REVIEW Lecture 17:

- Stability (Heuristic, Energy and von Neumann)
- Hyperbolic PDEs and Stability, CFL condition, Examples
- **Elliptic PDEs**
  - FD schemes: direct and iterative
  - Iterative schemes, 2D: Laplace, Poisson and Helmholtz equations
  - Boundary conditions, Examples
  - Higher order finite differences
  - Irregular boundaries: Dirichlet and von Neumann BCs
  - Internal boundaries
- **Parabolic PDEs and Stability**
  - Explicit schemes
    - Von Neumann
  - Implicit schemes: simple and Crank-Nicholson
    - Von Neumann
  - Examples
2.29 Numerical Fluid Mechanics
Fall 2011 – Lecture 18

REVIEW Lecture 17, Cont’d:

• Parabolic PDEs and Stability, Cont’d
  – Explicit schemes (1D-space)
    • Von Neumann
  – Implicit schemes (1D-space): simple and Crank-Nicholson
    • Von Neumann
  – Examples
  – Extensions to 2D and 3D
    • Explicit and Implicit schemes
    • Alternating-Direction Implicit (ADI) schemes

Finite Volume Methods

\[ \frac{d}{dt} \int_{CV_{\text{fixed}}} \rho \phi dV + \int_{CS} \rho \phi (\vec{v} \cdot \vec{n}) dA = -\int_{CS} \vec{q} \cdot \vec{n} dA + \sum \int_{CV_{\text{fixed}}} s_{\phi} dV \]

• Integral and conservative forms of the cons. laws
• Introduction

\[ \frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi \vec{v}) = -\nabla \cdot \vec{q} + s_{\phi} \]
TODAY (Lecture 18): FINITE VOLUME METHODS

• Introduction to FV Methods

• Approximations needed and basic elements of a FV scheme
  – FV grids
  – Approximation of surface integrals (leading to symbolic formulas)
  – Approximation of volume integrals (leading to symbolic formulas)

• Summary: Steps to step-up FV scheme

• Examples: One Dimensional examples
  – Generic equations
  – Linear Convection (Sommerfeld eqn.): convective fluxes
    • 2\textsuperscript{nd} order in space, 4\textsuperscript{th} order in space, links to CDS
  – Unsteady Diffusion equation: diffusive fluxes
    • Two approaches for 2\textsuperscript{nd} order in space, links to CDS
References and Reading Assignments


FINITE VOLUME METHODS: Introduction

• Finite Difference Methods are based on a discretization of the differential form of the conservation equations.

• Finite Volume Methods are based on a discretization of the integral forms of the conservation equations:

\[
\frac{d}{dt} \int_{CV} \rho \phi dV + \int_{CS} \rho \phi (\vec{v} \cdot \vec{n}) dA = \int_{CS} -q_{\phi} \cdot \vec{n} \ dA + \sum \int_{CV} s_{\phi} \ dV
\]

Advective (convective) fluxes Other transports (diffusion, etc) Sum of sources and sinks terms (reactions, etc)

• Basic ideas/steps to set-up a FV scheme:
  – Grid generation (CVs):
    • Divide the simulation domain into a set of discrete control volumes (CVs)
    • For maintenance of conservation, important that CVs don’t overlap
  – Discretize the integral/conservation equation on CVs:
    • Satisfy the integral form of the conservation law to some degree of approximation for each of the many contiguous control volumes
  – Solve the resultant discrete integral/flux equations
FV METHODS: Introduction

• FV approach has two main advantages:
  – Ensures that the discretization is conservative, locally and globally
    • Mass, Momentum and Energy are conserved in a discrete sense
    • In general, if discrete equations are summed over all CVs, the global conservation equation are retrieved (surface integrals cancel out)
    • These local/global conservations can be obtained from a Finite Difference (FD) formulation, but they are natural/direct for a FV formulation
  – Does not require a coordinate transformation to be applied to irregular meshes
    • Can be applied to unstructured meshes (arbitrary polyhedra in 3D or polygons in 2D)

• In our examples, we will work with

\[
\frac{d}{dt} \int_{V(t)} \rho \phi dV + \int_{S(t)} \rho \phi \cdot (\vec{v} \cdot \vec{n}) dA = -\int_{S(t)} \vec{q}_\phi \cdot \vec{n} dA + \int_{V(t)} s_\phi dV
\]

where \( V(t) \) is any discrete control volume. We will assume for now that they don’t vary in time: \( V(t) = V \)
FV METHODS
Several Approximations Needed

• To integrate discrete CV equation:

\[
\frac{d}{dt} \int_V \rho \phi dV + \int_S \rho \phi (\vec{v}.\vec{n}) dA = -\int_S q_\phi \vec{n} dA + \int_V S_\phi dV
\]

– A “time-marching method” needs to be used to integrate \( \Phi = \int_V \rho \phi dV \) to the next time step(s)

\[
\frac{d}{dt} \int_V \rho \phi dV = \frac{d\Phi}{dt}
\]

– Total flux estimate \( F_\phi \) required at the boundary of each CV

\[
\int_S F_\phi \vec{n} dA = \int_S \rho \phi (\vec{v}.\vec{n}) dA + \int_S q_\phi \vec{n} dA
\]

  e.g. \( F_\phi = \) advection + diffusion fluxes

– Total source term (sum of sources) must be integrated over each CV

\[
S_\phi = \int_V s_\phi dV
\]

• Hence cons. eqn. becomes:

\[
\frac{d\Phi}{dt} + \int_S F_\phi \vec{n} dA = S_\phi
\]

• These needs lead to basic elements of a FV scheme, but we need to relate \( \Phi \) and \( \phi \)
FV METHODS
Several Approximations Needed, Cont’d

• “Time-marching method” for CV equation: \[ \frac{d\Phi}{dt} + \int_s \overrightarrow{F}_\phi \cdot \vec{n} \, dA = S_\phi \]
  – The average of \( \phi \) over a CV cell, \( \bar{\Phi} = \frac{1}{V} \int_v \rho \phi dV \), satisfies

\[ V \frac{d\bar{\Phi}}{dt} + \int_s \overrightarrow{F}_\phi \cdot \vec{n} \, dA = S_\phi \]

(since \( \frac{d}{dt} \int_v \rho \phi dV = \frac{d}{dt} (\frac{1}{V} \int_v \rho \phi dV) \))

for \( V \) fixed in time.

– Hence, after discrete time-integration, we would have updated the cell-averaged quantities \( \bar{\Phi} \)

• For the total flux estimate \( F_\phi \) at CV boundary: “Reconstruction” of \( \phi \) from \( \bar{\Phi} \)
  – Fluxes are functions of \( \phi \) => to evaluate them, we need to represent \( \phi \) within the cell
  – This can be done by a piece-wise approximation which, when averaged over the CV, gives back \( \bar{\Phi} \)
  – But, each cell has a different piece-wise approximation => fluxes at boundaries can be discontinuous. Two example of remedies:
    • Take the average of these fluxes (this is a non-dissipative scheme, analogous to central differences)
    • Flux-difference splitting
FV METHODS
Basic Elements of FV Scheme

1. Given $\Phi$ for each CV, construct an approximation to $\phi(x, y, z)$ in each CV and evaluate fluxes $F_\phi$
   - Find $\phi$ at the boundary using this approximation, evaluate fluxes $F_\phi$
   - This generally leads to two distinct values of the flux for each boundary

2. Apply some strategy to resolve the flux discontinuity at the CV boundary to produce a single $F_\phi$ over the whole boundary

3. Integrate the flux $F_\phi$ to obtain $\int_S F_\phi \cdot \vec{n} \, dA$ : Surface Integrals

4. Compute $S_\phi$ by integration over each CV: Volume Integrals

5. Advance the solution in time to obtain the new values of $\Phi$

$$V \frac{d\Phi}{dt} + \int_S F_\phi \cdot \vec{n} \, dA = S_\phi$$

Time-Marching
Different Types of FV Grids

- Usual approach (used here):
  - Define CVs by a suitable grid
  - Assign computational node to CV center
  - Advantages: nodal values will represent the mean over the CV at high(er) accuracy (second order) since node is centroid of CV

- Other approach:
  - Define nodal locations first
  - Construct CVs around them (so that CV faces lie midway between nodes
  - Advantage: CDS approximations of derivatives (fluxes) at boundaries are more accurate (faces are midway between two nodes)
Different Types of FV Grids, Cont’d

- Other specialized variants
  - Cell centered vs. Cell vertex

- Structured:
  - All mesh points lie on intersection two/three lines

- vs. Unstructured:
  - Meshes formed of triangular or quadrilateral cells in 2D, or tetrahedra or pyramids in 3D
  - Cells are identified by their numbers (can not be identified by coordinate lines, e.g. \(i,j\))

- Remarks
  - Discretization principles the same for all grid variants
    - => For now, we work with (a): Cell centered (\(i,j\) is the center of the cell, similar to FD)
    - In 3D, a cell has a finite volume (but if unit distance perpendicular to plane is assumed, it behaves as 2D)
  - What changes are the relations between various locations on the grid and accuracies
Approximation of Surface Integrals

• Typical (cell centered) 2D and 3D Cartesian CV (see conventions on 2 figs)

• Total/Net flux through CV boundary
  – Is sum of integrals over four (2D) or six (3D) faces:
  \[ \int_S \vec{F}_\phi \cdot \vec{n} \, dA = \sum_k \int_{S_k} f_\phi \, dA \]
  – For now, we will consider a single typical CV surface, the one labeled ‘e’

• To compute surface integral, \( \phi \) is needed everywhere on surface, but \( \overline{\Phi} \) only known at nodal (CV center) values \( \Rightarrow \) two successive approximations needed:
  – Integral estimated based on values at one or more locations on the cell face
  – These cell faces values approximated in terms of nodal values
1D surfaces (2D CV)

- Goal: estimate \( F_e = \int_{S_e} f \phi \, dA \)
- Simplest approximation: 
  midpoint rule (2\textsuperscript{nd} order)

  - \( F_e \) is approximated as a product of the integrand at cell-face center (itself approximation of mean value over surface) and the cell-face area

\[
F_e = \int_{S_e} f \phi \, dA = \overline{f_e} S_e = f_e S_e + O(\Delta y^2) \approx f_e S_e
\]

  - Since \( f_e \) is not available, it has to be obtained by interpolation
    - Has to be computed with 2\textsuperscript{nd} order accuracy to preserve accuracy of midpoint rule
Approximation of Surface Integrals, Cont’d

- Goal: estimate \( F_e = \int_{S_e} f_\phi \, dA \)

- Another 2^{nd} order approximation:
  
  **Trapezoid rule**
  
  - \( F_e \) is approximated as:
    \[
    F_e = \int_{S_e} f_\phi \, dA \approx S_e \frac{f_{ne} + f_{se}}{2} + O(\Delta y^2)
    \]
    
    - In this case, it is the fluxes at the corners \( f_{ne} \) and \( f_{se} \) that need to be obtained by interpolation
      
      - Have to be computed with 2^{nd} order accuracy to preserve accuracy

- Higher-order approximation of surface integrals require more than 2 locations
  
  - Simpson’s rule (4^{th} order approximation):
    \[
    F_e = \int_{S_e} f_\phi \, dA \approx S_e \frac{f_{ne} + 4f_e + f_{se}}{6} + O(\Delta y^4)
    \]
    
    - Values needed at 3 locations
    
    - To keep accuracy of integral: e.g. use cubic polynomials to estimate these values from \( \Phi_p \)’s nearby

Notation used for a Cartesian 2D and 3D grid. Image by MIT OpenCourseWare.
Approximation of Surface Integrals, Cont’d

2D surface (for 3D problems)

• Goal: estimate \( F_e = \int_{S_e} f \phi \, dA \) for 3D CV

• Simplest approximation: still the midpoint rule (2\(^{nd}\) order)
  – \( F_e \) is approximated as:

\[
F_e = \int_{S_e} f \phi \, dA \approx S_e f_e + O(\Delta y^2, \Delta z^2)
\]

• Higher-order approximation (require values elsewhere e.g. at vertices) possible but more complicated to implement for 3D CV

• Integration easy if variation of \( f_e \) over 2D surface is assumed to have specific easy shape to integrate, e.g. 2D polynomial interpolation, then integration
Approximation of VOLUME Integrals

• Goal: estimate

\[ S_\phi = \int_V s_\phi \, dV \]

\[ \overline{\Phi} = \frac{1}{V} \int_V \rho \phi \, dV \]

• Simplest approximation: product of CV volume with the mean value of the integrand (approximated by the value at the center of the node \( P \))
  
  – \( S_\phi \) approximated as:

\[ S_\phi = \int_V s_\phi \, dV = \overline{s_\phi} \, V \approx s_\phi \, V \]

• Exact if \( s_\phi \) is constant or linear within CV

• 2\textsuperscript{nd} order accurate otherwise

• Higher order approximation require more locations than just the center
Approximation of VOLUME Integrals

- Goal: estimate \( S_\phi = \int_V s_\phi \, dV \)

\[ \Phi = \frac{1}{V} \int_V \rho \phi \, dV \]

- Higher order approximations:
  - Requires \( \Phi \) values at other locations than
  - Obtained either by interpolating nodal values or by using shape functions/polynomials

- Consider 2D case (volume integral is a surface integral) using shape functions
  - Bi-quadratic shape function leads to a 4\(^{th}\) order approximation (9 coefficients)
    \[ s(x, y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2 + a_5 xy + a_6 x^2 y + a_7 xy^2 + a_8 x^2 y^2 \]
  - 9 coefficients obtained by fitting \( s(x,y) \) to 9 node locations (center, corners, middles)
  - For Cartesian grid, this gives:
    \[ S_p = \int_V s_\phi \, dV = \Delta x \Delta y \left[ a_0 + \frac{a_3}{12} \Delta x^2 + \frac{a_4}{12} \Delta y^2 + \frac{a_8}{144} \Delta x^2 \Delta y^2 \right] \]

Only four coefficients (linear dependences cancel), but they still depend on the 9 nodal values.
Approximation of VOLUME Integrals, Cont’d
2D and 3D

• 2D case example, Cont’d
  – For a uniform Cartesian grid, one obtains the 2D integral as a function of the 9 nodal values:

\[
S_p = \int_V s_\phi \, dV = \frac{\Delta x \Delta y}{36} \left[ 16s_p + 4s_s + 4s_n + 4s_w + 4s_e + s_{se} + s_{sw} + s_{ne} + s_{nw} \right]
\]

  – Since only value at node P is available, one must interpolate to obtain values at surface locations
  – Has to be at least 4\textsuperscript{th} order accurate interpolation to retain order of integral approximation

• 3D case:
  – Techniques are similar to 2D case: above 4\textsuperscript{th} order approx directly extended
  – For Higher Order
    • Integral approximation formulas are more complex
    • Interpolation of node values are more complex
Approx. of Surface/Volume Integrals:
Classic symbolic formulas

• Surface Integrals \[ F_e = \int_{S_e} f_\phi \, dA \]

– 2D problems (1D surface integrals)
  • Midpoint rule (2nd order): \[ F_e = \int_{S_e} f_\phi \, dA = \bar{f}_e S_e = f_e S_e + O(\Delta y^2) \approx f_e S_e \]
  • Trapezoid rule (2nd order): \[ F_e = \int_{S_e} f_\phi \, dA \approx S_e \frac{(f_{ne} + f_{se})}{2} + O(\Delta y^2) \]
  • Simpson’s rule (4th order): \[ F_e = \int_{S_e} f_\phi \, dA \approx S_e \frac{(f_{ne} + 4f_e + f_{se})}{6} + O(\Delta y^4) \]

– 3D problems (2D surface integrals)
  • Midpoint rule (2nd order): \[ F_e = \int_{S_e} f_\phi \, dA \approx S_e f_e + O(\Delta y^2, \Delta z^2) \]
  • Higher order more complicated to implement in 3D

• Volume Integrals: \[ S_\phi = \int_V s_\phi \, dV, \quad \Phi = \frac{1}{V} \int_V \rho \phi dV \]

– 2D/3D problems, Midpoint rule (2nd order): \[ S_p = \int_V s_\phi \, dV = \bar{s}_p V \approx s_p V \]

– 2D, bi-quadratic (4th order, Cartesian): \[ S_p = \frac{\Delta y}{36} \left[ 16 s_p + 4 s_s + 4 s_a + 4 s_w + 4 s_e + s_{se} + s_{sw} + s_{ne} + s_{nw} \right] \]
Summary: 3 basic steps to set-up a FV scheme

• Grid generation ("create CVs")

• Discretize integral/conservation equation on CVs
  
  – This integral eqn. is:  \( \frac{d\Phi}{dt} + \int_S \overline{F}_\phi \cdot \vec{n} \, dA = S_\phi \)
  
  – Which becomes for \( V \) fixed in time:  \( V \frac{d\overline{\Phi}}{dt} + \int_S \overline{F}_\phi \cdot \vec{n} \, dA = S_\phi \)
  
  where  \( \overline{\Phi} = \frac{1}{V} \int_V \rho \phi dV \) and  \( S_\phi = \int_V s_\phi \, dV \)
  
  – This implies:
    
    • The discrete state variables are the averaged values over each cell (CV):  \( \overline{\Phi}_p \)'s
    
    • Need rules to compute surface/volume integrals as a function of \( \phi \) within CV
      
      • Evaluate integrals as a function of \( \phi_e \) values at points on and near CV.
      
      • Need to interpolate to obtain these \( \phi_e \) values on and near CV from averaged  \( \overline{\Phi}_p \)'s of nearby CVs
    
    • Other approach: impose piece-wise function \( \phi \) within CV, ensures that it satisfies  \( \overline{\Phi}_p \)'s constraints, then evaluate integrals (surface and volume)
    
    • Select scheme to resolve/address discontinuities

• Solve resultant discrete integral/flux eqns: (Linear) algebraic system for  \( \overline{\Phi}_p \)'s
One-Dimensional Examples: Generic 1D FV

• Grid generation (fixed CVs)
  – Consider equispaced grid: \( x_j = j\Delta x \)
  – Control volume \( j \) extends from \( x_{j-1/2} \) to \( x_{j+1/2} \)
  – Boundary values are: \( \phi_{j\pm1/2} = \phi(x_{j\pm1/2}) \)
  – Boundary total fluxes (convective+diffusive) are: \( f_{j\pm1/2} = f(\phi_{j\pm1/2}) \)
  – Average cell and source values:
    \[
    \bar{\Phi}_j(t) = \frac{1}{V} \int_V \rho \phi \, dV = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \phi(x,t) \, dx
    \]
    \[
    S_j(t) = \int_V s_{\phi_j} \, dV = \int_{x_{j-1/2}}^{x_{j+1/2}} s_{\phi}(x,t) \, dx
    \]

• Discretize generic integral/conservation equation on CVs
  – The integral form \( V \frac{d\bar{\Phi}}{dt} + \int_S \bar{F}_\phi \bar{n} \, dA = S_\phi \) becomes:
    \[
    \frac{d}{dt} \left( \Delta x \, \bar{\Phi}_j \right) + f_{j+1/2} - f_{j-1/2} = \int_{x_{j-1/2}}^{x_{j+1/2}} s_{\phi}(x,t) \, dx
    \]
One-Dimensional Examples, Cont’d

Note: Cell-average vs. Center value

• With $\xi = x - x_j$ and a Taylor series expansion

$$
\Phi_j(t) = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \phi(x,t)dx
= \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \left[ \phi_j + \xi \frac{\partial \phi}{\partial x} \bigg|_j + \frac{\xi^2}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_j + R_2 \right] d\xi
= \phi_j + \frac{\Delta x^2}{24} \frac{\partial^2 \phi}{\partial x^2} \bigg|_j + O(\Delta x^4)
$$

$\Rightarrow \quad \Phi_j(t) = \phi_j + O(\Delta x^2)$

• Thus: cell-average value and center value differ only by second order term
One-Dimensional Example I

Linear Convection (Sommerfeld) Eqn:

\[ \frac{\partial \phi(x,t)}{\partial t} + c \frac{\partial \phi(x,t)}{\partial x} = 0 \]

- With convection only, our generic 1D eqn.

\[ \frac{d(\Delta x \Phi_j)}{dt} + f_{j+1/2} - f_{j-1/2} = \int_{x_{j-1/2}}^{x_{j+1/2}} s_\phi(x,t) \, dx \]

becomes:

\[ \frac{d(\Delta x \Phi_j)}{dt} + f_{j+1/2} - f_{j-1/2} = 0 \]

- Compute surface/volume integrals as a function of \( \phi \) within CV
  - Here impose/choose first piecewise-constant approximation to \( \phi(x) \):
    \[ \phi(x) = \Phi_j \quad \forall \ x_{j-1/2} \leq x \leq x_{j+1/2} \]
  - This gives simple flux terms. The only issue is that they differ depending on the cell from which the flux is computed:
    \[ f_{j+1/2}^L = f(\Phi_{j+1/2}^L) = c\Phi_j \]
    \[ f_{j+1/2}^R = f(\Phi_{j+1/2}^R) = c\Phi_{j+1} \]
    \[ f_{j-1/2}^L = f(\Phi_{j-1/2}^L) = c\Phi_{j-1} \]
    \[ f_{j-1/2}^R = f(\Phi_{j-1/2}^R) = c\Phi_j \]
One-Dimensional Example I
Linear Convection (Sommerfeld) Eqn, Cont’d

• Now, we have obtained the fluxes at the CV boundaries in terms of the CV-averaged values

• We need to resolve the flux discontinuity ⇒ average values of the fluxes on either side, leading the (2nd order) estimates:

\[ \hat{f}_{j-1/2} = \frac{f_{j-1/2}^L + f_{j-1/2}^R}{2} = \frac{c\phi_{j-1} + c\phi_j}{2} \]

\[ \hat{f}_{j+1/2} = \frac{f_{j+1/2}^L + f_{j+1/2}^R}{2} = \frac{c\phi_j + c\phi_{j+1}}{2} \]

• Substitute into integral equation

\[ \frac{d}{dt}(\Delta x \bar{\phi}_j) + f_{j+1/2} - f_{j-1/2} \approx \frac{d}{dt}(\Delta x \bar{\phi}_j) + \hat{f}_{j+1/2} - \hat{f}_{j-1/2} = \frac{d}{dt}(\Delta x \bar{\phi}_j) + \frac{c\phi_j + c\phi_{j+1} - c\phi_{j-1} + c\phi_j}{2} \]

\[ \Rightarrow \Delta x \frac{d\phi_j}{dt} + \frac{c\phi_{j+1} - c\phi_{j-1}}{2} = 0 \]

• With periodic BCs, storing all cell-averaged values into a vector \( \bar{\Phi} \)

\[ d \frac{\bar{\Phi}}{dt} + \frac{c}{2\Delta x} B_p(-1,0,1)\bar{\Phi} = 0 \]

(where \( B_p \) is a circulant tri-diagonal matrix, P for periodic)
• The resultant linear algebraic system is circulant tri-diagonal (for periodic BCs)

\[ \frac{d}{dt} \Phi + \frac{c}{2\Delta x} B_\rho((-1,0,1))\Phi = 0 \]

• This is as the 2\textsuperscript{nd} order CDS!, except that it is written in terms of cell averaged values instead of center values
  – It is also 2\textsuperscript{nd} order in space
  – Has same properties as classic CDS:
    • Non-dissipative (check Fourier analysis or eigenvalues of \( B_\rho \), which are imaginary), but can provide oscillatory errors
    • Stability (recall tables for FD schemes, linear convection eqn.) of time-marching
      – If centered in time, centered in space, explicit: stable with CFL condition: \( \frac{c \Delta t}{\Delta x} \leq 1 \)
      – If implicit in time: unconditionally stable for all \( \Delta t, \Delta x \)
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