



2.29 Numerical Fluid Mechanics

Fall 2011 – Lecture 21

REVIEW Lecture 20: Time-Marching Methods and ODEs–IVPs

- Time-Marching Methods and ODEs – Initial Value Problems

$$\frac{d \bar{\Phi}}{dt} = \mathbf{B} \bar{\Phi} + (\mathbf{bc}) \quad \text{or} \quad \frac{d \bar{\Phi}}{dt} = \mathbf{B}(\bar{\Phi}, t) ; \quad \text{with } \bar{\Phi}(t_0) = \bar{\Phi}_0$$

- Euler’s method

- Taylor Series Methods

- Error analysis: for two time-levels, if truncation error is of $O(h^n)$, the global error is of $O(h^{n-1})$

- Simple 2nd order methods

- Heun’s Predictor-Corrector and Midpoint Method (part of Runge-Kutta’s methods)

- To achieve higher accuracy in time: utilize information (known values of the derivative in time, i.e. the RHS f) at more points in time

- Runge-Kutta Methods

- Additional points are between t_n and t_{n+1}

$$\phi^{n+1} - \phi^n = \int_{t_n}^{t_{n+1}} f(t, \phi) dt$$

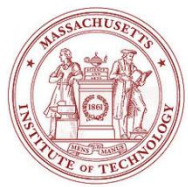
- Multistep/Multipoint Methods: Adams Methods

- Additional points are at past time steps

- Practical CFD Methods

- Implicit Nonlinear systems

- Deferred-correction Approach



TODAY (Lecture 21): End of Time-Marching Methods, Grid Generation and Complex Geometries

- Time-Marching Methods and ODEs – IVPs: End
 - Multistep/Multipoint Methods
 - Implicit Nonlinear systems
 - Deferred-correction Approach
- Complex Geometries
 - Different types of grids
 - Choice of variable arrangements
- Grid Generation
 - Basic concepts and structured grids
 - Stretched grids
 - Algebraic methods
 - General coordinate transformation
 - Differential equation methods
 - Conformal mapping methods
 - Unstructured grid generation
 - Delaunay Triangulation
 - Advancing Front method



References and Reading Assignments

- Chapters 25 and 26 of “Chapra and Canale, *Numerical Methods for Engineers*, 2010/2006.”
- Chapter 6 (end) and Chapter 8 on “Complex Geometries” of “J. H. Ferziger and M. Peric, *Computational Methods for Fluid Dynamics*. Springer, NY, 3rd edition, 2002”
- Chapter 6 (end) on “Time-Marching Methods for ODE’s” of “H. Lomax, T. H. Pulliam, D.W. Zingg, *Fundamentals of Computational Fluid Dynamics (Scientific Computation)*. Springer, 2003”
- Chapter 9 on “Grid Generation” of T. Cebeci, J. P. Shao, F. Kafyeke and E. Laurendeau, *Computational Fluid Dynamics for Engineers*. Springer, 2005.
- Ref on Grid Generation only:
 - Thompson, J.F., Warsi Z.U.A. and C.W. Mastin, “Numerical Grid Generation, Foundations and Applications”, North Holland, 1985



Multistep/Multipoint Methods

- Additional points are at time steps at which data has already been computed
- Adams Methods: fitting a (Lagrange) polynomial to the derivatives at a number of points in time

- Explicit in time (up to t_n): Adams-Bashforth methods

$$\phi^{n+1} - \phi^n = \sum_{k=n-K}^n \beta_k f(t_k, \phi^k) \Delta t$$

- Implicit in time (up to t_{n+1}): Adams-Moulton methods

$$\phi^{n+1} - \phi^n = \sum_{k=n-K}^{n+1} \beta_k f(t_k, \phi^k) \Delta t$$

- Coefficients β_k 's can be estimated by Taylor Tables:
 - Fit Taylor series so as to cancel higher-order terms



Example: Taylor Table for the Adams-Moulton 3-steps (4 time-nodes) Method

Denoting $h \equiv \Delta t$, $\phi \equiv u$, $\frac{du}{dt} = u' = f(t, u)$ and $u'_n = f(t_n, u^n)$, one obtains for $K = 2$:

$$u^{n+1} - u^n = \sum_{k=-K}^1 \beta_k f(t_{n+k}, u^{n+k}) \Delta t = h \left[\beta_1 f(t_{n+1}, u^{n+1}) + \beta_0 f(t_n, u^n) + \beta_{-1} f(t_{n-1}, u^{n-1}) + \beta_{-2} f(t_{n-2}, u^{n-2}) \right]$$

Taylor Table:

- The first row (Taylor series) + the last 5 rows (Taylor series for each term) must sum to zero
- This can be satisfied up to the 5th column (4th order term)
- Hence, the AM method with 4-time levels is 4th order accurate

	u_n	$h \cdot u'_n$	$h^2 \cdot u''_n$	$h^3 \cdot u'''_n$	$h^4 \cdot u''''_n$
u_{n+1}	1	1	$\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{24}$
$-u_n$	-1				
$-h\beta_1 u'_{n+1}$		$-\beta_1$	$-\beta_1$	$-\beta_1 \frac{1}{2}$	$-\beta_1 \frac{1}{6}$
$-h\beta_0 u'_n$		$-\beta_0$			
$-h\beta_{-1} u'_{n-1}$		$-\beta_{-1}$	β_{-1}	$-\beta_{-1} \frac{1}{2}$	$\beta_{-1} \frac{1}{6}$
$-h\beta_{-2} u'_{n-2}$		$-(-2)^0 \beta_{-2}$	$-(-2)^1 \beta_{-2}$	$-(-2)^2 \beta_{-2} \frac{1}{2}$	$-(-2)^3 \beta_{-2} \frac{1}{6}$

solving for the β_k 's $\Rightarrow \beta_1 = 9/24$, $\beta_0 = 19/24$, $\beta_{-1} = -5/24$ and $\beta_{-2} = 1/24$



Example of Adams Methods for Time-Integration

Explicit Methods. (Adams-Bashforth, with AB n meaning n^{th} order AB)

$$\begin{aligned}u_{n+1} &= u_n + hu'_n && \text{Euler} \\u_{n+1} &= u_{n-1} + 2hu'_n && \text{Leapfrog} \\u_{n+1} &= u_n + \frac{1}{2}h[3u'_n - u'_{n-1}] && \text{AB2} \\u_{n+1} &= u_n + \frac{h}{12}[23u'_n - 16u'_{n-1} + 5u'_{n-2}] && \text{AB3}\end{aligned}$$

Implicit Methods. (Adams-Moulton, with AM n meaning n^{th} order AM)

$$\begin{aligned}u_{n+1} &= u_n + hu'_{n+1} && \text{Implicit Euler} \\u_{n+1} &= u_n + \frac{1}{2}h[u'_n + u'_{n+1}] && \text{Trapezoidal (AM2)} \\u_{n+1} &= \frac{1}{3}[4u_n - u_{n-1} + 2hu'_{n+1}] && \text{2nd-order Backward} \\u_{n+1} &= u_n + \frac{h}{12}[5u'_{n+1} + 8u'_n - u'_{n-1}] && \text{AM3}\end{aligned}$$



Practical Time-Integration Methods for CFD

- High-resolution CFD requires large discrete state vector sizes to store the spatial information
- This means that up to two times (one on each side of the current time step) have often been utilized (3 time-nodes): $u^{n+1} - u^n = h \left[\beta_1 f(t_{n+1}, u^{n+1}) + \beta_0 f(t_n, u^n) + \beta_{-1} f(t_{n-1}, u^{n-1}) \right]$
- Rewriting this equations in a way such that differences wrt. the Euler's method are easily seen, one obtains ($\theta = 0$ for explicit schemes):

$$(1 + \xi) u^{n+1} = \left[(1 + 2\xi) u^n - \xi u^{n-1} \right] + h \left[\theta f(t_{n+1}, u^{n+1}) + (1 - \theta + \varphi) f(t_n, u^n) - \varphi f(t_{n-1}, u^{n-1}) \right]$$

θ	ξ	φ	Method	Order
0	0	0	Euler	1
1	0	0	Implicit Euler	1
1/2	0	0	Trapezoidal or AM2	2
1	1/2	0	2nd-order Backward	2
3/4	0	-1/4	Adams type	2
1/3	-1/2	-1/3	Lees	2
1/2	-1/2	-1/2	Two-step trapezoidal	2
5/9	-1/6	-2/9	A-contractive	2
0	-1/2	0	Leapfrog	2
0	0	1/2	AB2	2
0	-5/6	-1/3	Most accurate explicit	3
1/3	-1/6	0	Third-order implicit	3
5/12	0	1/12	AM3	3
1/6	-1/2	-1/6	Milne	4



Implementation of Implicit Time-Marching Methods: Nonlinear Systems and Larger dimensions

- Consider the nonlinear system (discrete in space):

$$\frac{d \Phi}{dt} = \mathbf{B}(\Phi, t) ; \text{ with } \Phi(t_0) = \Phi_0$$

- For an explicit method in time, solution is straightforward

- For explicit Euler: $\Phi^{n+1} = \Phi^n + \mathbf{B}(\Phi^n, t^n) \Delta t$
- More general, e.g. AB: $\Phi^{n+1} = \mathbf{F}(\Phi^n, \Phi^{n-1}, \dots, \Phi^{n-K}, t^n) \Delta t$

- For an implicit method

- For Implicit Euler: $\Phi^{n+1} = \Phi^n + \mathbf{B}(\Phi^{n+1}, t^{n+1}) \Delta t$
- More general: $\Phi^{n+1} = \mathbf{F}(\Phi^{n+1}, \Phi^n, \Phi^{n-1}, \dots, \Phi^{n-K}, t^{n+1}) \Delta t$ or
 $\tilde{\mathbf{F}}(\Phi^{n+1}, \Phi^n, \Phi^{n-1}, \dots, \Phi^{n-K}, t^{n+1}) = 0 ;$ with $\tilde{\mathbf{F}} = \mathbf{F}\Delta t - \Phi^{n+1}$

=> a nontrivial scheme is needed to obtain Φ^{n+1}



Implementation of Implicit Time-Marching Methods: Larger dimensions and Nonlinear systems

• Two main options for an implicit method, either:

1. Linearize the RHS at t^n :

• Taylor Series: $\mathbf{B}(\Phi, t) = \mathbf{B}(\Phi^n, t^n) + \mathbf{J}^n (\Phi - \Phi^n) + \left. \frac{\partial \mathbf{B}}{\partial t} \right|^n (t - t^n) + O(\Delta t^2)$ for $t^n \leq t \leq t^{n+1}$

where $\mathbf{J}^n = \left. \frac{\partial \mathbf{B}}{\partial \Phi} \right|^n$; i.e. $[\mathbf{J}^n]_{ij} = \frac{\partial \mathbf{B}_i}{\partial \Phi_j}$ (Jacobian Matrix)

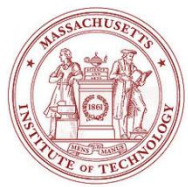
• Hence, the linearized system (for the frequent case of system not explicitly function of t):

$$\frac{d \Phi}{dt} = \mathbf{B}(\Phi) \Rightarrow \frac{d \Phi}{dt} = \mathbf{J}^n \Phi + [\mathbf{B}(\Phi^n) - \mathbf{J}^n \Phi^n]$$

2. Use an iteration scheme at each time step, e.g. fixed point iteration (direct), Newton-Raphson or secant method

• Newton-Raphson: $x_{r+1} = x_r - \frac{1}{f'(x_r)} f(x_r) \Rightarrow \Phi_{r+1}^{n+1} = \Phi_r^{n+1} - \left(\left. \frac{\partial \tilde{\mathbf{F}}}{\partial \Phi^{n+1}} \right|_r \right)^{-1} \tilde{\mathbf{F}}(\Phi_r^{n+1}, t^{n+1})$

• Iteration often rapidly convergent since initial guess to start iteration at t^n close to unknown solution at t^{n+1}



Deferred-Correction Approaches

- Size of computational molecule affects both storage requirements and effort needed to solve the algebraic system at each time-step
 - Usually, we wish to keep only the nearest neighbors of the center node P in the LHS of equations (leads to tri-diagonal matrix or something close to it) \Rightarrow easier to solve linear/nonlinear system
 - But, approximations that produce such molecules are often not accurate enough
- Way around this issue?
 - Leave only the terms containing the nearest neighbors in the LHS and bring all other more-remote terms to the RHS
 - This requires that these terms be evaluated with previous or old values, which may lead to divergence of the iterative scheme
- Better approach?



Deferred-Correction Approaches, Cont'd

- Better Approach

- Compute the terms that are approximated with a high-order approximation explicitly and put them in the RHS
- Take a simpler approximation to these terms (that give a small computational molecule). Insert it twice in the equation, with a + and - sign
- One of these two simpler approximation, keep it in the LHS of the equations (with unknown variables values, e.g. implicit/new). Move the other to the RHS (e.g. computing it explicitly using existing/old values)
- The RHS now contains the difference between two explicit approximations of the same term, and is likely to be small \Rightarrow
 - Likely no convergence problems to an iteration scheme (Jacobi, GS, SOR, etc) or gradient descent (CG, etc)
- Once the iteration converges, the low order approximation terms (one explicit, the other implicit) drop out and the solution corresponds to the higher-order approximation

- \Rightarrow Using H & L for high & low orders:

$$\mathbf{A}^H \mathbf{x} = \mathbf{b} \quad \rightarrow \quad \mathbf{A}^L \mathbf{x} = \mathbf{b} - \left[\mathbf{A}^H \mathbf{x} - \mathbf{A}^L \mathbf{x} \right]^{\text{old}}$$



Deferred-Correction Approaches, Cont'd

- This approach can be very powerful and general
 - Used when treating higher-order approximations, non-orthogonal grids, corrections needed to avoid oscillation effects, etc
 - Since RHS can be viewed as a correction \Rightarrow called deferred-correction
 - Note: both L&H terms could be implicit in time (use L&H implicit starter to get first values and then most recent old values in bracket during iterations)
 - Explicit for H (high-order) term, implicit for L (low-order) term

$$\mathbf{A}^H \mathbf{x} = \mathbf{b} \rightarrow \mathbf{A}^L \mathbf{x}_{\text{implicit}} = \mathbf{b} - \left[\mathbf{A}^H \mathbf{x}_{\text{explicit}} - \mathbf{A}^L \mathbf{x}_{\text{implicit}} \right]^{\text{old}}$$

- Implicit for both L and H terms

$$\mathbf{A}^H \mathbf{x} = \mathbf{b} \rightarrow \mathbf{A}^L \mathbf{x}_{\text{implicit}} = \mathbf{b} - \left[\mathbf{A}^H \mathbf{x}_{\text{implicit}} - \mathbf{A}^L \mathbf{x}_{\text{implicit}} \right]^{\text{old}}$$



Deferred-Correction Approaches, Cont'd

• Example 1: FD methods with High-order Pade' schemes

- One can use the PDE itself to express implicit Pade' time derivative $\left(\frac{\partial\phi}{\partial t}\right)_{n+1}$ as a function of ϕ^{n+1} (see homework 6)
- Or, use deferred-correction (within an iteration scheme of index r):

- In time:
$$\left(\frac{\partial\phi}{\partial t}\right)_n^{r+1} = \left(\frac{\phi_{n+1} - \phi_{n-1}}{2\Delta t}\right)^{r+1} + \left[\left(\frac{\partial\phi}{\partial t}\right)_n^{\text{Pade}'} - \frac{\phi_{n+1} - \phi_{n-1}}{2\Delta t}\right]^r$$

- In space:
$$\left(\frac{\partial\phi}{\partial x}\right)_i^{r+1} = \left(\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}\right)^{r+1} + \left[\left(\frac{\partial\phi}{\partial x}\right)_i^{\text{Pade}'} - \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}\right]^r$$

- The complete 2nd order CDS would be used on the LHS. The RHS would be the bracket term: the difference between the Pade' scheme and the "old" CDS. When the CDS becomes as accurate as Pade', this term in the bracket is zero

- Note: Forward/Backward DS could have been used instead of CDS, e.g. in

time,
$$\left(\frac{\partial\phi}{\partial t}\right)_{n+1}^{r+1} = \left(\frac{\phi_{n+1} - \phi_n}{\Delta t}\right)^{r+1} + \left[\left(\frac{\partial\phi}{\partial t}\right)_{n+1}^{\text{Pade}'} - \frac{\phi_{n+1} - \phi_n}{\Delta t}\right]^r$$



Deferred-Correction Approaches, Cont'd

• Example 2 with FV methods: Higher-order Flux approximations

- *Higher-order* flux approximations are computed with “old values” and a lower order approximation is used with “new values” (implicitly) in the linear system solver:

$$F_e = F_e^L + [F_e^H - F_e^L]^{\text{old}}$$

where F_e is the flux. The Low order approximation can be UDS or CDS.

- Convergence and stability properties are close to those of the Low order implicit term since the bracket is often small compared to this implicit term
 - In addition, since bracket term is small, the iteration in the algebraic equation solver can converge to the accuracy of higher-order scheme
 - Additional numerical effort is explicit with “old values” and thus much smaller than the full implicit treatment of the higher-order terms
- A factor can be used to produce a mixture of pure low and pure high order. This can be used to remove undesired properties, e.g. oscillations of high-order schemes

$$F_e = \omega F_e^L + (1 - \omega) [F_e^H - F_e^L]^{\text{old}}$$



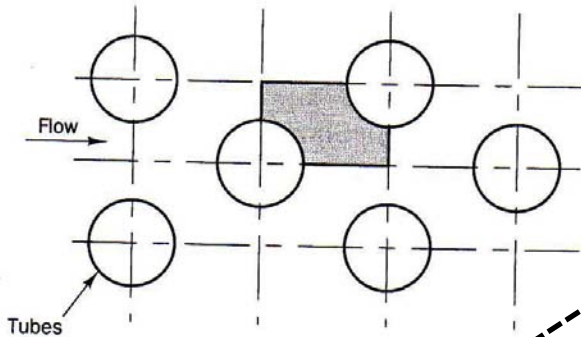
Grid Generation and Complex Geometries: Introduction

- Many flows in engineering and science involve complex geometries
- This requires some modifications of the algorithms:
 - Ultimately, properties of the numerical solver depend on the:
 - Choice of the grid
 - Vector/tensor components (e.g. Cartesian or not)
 - Arrangement of the variables on the grid
- Different types of grids:
 - Structured grids: families of grid lines such that members of the same family do not cross each other and cross each member of other families only once
 - Advantages: simpler to program, neighbor connectivity, resultant algebraic system has a regular structure => efficient solvers
 - Disadvantages: can be used only for simple geometries, difficult to control the distribution of grid points on the domain (e.g. concentrate in specific areas)
 - Three types (names derived from the shape of the grid):
 - H-grid: a grid which can map into a rectangle
 - O-grid: one of the coordinate lines wraps around or is “endless”. One introduces an artificial cut at which the grid numbering jumps
 - C-grid: points on portions of one grid line coincide (used for body with sharp edges)



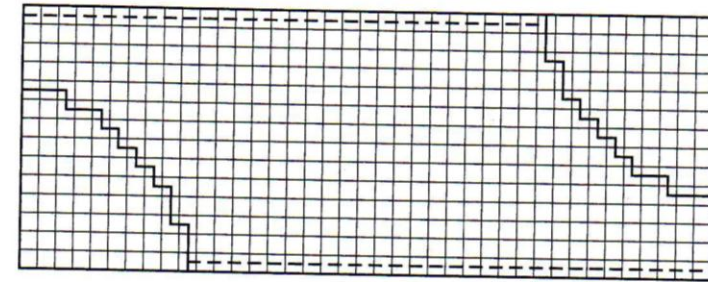
Grid Generation and Complex Geometries: Structured Grids

- Example: create a grid for the flow over a heat exchanger tube bank (only part of it is shown)

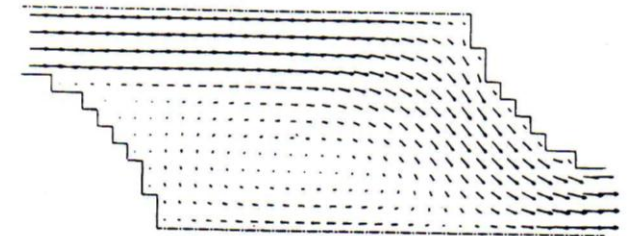


- Stepwise 2D Cartesian grid
 - Number of points non constant or use masks
 - Steps at boundary introduce errors
- vs. non-orthogonal, structured grid

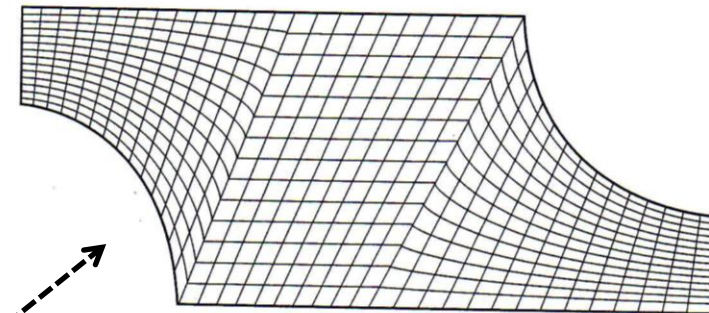
H-Type grids



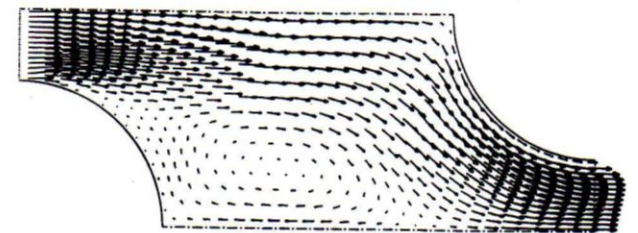
(a)



(b)



(a)



(b)

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Grid Generation and Complex Geometries: Block-Structured Grids

- Grids for which there is one or more level subdivisions of the solution domain
 - Can match at interfaces or not
 - Can overlap or not
- Block structured grids with overlapping blocks are sometimes called “*composite*” or “*Chimera*” grids
 - Interpolation used from one grid to the other
 - Useful for moving bodies (one block attached to it and the other is a stagnant grid)
- Special case: Embedded or Nested grids, which can use different dynamics at different scales

Grid with 3 Blocks, with an O-Type grid (for coordinates around the cylinder)

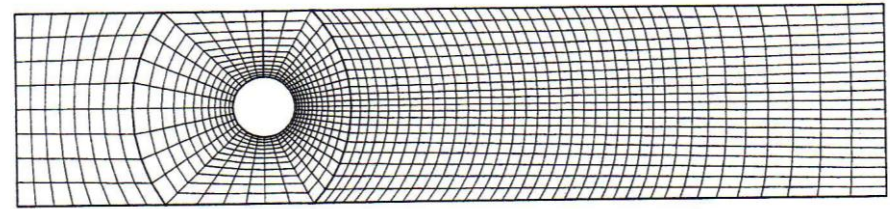


Fig. 2.2. Example of a 2D block-structured grid which matches at interfaces, used to calculate flow around a cylinder in a channel

Grid with 5 blocks, including H-Type and C-Type, and non-matching interface:

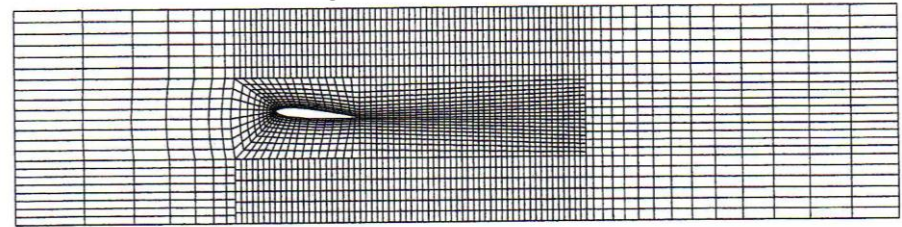


Fig. 2.3. Example of a 2D block-structured grid which does not match at interfaces, designed for calculation of flow around a hydrofoil under a water surface

“composite” or Chimera” Grid

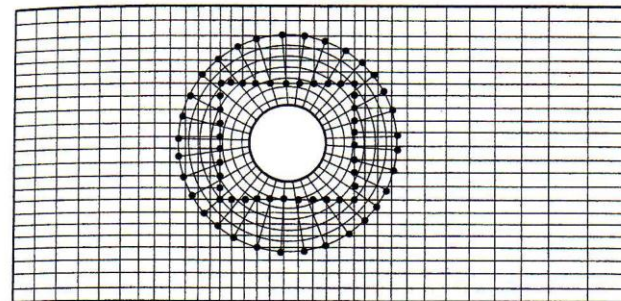


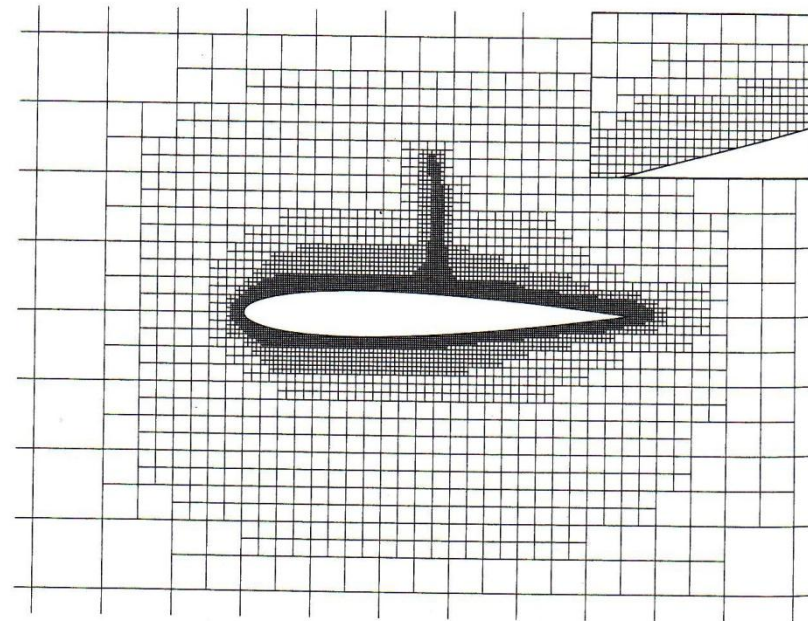
Fig. 2.4. A composite 2D grid, used to calculate flow around a cylinder in a channel

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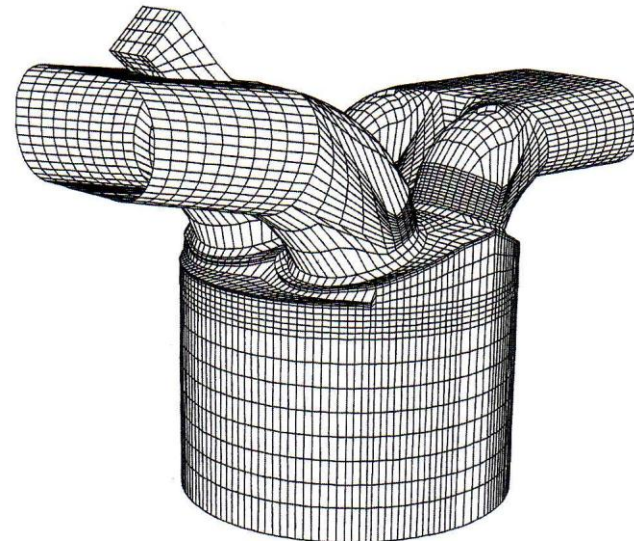
Grid Generation and Complex Geometries:

Other examples of Block-structured Grids



Cartesian grid for NACA 0012 aerofoil. Inset shows cut cells near aerofoil surface. Courtesy of Andreas Haselbacher. Figure 1.7 in "A grid-transparent numerical method for compressible viscous flows on mixed unstructured grids." © Andreas Haselbacher, 1999.

Figure 11.10 Block-structured mesh arrangement for an engine geometry, including inlet and exhaust ports, used in engine simulations with KIVA-3V

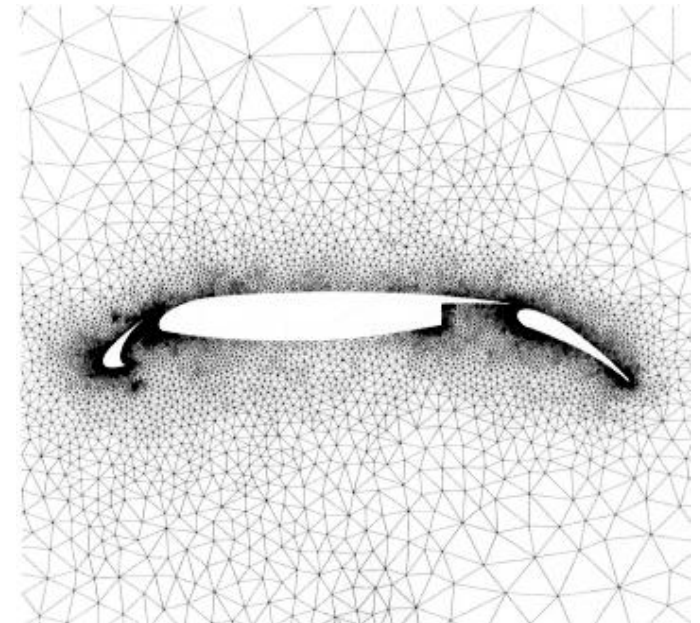


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Grid Generation and Complex Geometries: Unstructured Grids

- For very complex geometries, most flexible grid is one for which one can fit any physical domain: i.e. unstructured
- Can be used with any discretization scheme, but best adapted to FV and FE methods
- Grid most often made of:
 - Triangles or quadrilaterals in 2D
 - Tetrahedra or hexahedra in 3D
- Advantages
 - Unstructured grid can be made orthogonal if needed
 - Aspect ratio easily controlled
 - Grid may be easily refined
- Disadvantages:
 - Irregularity of the data structure: nodes locations and neighbor connections need to be specified explicitly
 - The matrix to be solved is not regular anymore and the size of the band needs to be controlled by node ordering



Triangular grid for three-element airfoil. Courtesy of Andreas Haselbacher. Used with permission. Figure 1.5 in "A grid-transparent numerical method for compressible viscous flows on mixed unstructured grids." © Andreas Haselbacher, 1999.



Unstructured Grids Examples:

Multi-element grids

- For FV methods, what matters is the angle between the vector normal to the cell surface and the line connecting the CV centers \Rightarrow
 - 2D equilateral triangles are equivalent to a 2D orthogonal grid
- Cell topology is important:
 - If cell faces parallel, remember that certain terms in Taylor expansion can cancel \Rightarrow higher accuracy
 - They nearly cancel if topology close to parallel
- Ratio of cells' sizes should be smooth
- Generation of triangles or tetrahedra is easier and can be automated, but lower accuracy
- Hence, more regular grid (prisms, quadrilaterals or hexahedra) often used near boundary where solution often vary rapidly

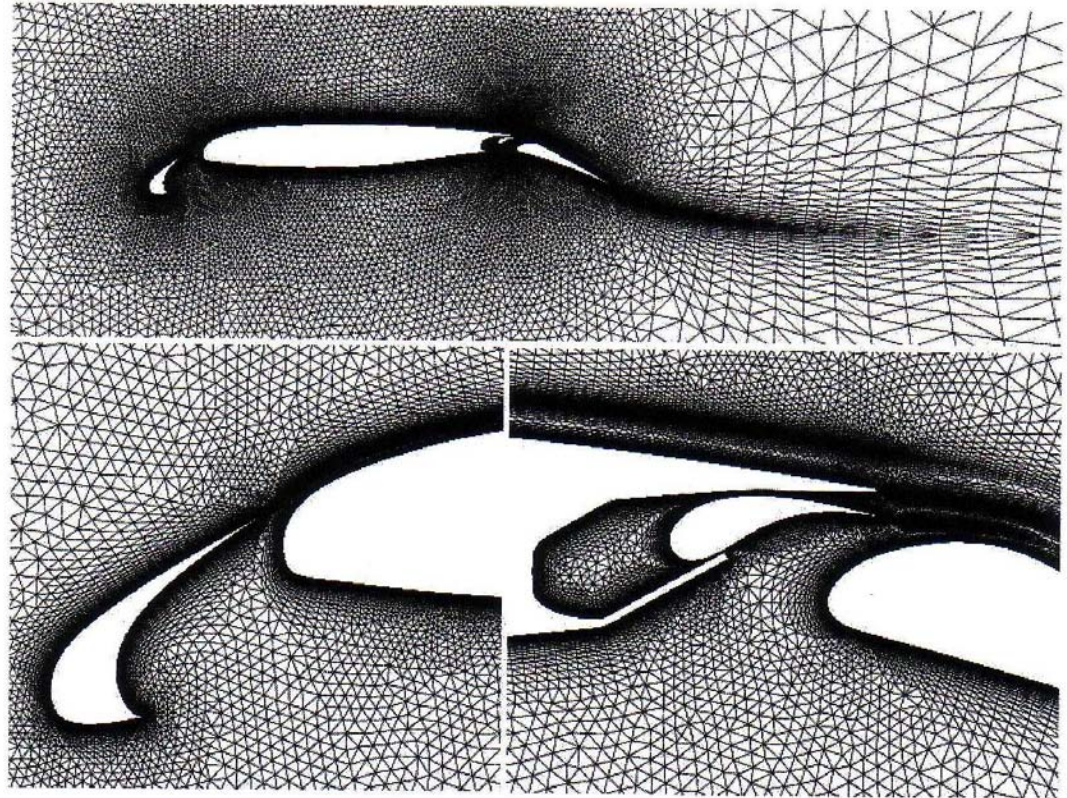


Fig. 9.16. 2D Unstructured grid for Navier–Stokes computations of a multi-element airfoil generated with the hybrid advancing front Delaunay method of Mavriplis [6].

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Complex Geometries: The choice of velocity (vector) components

- Cartesian (used in this course)
 - With FD, one only needs to employ modified equations to take into account of non-orthogonal coordinates (change of derivatives due to change of spatial coordinates from Cartesian to non-orthogonal)
 - In FV methods, normally, no need for coordinate transformations in the PDEs: a local coordinate transformation can be used for the gradients normal to the cell faces
- Grid-oriented:
 - Non-conservative source terms appear in the equations (they account for the re-distribution of momentum between the components)
 - For example, in polar-cylindrical coordinates, in the momentum equations:
 - Apparent centrifugal force and apparent Coriolis force



Complex Geometries: The choice of variable arrangement

- Staggered arrangements

- Improves coupling $u \leftrightarrow p$
- For Cartesian components when grid lines change by 90 degrees, the velocity component stored at the cell face makes no contribution to the mass flux through that face
- Difficult to use Cartesian components in these cases
- Hence, for non-orthogonal grids, grid-oriented velocity components often used

- Collocated arrangements (mostly used here)

- The simplest one: all variables share the same CV
- Requires more interpolation

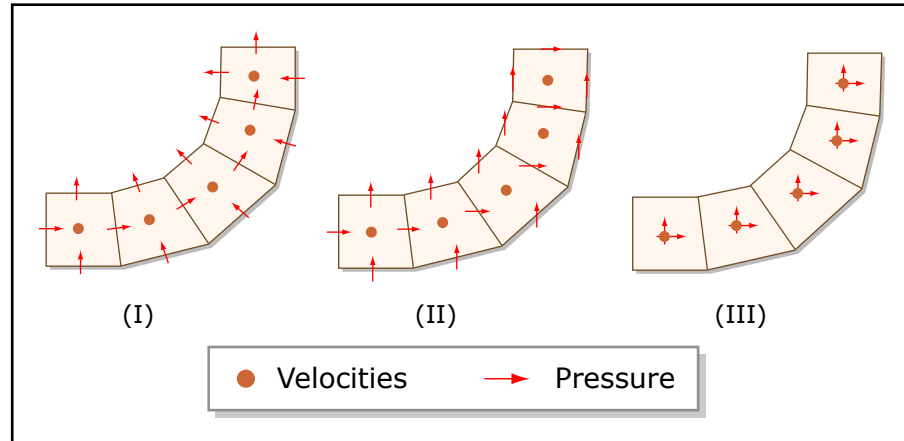


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Variable arrangements on a non-orthogonal grid. Illustrated are a staggered arrangement with (i) contravariant velocity components and (ii) Cartesian velocity components, and (iii) a collocated arrangement with Cartesian velocity components.



Classes of Grid Generation

- An arrangement of discrete set of grid points or cells needs to be generated for the numerical solution of PDEs (fluid conservation equations)
 - Finite volume methods:
 - Can be applied to uniform and non-uniform grids
 - Finite difference methods:
 - Require a coordinate transformation to map the irregular grid in the spatial domain to a regular one in the computational domain
 - Difficult to do this in complex 3D spatial geometries
 - So far, only used with structured grid (could be used with unstructured grids with polynomials ϕ defining the shape of ϕ around a grid point)
- Three major classes of grid generation: i) algebraic methods, ii) differential equation methods and iii) conformal mapping methods
- Grid generation and solving PDE can be independent
 - A numerical (flow) solver can in principle be developed independently of the grid
 - A grid generator then gives the metrics (weights) and the one-to-one correspondence between the spatial-grid and computational-grid

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2.29 Numerical Fluid Mechanics

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