OpenFOAM

http://www.opencfd.co.uk

A Code Independent Notation for Finite Volume Algorithms

23rd Feb 2005

OpenCFD

Technical Report
TR/HGW/01
23rd Feb 2005

The Mews, Picketts Lodge,
Picketts Lane, Salfords,
Surrey, RH1 5RG,
United Kingdom.
Tel: +44 (0)1293 821 272

Abstract

The continuing increase in the complexity of problems being solved using the finite volume method and the additional algorithm complexity required is causing difficulties in transferring ideas between researchers in a clear and unambiguous way. It now appears that a special notation would be useful, which is concise, unambiguous, code-independent and makes it as easy as possible to understand an algorithm and to implement it in the code of choice. This report describes one possibility. No attempt is made here to describe implementations of the finite-volume operations merely a notation to represent them. It would be interesting to extend this notation in the future such that particular code implementations may be described in a similar fashion.

Currently this notation is still under development and may require significant revision. In particular, it is understood that the author's particular experience may have led to a notation which is better able to describe algorithms currently implemented in the authors own code OpenFOAM, rather than any other code. If it is felt that anything covered here may be affected by such a bias or if any of the terms are not clear or you have any suggestions please contact the author by Email at H.Weller@OpenCFD.co.uk.

The Mews, Picketts Lodge,
Picketts Lane, Salfords,
Surrey, RH1 5RG,
United Kingdom.
Tel: +44 (0)1293 821 272

1 Cell Geometry

In finite-volume discretisation the computational cell is typically described i.t.o. its volume and face area vectors. This is sufficient information to apply Gauss' theorem and obtain second-order accurate derivatives, but not for more complex operations or higher-order accurate approximations. For the current purpose this basic set of cell information is sufficient and the following notation will be used:

Cell volume	V
Cell face area vector	$\mathbf{s}_f$
Cell face area magnitude	$\lvert\mathbf{s}_f\rvert$ or S_f

2 Face Interpolation

Interpolating fields from the cell centres to the cell faces is fundamental to the finite-volume method and many schemes have been devised for this purpose. Linear interpolation between the cell centres (central differencing) may be used under many circumstances but not for convection terms if boundedness is a requirement. For such cases first-order upwind differencing is often used, in which the weighting factors are obtained purely from the flow direction. For cases in which upwind differencing is not accurate enough NVD or TVD schemes may be appropriate. All of these schemes use at least the face-flux to determine the interpolation weighting factors but may require other information *e.g.* a blending coefficient. To support all of the interpolation possibilities a simple extensible notation is used in which a subscript f denotes face interpolation and arguments are given to specify the scheme and the parameters required by the scheme *e.g.*

Central differencing face value of $\mathbf{Q}$	$\mathbf{Q}_f$
Interpolated face value of $\mathbf{Q}$ using scheme S with coefficient γ	$\mathbf{Q}_{f(\phi,S,\gamma)}$
e.g. Upwind differencing face value of $\mathbf{Q}$	$\mathbf{Q}_{f(\phi,UD,\gamma)}$
Blended differencing face value of $\mathbf{Q}$	$\mathbf{Q}_{f(\phi,BD,\gamma)}$
Gamma differencing face value of $\mathbf{Q}$	$\mathbf{Q}_{f(\phi,\Gamma,\gamma)}$

3 Face Flux

In finite-volume discretisation, conservation is guaranteed by convecting properties between cells using face fluxes which represent the integral of the velocity (or momentum in the case of a mass flux) across a face. A second-order approximation to these fluxes may be obtained from the face-interpolate of the velocity and the face-area vector thus

Face flux for velocity $\mathbf{U}$	$\phi = \mathbf{s}_f \bullet \mathbf{U}_f$
Face mass flux for velocity $\mathbf{U}$	$\phi = \mathbf{s}_f \bullet (\rho_f \mathbf{U}_f)$.

Alternatively, these fluxes may be obtained from the solution of a pressure equation as in

The Mews, Picketts Lodge,
Picketts Lane, Salfords,
Surrey, RH1 5RG,
United Kingdom.
Tel: +44 (0)1293 821 272

the SIMPLE or PISO algorithms.

4 Explicit Differential Operators

The notation used for explicit implementations of differential operators is generally the same as that used in the original differential equations *e.g.*

Time derivative of field $\mathbf{Q}$	$\frac{\partial \mathbf{Q}}{\partial t}$.
Tensorial derivative of field $\mathbf{Q}$	$\nabla \mathbf{Q}$
e.g. divergence of field $\mathbf{Q}$	$\nabla \bullet \mathbf{Q}$

Due to the common use of face-fluxes in the finite-volume method it is convenient to allow $\nabla \bullet \phi$ to represent $\nabla \bullet \mathbf{U}$ where $\phi = \mathbf{s}_f \bullet \mathbf{U}_f$ despite the fact that ϕ is an extensive scalar field. Other possible notations are being considered and feedback on this point would be appreciated. Another departure from standard differential calculus is the concept of face-gradient:

Face-gradient of field $\mathbf{Q}$	$\nabla_f \mathbf{Q}$
Face-normal gradient of field $\mathbf{Q}$	$\nabla_f^\perp \mathbf{Q} = \widehat{\mathbf{S}}_f \bullet \nabla_f \mathbf{Q}$

which, if implemented using a smaller computational molecule than that implied by interpolating the cell-centre gradients, may improve accuracy and stability of some algorithms.

5 Averaging

Under some circumstances it may be necessary to create an average of a field over some region of space *e.g.* for smoothing or for numerical stability. Such averaging procedures are denoted

Average of field $\mathbf{Q}$ over region $\square$	$\langle \mathbf{Q} \rangle_\square$
e.g. average of field $\mathbf{Q}$ over the computational molecule of ∇	$\langle \mathbf{Q} \rangle_\nabla$.

A particularly problematic term in phase-intensive conditionally-averaged equations has the form $\frac{\nabla \varphi}{\varphi}$ which cannot be evaluated in the limit of $\varphi \rightarrow 0$ even if the gradient also approaches zero. The greatest difficulty with this term is when the cell centre value of φ is zero but a neighbour cell value is not, in which case it is not possible to divide by the cell-centre value. This problem can be avoided if the denominator is averaged over the computational molecule of the ∇ operator and a small stabilising factor δ added.

The Mews, Picketts Lodge,
Picketts Lane, Salfords,
Surrey, RH1 5RG,
United Kingdom.
Tel: +44 (0)1293 821 272

6 Matrices

Matrices are composed of both the matrix coefficients and the source vector. This encapsulation is very convenient when describing the matrices generated by discretisation which often creates both matrix coefficients and source contributions. Given

Matrix from differential operator $\mathcal{L}$ operating on the field $\mathbf{Q}$	$[\![\mathcal{L}[\mathbf{Q}]]\!]$
Matrix coefficients	$[\![\mathcal{L}[\mathbf{Q}]]\!]_A$
Source vector	$[\![\mathcal{L}[\mathbf{Q}]]\!]_S$

then

$$[\![\mathcal{L}[\mathbf{Q}]]\!] \equiv [\![\mathcal{L}[\mathbf{Q}]]\!]_A \mathbf{Q} - [\![\mathcal{L}[\mathbf{Q}]]\!]_S . \tag{1}$$

Matrices are decomposed into parts using the notation

diagonal part of	$[\![\mathcal{L}[\mathbf{Q}]]\!]$	$[\![\mathcal{L}[\mathbf{Q}]]\!]_D$
upper part of	$[\![\mathcal{L}[\mathbf{Q}]]\!]$	$[\![\mathcal{L}[\mathbf{Q}]]\!]_U$
lower part of	$[\![\mathcal{L}[\mathbf{Q}]]\!]$	$[\![\mathcal{L}[\mathbf{Q}]]\!]_L$
"H" part of	$[\![\mathcal{L}[\mathbf{Q}]]\!]$	$[\![\mathcal{L}[\mathbf{Q}]]\!]_H \equiv [\![\mathcal{L}[\mathbf{Q}]]\!]_D \mathbf{Q} - [\![\mathcal{L}[\mathbf{Q}]]\!]$

which is used in many numerical schemes to provide a simple way of obtaining an approximate solution to the equation

$$[\![\mathcal{L}[\mathbf{Q}]]\!] = 0 \tag{2}$$

by

$$\mathbf{Q} \approx \frac{[\![\mathcal{L}[\mathbf{Q}]]\!]_H}{[\![\mathcal{L}[\mathbf{Q}]]\!]_D}. \tag{3}$$

7 Implicit Differential Operators

The notation for implicit implementations of differential operators uses the matrix notation from the previous section in conjunction with that used in the original differential equations *e.g.*

Time derivative of field $\mathbf{Q}$	$\left[\!\!\left[\frac{\partial[\mathbf{Q}]}{\partial t}\right]\!\!\right]$
Tensorial derivative of field $\mathbf{Q}$	$[\![\nabla[\mathbf{Q}]]\!]$
e.g. divergence of field $\mathbf{Q}$	$[\![\nabla \bullet [\mathbf{Q}]]\!]$