If we estimate the turbulent length scale l to be 10% of the width of the inlet then

$$\varepsilon = \frac{C_\mu^{0.75} k^{1.5}}{l} = \frac{0.09^{0.75} 0.375^{1.5}}{0.1 \times 25.4 \times 10^{-3}} = 14.855 \, \text{m}^2/\text{s}^3 \tag{3.7}$$

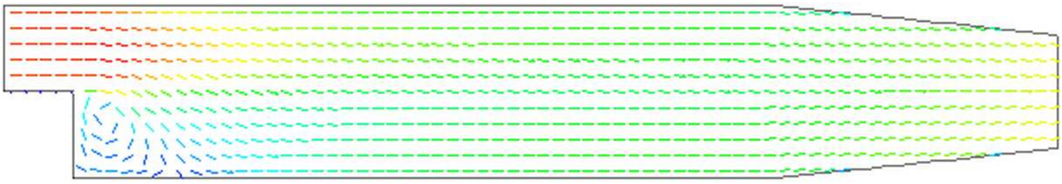
At the outlet we need only specify the pressure $p = 0$Pa.

3.2.4 Case control

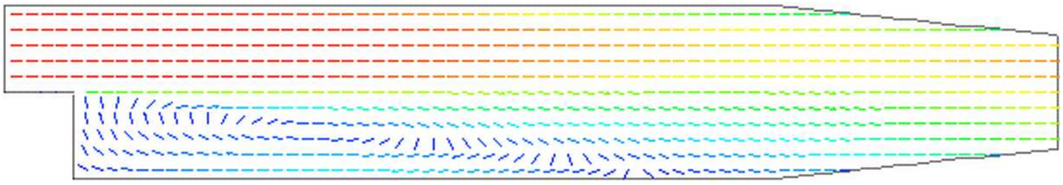
The choices of *fvSchemes* are as follows: the `timeScheme` should be `SteadyState`; the `gradScheme` and `laplacianScheme` should be set as default to `Gauss`; and, the `divScheme` should be set to `UD` to ensure boundedness.

Special attention should be paid to the settings of *fvTolerances*. Although the top level simpleFoam code contains only equations for p and $\mathbf{U}$, the turbulent model solves equations for k, ε and $\mathbf{R}$, and tolerance settings are required for all 5 equations. A `solverTolerance` of 10^{-5} and `solverRelativeTolerance` of 0.1 are acceptable for all variables with the exception of p when 10^{-6} and 0.01 are recommended. Under-relaxation of the solution is required since the problem is steady. A `relaxationFactor` of 0.7 is acceptable for $\mathbf{U}$, k, ε and $\mathbf{R}$ but 0.3 is required for p to avoid numerical instability.

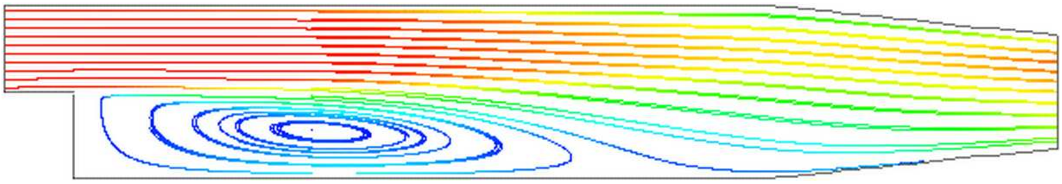
Finally, in *controlDict*, the time step `deltaT` should be set to 1 since in steady state cases such as this is effectively an iteration counter. With benefit of hindsight we know that the solution requires 1000 iterations reach reasonable convergence, hence `endTime` is set to 1000. Ensure that the `writeFrequency` is sufficiently high, *e.g.* 50, that you will not fill the hard disk with data during run time.



(a) Velocity vectors after 50 iterations



(b) Velocity vectors at 1000 iterations



(c) Streamlines at 1000 iterations

Figure 3.6: Development of a vortex in the backward-facing step.

3.2.5 Running the case and post-processing

Run the case and post-process the results. After a few iterations, *e.g.* 50, a vortex develops beneath the corner of the step that is the height of the step but narrow in the x-direction as shown by the vector plot of velocities is shown Figure 3.6(a). Over several iterations the vortex stretches in the x-direction from the step to the outlet until at 1000 iterations the system reaches a steady-state in which the vortex is fully developed as shown in Figure 3.6(b-c).

3.3 Supersonic flow over a forward-facing step

In this example we shall investigate supersonic flow over a forward-facing step. The problem description involves a flow of Mach 3 at an inlet to a rectangular geometry with a step near the inlet region that generates shock waves.

This example introduces the following OpenFOAM features for the first time:

- supersonic flow;

3.3.1 Problem specification

The problem is defined as follows:

Solution domain The domain is 2 dimensional and consists of a short inlet section followed by a forward-facing step of 20% the height of the section as shown in Figure 3.7

Governing equations

- Mass continuity

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{U}) = 0 \tag{3.8}$$

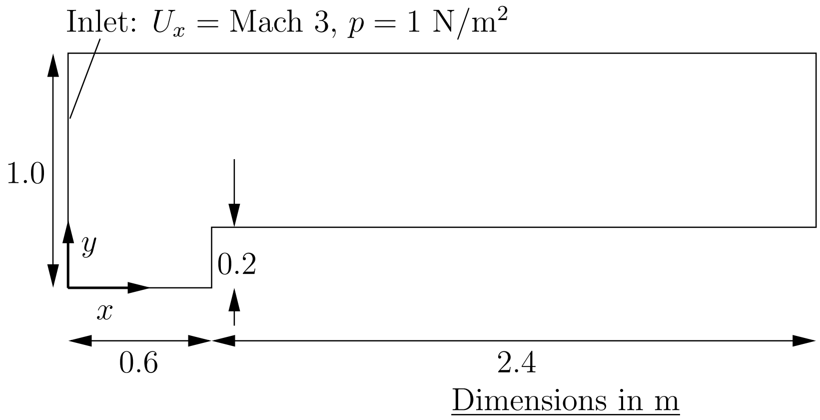


Figure 3.7: Geometry of the forward step geometry

- Ideal gas

$$p = \rho RT \tag{3.9}$$

- Momentum equation for Newtonian fluid

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) - \nabla \cdot \mu \nabla \mathbf{U} = -\nabla p \tag{3.10}$$

- Energy equation for fluid (ignoring some viscous terms), $e = C_v T$, with Fourier's Law $\mathbf{q} = -k\nabla T$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho \mathbf{U} e) - \nabla \cdot \left(\frac{k}{C_v}\right) \nabla e = p \nabla \cdot \mathbf{U} \tag{3.11}$$

Initial conditions $U = 0$ m/s, $p = 1$ Pa, $T = 1$ K.

Boundary conditions

- Inlet (left) with fixedValue for velocity $U = 3$ m/s = Mach 3, pressure $p = 1$ Pa and temperature $T = 1$ K;
- Outlet (right) with zeroGradient on U, p and T;
- No-slip adiabatic wall (bottom);
- Symmetry plane (top).

Transport properties

- Dynamic viscosity of air $\mu =$ 18.1μPa s

Thermodynamic properties

- Specific heat at constant volume $C_v = 1.78571$ J/kg K
- Gas constant $R = 0.714286$ J/kg K
- Conductivity $k = 32.3$ μW/m K

Case name *forwardStep* case located in the *$FOAM_TUTORIALS/sonicFoam* directory.

Solver name sonicFoam: an implementation for compressible trans-sonic/supersonic laminar gas flow.

The case is designed such that the speed of sound of the gas $c = \sqrt{\gamma RT} = 1$ m/s, the consequence being that the velocities are directly equivalent to the Mach number, *e.g.* the inlet velocity of 3 m/s is equivalent to Mach 3. This speed of sound calculation can be verified using the relationship for a perfect gas, $C_p - Cv = R$, *i.e.* the ratio of specific heats

$$\gamma = C_p/C_v = \frac{R}{C_v} + 1 \tag{3.12}$$

3.3.2 Mesh generation

The mesh used in this case is relatively simple, specified with uniform rectangular cells of length 0.06 m in the x direction and 0.05 m in the y direction. The geometry can simply be divided into 3 blocks, one below the top of the step, and two above the step, one either side of the step front. The full set of vertices and blocks are given in the mesh description file below:

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      blockMeshDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

convertToMeters 1;

vertices
(
    (0 0 -0.05)
    (0.6 0 -0.05)
    (0 0.2 -0.05)
    (0.6 0.2 -0.05)
    (3 0.2 -0.05)
    (0 1 -0.05)
    (0.6 1 -0.05)
    (3 1 -0.05)
    (0 0 0.05)
    (0.6 0 0.05)
    (0 0.2 0.05)
    (0.6 0.2 0.05)
    (3 0.2 0.05)
    (0 1 0.05)
    (0.6 1 0.05)
    (3 1 0.05)
);

blocks
(
    hex (0 1 3 2 8 9 11 10) (25 10 1) simpleGrading (1 1 1)
    hex (2 3 6 5 10 11 14 13) (25 40 1) simpleGrading (1 1 1)
    hex (3 4 7 6 11 12 15 14) (100 40 1) simpleGrading (1 1 1)
);

edges
(
);

boundary
(
    inlet
    {
        type patch;
        faces
        (
            (0 8 10 2)
            (2 10 13 5)
```

```
        );
    }
    outlet
    {
        type patch;
        faces
        (
            (4 7 15 12)
        );
    }
    bottom
    {
        type symmetryPlane;
        faces
        (
            (0 1 9 8)
        );
    }
    top
    {
        type symmetryPlane;
        faces
        (
            (5 13 14 6)
            (6 14 15 7)
        );
    }
    obstacle
    {
        type patch;
        faces
        (
            (1 3 11 9)
            (3 4 12 11)
        );
    }
);

mergePatchPairs
(
);

// ************************************************************************* //
```

3.3.3 Running the case

The case approaches a steady-state at some time after 5 s. The results for pressure at 10 s are shown in Figure 3.8. The results clearly show discontinuities in pressure, *i.e.* shock waves, emanating from ahead of the base of the step.

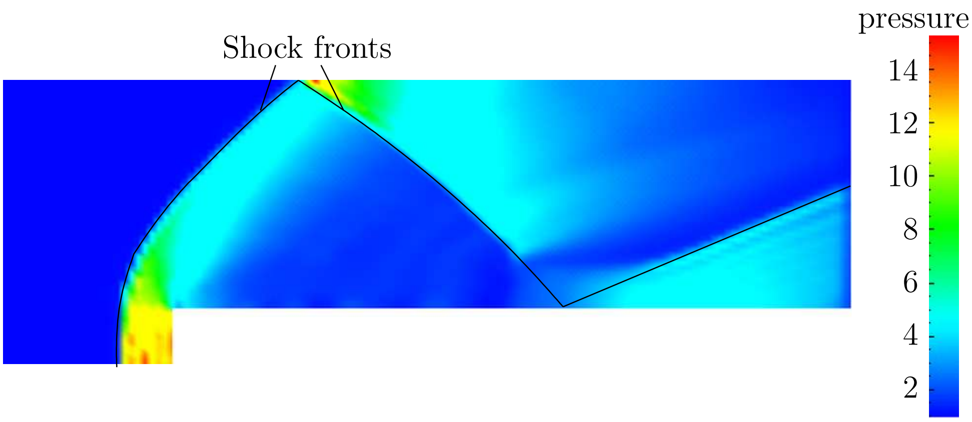


Figure 3.8: Shock fronts in the forward step problem

3.3.4 Exercise

The user can examine the effect on the solution of increasing the inlet velocity.

3.4 Decompression of a tank internally pressurised with water

In this example we shall investigate a problem of rapid opening of a pipe valve close to a pressurised liquid-filled tank. The prominent feature of the result in such cases is the propagation of pressure waves which must therefore be modelled as a compressible liquid.

This tutorial introduces the following OpenFOAM features for the first time:

- Mesh refinement
- Pressure waves in liquids

3.4.1 Problem specification

Solution domain The domain is 2 dimensional and consists of a tank with a small outflow pipe as shown in Figure 3.9

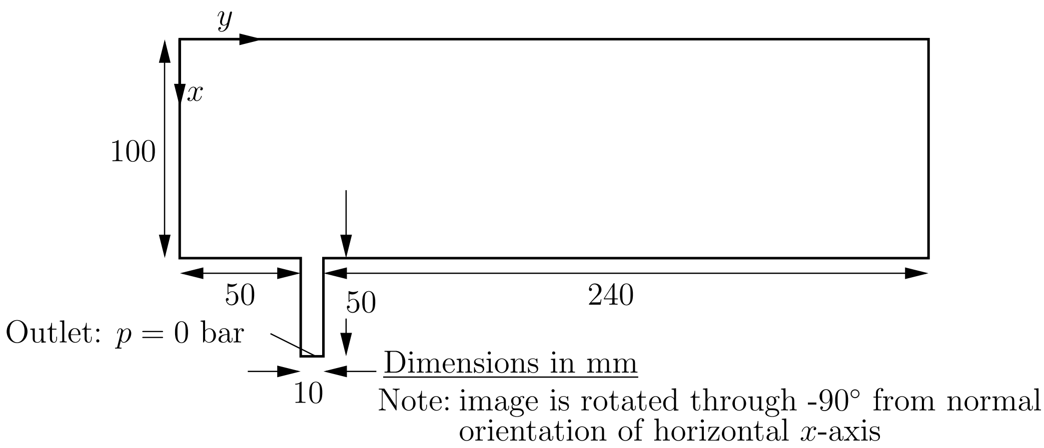


Figure 3.9: Geometry of a tank with outflow pipe

Governing equations This problem requires a model for compressibility ψ in the fluid in order to be able to resolve waves propagating at a finite speed. A barotropic relationship is used to relate density ρ and pressure p are related to ψ.

- Mass continuity

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{U}) = 0 \tag{3.13}$$

- The barotropic relationship

$$\frac{\partial \rho}{\partial p} = \frac{\rho}{K} = \psi \tag{3.14}$$

  where K is the bulk modulus

- Equation 3.14 is linearised as

$$\rho \approx \rho_0 + \psi\left(p - p_0\right) \tag{3.15}$$

  where ρ_0 and p_0 are the reference density and pressure respectively such that $\rho(p_0) = \rho_0$.

- Momentum equation for Newtonian fluid

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \bullet (\rho \mathbf{U}\mathbf{U}) - \nabla \bullet \mu \nabla \mathbf{U} = -\nabla p \tag{3.16}$$

Boundary conditions Using FoamX the following physical boundary conditions can be set:

- `outerWall` is specified the wall condition;
- `axis` is specified as the symmetryPlane;
- `nozzle` is specified as a pressureOutlet where $p = 0$ bar.
- `front` and `back` boundaries are specified as empty.

Initial conditions $\mathbf{U} = \mathbf{0}$ m/s, $p = 100$ bar.

Transport properties

- Dynamic viscosity of water $\mu = 1.0$ mPa s

Thermodynamic properties

- Density of water $\rho = 1000$ kg/m^3
- Reference pressure $p_0 = 1$ bar
- Compressibility of water $\psi = 4.54 \times 10^{-7}$ s^2/m^2

Solver name sonicLiquidFoam: a compressible sonic laminar liquid flow code.

Case name *decompressionTank* case located in the *$FOAM_TUTORIALS/sonicLiquidFoam* directory.

3.4.2 Mesh Generation

The full geometry is modelled in this case; the set of vertices and blocks are given in the mesh description file below:

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      blockMeshDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

convertToMeters 0.1;

vertices
(
    (0 0 -0.1)
    (1 0 -0.1)
    (0 0.5 -0.1)
    (1 0.5 -0.1)
    (1.5 0.5 -0.1)
    (0 0.6 -0.1)
    (1 0.6 -0.1)
    (1.5 0.6 -0.1)
    (0 3 -0.1)
    (1 3 -0.1)
```

```
    (0 0 0.1)
    (1 0 0.1)
    (0 0.5 0.1)
    (1 0.5 0.1)
    (1.5 0.5 0.1)
    (0 0.6 0.1)
    (1 0.6 0.1)
    (1.5 0.6 0.1)
    (0 3 0.1)
    (1 3 0.1)
);

blocks
(
    hex (0 1 3 2 10 11 13 12) (30 20 1) simpleGrading (1 1 1)
    hex (2 3 6 5 12 13 16 15) (30 5 1) simpleGrading (1 1 1)
    hex (3 4 7 6 13 14 17 16) (25 5 1) simpleGrading (1 1 1)
    hex (5 6 9 8 15 16 19 18) (30 95 1) simpleGrading (1 1 1)
);

edges
(
);

boundary
(
    outerWall
    {
        type wall;
        faces
        (
            (0 1 11 10)
            (1 3 13 11)
            (3 4 14 13)
            (7 6 16 17)
            (6 9 19 16)
            (9 8 18 19)
        );
    }
    axis
    {
        type symmetryPlane;
        faces
        (
            (0 10 12 2)
            (2 12 15 5)
            (5 15 18 8)
        );
    }
    nozzle
    {
        type patch;
        faces
        (
            (4 7 17 14)
        );
    }
    back
    {
        type empty;
        faces
        (
            (0 2 3 1)
            (2 5 6 3)
            (3 6 7 4)
            (5 8 9 6)
        );
    }
    front
    {
        type empty;
        faces
        (
            (10 11 13 12)
            (12 13 16 15)
            (13 14 17 16)
            (15 16 19 18)
        );
    }
);

mergePatchPairs
(
);

```

```
// ************************************************************************* //
```

In order to improve the numerical accuracy, we shall use the reference level of 1 bar for the pressure field. Note that both the internal field level and the boundary conditions are offset by the reference level.

3.4.3 Preparing the Run

Before we commence the setup of the calculation, we need to consider the characteristic velocity of the phenomenon we are trying to capture. In the case under consideration, the fluid velocity will be very small, but the pressure wave will propagate with the speed of sound in water. The speed of sound is calculated as:

$$c = \sqrt{\frac{1}{\psi}} = \sqrt{\frac{1}{4.54 \times 10^{-7}}} = 1483.2\text{m/s}. \tag{3.17}$$

For the mesh described above, the characteristic mesh size is approximately 2 mm (note the scaling factor of 0.1 in the *blockMeshDict* file). Using

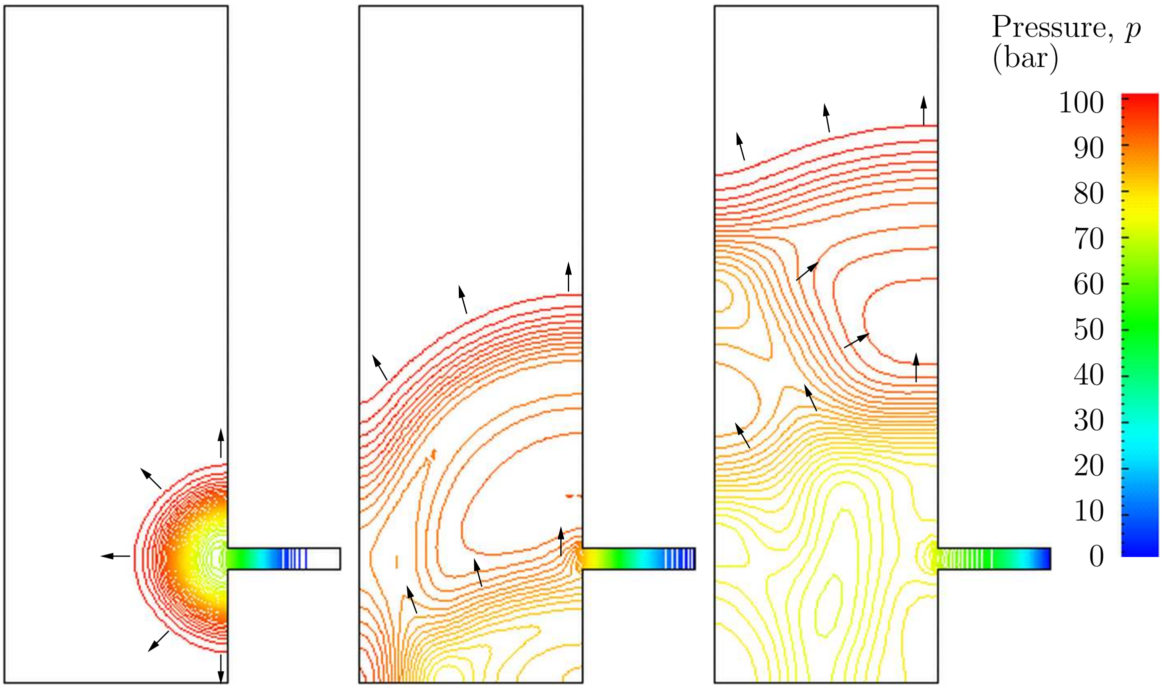
$$Co = \frac{U\,\Delta t}{\Delta x} \tag{3.18}$$

a reasonable time step is around $\Delta t = 5 \times 10^{-7}$s, giving the Co number of 0.35, based on the speed of sound. Also, note that the reported Co number by the code (associated with the convective velocity) will be two orders of magnitude smaller. As we are interested in the pressure wave propagation, we shall set the simulation time to 0.25 ms. For reference, the *controlDict* file is quoted below.

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "system";
    object      controlDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

application     sonicLiquidFoam;

startFrom       startTime;

startTime       0;

stopAt          endTime;

endTime         0.0001;

deltaT          5e-07;

writeControl    timeStep;

writeInterval   20;

purgeWrite      0;

writeFormat     ascii;

writePrecision  6;

writeCompression off;

```

```
timeFormat      general;

timePrecision   6;

runTimeModifiable true;


// ************************************************************************* //
```

3.4.4 Running the case



(a) At $t = 50$ µs (b) At $t = 100$ µs (c) At $t = 150$ µs

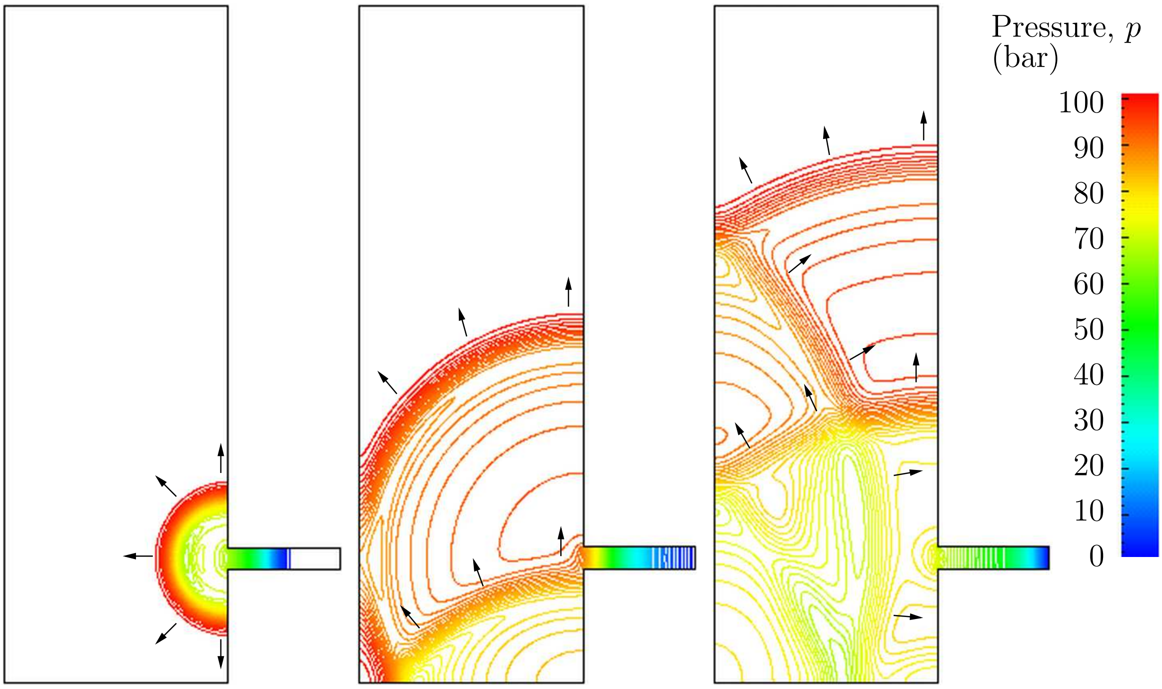
Figure 3.10: Propagation of pressure waves

The user can run the case and view results in dxFoam. The liquid flows out through the nozzle causing a wave to move along the nozzle. As it reaches the inlet to the tank, some of the wave is transmitted into the tank and some of it is reflected. While a wave is reflected up and down the inlet pipe, the waves transmitted into the tank expand and propagate through the tank. In Figure 3.10, the pressures are shown as contours so that the wave fronts are more clearly defined than if plotted as a normal isoline plot.

If the simulation is run for a long enough time for the reflected wave to return to the pipe, we can see that negative absolute pressure is detected. The modelling permits this and has some physical basis since liquids can support tension, *i.e.* negative pressures. In reality, however, impurities or dissolved gases in liquids act as sites for cavitation, or vapourisation/boiling, of the liquid due to the low pressure. Therefore in practical situations, we generally do not observe pressures falling below the vapourisation pressure of the liquid; not at least for longer than it takes for the cavitation process to occur.

3.4.5 Improving the solution by refining the mesh

Looking at the evolution of the resulting pressure field in time, we can clearly see the propagation of the pressure wave into the tank and numerous reflections from the inside walls. It is also obvious that the pressure wave is smeared over a number of cells. We shall



(a) At $t = 50$ µs (b) At $t = 100$ µs (c) At $t = 150$ µs

Figure 3.11: Propagation of pressure waves with refined mesh

now refine the mesh and reduce the time step to obtain a sharper front resolution. Simply edit the *blockMeshDict* and increase the number of cells by a factor of 4 in the x and y directions, *i.e.* block 0 becomes `(120 80 1)` from `(30 20 1)` and so on. Run blockMesh on this file. In addition, in order to maintain a Courant number below 1, the time step must be reduced accordingly to $\Delta t = 10^{-7}$ s. The second simulation gives considerably better resolution of the pressure waves as shown in Figure 3.11.

3.5 Magnetohydrodynamic flow of a liquid

In this example we shall investigate an flow of an electrically-conducting liquid through a magnetic field. The problem is one belonging to the branch of fluid dynamics known as magnetohydrodynamics (MHD) that uses mhdFoam.

3.5.1 Problem specification

The problem is known as the Hartmann problem, chosen as it contains an analytical solution with which mhdFoam can be validated. It is defined as follows:

Solution domain The domain is 2 dimensional and consists of flow along two parallel plates as shown in Fig. 3.12.

Governing equations

- Mass continuity for incompressible fluid

$$\nabla \cdot \mathbf{U} = 0 \tag{3.19}$$

- Momentum equation for incompressible fluid

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\mathbf{U}\mathbf{U}) + \nabla \cdot (2\mathbf{B}\Gamma_{\mathbf{BU}}\mathbf{B}) + \nabla \cdot (\nu \mathbf{U}) + \nabla (\Gamma_{\mathbf{BU}}\mathbf{B} : \mathbf{B}) = -\nabla p \tag{3.20}$$

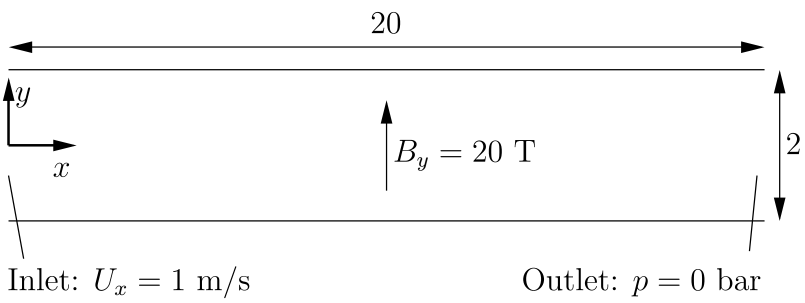


Figure 3.12: Geometry of the Hartmann problem

where $\mathbf{B}$ is the magnetic flux density, $\Gamma_{\mathbf{BU}} = (2\mu\rho)^{-1}$.

- Maxwell's equations

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{3.21}$$

where $\mathbf{E}$ is the electric field strength.

$$\nabla \bullet \mathbf{B} = 0 \tag{3.22}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J} \tag{3.23}$$

assuming $\partial \mathbf{D}/\partial t \ll \mathbf{J}$. Here, $\mathbf{H}$ is the magnetic field strength, $\mathbf{J}$ is the current density and $\mathbf{D}$ is the electric flux density.

- Charge continuity

$$\nabla \bullet \mathbf{J} = 0 \tag{3.24}$$

- Constitutive law

$$\mathbf{B} = \mu \mathbf{H} \tag{3.25}$$

- Ohm's law

$$\mathbf{J} = \sigma \left(\mathbf{E} + \mathbf{U} \times \mathbf{B} \right) \tag{3.26}$$

- Combining Equation 3.21, Equation 3.23, Equation 3.26, and taking the curl

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \bullet (\mathbf{U}\mathbf{B}) - \nabla \bullet (\phi_{\mathbf{B}} \mathbf{U}) - \nabla \bullet (\Gamma_{\mathbf{B}} \mathbf{B}) = 0 \tag{3.27}$$

Boundary conditions

- `inlet` is specified the inlet condition with fixed velocity $\mathbf{U} = (1, 0, 0)$ m/s;
- `outlet` is specified as the outlet with with fixed pressure $p = 0$ Pa;
- `upperWall` is specified as a wall where $\mathbf{B} = (0, 20, 0)$ T.
- `lowerWall` is specified as a wall where $\mathbf{B} = (0, 20, 0)$ T.
- `front` and `back` boundaries are specified as empty.

Initial conditions $\mathbf{U} = \mathbf{0}$ m/s, $p = 100$ Pa, $\mathbf{B} = (0, 20, 0)$ T.

Transport properties

- Kinematic viscosity $\nu = 1$ Pa s
- Density $\rho = 1$ kg m/s
- Electrical conductivity $\sigma = 1$ $(\Omega\,\mathrm{m})^{-1}$
- Permeability $\mu = 1$ H/m

Solver name mhdFoam: an incompressible laminar magneto-hydrodynamics code.

Case name *hartmann* case located in the *$FOAM_TUTORIALS/mhdFoam* directory.

3.5.2 Mesh generation

The geometry is simply modelled with 100 cells in the x-direction and 40 cells in the y-direction; the set of vertices and blocks are given in the mesh description file below:

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.0.0                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.com                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    object      blockMeshDict;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

convertToMeters 1;

vertices
(
    (0 -1 0)
    (20 -1 0)
    (20 1 0)
    (0 1 0)
    (0 -1 0.1)
    (20 -1 0.1)
    (20 1 0.1)
    (0 1 0.1)
);

blocks
(
    hex (0 1 2 3 4 5 6 7) (100 40 1) simpleGrading (1 1 1)
);

edges
(
);

boundary
(
    inlet
    {
        type patch;
        faces
        (
            (0 4 7 3)
        );
    }
    outlet
    {
        type patch;
        faces
        (
            (2 6 5 1)
        );
    }
    lowerWall
    {
```

```
            type patch;
            faces
            (
                (1 5 4 0)
            );
        }
        upperWall
        {
            type patch;
            faces
            (
                (3 7 6 2)
            );
        }
        frontAndBack
        {
            type empty;
            faces
            (
                (0 3 2 1)
                (4 5 6 7)
            );
        }
);

mergePatchPairs
(
);

// ************************************************************************* //
```

3.5.3 Running the case

The user can run the case and view results in dxFoam. It is also useful at this stage to run the Ucomponents utility to convert the **U** vector field into individual scalar components. MHD flow is governed by, amongst other things, the Hartmann number which is a measure of the ratio of electromagnetic body force to viscous force

$$M = BL\sqrt{\frac{\sigma}{\rho\nu}} \tag{3.28}$$

where L is the characteristic length scale. In this case with $B_y = 20$ T, $M = 20$ and the electromagnetic body forces dominate the viscous forces. Consequently with the flow fairly steady at $t = 2$ s the velocity profile is almost planar, viewed at a cross section midway along the domain $x = 10$ m. The user can plot a graph of the profile of U_x in dxFoam. Now the user should reduce the magnetic flux density **B** to 1 Tand re-run the code and Ucomponents. In this case, $M = 1$ and the electromagnetic body forces no longer dominate. The velocity profile consequently takes on the parabolic form, characteristic of Poiseuille flow as shown in Figure 3.13. To validate the code the analytical solution for the velocity profile U_x is superimposed in Figure 3.13, given by:

$$\frac{U_x(y)}{U_x(0)} = \frac{\cosh M - \cosh M(y/L)}{\cosh M - 1} \tag{3.29}$$

where the characteristic length L is half the width of the domain, *i.e.* 1 m.

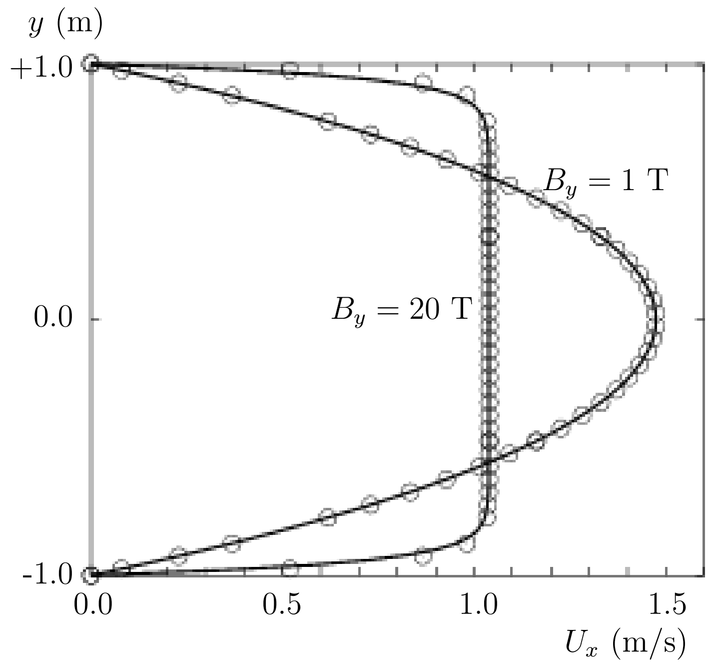


Figure 3.13: Velocity profile in the Hartmann problem for $B_y = 1$ T and $B_y = 20$ T.

Index

Symbols Numbers A B C D E F G H I J K L M N O P Q R S T U V W X Z

C

G

L

N

T

X

Y

Z