Geometry and Grids

Larry Caretto
Mechanical Engineering 692

Computational Fluid Dynamics

April 26, 2010

California State University Northridge

Outline

- Review last lecture
- Problem of treating realistic geometry
- Use of partial grid cells
- Boundary fitted coordinates
- Unstructured grids
- Grids where all variables are located at the same point

California State University Northridge 2

Density-based Solvers

- Density-based solvers traditionally used for compressible flows
  - Not accurate for low Mach numbers
  - Fluent uses a transformation to allow density based solvers for low Mach number flows
- Density-based solvers can be implicit or explicit
  - Implicit allows longer time steps while preserving stability at higher Courant numbers

California State University Northridge 3

Pressure-based Solvers

- Transient finite-volume equation

$$\frac{\left[(\rho\phi)_{P,t+\Delta t} - (\rho\phi)_{P,t}\right]\Delta V}{\Delta t} = \overline{a_N}\;\overline{\phi_N} + \overline{a_S}\;\overline{\phi_S} + \overline{a_E}\;\overline{\phi_E} + \overline{a_W}\;\overline{\phi_W} - \overline{a_P}\;\overline{\phi_P} + \overline{S^{(\phi)}}$$

$$\overline{a_N}\;\overline{\phi_N} + \overline{a_S}\;\overline{\phi_S} + \overline{a_E}\;\overline{\phi_E} + \overline{a_W}\;\overline{\phi_W} - \overline{a_{P,transient}}\;\overline{\phi_P} + \overline{S^{(\phi)}_{transient}} = 0$$

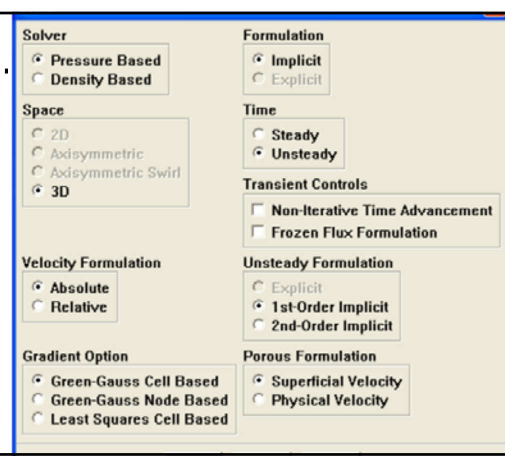
$$\overline{a_{P,transient}} = \overline{a_P} + \frac{\rho_{P,t+\Delta t}\Delta V}{\Delta t} \qquad \overline{S^{(\phi)}_{transient}} = \overline{S^{(\phi)}} + \frac{\rho\phi_{P,t}\Delta V}{\Delta t}$$

California State University Northridge 4

What is Time Average?

- Have same choices used for conduction equation
  - Explicit – use values at old time step
  - Implicit – use values at new time step
  - Crank-Nicholson – use average of values at old and new time steps
- Can also use more accurate time derivatives
- Fluent has various options

California State University Northridge 5



Explicit or Implicit?

- Explicit stability limits on time step (set by the local Courant number, $u\Delta x/\alpha$)
- The Δt required for stability is usually much lower than the Δt for accuracy
- Implicit algorithms will generally take less computer time
- Moving waves (*e. g*. shock waves) require small time steps so that explicit algorithms are preferred here
  – Available in Fluent only with density solver

California State University Northridge 7

Other Fluent Options

- Non-iterative time advancement – simplifies iterations to reduce computer time for solution
  – Does not do “outer” iteration
- Frozen-flux formulation uses a_K coefficients from previous time step
  – Does not update during iterations
  – Another item to save computer time

California State University Northridge 8

Geometry

- CFD problems applied to a variety of complex geometries: aircraft, engine coolant and valve passages, gas turbine combustors, rocket engines, etc.
- Accurate modeling of flows requires accurate specification of geometries
- Development of geometry model and mesh are usually the most time consuming part of a CFD calculation

California State University Northridge 9

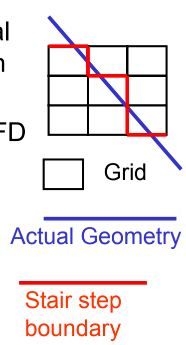
Approaches to Geometry

- Approaches leaving a regular gird
  – Stair step approach giving an approximate boundary
  – Special grid cells near boundary
- Approaches using coordinate transformations
  – Boundary fitted coordinates with transformed differential equations
  – Local coordinate transformations in a finite-volume approach

California State University Northridge 10

Stair Step Approach

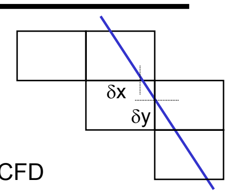
- Only mentioned for historical reasons and to contrast with next method
- Sometimes used in early CFD calculations
- Not used in any realistic codes
- Quick and dirty way to get different geometry in new codes.



California State University Northridge 11

Boundary Crosses Grid

- Define new δx and δy to define boundary
- Use derivative expressions for uneven grid
  – Usually used anyway for CFD
- Programming problems when two boundary values have to be stored at one node as in example here
- Gradient boundary conditions must be split into components



California State University Northridge 12

Boundary Crosses Grid II

- Grid spacing near boundary will have smaller steps than remainder of grid
  - Will decrease allowed time step in procedures with stability limits
- More accurate than stair step approach
- Generally not favored
  - Exception is Flow-3D software by C. W. "Tony" Hirt who recommends this procedure
  - http://www.flow3d.com/CFD-101/fvsbfc.htm

California State University Northridge 13

Boundary-Fitted Coordinates

- Grid lines are determined by physical geometry of object
- Dimensionless coordinate system, $\xi_i = i$, $\eta_j = j$, and $\zeta_k = k$ retains i, j, k notation
- Physical locations corresponding to a given (ξ_i, η_j, ζ_k) location determined by a grid generation program
- Necessary to transform differential equations to general coordinate system

California State University Northridge 14

Boundary-Fitted Coordinates II

- To transform Cartesian coordinates, x, y, z, into computational ones, ξ, η, ζ
  - Write Cartesian coordinates as x_1, x_2, and x_3, and computational coordinates as ξ_1, ξ_2, and ξ_3
  - Grid (mesh) generation programs define physical coordinates x_1, x_2, and x_3, as functions of ξ_1, ξ_2, and ξ_3
  - Differential equations modified by coordinate transformations include terms like $\partial\xi_i/\partial x_j$

California State University Northridge 15

Coordinate Transformations

- Mesh generation gives the x, y, and z at each point in the computational grid
- It is easy to compute finite difference expressions for derivatives like $\partial x_i/\partial\xi_j$
  - E.g. $\partial z/\partial\eta = (z_{ij+1k} - z_{ij-1k})/(2\Delta\eta)$
- Transformed differential equations require derivatives like $\partial\xi_i/\partial x_j$
  - Coordinate transformations required for these derivatives
    - Involve Jacobian determinant, J

California State University Northridge 16

Coordinate Transformations II

- Details in online notes and slides at end of presentation
- Matrix based result
- Typical equation below
- Have nine such equations in 3D (four in 2D)

$$J = \begin{vmatrix} \frac{\partial x_1}{\partial \xi_1} & \frac{\partial x_1}{\partial \xi_2} & \frac{\partial x_1}{\partial \xi_3} \\ \frac{\partial x_2}{\partial \xi_1} & \frac{\partial x_2}{\partial \xi_2} & \frac{\partial x_2}{\partial \xi_3} \\ \frac{\partial x_3}{\partial \xi_1} & \frac{\partial x_3}{\partial \xi_2} & \frac{\partial x_3}{\partial \xi_3} \end{vmatrix}$$

$$\frac{\partial \xi_2}{\partial x_3} = \frac{1}{J}\left[\frac{\partial x_1}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_3} - \frac{\partial x_1}{\partial \xi_3}\frac{\partial x_2}{\partial \xi_1}\right]$$

$$\frac{\partial \eta}{\partial z} = \frac{1}{J}\left[\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \zeta} - \frac{\partial x}{\partial \zeta}\frac{\partial y}{\partial \xi}\right] = \frac{x_\xi y_\zeta - x_\zeta y_\xi}{J}$$

California State University Northridge 17

Transformed Transport Equation

- Original equation and transformed result shown below
  - Summation convention hides complexity

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = \frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} + S^{(\phi)}$$

$$\frac{\partial \rho\phi}{\partial t} + \frac{1}{J}\frac{\partial \rho U_j \phi}{\partial \xi_j} = \frac{1}{J}\frac{\partial}{\partial \xi_k}\left(B_{kj}\Gamma^{(\phi)}\frac{\partial \phi}{\partial \xi_j}\right) + S^{(\phi)}$$

$$U_j = J\frac{\partial \xi_j}{\partial x_i}u_i \qquad B_{kj} = J\frac{\partial \xi_k}{\partial x_i}\frac{\partial \xi_j}{\partial x_i}$$

California State University Northridge 18

Transformed Convection Terms

$$\frac{1}{J}\frac{\partial \rho U_j \phi}{\partial \xi_j} = \frac{1}{J}\frac{\partial \rho}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial x_i}u_i\phi\right) =$$

$$\frac{1}{J}\left\{\frac{\partial}{\partial \xi_1}\rho J\left[\left(\frac{\partial \xi_1}{\partial x_1}u_1\phi\right)+\left(\frac{\partial \xi_1}{\partial x_2}u_2\phi\right)+\left(\frac{\partial \xi_1}{\partial x_3}u_3\phi\right)\right]\right.$$

$$+\frac{\partial}{\partial \xi_2}\rho J\left[\left(\frac{\partial \xi_2}{\partial x_1}u_1\phi\right)+\left(\frac{\partial \xi_2}{\partial x_2}u_2\phi\right)+\left(\frac{\partial \xi_2}{\partial x_3}u_3\phi\right)\right]+$$

$$\left.\frac{\partial}{\partial \xi_3}\rho J\left[\left(\frac{\partial \xi_3}{\partial x_1}u_1\phi\right)+\left(\frac{\partial \xi_3}{\partial x_2}u_2\phi\right)+\left(\frac{\partial \xi_3}{\partial x_3}u_3\phi\right)\right]\right\}$$

Transformed Diffusion Terms

- Have mixed second derivatives that will become part of “source” term

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{1}{J}\left\{\frac{\partial}{\partial \xi_1}\Gamma^{(\phi)}B_{11}\frac{\partial \phi}{\partial \xi_1}+\frac{\partial}{\partial \xi_1}\Gamma^{(\phi)}B_{21}\frac{\partial \phi}{\partial \xi_2}+\frac{\partial}{\partial \xi_1}\Gamma^{(\phi)}B_{31}\frac{\partial \phi}{\partial \xi_3}\right.$$

$$+\frac{\partial}{\partial \xi_2}\Gamma^{(\phi)}B_{12}\frac{\partial \phi}{\partial \xi_1}+\frac{\partial}{\partial \xi_2}\Gamma^{(\phi)}B_{22}\frac{\partial \phi}{\partial \xi_2}+\frac{\partial}{\partial \xi_2}\Gamma^{(\phi)}B_{32}\frac{\partial \phi}{\partial \xi_3}+$$

$$\left.\frac{\partial}{\partial \xi_3}\Gamma^{(\phi)}B_{13}\frac{\partial \phi}{\partial \xi_1}+\frac{\partial}{\partial \xi_3}\Gamma^{(\phi)}B_{23}\frac{\partial \phi}{\partial \xi_2}+\frac{\partial}{\partial \xi_3}\Gamma^{(\phi)}B_{33}\frac{\partial \phi}{\partial \xi_3}\right\}$$

$$B_{kj} = J\left(\frac{\partial \xi_k}{\partial x_1}\frac{\partial \xi_j}{\partial x_1}+\frac{\partial \xi_k}{\partial x_2}\frac{\partial \xi_j}{\partial x_2}+\frac{\partial \xi_k}{\partial x_3}\frac{\partial \xi_j}{\partial x_3}\right)$$

From BFC to Finite Volumes

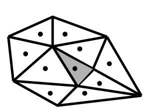
- Originally for finite-difference approaches in complex geometries
- Alternative of finite elements has natural system for complex geometries
- Finite-volume approach uses grid management systems of finite elements with gradients from finite differences
- Fluent gets gradients from vector calculus approaches

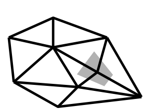
Unstructured Grids

- Grids that do not follow i, j, k relationship among neighboring nodes
- Require more bookkeeping for set of algebraic equations to be solved
  - Equations have more complex structure
- Also requires correct determination of average values and gradients
- Generally favored for flexibility in applications to complex geometries

Choice of Control Volumes

- Control volumes can be an individual cell with nodes at the center of the control volume
- An alternative, vertex-centered, is to construct control volumes around the nodes, which are located on the vertices of the grid



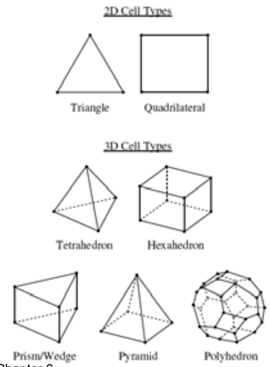


Finite-Volume Equations

- Finite-volume equations for unstructured grids derived in same way as for structured grids
- Have to consider geometries that are not at right angles
- See text for details of convection and diffusion terms
- Operations similar to those for boundary-fitted coordinates, but in a discrete sense

Fluent Finite-volume Cells

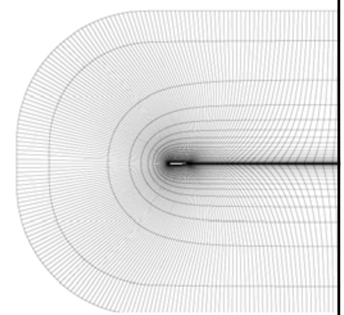
- Finite volumes or cells can have different shapes
- Figures at right are those available in Fluent
  - Similar to types available in general CFD or other analysis codes



California State University Northridge
Fluent Users Manual, September 29, 2006, Chapter 6

Structured Airfoil Grid

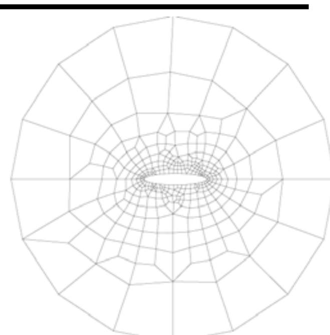
- Structured girds have fixed relationship between ξ_i, η_j, and ζ_k generalized coordinates to fit problem geometry



California State University Northridge
Fluent Users Manual, September 29, 2006, Chapter 6
26

Unstructured Airfoil Grid

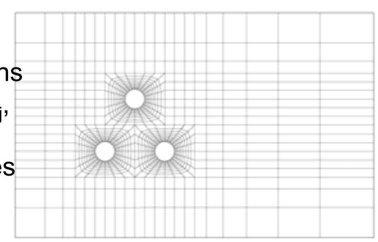
- Unstructured grids have no relationship between ξ_i, η_j, and ζ_k coordinates
- Geometry coding more complex



California State University Northridge
Fluent Users Manual, September 29, 2006, Chapter 6
27

Multiblock Structured Grid

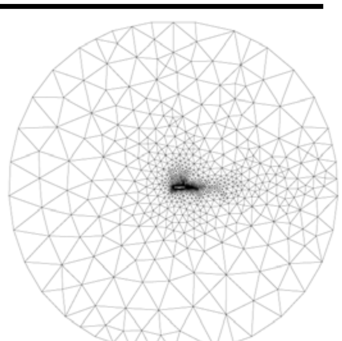
- Overall problem geometry has main grid with subdivisions
- Both main grid and subdivisions have ξ_i, η_j, and ζ_k coordinates



California State University Northridge
Fluent Users Manual, September 29, 2006, Chapter 6
28

Unstructured Airfoil Grid

- All visible elements in this grid appear to be triangular elements
  - Most flexible form for a 2D grid



California State University Northridge
Fluent Users Manual, September 29, 2006, Chapter 6
29

Unstructured Tetrahedral

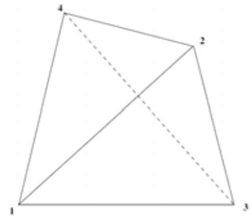
- Tetrahedron (solid surface with four sides) is three-dimensional analog of triangle for gridding
  - Most flexible for complex three-dimensional geometries

California State University Northridge
Fluent Users Manual, September 29, 2006, Chapter 6
30

Tetrahedral Cell Numbering

- In unstructured grids there is no natural i, j, k numbering system
- Cells have nodes and faces
- Local numbering system

Face 1	Nodes 3-2-4
Face 2	Nodes 4-1-3
Face 3	Nodes 2-1-4
Face 4	Nodes 3-1-2



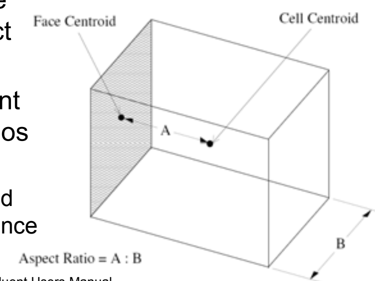
California State University Northridge

Fluent Users Manual, September 29, 2006, Chapter 6

31

Aspect Ratio

- Measure of cell “stretching”
- For square cell, aspect ratio = 1
- Do not want aspect ratios too large
  - Errors and convergence problems



California State University Northridge

Fluent Users Manual, September 29, 2006, Chapter 6

32

Finite-Volume Approaches

- Use integral equations
- Grid generation approaches more closely related to finite elements
  - Different types of mesh elements allowed
    - Finite differences result in quadrilaterals in two dimensions and hexahedrons in three
    - Finite-element and finite-volume can use triangles in two dimensions and tetrahedrons in three dimensions
- Apply gird transformations locally

California State University Northridge

33

Finite Volume Approaches II

- General integral balance equation over volume, Ω, enclosed by surface, Σ

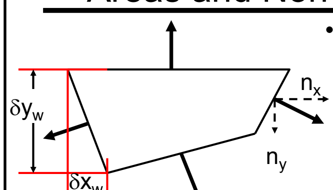
$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial t}\int_{\Omega} \rho\varphi dV = -\int_{\Sigma} \rho\varphi \mathbf{v}\cdot\mathbf{n} dS - \int_{\Sigma} \mathbf{d}_{\varphi}\cdot\mathbf{n} dS + \int_{\Omega} S_{\varphi} dV$$

- $\mathbf{d}_\phi$ is diffusive flux of $\phi = -\Gamma^{(\phi)}$ grad ϕ
- **n** is outward pointing unit normal
  - Must construct **n** for each finite volume cell face in complex geometry

California State University Northridge

34

Areas and Normal Vectors



- Normals are perpendicular to surface, pointing outward from enclosed area and have unit length
- Grid coordinates known from mesh generation routines
- Compute δx and δy terms to compute surface “area”
  - For 2D area found as $(\delta S)^2 = (\delta x)^2 + (\delta y)^2$

California State University Northridge

35

Convection Terms

- Evaluate this integral for each cell face $\int_{\Sigma} \rho\varphi\mathbf{v}\cdot\mathbf{n}dS$
- The **v·n** term is found from basic u and v velocity components as ±u cos θ ± v sin θ where $\theta = \tan^{-1}(dx/dy)$
  - Use plus sign of ± for east and north faces and minus sign for west and south faces
- Use midpoint rule to approximate integral $\int_{\Sigma} \rho\varphi\mathbf{v}\cdot\mathbf{n}dS \approx (\rho\varphi\mathbf{v}\cdot\mathbf{n})_{center}\delta S$

California State University Northridge

36

Convection Terms II

- With midpoint rule result we have to interpolate values to cell face from surrounding nodes $\int_{\Sigma} \rho\varphi \mathbf{v}\cdot\mathbf{n}dS \approx (\rho\varphi\mathbf{v}\cdot\mathbf{n})_{center}\delta S$
- Use interpolation for velocity (**v·n**)
- Choose differencing scheme (central, upwind, QUICK, etc.)for ϕ a
- Consider higher order interpolation if face midpoint is not on line with cell centers

California State University Northridge 37

Diffusion Terms

- Use midpoint rule for integral

$$-\int_{\Sigma}\mathbf{d}_{\varphi}\cdot\mathbf{n}dS = \int_{\Sigma}\Gamma^{(\phi)} grad\,\phi\cdot\mathbf{n}dS \approx \left(\Gamma^{(\phi)} grad\,\phi\cdot\mathbf{n}\right)_{center}\delta S$$

- Use Cartesian coordinates for gradient

$$\left(\Gamma^{(\phi)} grad\,\phi\cdot\mathbf{n}\right) = \frac{\partial\phi}{\partial x}n_x + \frac{\partial\phi}{\partial y}n_y$$

- Interpolate both ϕ and coordinates to get Cartesian derivatives
- Variety of possible approaches

California State University Northridge 38

Other Computations

- Can get more accurate expressions by considering vector analysis to get gradients
- Requires cross diffusion terms, similar to terms in boundary-fitted coordinates, but done in finite difference form
- Have to analyze geometry of adjacent cells to compute gradients and convective fluxes

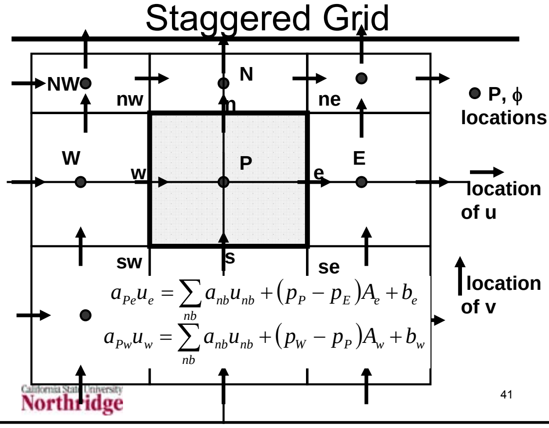
California State University Northridge 39

Non-Staggered (Colocated) Grids

- Staggered grids are convenient way to handle pressure in simple finite-difference grids
- These become difficult in boundary-fitted coordinates and unstructured grids
- Alternative approach uses colocated variables (all variables at same point)
- Need interpolation method to avoid problems with pressure

California State University Northridge 40

Staggered Grid

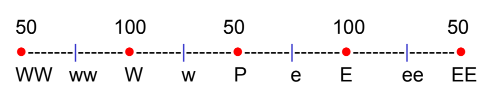


$$a_{Pe}u_e = \sum_{nb} a_{nb}u_{nb} + (p_P - p_E)A_e + b_e$$

$$a_{Pw}u_w = \sum_{nb} a_{nb}u_{nb} + (p_W - p_P)A_w + b_w$$

California State University Northridge 41

Colocated Grid Problem



- Oscillating pressures seen if equation for u_P has pressure gradient $(p_E - p_P)/\delta x$
- Staggered grid solves problem by placing u velocities at "e" and "w" node
- Real importance is for continuity-momentum combination used to solve for pressure

California State University Northridge 42

Colocated Grid

- All variables (u, v, p) stored at nodes WW, W, P, E, EE

●-------|-------●-------|-------●-------|-------●-------|-------●

WW ww W w P e E ee EE

$$a_{P_P} u_P = \sum_{nb} a_{nb} u_{nb} + (p_w - p_e) A_P + b_P$$

- Find p_e and p_w by interpolation

$$p_w - p_e = \frac{p_W + p_P}{2} - \frac{p_P + p_E}{2} = \frac{p_W - p_E}{2}$$

$$a_{P_P} u_P = \sum_{nb} a_{nb} u_{nb} + \frac{p_W - p_E}{2} A_P + b_P$$

Colocated Grid II

$$u_P = \frac{\sum_{nb} a_{nb} u_{nb} + b_P}{a_{P_P}} + \frac{p_W - p_E}{2} \frac{A_P}{a_{P_P}} = \frac{\sum_{nb} a_{nb} u_{nb} + b_P}{a_{P_P}} + \frac{p_W - p_E}{2} d_P$$

- Have similar equation for u_E

$$u_E = \frac{\sum_{nb} a_{nb} u_{nb} + b_E}{a_{P_E}} + \frac{p_{EE} - p_P}{2} \frac{A_E}{a_{P_E}} = \frac{\sum_{nb} a_{nb} u_{nb} + b_E}{a_{P_E}} + \frac{p_{EE} - p_P}{2} d_E$$

- Continuity equation needs u_e
- Need interpolation for relation of this velocity to pressure

Rhie and Chow Interpolation

$$u_e = \frac{u_P + u_E}{2} + \frac{d_E + d_P}{2}(p_P - p_E) - \frac{d_P}{4}(p_W - p_E) - \frac{d_E}{4}(p_P - p_{EE})$$

- Can show that added terms amount to a third-order error in pressure
  - Examine constant d for simplicity

$$\frac{T}{4} = \frac{d + d}{2}(p_P - p_E) - \frac{d}{4}(p_W - p_E) - \frac{d}{4}(p_P - p_{EE})$$

$$T = 4d(p_P - p_E) - d(p_W - p_E) - d(p_P - p_{EE}) = d(p_{EE} - 3p_E + 3p_P - p_W)$$

- Third derivative as first derivative of second derivative in finite-difference form

$$\left.\frac{\partial^3 p}{\partial x^3}\right|_e = \left(\frac{\partial}{\partial x}\frac{\partial^2 p}{\partial x^2}\right)_e = \frac{\left.\frac{\partial^2 p}{\partial x^2}\right|_E - \left.\frac{\partial^2 p}{\partial x^2}\right|_P}{2\frac{\Delta x}{2}}$$

Rhie and Chow Interpolation II

$$\left.\frac{\partial^3 p}{\partial x^3}\right|_e = \frac{\left.\frac{\partial^2 p}{\partial x^2}\right|_E - \left.\frac{\partial^2 p}{\partial x^2}\right|_P}{2\frac{\Delta x}{2}} = \frac{\frac{p_P + p_{EE} - 2p_E}{(\Delta x)^2} - \frac{p_W + p_E - 2p_P}{(\Delta x)^2}}{\Delta x} = \frac{3p_P + p_{EE} - 3p_E - p_W}{(\Delta x)^3}$$

- Compare to previous equation

$$u_e = \frac{u_P + u_E}{2} + \frac{d_E + d_P}{2}(p_P - p_E) - \frac{d_P}{4}(p_W - p_E) - \frac{d_E}{4}(p_P - p_{EE})$$

$$= \frac{u_P + u_E}{2} + \frac{d}{4}(3p_P + p_{EE} - 3p_E - p_W) = \frac{u_P + u_E}{2} + \frac{d}{4}\left.\frac{\partial^3 p}{\partial x^3}\right|_e (\Delta x)^3$$

- Added pressure terms are equivalent to adding a third-order error in pressure
  - Higher order than usual first or second order error in finite-volume approaches

Grid Quality

- Non-structured meshes have equations that are exact for orthogonal cells, but have errors as cells depart from orthogonal
- Triangular cells are best when they are equilateral triangles
- Use code indicators of mesh quality to ensure that meshes are not badly structured in your grid

Summary

- CFD codes must be able to handle complex geometries
- Flow-3D uses FAVOR™ method in which boundaries cross grid lines
- Most other codes use boundary fitted coordinates or fractional volume methods
- Finite-element codes, not considered here, have own approaches
- Check mesh quality

Material Not Covered in Class

- The following slides discuss the basic coordinate transformations used in boundary-fitted coordinates
- These will not be covered in class
- Additional material is available in online notes on coordinate transformations
- This is mostly mathematical material to provide background for coordinate transformations

California State University Northridge 49

Coordinate Transformations

- Transform Cartesian coordinates, x, y, z, into computational ones, ξ, η, ζ
  - For derivations, write Cartesian coordinates as x_1, x_2, and x_3, and computational coordinates as ξ_1, ξ_2, and ξ_3
  - Grid (mesh) generation programs define physical coordinates x_1, x_2, and x_3, as functions of ξ_1, ξ_2, and ξ_3
  - In principle have two sets of relations: $\xi_i = \xi_i(x_1, x_2, x_3)$ and $x_i = x_i(\xi_1,\xi_2,\xi_3)$

California State University Northridge 50

Coordinate Transformations II

- The mesh generation step will give the values of x, y, and z at each point in the computational grid
- From these it is easy to compute finite difference expressions for derivatives like $\partial x_i/\partial \xi_j$
  - E.g. $\partial z/\partial \eta = (z_{ijk+1} - z_{ijk-1})/(2\Delta\eta)$
- Some transformations require derivatives like $\partial \xi_i/\partial x_j$
  - How do we get these derivatives?

California State University Northridge 51

Derivative Relationships

- General equation for total differentials can use summation convention

$$d\xi_i = \frac{\partial \xi_i}{\partial x_1}dx_1 + \frac{\partial \xi_i}{\partial x_2}dx_2 + \frac{\partial \xi_i}{\partial x_3}dx_3 \; or \; d\xi_i = \frac{\partial \xi_i}{\partial x_j}dx_j \; i = 1,2,3$$

$$dx_i = \frac{\partial x_i}{\partial \xi_1}d\xi_1 + \frac{\partial x_i}{\partial \xi_2}d\xi_2 + \frac{\partial x_i}{\partial \xi_3}d\xi_3 \quad or \quad dx_i = \frac{\partial x_i}{\partial \xi_j}d\xi_j$$

- Use these equations to get relationship between $\partial x_i/\partial \xi_j$ and $\partial \xi_i/\partial x_j$
  - Write equations in matrix form

California State University Northridge 52

Derivative Relationships II

$$\begin{bmatrix} d\xi_1 \\ d\xi_2 \\ d\xi_3 \end{bmatrix} = \begin{bmatrix} \frac{\partial \xi_1}{\partial x_1} & \frac{\partial \xi_1}{\partial x_2} & \frac{\partial \xi_1}{\partial x_3} \\ \frac{\partial \xi_2}{\partial x_1} & \frac{\partial \xi_2}{\partial x_2} & \frac{\partial \xi_2}{\partial x_3} \\ \frac{\partial \xi_3}{\partial x_1} & \frac{\partial \xi_3}{\partial x_2} & \frac{\partial \xi_3}{\partial x_3} \end{bmatrix} \begin{bmatrix} dx_1 \\ dx_2 \\ dx_3 \end{bmatrix}$$

- The matrices must be inverses of each other for both equations to be correct

$$\begin{bmatrix} dx_1 \\ dx_2 \\ dx_3 \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial \xi_1} & \frac{\partial x_1}{\partial \xi_2} & \frac{\partial x_1}{\partial \xi_3} \\ \frac{\partial x_2}{\partial \xi_1} & \frac{\partial x_2}{\partial \xi_2} & \frac{\partial x_2}{\partial \xi_3} \\ \frac{\partial x_3}{\partial \xi_1} & \frac{\partial x_3}{\partial \xi_2} & \frac{\partial x_3}{\partial \xi_3} \end{bmatrix} \begin{bmatrix} d\xi_1 \\ d\xi_2 \\ d\xi_3 \end{bmatrix}$$

California State University Northridge 53

Derivative Relationships III

- Inverse matrix relationship

$$\begin{bmatrix} \frac{\partial \xi_1}{\partial x_1} & \frac{\partial \xi_1}{\partial x_2} & \frac{\partial \xi_1}{\partial x_3} \\ \frac{\partial \xi_2}{\partial x_1} & \frac{\partial \xi_2}{\partial x_2} & \frac{\partial \xi_2}{\partial x_3} \\ \frac{\partial \xi_3}{\partial x_1} & \frac{\partial \xi_3}{\partial x_2} & \frac{\partial \xi_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial \xi_1} & \frac{\partial x_1}{\partial \xi_2} & \frac{\partial x_1}{\partial \xi_3} \\ \frac{\partial x_2}{\partial \xi_1} & \frac{\partial x_2}{\partial \xi_2} & \frac{\partial x_2}{\partial \xi_3} \\ \frac{\partial x_3}{\partial \xi_1} & \frac{\partial x_3}{\partial \xi_2} & \frac{\partial x_3}{\partial \xi_3} \end{bmatrix}^{-1}$$

- Use analytical formula for calculating the components of an inverse matrix to get necessary derivative relationships

California State University Northridge 54

Derivative Relationships IV

- Formula for matrix inversion, **B** = **A**$^{-1}$
- $b_{ij} = (-1)^{i+j} M_{ji} / \det(\mathbf{A})$
- M_{ij} is minor determinant found by eliminating row i and column j
- Determinant, called Jacobian J, is the ratio of volume elements in the two coordinate systems

$$J = \begin{vmatrix} \frac{\partial x_1}{\partial \xi_1} & \frac{\partial x_1}{\partial \xi_2} & \frac{\partial x_1}{\partial \xi_3} \\ \frac{\partial x_2}{\partial \xi_1} & \frac{\partial x_2}{\partial \xi_2} & \frac{\partial x_2}{\partial \xi_3} \\ \frac{\partial x_3}{\partial \xi_1} & \frac{\partial x_3}{\partial \xi_2} & \frac{\partial x_3}{\partial \xi_3} \end{vmatrix}$$

California State University Northridge 55

Derivative Relationships V

- Example of matrix inverse component

$$\begin{bmatrix} \frac{\partial \xi_1}{\partial x_1} & \frac{\partial \xi_1}{\partial x_2} & \frac{\partial \xi_1}{\partial x_3} \\ \frac{\partial \xi_2}{\partial x_1} & \frac{\partial \xi_2}{\partial x_2} & \frac{\partial \xi_2}{\partial x_3} \\ \frac{\partial \xi_3}{\partial x_1} & \frac{\partial \xi_3}{\partial x_2} & \frac{\partial \xi_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial \xi_1} & \frac{\partial x_1}{\partial \xi_2} & \frac{\partial x_1}{\partial \xi_3} \\ \frac{\partial x_2}{\partial \xi_1} & \frac{\partial x_2}{\partial \xi_2} & \frac{\partial x_2}{\partial \xi_3} \\ \frac{\partial x_3}{\partial \xi_1} & \frac{\partial x_3}{\partial \xi_2} & \frac{\partial x_3}{\partial \xi_3} \end{bmatrix}^{-1}$$

- To compute $\partial\xi_2/\partial x_3$, we need M_{32}

$$\frac{\partial \xi_2}{\partial x_3} = \frac{(-1)^{2+3} M_{32}}{J} = -\frac{1}{J}\left[\frac{\partial x_1}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_3} - \frac{\partial x_1}{\partial \xi_3}\frac{\partial x_2}{\partial \xi_1}\right]$$

California State University Northridge 56

Derivative Relationships VI

- Have nine relationships like the one at the bottom of the previous slide
- See coordinate transformation notes, page four
- Note alternative notations

$$\frac{\partial \xi_2}{\partial x_3} = \frac{1}{J}\left[\frac{\partial x_1}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_3} - \frac{\partial x_1}{\partial \xi_3}\frac{\partial x_2}{\partial \xi_1}\right]$$

$$\frac{\partial \eta}{\partial z} = \frac{1}{J}\left[\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \zeta} - \frac{\partial x}{\partial \zeta}\frac{\partial y}{\partial \xi}\right] = \frac{x_\xi y_\zeta - x_\zeta y_\xi}{J}$$

California State University Northridge 57

Transform Transport Equation

- We need to transform the convection and diffusion terms in the general transport equation

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = \frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} + S^{(\phi)}$$

- Look at general first derivative term (with implied summation) $\partial F_i/\partial x_i$
- For convection terms $F_i = \rho u_i \phi$

California State University Northridge 58

Transform Transport Equation II

- Required transformation equation

$$\frac{\partial}{\partial x_i} = \frac{\partial \xi}{\partial x_i}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x_i}\frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial x_i}\frac{\partial}{\partial \zeta} \quad or \quad \frac{\partial}{\partial x_i} = \frac{\partial \xi_j}{\partial x_i}\frac{\partial}{\partial \xi_j} \qquad i = 1,2,3$$

$$\frac{\partial F_i}{\partial x_i} = \frac{\partial \xi_j}{\partial x_i}\frac{\partial F_i}{\partial \xi_j}$$

- Two repeated indices (i and j) give two implied summations
- Next step is not obvious – multiply by J

California State University Northridge 59

Transform Transport Equation III

- Apply product rule for derivatives

$$J\frac{\partial F_i}{\partial x_i} = J\frac{\partial \xi_j}{\partial x_i}\frac{\partial F_i}{\partial \xi_j} = \frac{\partial}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial x_i}F_i\right) - F_i\frac{\partial}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial x_i}\right)$$

$$AdF \quad = \quad d(AF) \quad - \quad FdA$$

- Can show that last term vanishes
- See pages 6 and 7 in notes
  - Show that this term is zero for i = 1
  - Requires substitution of matrix inversion relationships for $\partial\xi_i/\partial x_j$ in terms of $\partial x_i/\partial\xi_j$

California State University Northridge 60

Transform Transport Equation IV

- Result for $\partial F_i/\partial x_i$

$$J\frac{\partial F_i}{\partial x_i} = \frac{\partial}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial x_i}F_i\right) \quad \Rightarrow \quad \frac{\partial F_i}{\partial x_i} = \frac{1}{J}\frac{\partial}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial x_i}F_i\right)$$

- For convection terms $F_i = \rho u_i \phi$
- Define $U_j = J u_i \partial\xi_i/\partial x_j$ (implied summation) to give following result for convection

$$\frac{\partial \rho u_i \phi}{\partial x_i} = \frac{1}{J}\frac{\partial \rho U_j \phi}{\partial \xi_j}$$

Transform Transport Equation V

- Handle diffusion terms next
- Have analog to convection terms

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{\partial F_i}{\partial x_i} \quad with \quad F_i = \Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i}$$

- We can use result just found for $\partial F_i/\partial x_i$ in analysis of convection terms
- Basic transformation equation for $\partial\phi/\partial x_i$

$$\frac{\partial \phi}{\partial x_i} = \frac{\partial \xi_j}{\partial x_i}\frac{\partial \phi}{\partial \xi_j} \qquad i = 1,2,3$$

Transform Transport Equation V

- Combine results from previous chart

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{\partial F_i}{\partial x_i} \quad with \quad F_i = \Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \Gamma^{(\phi)}\frac{\partial \xi_j}{\partial x_i}\frac{\partial \phi}{\partial \xi_j}$$

- With convection terms analysis result

$$\frac{\partial F_i}{\partial x_i} = \frac{1}{J}\frac{\partial}{\partial \xi_k}\left(J\frac{\partial \xi_k}{\partial x_i}F_i\right)$$

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{1}{J}\frac{\partial}{\partial \xi_k}\left(J\frac{\partial \xi_k}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \xi_j}{\partial x_i}\frac{\partial \phi}{\partial \xi_j}\right)$$

Transform Transport Equation VI

- Define coefficients B_{kj} to simplify diffusion terms

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{1}{J}\frac{\partial}{\partial \xi_k}\left(\Gamma^{(\phi)}J\frac{\partial \xi_k}{\partial x_i}\frac{\partial \xi_j}{\partial x_i}\frac{\partial \phi}{\partial \xi_j}\right)$$

$$B_{kj} = J\frac{\partial \xi_k}{\partial x_i}\frac{\partial \xi_j}{\partial x_i} = J\left[\frac{\partial \xi_k}{\partial x_1}\frac{\partial \xi_j}{\partial x_1} + \frac{\partial \xi_k}{\partial x_2}\frac{\partial \xi_j}{\partial x_2} + \frac{\partial \xi_k}{\partial x_3}\frac{\partial \xi_j}{\partial x_3}\right]$$

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{1}{J}\frac{\partial}{\partial \xi_k}\left(\Gamma^{(\phi)}B_{kj}\frac{\partial \phi}{\partial \xi_j}\right)$$

Transform Transport Equation VII

- Transformed diffusion terms now have mixed second derivatives
- Full set of diffusion terms shown below

$$\frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} = \frac{1}{J}\left\{\frac{\partial}{\partial \xi_1}\Gamma^{(\phi)}B_{11}\frac{\partial \phi}{\partial \xi_1} + \frac{\partial}{\partial \xi_1}\Gamma^{(\phi)}B_{21}\frac{\partial \phi}{\partial \xi_2} + \frac{\partial}{\partial \xi_1}\Gamma^{(\phi)}B_{31}\frac{\partial \phi}{\partial \xi_3}\right.$$
$$+ \frac{\partial}{\partial \xi_2}\Gamma^{(\phi)}B_{12}\frac{\partial \phi}{\partial \xi_1} + \frac{\partial}{\partial \xi_2}\Gamma^{(\phi)}B_{22}\frac{\partial \phi}{\partial \xi_2} + \frac{\partial}{\partial \xi_2}\Gamma^{(\phi)}B_{32}\frac{\partial \phi}{\partial \xi_3} +$$
$$\left.\frac{\partial}{\partial \xi_3}\Gamma^{(\phi)}B_{13}\frac{\partial \phi}{\partial \xi_1} + \frac{\partial}{\partial \xi_3}\Gamma^{(\phi)}B_{23}\frac{\partial \phi}{\partial \xi_2} + \frac{\partial}{\partial \xi_3}\Gamma^{(\phi)}B_{33}\frac{\partial \phi}{\partial \xi_3}\right\}$$

Final Transformed Equation

- Substitute transformed convection and diffusion terms into general transport equation

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = \frac{\partial}{\partial x_i}\Gamma^{(\phi)}\frac{\partial \phi}{\partial x_i} + S^{(\phi)}$$

$$\frac{\partial \rho \phi}{\partial t} + \frac{1}{J}\frac{\partial \rho U_j \phi}{\partial \xi_j} = \frac{1}{J}\frac{\partial}{\partial \xi_k}\left(B_{kj}\Gamma^{(\phi)}\frac{\partial \phi}{\partial \xi_j}\right) + S^{(\phi)}$$

$$U_j = J\frac{\partial \xi_j}{\partial x_i}u_i \qquad\qquad B_{kj} = J\frac{\partial \xi_k}{\partial x_i}\frac{\partial \xi_j}{\partial x_i}$$

Using the Transformed Equation

- Have to store a lot of additional information about grid coordinates, derivatives, J and B_{jk}
- Differential equations more complex
- Coordinates fit boundaries and give good representation of geometry
  - Models gradient fluxes well
- Can have grids with bad aspect ratios
- Small sizes extend throughout grid

California State University Northridge 67