Numerical Methods

Possibilities and Limitations

- Bear in mind that numerical results are always approximate. Errors arise from:
  - The differential equations may contain approximations of idealizations.
    - For many phenomena (e.g., turbulence, combustion, multi-phase, …), the exact equations are not available or numerical solution is not feasible, thus modeling is necessary.
  - Approximations are made in the discretization process.
    - Discretization errors can be reduced by using more accurate interpolation or approximations or by applying the approximations to smaller regions.
  - In solving the discretized equations, iterative methods are used.
    - Errors due to stopping the iteration process too soon need to be taken into account.

Components of Numerical Solution Method

- Mathematical model
  - Sets of partial differential or integro-differential equations and BCs.
  - This model may include simplifications of the exact conservation.
- Discretization method
  - Method of approximating the differential equations by a system of algebraic equations for the variables at some set of discrete locations in space and time.
  - Most important types are FD, FV, and FE.
  - Each type of method yields the same solution if the grid is very fine.

Components – Cont.

- Coordinate and basis vector systems
  - Cartesian, cylindrical, spherical, curvilinear orthogonal or non-orthogonal coordinate systems.
  - Depending on the choice, the velocity vector and stress tensor can be expressed in terms of e.g. Cartesian, covariant or contra-variant, physical or non-physical coordinate-oriented components.

Components – Cont.

- Numerical grid
  - Discrete representation of the geometric domain on which the problem is to be solved, i.e., at which the variables are to be calculated.
  - Structured (regular) grid
    - Consists of families of grid lines with the property that members of a single family do not cross each other and cross each member of other families only once.
    - Simplest grid structure. Logically equivalent to Cartesian grid.
    - Disadvantages
      - Can be used only for geometrically simple solution domains.
      - Difficult to control the distribution of the grid points.
    - H-, O-, or C-types

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Components – Cont.

- Structured (regular) grid

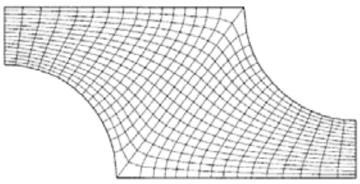

Fig. 2.1. Example of a 2D, structured, non-orthogonal grid, designed for calculation of flow in a symmetry segment of a staggered tube bank

- Block-structured grid
  - Two or more level subdivision of solution domain.

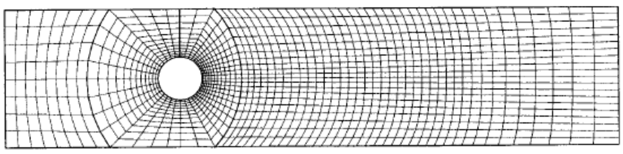

Fig. 2.2. Example of a 2D block-structured grid which matches at interfaces, used to calculate flow around a cylinder in a channel

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Components – Cont.

- Block-structured grid
  - With non-matching interface

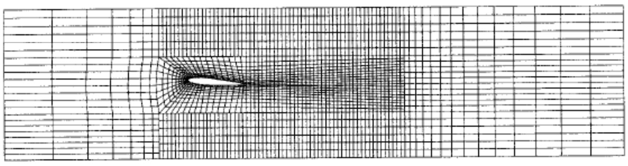

Fig. 2.3. Example of a 2D block-structured grid which does not match at interfaces, designed for calculation of flow around a hydrofoil under a water surface

  - Composite or Chimera grids – with over-lapping blocks

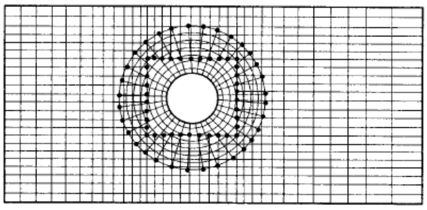

Fig. 2.4. A composite 2D grid, used to calculate flow around a cylinder in a channel

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Components – Cont.

- Unstructured grid
  - The most flexible type
  - Triangles or quadrilaterals in 2D
  - Tetrahedra or hexahedra in 3D

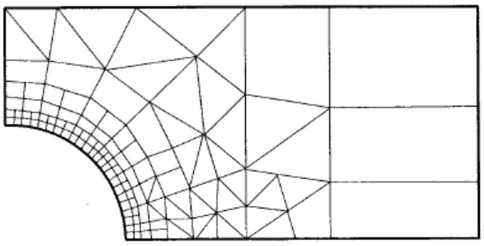

Fig. 2.5. Example of a 2D unstructured grid

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Components – Cont.

- Finite approximations
  - Depending on the grid type, select the approximations to be used in the discretization process.
  - FD – how to approximate the derivatives at grid points
  - FV – how to approximate surface and volume integrals
  - FE – choose the shape functions (elements) and weighting functions
- Solution method
  - Successive linearization of the equations and the resulting linear systems are solved by iterative techniques.

Components – Cont.

- Convergence criteria
  - Two levels of iterations
    - Inner iterations: linear equations are solved
    - Outer iterations: deal with non-linearity and coupling of the equations

Properties of Numerical Solution Methods

- Consistency
  - The discretization should become exact as the grid spacing tends to zero.
  - For a method to be consistent, the truncation error must become zero when the mesh spacing $\Delta t \rightarrow 0$ and/or $\Delta x_i \rightarrow 0$.
  - The difference between the discretized equation and the exact one is called the truncation error.
  - Even if the approximations are consistent, it does not necessarily mean that the solution of the discretized equation system will become the exact solution of the differential equation in the limit of small step size. For this to happen, the solution method has to be stable.

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Properties – Cont.

- Stability
  - A numerical solution method is said to be stable if it does not magnify the errors that appear in the course of numerical solution process.
  - For iterative methods, a stable method is one that does not diverge.
  - The most widely used approach to studying stability of numerical schemes is the von Neumann's method (HW).
  - When solving complicated, non-linear and coupled equations with complicated BCs, there are few stability results so we may have to rely on experience and intuition.

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Properties – Cont.

- Convergence
  - A numerical solution method is said to be convergent if the solution of the discretized equations tend to the exact solution of the differential equation as the grid spacing tends to zero.
  - For linear IVP, the Lax equivalence theorem states that "given a properly posed linear IVP and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence."
  - Convergence is usually checked using numerical experiments, i.e., repeating the calculation on a series of successfully refined grids.

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Properties – Cont.

- Conservation
  - At steady state and in the absence of sources, the amount of a conserved quantity leaving a closed CV is equal to the amount entering that volume.
  - If the strong conservation form of equations and a finite volume method are used, this is guaranteed for each individual CV and for the solution domain as a whole.
  - Non-conservative schemes can produce artificial sources and sinks, changing the balance both locally and globally.

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Properties – Cont.

- Boundedness
  - Numerical solutions should lie within proper bounds.
  - Boundedness is difficult to guarantee. Only some first order schemes guarantee this property.
  - The problem is that schemes prone to producing unbounded solutions may have stability and convergence problems.
- Realizability
  - This is not a numerical issue per se, but models that are not realizable may result in unphysical solutions or cause numerical methods to diverge.

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Properties – Cont.

- Accuracy
  - Numerical solutions always include three kinds of systematic errors:
    - Modeling errors: difference between the actual flow and the exact solution of the mathematical model
      - Depend on the assumptions made in deriving the transport equations for the variables
      - Introduced by simplifying the geometry of the solution domain, by simplifying BCs, etc.

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Properties – Cont.

- Discretization errors: difference between the exact solution of the conservation equations and the exact solution of the algebraic system of equations obtained by discretizing these equations
  - On a given grid, methods of the same order may produce solution errors which differ by as much as an order of magnitude. This is because the order only tells us the rate at which the error decreases as the mesh spacing is reduced.
- Iteration errors: difference between the iterative and exact solutions of the algebraic equations systems

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Discretization Approaches

- Finite difference method
- Finite volume method
- Finite element method

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