Numerical Simulation Methods
Part 2 - Applied Concepts

Lecture 11: The Finite-Volume Method

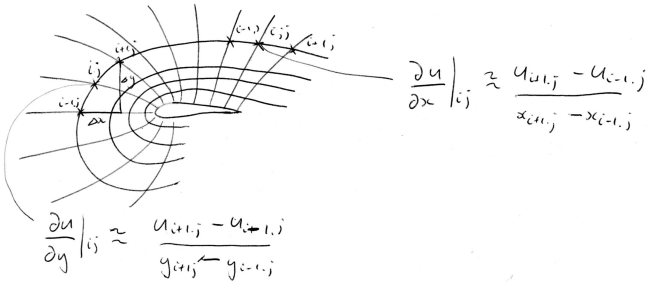
Roadmap

Applied Concepts

- Introduction to meshing
- **Today**
  - **Coordinate transform**
  - **Introduction to finite volume method**
- Next Lecture: Evaluation of fluxes and Jameson's scheme
- Solution storage approaches and their implications
- Advanced implicit methods
- Introduction to computer hardware and high performance computing
- Parallel decomposition and efficiency

Coordinate Transform

For general body-fitted meshes, the mesh lines are not aligned to the global x, y, or z directions - so how can we apply finite differences? We need to transform our coordinates.



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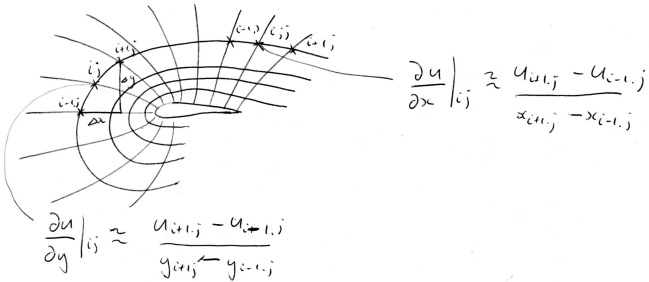


Coordinate transform

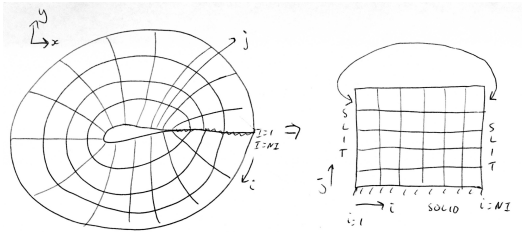
Transformation of coordinates from the physical domain to a computational domain, where in the computational domain all mesh lines are equally spaced.

- The coordinate transformation is applied to the PDEs ; the transformed equations are solved in the equally-spaced computational domain

Coordinate Transform

The original PDE is:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = 0 \qquad (1)$$



Under the coordinate $\tau = \tau(t)$, $\xi = \xi(x, y, t)$, $\eta = \eta(x, y, t)$ transformation this becomes (with $\mathbf{U}_{\xi\eta} = J\mathbf{U}$ and $\mathbf{F}_{\xi\eta} = J\mathbf{F}\xi_x + J\mathbf{G}\xi_y$ and $\mathbf{G}_{\xi\eta} = J\mathbf{F}\eta_x + J\mathbf{J}\mathbf{G}\eta_y$:

$$\frac{\partial \underline{\mathbf{U}}_{\xi\eta}}{\partial t} + \frac{\partial \underline{\mathbf{F}}_{\xi\eta}}{\partial \xi} + \frac{\partial \underline{\mathbf{G}}_{\xi\eta}}{\partial \eta} = 0 \qquad (2)$$

- It turns out that is is possible to write the system in the same conservative form as the original equations, after some manipulation (chapter 5 of Anderson if interested - it is a little fiddly)
- The geometry of the mesh is 'encoded' in the coordinate transform

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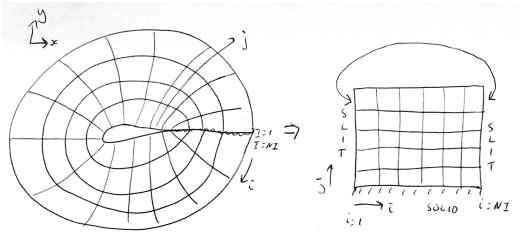

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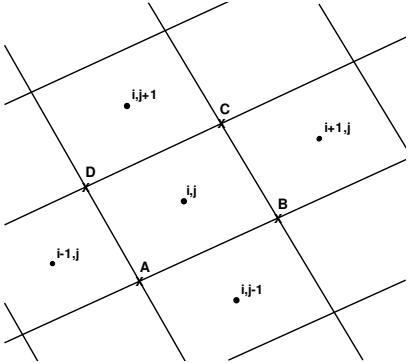
- It turns out that is is possible to write the system in the same conservative form as the original equations, after some manipulation (chapter 5 of Anderson if interested - it is a little fiddly)
- The geometry of the mesh is 'encoded' in the coordinate transform
- The coordinate transform requires **much extra work** to implement - mistakes are easily

The Finite-Volume Method - Overview

Finite-differences are restrictive for general problems: they require structured meshes and an involved coordinate transformation. Hence, the majority of CFD codes are now **finite-volume based**.

The Finite-Volume Method

- Assume a constant variation of the solution across each cell
- Discretise and solve the **integral form** of our PDEs
- We use **Greens Theorem** to transform our volume integrals into boundary integrals



The Finite-Volume Method - The temporal term

The differential form of a system of equations is:

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Integrating the equation throughout the entire volume/area of a computational cell:

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$$\int \int_A \frac{\partial \underline{\mathbf{U}}}{\partial t} dA = \frac{\partial}{\partial t} \int \int_A \underline{\mathbf{U}} dA \qquad (5)$$

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$$\overline{\underline{\mathbf{U}}} = \frac{1}{A} \int \int_A \underline{\mathbf{U}} dA \qquad (6)$$

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therefore

$$\int\int_A \frac{\partial \underline{\mathbf{U}}}{\partial t} dA = A \frac{\partial \overline{\underline{\mathbf{U}}}}{\partial t} \qquad (7)$$

The Finite-Volume Method - The flux integral

Collect the flux functions generally as $\mathbf{F} = [\underline{\mathbf{F}}, \underline{\mathbf{G}}, \underline{\mathbf{0}}]^T$, so that:

$$\int\int_A \left(\frac{\partial \underline{\mathbf{U}}}{\partial t} + \frac{\partial \underline{\mathbf{F}}}{\partial x} + \frac{\partial \underline{\mathbf{G}}}{\partial y} \right) dA = A \frac{\partial \overline{\underline{\mathbf{U}}}}{\partial t} + \int\int_A \nabla . \mathbf{F} dA = 0 \tag{8}$$

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The volume flux integral ($\int \int_A$) is awkward, so we change it using Greens theorem which relates a volume integral to a boundary integral.

Greens Theorem (2D)

$$\int \int_A \nabla . \mathbf{F} dA = \int_c \mathbf{F} . \underline{\mathbf{n}} ds \tag{9}$$

where c is the domain boundary, i.e. the contour around the edge of the cell, ds is an elemental length of it, and $\underline{\mathbf{n}}$ is the outward unit normal to the boundary.

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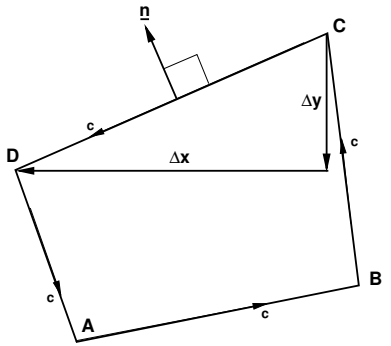
So the integral form of the equations is

$$A \frac{\partial \overline{\underline{\mathbf{U}}}}{\partial t} + \int_c \mathbf{F} . \underline{\mathbf{n}} ds = 0 \tag{10}$$

c is defined as positive anticlockwise. **This is still an exact form of the equations.**

The Finite-Volume Method - Expand for 2D

$$A\frac{\partial \overline{\mathbf{U}}}{\partial t} + \int_c \mathbf{F}.\underline{\mathbf{n}} ds = 0 \tag{11}$$



But, $d\underline{\mathbf{s}} = [dx, dy, 0]^T$ and so

$$\underline{\mathbf{n}} = \frac{d\underline{\mathbf{s}} \times \underline{\mathbf{k}}}{|d\underline{\mathbf{s}}|} = \frac{[dy, -dx, 0]^T}{|d\underline{\mathbf{s}}|} \tag{12}$$

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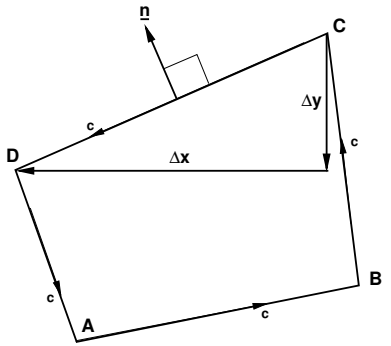

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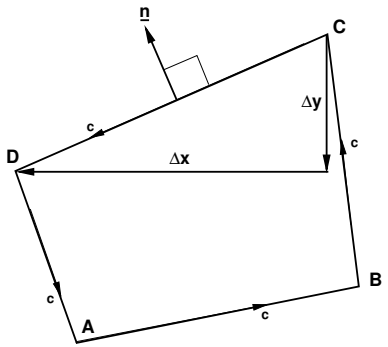

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Hence,

$$A\frac{\partial \overline{\mathbf{U}}}{\partial t} + \int_c \underline{\mathbf{F}} dy - \underline{\mathbf{G}} dx = 0 \tag{14}$$

The Finite-Volume Method - Discretise in space

So we now have:

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We take $\overline{\underline{\mathbf{U}}}$ to be represented by the ACTUAL VALUE of $\underline{\mathbf{U}}_{i,j}$ in the centre of the discrete cell i, j. **i.e. we assume the solution is constant across a single cell.**

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$$\frac{\partial \overline{\underline{\mathbf{U}}}}{\partial t} \rightarrow \frac{d\underline{\mathbf{U}}_{i,j}}{dt} \tag{16}$$

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$$\frac{d\underline{\mathbf{U}}_{i,j}}{dt} = -\frac{1}{A}\int_c \underline{\mathbf{F}} dy - \underline{\mathbf{G}} dx \tag{17}$$

This equation is solved in each cell to give the cell-centred solution in each cell.

The Finite-Volume Method - Discretise in time

So we now have:

$$\frac{d\underline{\mathbf{U}}_{i,j}}{dt} = -\frac{1}{A}\int_c \underline{\mathbf{F}}dy - \underline{\mathbf{G}}dx \tag{18}$$

This is the general form of a FINITE-VOLUME scheme. There are many ways to solve this equation. The method used to compute the flux integral depends on the spatial discretisation scheme chosen. The flux integral is the RESIDUAL for each cell, known as $\underline{\mathbf{R}}_{i,j}$,

$$\underline{\mathbf{R}}_{i,j} = \frac{1}{A}\int_c \underline{\mathbf{F}}dy - \underline{\mathbf{G}}dx \tag{19}$$

A first-order explicit approximation for the temporal derivative (as usual) would be

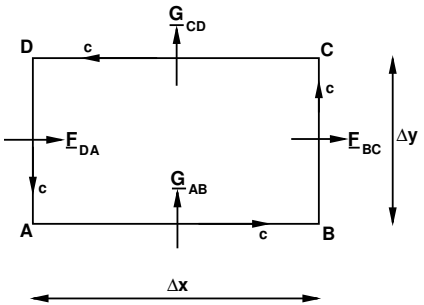
$$\frac{\underline{\mathbf{U}}^{n+1}_{i,j} - \underline{\mathbf{U}}^{n}_{i,j}}{\Delta t} = \frac{d\underline{\mathbf{U}}_{i,j}}{dt} + O(\Delta t) \tag{20}$$

and this would lead to

$$\underline{\mathbf{U}}^{n+1}_{i,j} = \underline{\mathbf{U}}^{n}_{i,j} - \Delta t\underline{\mathbf{R}}_{i,j} \tag{21}$$

Evaluation of the Flux Integral - Cartesian Cells

To compute the flux integral (residual), it is assumed that the flux values $\underline{\mathbf{F}}$ and $\underline{\mathbf{G}}$ do not vary across each face. Consider a structured cartesian cell for simplicity



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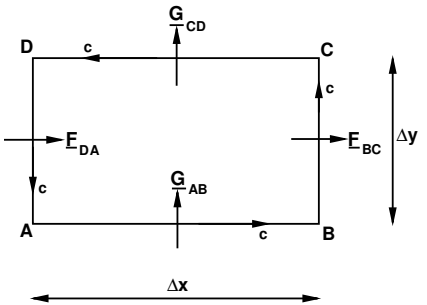

$$\begin{aligned}\frac{1}{A}\int_c \underline{\mathbf{F}}dy - \underline{\mathbf{G}}dx &= \frac{1}{A}\int_c \underline{\mathbf{F}}dy - \underline{\mathbf{G}}dx \\ &= \frac{1}{A}\left(-\underline{\mathbf{G}}_{AB}\Delta x + \underline{\mathbf{F}}_{BC}\Delta y + \underline{\mathbf{G}}_{CD}\Delta x - \underline{\mathbf{F}}_{DA}\Delta y\right)\end{aligned} \tag{22}$$

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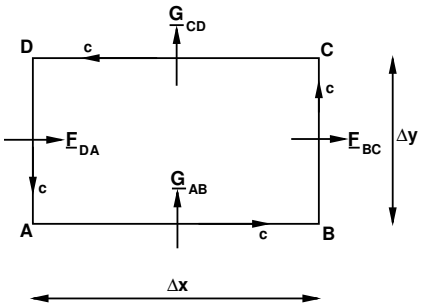

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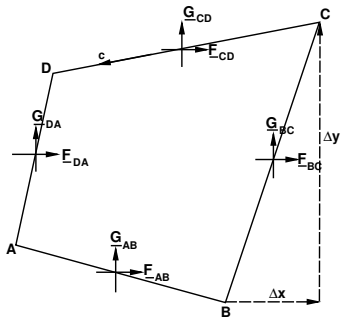
For cartesian cell $A = \Delta x \times \Delta y$, so:

$$\frac{\underline{\mathbf{F}}_{BC} - \underline{\mathbf{F}}_{DA}}{\Delta x} + \frac{\underline{\mathbf{G}}_{CD} - \underline{\mathbf{G}}_{AB}}{\Delta y} \tag{23}$$

i.e., same as a finite-difference scheme. However, this is only the case for cartesian cells.

Evaluation of the Flux Integral - General Cells

For general structured cells we have



$$\frac{1}{A}\int_c \underline{\mathbf{F}}dy - \underline{\mathbf{G}}dx = \frac{1}{A}(\underline{\mathbf{F}}_{AB}\Delta y_{AB} - \underline{\mathbf{G}}_{AB}\Delta x_{AB} + \underline{\mathbf{F}}_{BC}\Delta y_{BC} - \underline{\mathbf{G}}_{BC}\Delta x_{BC} + \underline{\mathbf{F}}_{CD}\Delta y_{CD} - \underline{\mathbf{G}}_{CD}\Delta x_{CD} + \underline{\mathbf{F}}_{DA}\Delta y_{DA} - \underline{\mathbf{G}}_{DA}\Delta x_{DA}) \quad (24)$$

Hence, if we know the flux functions at each cell face, $\underline{\mathbf{F}}_{AB}$ etc, we can evaluate the flux integral (at least approximately).

To evaluate the flux functions at each cell face we need the value of $\underline{\mathbf{U}}$ at each cell face, and how this is computed depends on the spatial discretisation chosen - there are many options.

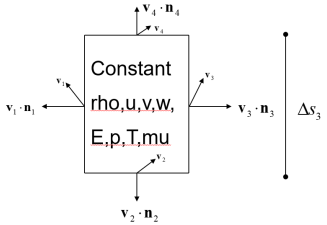


Figure: A finite volume

$$\int_\Omega \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} dv = \int_\Omega \frac{\partial \rho}{\partial t} dv + \int_{\partial\Omega} \rho \mathbf{v} \cdot \mathbf{n} ds$$

$$\int_\Omega \nabla \cdot \rho \mathbf{v} dv = \int_{\partial\Omega} \rho \mathbf{v} \cdot \mathbf{n} ds$$

$$\int_\Omega \frac{\partial \rho}{\partial t} dv = -\int_{\partial\Omega} \rho \mathbf{v} \cdot \mathbf{n} ds \approx -\sum_{i=1}^{i=4} \rho_i \mathbf{v}_i \cdot \mathbf{n}_i \Delta S_i$$

Can do a similar approach for momentum (here just in x)

$$\int_\Omega \frac{\partial \rho u}{\partial t} + \nabla \cdot \rho u \mathbf{v} + \nabla p_x dv = \int_\Omega \frac{\partial \rho u}{\partial t} dv + \int_{\partial\Omega} \rho u \mathbf{v} \cdot \mathbf{n} ds + \int_{\partial\Omega} p \mathbf{n} \cdot \mathbf{i} ds$$

and can also write for all coordinate directions in one go as

$$\int_\Omega \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v}\mathbf{v} + \nabla p dv = \int_\Omega \frac{\partial \rho \mathbf{v}}{\partial t} dv + \int_{\partial\Omega} \rho \mathbf{v} \left(\mathbf{v} \cdot \mathbf{n} \right) ds + \int_{\partial\Omega} p \mathbf{n} ds$$

```
!$OMP PARALLEL REDUCTION(+:R) PRIVATE(ed,FLXL,FLXR,FLXFACE,fvell,norml)   SHARED(R)
do edcnt=1,nedgei

  !print *, "EDGE",ed

  ed=edgei(edcnt)

  !FLXL=0.0
  !FLXR=0.0

  aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa
    norml=norm(ed,:)
    fvell=fvel(ed,:)
    call GETFLX(rho(edge(ed,1)),u(edge(ed,1)),                    &
&     v(edge(ed,1)),w(edge(ed,1)),E(edge(ed,1)),p(edge(ed,1)),    &
&     fvell,norml,FLXL)

    !bc="int"

    call GETFLX(rho(edge(ed,2)),u(edge(ed,2)),                    &
&     v(edge(ed,2)),w(edge(ed,2)),E(edge(ed,2)),p(edge(ed,2)),    &
&     fvell,norml,FLXR)

    !bc="int"

  FLXFACE(:)=0.5*(FLXL(:)+FLXR(:))*cfa(ed)

  R(edge(ed,1),:)=R(edge(ed,1),:)+FLXFACE(:)
  R(edge(ed,2),:)=R(edge(ed,2),:)-FLXFACE(:)
  aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa

enddo
!$OMP END PARALLEL
```

```
!*****************************************************
subroutine GETFLX(rho,u,v,w,E,p,fvel,norm,FLX)

implicit none

real,intent(in)::rho,u,v,w,E,p
real,intent(in),dimension(3)::norm
real,intent(in),dimension(3)::fvel
real,intent(out),dimension(5)::FLX
real::cvel,nvel
integer::dimnum
real,dimension(3)::vel

vel(1)=u
vel(2)=v
vel(3)=w

dimnum=3

call DOTPROD(dimnum,norm,vel-fvel,cvel)
call DOTPROD(dimnum,norm,vel,nvel)

!write(456,*) "cvel",cvel,nvel
!write(456,*) "comp",vel(1),vel(2),vel(3)
!write(456,*) "norm",norm(1),norm(2),norm(3)
!write(456,*) "fvel",fvel(1),fvel(2),fvel(3)

FLX(1)=rho*cvel
FLX(2)=rho*u*cvel+p*norm(1)
FLX(3)=rho*v*cvel+p*norm(2)
FLX(4)=rho*w*cvel+p*norm(3)
FLX(5)=rho*cvel*E+nvel*p

end subroutine GETFLX
!*****************************************************
```

Summary

- Coordinate transform
  - Necessary for applying finite differences to curvilinear structured grids
  - Coordinate transform requires extra work to transform PDEs
  - Finite differences still limited to structured meshes
- Finite Volume Method
  - A more general approach to solving PDEs (can use unstructured meshes)
  - Solve the **integral form** of our equations
  - Use Green's Theorem to transform awkward volume integral to an integral around the cell boundary
  - Spatial discretisation assumes that solution is constant across each cell; hence we can say that $\overline{\underline{\mathbf{U}}} = \underline{\mathbf{U}}_{i,j}$

Next Lecture: How do we evaluate the fluxes at the faces and Jameson's scheme