2.29 Numerical Fluid Mechanics
Fall 2011 – Lecture 19

REVIEW Lecture 18:

- Finite Volume Methods
  - Integral and conservative forms of the cons. laws
  - Introduction
  - Approximations needed and basic elements of a FV scheme
    - Time-Marching and Grid generation
    - FV grids: Cell centered (Nodes or CV-faces) vs. Cell vertex; Structured vs. Unstructured
    - Approximation of surface integrals (leading to symbolic formulas)
    - Approximation of volume integrals (leading to symbolic formulas)
    - Summary: Steps to step-up a FV scheme
  - One Dimensional examples
    - Generic equation: $\frac{d\left(\Delta x\,\bar{\Phi}_j\right)}{dt} + f_{j+1/2} - f_{j-1/2} = \int_{x_{j-1/2}}^{x_{j+1/2}} s_\phi(x,t)\,dx$
    - Linear Convection (Sommerfeld eqn): convective fluxes
      - 2^{nd} order in space

Summary: 3 basic steps to set-up a FV scheme

- Grid generation (CVs)
- Discretize integral/conservation equation on CVs
  - This integral is: $\frac{d\Phi}{dt} + \int_S \vec{F}_\phi . \vec{n}\, dA = S_\phi$
  - Which becomes for V fixed in time: $V\frac{d\bar{\Phi}}{dt} + \int_S \vec{F}_\phi . \vec{n}\, dA = S_\phi$

    where $\bar{\Phi} = \frac{1}{V}\int_V \rho\phi dV$ and $S_\phi = \int_{V(t)} s_\phi \, dV$
  - This implies:
    - The discrete state variables are the averaged values over each cell (CV): $\bar{\Phi}_P$'s
    - Need rules to compute surface/volume integrals as a function of ϕ within CV
      - Evaluate integrals as a function of ϕ_e values at points on and near CV.
      - Need to interpolate to obtain these ϕ_e values on and near CV from averaged $\bar{\Phi}_P$'s of nearby CVs
    - Other approach: impose piece-wise function ϕ within CV, ensures that it satisfies $\bar{\Phi}_P$'s constraints, then evaluate integrals (surface and volume)
    - Select scheme to resolve/address discontinuities
- Solve resultant discrete integral/flux eqns: (Linear) algebraic system for $\bar{\Phi}_P$'s

FV METHODS
Basic Elements of FV Scheme

1. Given $\bar{\Phi}$ for each CV, construct an approximation to $\phi(x, y, z)$ in each CV and evaluate fluxes F_ϕ
   - Find ϕ at the boundary using this approximation, evaluate fluxes F_ϕ
   - 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_ϕ over the whole boundary
3. Integrate the flux F_ϕ to obtain $\int_S \vec{F}_\phi . \vec{n}\, dA$: Surface Integrals
4. Compute S_ϕ by integration over each CV: Volume Integrals
5. Advance the solution in time to obtain the new values of $\bar{\Phi}$

$$V \frac{d\bar{\Phi}}{dt} + \int_S \vec{F}_\phi . \vec{n}\, dA = S_\phi$$

Time-Marching

TODAY (Lecture 19): FINITE VOLUME METHODS

- Summary: Steps to step-up a FV scheme
- Examples: One Dimensional examples
  - Generic equations
  - Linear Convection (Sommerfeld eqn): convective fluxes
    - 2^{nd} order in space, 4^{th} order in space, links to CDS
  - Unsteady Diffusion equation: diffusive fluxes
    - Two approaches for 2^{nd} order in space, links to CDS
- Approximation of surface integrals and volume integrals revisited
- Interpolations and differentiations
  - Upwind interpolation (UDS)
  - Linear Interpolation (CDS)
  - Quadratic Upwind interpolation (QUICK)
  - Higher order (interpolation) schemes
- Time-Marching Methods: Euler's methods

References and Reading Assignments

- Chapter 29.4 on “The control-Volume approach for Elliptic equations” of “Chapra and Canale, Numerical Methods for Engineers, 2010/2006.”
- Chapter 4 on “Finite Volume Methods” of “J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd edition, 2002”
- Chapter 5 on “Finite Volume Methods” of “H. Lomax, T. H. Pulliam, D.W. Zingg, *Fundamentals of Computational Fluid Dynamics (Scientific Computation).* Springer, 2003”
- Chapter 5.6 on “Finite-Volume Methods” of T. Cebeci, J. P. Shao, F. Kafyeke and E. Laurendeau, Computational Fluid Dynamics for Engineers. Springer, 2005.

One-Dimensional Example II
Linear Convection (Sommerfeld) Eqn: **4^{th} order approx.**

- 1D exact integral equation still

$$\frac{d\left(\Delta x\,\bar{\Phi}_j\right)}{dt} + f_{j+1/2} - f_{j-1/2} = 0$$

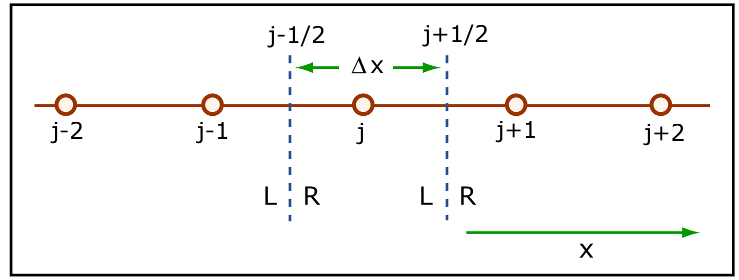


Image by MIT OpenCourseWare.

- Use 4^{th} order accurate surface/volume integrals
  - Replace piecewise-constant approx. to $\phi(x)$ with piece-wise quadratic approx ($\xi = x - x_j$): $\phi(\xi) = a\xi^2 + b\xi + c$
  - Satisfy $\bar{\Phi}_P$'s (average) constraints, i.e. choose a, b, c so that:

$$\frac{1}{\Delta x}\int_{-3\Delta x/2}^{-\Delta x/2} \phi(\xi)\, d\xi = \bar{\phi}_{j-1}\,, \quad \frac{1}{\Delta x}\int_{-\Delta x/2}^{+\Delta x/2} \phi(\xi)\, d\xi = \bar{\phi}_j\,, \quad \frac{1}{\Delta x}\int_{\Delta x/2}^{3\Delta x/2} \phi(\xi)\, d\xi = \bar{\phi}_{j+1}$$

  - This gives:

$$a = \frac{\bar{\phi}_{j+1} - 2\bar{\phi}_j + \bar{\phi}_{j-1}}{2\Delta x^2}, \quad b = \frac{\bar{\phi}_{j+1} - \bar{\phi}_{j-1}}{2\Delta x}, \quad c = \frac{-\bar{\phi}_{j-1} + 26\bar{\phi}_j - \bar{\phi}_{j+1}}{24}$$

  - We still need to evaluate the values of $\phi(x)$ at the boundaries so as to compute the advective fluxes at these boundaries: $f^L_{j-1/2}\,,\ f^R_{j-1/2},\ f^L_{j+1/2}\,,\ f^R_{j+1/2}$

One-Dimensional Example II
Linear Convection (Sommerfeld) Eqn: 4th order approx.

- Since $f = c\phi \Rightarrow$ compute ϕ at surfaces:

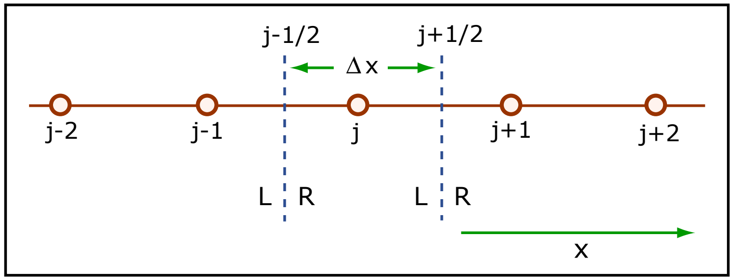


Image by MIT OpenCourseWare.

$$\phi^L_{j-1/2} = \frac{2\bar{\phi}_j + 5\bar{\phi}_{j-1} - \bar{\phi}_{j-2}}{6}, \quad \phi^L_{j+1/2} = \frac{2\bar{\phi}_{j+1} + 5\bar{\phi}_j - \bar{\phi}_{j-1}}{6},$$

$$\phi^R_{j-1/2} = \frac{-\bar{\phi}_{j+1} + 5\bar{\phi}_j + 2\bar{\phi}_{j-1}}{6}, \quad \phi^R_{j+1/2} = \frac{-\bar{\phi}_{j+2} + 5\bar{\phi}_{j+1} + 2\bar{\phi}_j}{6}$$

- Resolve flux discontinuity $\Rightarrow$ again, use average values

$$\hat{f}_{j-1/2} = \frac{f^L_{j-1/2} + f^R_{j-1/2}}{2} = \frac{c\phi^L_{j-1/2} + c\phi^R_{j-1/2}}{2} \qquad \hat{f}_{j+1/2} = \frac{f^L_{j+1/2} + f^R_{j+1/2}}{2} = \frac{c\phi^L_{j+1/2} + c\phi^R_{j+1/2}}{2}$$

$$\Rightarrow \hat{f}_{j-1/2} = c\frac{-\bar{\phi}_{j+1} + 7\bar{\phi}_j + 7\bar{\phi}_{j-1} - \bar{\phi}_{j-2}}{12} \qquad \Rightarrow \hat{f}_{j+1/2} = c\frac{-\bar{\phi}_{j+2} + 7\bar{\phi}_{j+1} + 7\bar{\phi}_j - \bar{\phi}_{j-1}}{12}$$

- Done with integrals $\Rightarrow$ we can substitute in 1D conv. eqn:

$$\frac{d\left(\Delta x\, \bar{\Phi}_j\right)}{dt} + f_{j+1/2} - f_{j-1/2} \approx \frac{d\left(\Delta x\, \bar{\phi}_j\right)}{dt} + \hat{f}_{j+1/2} - \hat{f}_{j-1/2} \quad \Rightarrow \quad \Delta x \frac{d\bar{\phi}_j}{dt} + c\frac{-\bar{\phi}_{j+2} + 8\bar{\phi}_{j+1} - 8\bar{\phi}_{j-1} + \bar{\phi}_{j-2}}{12} = 0$$

- For periodic domains: $\frac{d\,\bar{\mathbf{\Phi}}}{dt} + \frac{c}{2\Delta x}\mathbf{B}_P(-1,-8,0,8,1)\,\bar{\mathbf{\Phi}} = 0$

(from Lecture 12)

Centered Differences

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

One-Dimensional Example III
2nd order approx. of diffusion equation:

$$\frac{\partial \phi(x,t)}{\partial t} = \nu \frac{\partial^2 \phi(x,t)}{\partial x^2}$$

- 1D exact integral equation same form!

$$\frac{d\left(\Delta x\, \bar{\Phi}_j\right)}{dt} + f_{j+1/2} - f_{j-1/2} = 0$$

but with: $f = -\nu \nabla \phi = -\nu \frac{\partial \phi}{\partial x}$

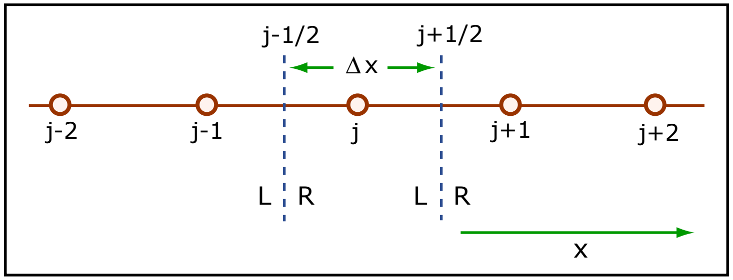


Image by MIT OpenCourseWare.

- Approximation of surface (flux) integral: Approach 1
  - Direct: we know that to second-order (since $\bar{\phi}_j = \phi_j + O(\Delta x^2)$ and CDS)

$$f_{j+1/2} = -\nu \left.\frac{\partial \phi}{\partial x}\right|_{j+1/2} = -\nu \frac{\bar{\phi}_{j+1} - \bar{\phi}_j}{\Delta x} + O(\Delta x^2) \quad \Rightarrow \quad \hat{f}_{j+1/2} = -\nu \frac{\bar{\phi}_{j+1} - \bar{\phi}_j}{\Delta x} \text{ and } \hat{f}_{j-1/2} = -\nu \frac{\bar{\phi}_j - \bar{\phi}_{j-1}}{\Delta x}$$

  - Substitute into integral equation:

$$\frac{d\left(\Delta x\, \bar{\phi}_j\right)}{dt} + \hat{f}_{j+1/2} - \hat{f}_{j-1/2} = \Delta x \frac{d\, \bar{\phi}_j}{dt} + \nu \frac{\bar{\phi}_{j-1} - 2\bar{\phi}_j + \bar{\phi}_{j+1}}{\Delta x} = 0$$

  - In the matrix form, with Dirichlet BCs:
    - Semi-discrete FV scheme is as CDS in space, but in terms of cell-averaged data

$$\frac{d\, \bar{\mathbf{\Phi}}}{dt} = \frac{\nu}{\Delta x^2} \mathbf{B}(1,-2,1)\, \bar{\mathbf{\Phi}} + (\mathbf{bc})$$

One-Dimensional Example III
2nd order approx. of diffusion equation:

$$\frac{\partial \phi(x,t)}{\partial t} = \nu \frac{\partial^2 \phi(x,t)}{\partial x^2}$$

- Approximation of surface (flux) integral: Approach 2
  - Use a piece-wise quadratic approx.: $\phi(\xi) = a\xi^2 + b\xi + c \quad \Rightarrow \quad \frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial \xi} = 2a\xi + b$
    - Note that a, b, c remain as before, they are set by the volume average constraints
    - Since a, b are symmetric:

$$f^R_{j+1/2} = f^L_{j+1/2} = -\nu \left.\frac{\partial \phi}{\partial x}\right|_{j+1/2} = -\nu \frac{\bar{\phi}_{j+1} - \bar{\phi}_j}{\Delta x} + O(\Delta x^2)$$

$$f^R_{j-1/2} = f^L_{j-1/2} = -\nu \left.\frac{\partial \phi}{\partial x}\right|_{j-1/2} = -\nu \frac{\bar{\phi}_j - \bar{\phi}_{j-1}}{\Delta x} + O(\Delta x^2)$$

    - There are no flux discontinuities in this case
  - Substitute into integral equation:

$$\frac{d\left(\Delta x\, \bar{\phi}_j\right)}{dt} + \hat{f}_{j+1/2} - \hat{f}_{j-1/2} = \Delta x \frac{d\, \bar{\phi}_j}{dt} + \nu \frac{\bar{\phi}_{j-1} - 2\bar{\phi}_j + \bar{\phi}_{j+1}}{\Delta x} = 0$$

  - In the matrix form, with Dirichlet BCs:
    - Semi-discrete FV scheme is as CDS in space, but in terms of cell-averaged data

$$\frac{d\, \bar{\mathbf{\Phi}}}{dt} = \frac{\nu}{\Delta x^2} \mathbf{B}(1,-2,1)\, \bar{\mathbf{\Phi}} + (\mathbf{bc})$$

Expressing fluxes at the surface based on cell-averaged (nodal) values: Summary of Two Approaches and Boundary Conditions

- Set-up of surface/volume integrals: 2 approaches (do things in opposite order)
  1. (i) Evaluate integrals using classic rules (symbolic evaluation); (ii) Then, to obtain the unknown symbolic values, interpolate based on cell-averaged (nodal) values

$$\left.\begin{array}{l}(i)\ F_e = \int_{S_e} f_\phi \, dA \quad \Rightarrow \quad F_e = G(\phi_e) \\ (ii)\ \phi_e = H\ (\bar{\phi}_P\ 's) \equiv H\ (\phi_P\ 's)\end{array}\right\} \Rightarrow F_e = F\ (\bar{\phi}_P\ 's)$$

Similar for other integrals:

$$(S_\phi = \int_V s_\phi \, dV\ ,\ \bar{\Phi} = \frac{1}{V}\int_V \rho\phi dV\ , etc)$$

  2. (i) Select shape of solution within CV (piecewise approximation); (ii) impose volume constraints to express coefficients in terms of nodal values; and (iii) then integrate. (this approach was used in the examples).

$$\left.\begin{array}{l}\left.\begin{array}{l}(i)\ \phi_{a_i}(x) \equiv J_{\ a_i}(x) \\ (ii)\ \int_{V_P} \phi_{a_i}(x) \equiv \bar{\phi}_P\end{array}\right\} \Rightarrow \phi_{a_i}(x) \equiv \phi_{\bar{\phi}_P}(x) \\ (iii)\ F_e = \int_{S_e} f_{\phi_{\bar{\phi}_P}} \, dA\end{array}\right\} \Rightarrow F_e = F\ (\bar{\phi}_P\ 's)$$

Similar for higher dimensions:

$$\phi(x, y) \equiv J_{\ a_i}(x, y); \quad etc$$

$$\phi_{a_i}(x_P, y_P) \equiv \phi_P; \quad etc$$

- Boundary conditions:
  - Directly imposed for convective fluxes
  - One-side differences for diffusive fluxes

Approach 1: Evaluate integrals symbolically, then interpolate based on neighboring cell-averages

- Surface/Volume integrals: Approach 1
  (i) Evaluate integrals based on classic rules (symbolic evaluation)
  (ii) Then, to obtain the unknown symbolic values, interpolate based on neighboring cell-averaged (nodal) values

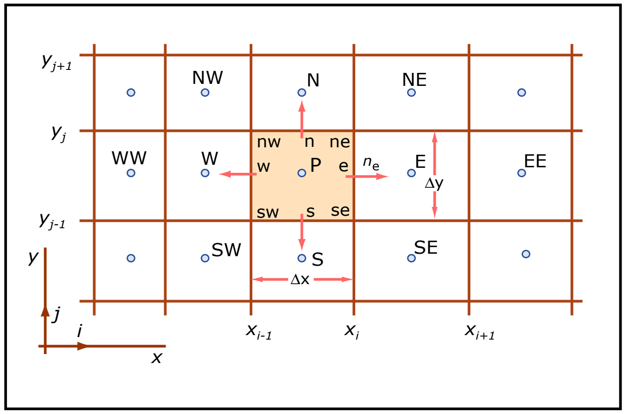
- If we utilize the first approach
  - Symbolic evaluation:
    - To evaluate total surface fluxes (convective + diffusive),

$$\int_S \vec{F}_\phi . \vec{n} \, dA = \int_S \underline{\rho\phi \, (\vec{v}.\vec{n})} dA + \int_S \underline{\vec{q}_\phi} . \vec{n} \, dA$$

      values of ϕ and its gradient normal to the cell face at one or more locations on that face are needed. They have to be expressed as a function of nodal values.

    - Similar for volume integrals
  - Next is interpolation:
    - Express the ϕ's as a function of nodal values. Numerous possibilities. Only most common mentioned next.

Approx. of Surface/Volume Integrals: Classic symbolic formulas



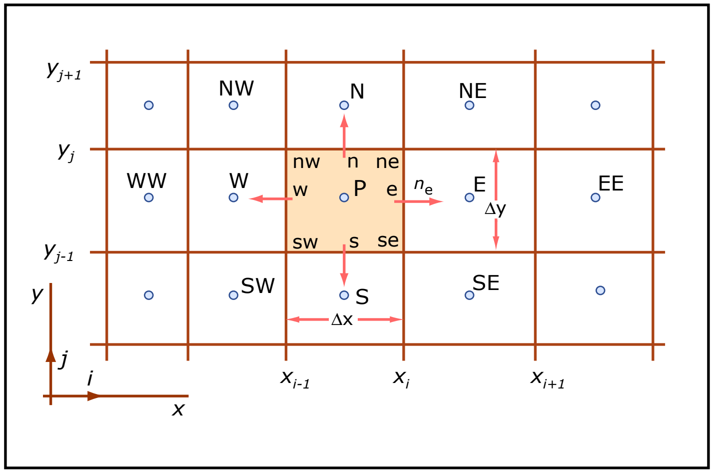
Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

- Surface Integrals $F_e = \int_{S_e} f_\phi \, dA$
  - 2D problems (1D surface integrals)
    - Midpoint rule (2nd order): $F_e = \int_{S_e} f_\phi \, dA = \overline{f_e} S_e = f_e S_e + O(\Delta y^2) \approx f_e S_e$
    - Trapezoid rule (2nd order): $F_e = \int_{S_e} f_\phi \, dA \approx S_e \dfrac{(f_{ne} + f_{se})}{2} + O(\Delta y^2)$
    - Simpson's rule (4th order): $F_e = \int_{S_e} f_\phi \, dA \approx S_e \dfrac{(f_{ne} + 4 f_e + f_{se})}{6} + O(\Delta y^4)$
  - 3D problems (2D surface integrals)
    - Midpoint rule (2nd order): $F_e = \int_{S_e} f_\phi \, dA \approx S_e f_e \quad + O(\Delta y^2, \Delta z^2)$
    - Higher order more complicated to implement in 3D
- Volume Integrals:
  - 2D/3D problems, Midpoint rule (2nd order): $S_P = \int_V s_\phi \, dV = \overline{s}_P V \approx s_P V$
  - 2D, bi-quadratic (4th order, Cartesian): $S_P = \dfrac{\Delta x \, \Delta y}{36} [16 s_P + 4 s_s + 4 s_n + 4 s_w + 4 s_e + s_{se} + s_{sw} + s_{ne} + s_{nw}]$

Interpolations and Differentiations

(to obtain fluxes "F_e" as a function of cell-average values)

- Upwind Interpolation (UDS) for convective fluxes
  - Approximates ϕ_e by its value at the node upstream of "e". This is equivalent to using backward or forward-difference approx for a first derivative (depends on direction of flow) => Upwind Differencing Scheme, which is also called or Donor-cell.



Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

$$\phi_e = \begin{cases} \phi_P \text{ if } \left(\vec{v}.\vec{n}\right)_e > 0 \\ \phi_E \text{ if } \left(\vec{v}.\vec{n}\right)_e < 0 \end{cases}$$

  - This approximation never yields oscillatory solutions (boundedness criterion), but it is numerically diffusive:
    - Taylor expansion about x_P: $\phi_e = \phi_P + (x_e - x_P)\left.\frac{\partial \phi}{\partial x}\right|_P + \frac{(x_e - x_P)^2}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_P + R_2$
    - UDS retains only first term: 1st order scheme in space

$$\hat{f}_e = \rho\,\phi_e\left(\vec{v}.\vec{n}\right)_e \approx \rho\phi_P\left(\vec{v}.\vec{n}\right)_e \qquad \Rightarrow \qquad \tau_{\Delta x} = \rho\left(\vec{v}.\vec{n}\right)_e \Delta x \left.\frac{\partial \phi}{\partial x}\right|_P + \ldots$$

    - Leading truncation error is "diffusive", it has the form of a diffusive flux
    - The numerical diffusion is $\rho\left(\vec{v}.n\right)_e \Delta x$ (has 2 components when flow is oblique to the grid)

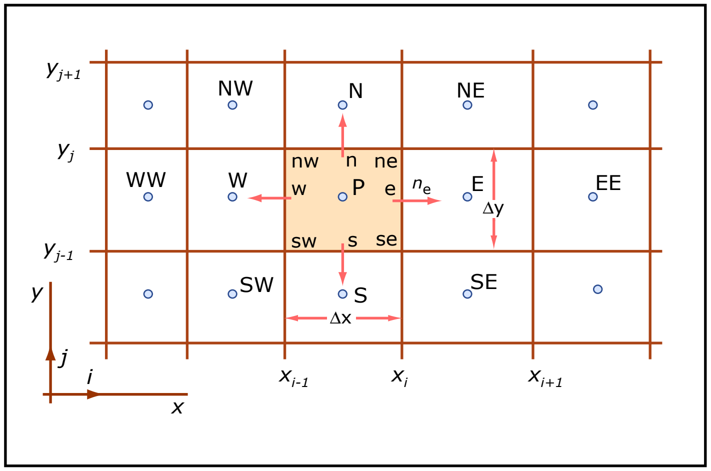
Interpolations and Differentiations

(to obtain fluxes "F_e" as a function of cell-average values)

- Linear Interpolation (CDS) for convective/diffusive
  - Approximates ϕ_e (value at face center) by its linear interpolation between two nearest nodes:

$$\phi_e = \phi_E \lambda_e + \phi_P (1-\lambda_e) \qquad \text{where } \lambda_e = \frac{x_e - x_P}{x_E - x_P}$$

    - λ_e is the interpolation factor



Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

  - This approx. is 2nd order accurate (for convective fluxes):
    - Taylor expansion of ϕ_E about x_P to eliminate first derivative:

$$\phi_E = \phi_P + (x_E - x_P)\left.\frac{\partial \phi}{\partial x}\right|_P + \frac{(x_E - x_P)^2}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_P + R_2 \quad \Rightarrow \left.\frac{\partial \phi}{\partial x}\right|_P = \frac{\phi_E - \phi_P}{x_E - x_P} - \frac{(x_E - x_P)}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_P - \frac{R_2}{x_E - x_P}$$

$$\Rightarrow \phi_e = \phi_P + (x_e - x_P)\left.\frac{\partial \phi}{\partial x}\right|_P + \frac{(x_e - x_P)^2}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_P + R_2 = \phi_E \lambda_e + \phi_P(1-\lambda_e) - \frac{(x_e - x_P)(x_E - x_e)}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_P + R'_2$$

    - Truncation error is proportional to square of grid spacing, on uniform/non-uniform grids.
    - As all approximations of order higher than one, this scheme can provide oscillatory solutions
    - Corresponds to central differences, hence its CDS name

Interpolations and Differentiations

(to obtain fluxes "F_e" as a function of cell-average values)

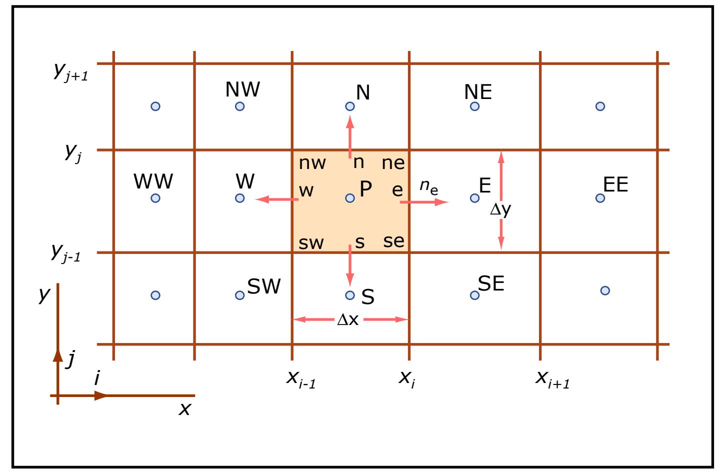
- Linear Interpolation (CDS) for convective/diffusive fluxes
  - Linear profile between two nearest nodes leads to simplest approx. of gradient (diffusive fluxes)

$$\phi \quad {}_{E} \quad {}_{P}(1 \quad)$$

$$\left.\frac{\partial\phi}{\partial x}\right|_e \approx \frac{\phi_E - \phi_P}{x_E - x_P}$$

  - Taylor expansions of ϕ's around x_e, one obtains:

$$\tau_{\Delta x} = \frac{(x_e - x_P)^2 - (x_E - x_e)^2}{2\,(x_E - x_P)} \left.\frac{\partial^2\phi}{\partial x^2}\right|_e - \frac{(x_e - x_P)^3 + (x_E - x_e)^3}{6\,(x_E - x_P)} \left.\frac{\partial^3\phi}{\partial x^3}\right|_e + R_3$$

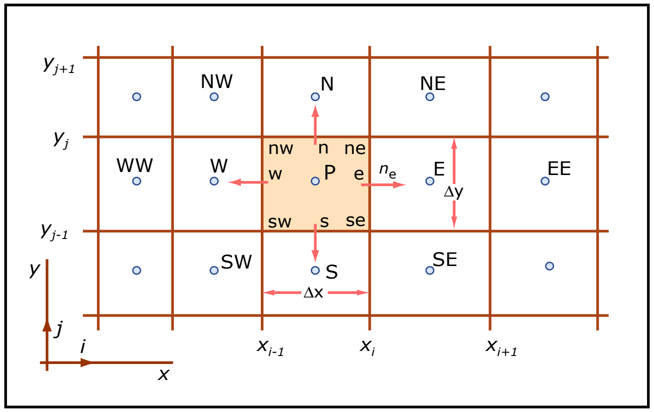


Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

  - Approximation is 2nd order accurate if e is midway between P and E (e.g. uniform grid)
  - When the grid is non-uniform, the formal accuracy is 1st order, but error reduction when grid is refined is asymptotically 2nd order

Interpolations and Differentiations
(to obtain fluxes "F_e" as a function of cell-average values)

- Quadratic Upwind Interpolation (QUICK)
  - Approx. by quadratic profile between two nearest nodes.
  - In accord with convection, third point chosen on upstream side:
    - i.e. chose W if flow is from P to E, or EE if flow from E to P.



Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

This gives:

$$\phi_e = \phi_U + g_1\,(\phi_D - \phi_U) + g_2\,(\phi_U - \phi_{UU})$$

where D, U and UU denote the downstream, first upstream and second downstream, respectively

  - Coefficients in terms of nodal coordinates: $g_1 = \dfrac{(x_e - x_U)\,(x_e - x_{UU})}{(x_D - x_U)\,(x_D - x_{UU})}$; $g_2 = \dfrac{(x_e - x_U)\,(x_D - x_e)}{(x_U - x_{UU})\,(x_D - x_{UU})}$
  - Uniform grids: coefficients of ϕ's are 3/8 for node D, 6/8 for node U and -1/8 for node UU
  - Somewhat more complex scheme than CDS (larger computational molecules by one node in each direction)
  - Approximation is 3[rd] order accurate on both uniform and non-uniform grids. For uniform grids:

$$\phi_e = \frac{6}{8}\phi_U + \frac{3}{8}\phi_D - \frac{1}{8}\phi_{UU} - \frac{3\Delta x^3}{48}\left.\frac{\partial^3 \phi}{\partial x^3}\right|_U + R_3$$

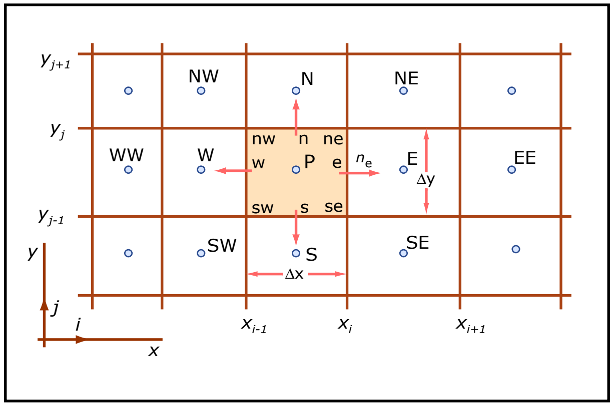
    - But, when this interpolation scheme is used with midpoint rule for surface integral, becomes 2[nd] order

Interpolations and Differentiations

(to obtain fluxes "$F_e = f(\phi_e)$" as a function of cell-average values)

- Higher Order Schemes (for convective/diffusive fluxes)
  - Interpolations of order higher than 3 make sense if integrals are also approximated with higher order formulas
  - In 1D problems, if Simpson's rule (4th order error) is used for the integral, a polynomial interpolation of order 3 can be used:

$$\phi(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$



Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

=> 4 unknowns, hence 4 nodal values (W, P, E and EE) needed
= Symmetric formula for ϕ_e (no need for "upwind" as with 0th or 2nd order polynomials)

  - With $\phi(x)$, one can insert in the symbolic integral formula. For a uniform Cartesian grid:
    - Convective Fluxes: $\phi_e = \dfrac{27\phi_P + 27\phi_E - 3\phi_W - 3\phi_{EE}}{48}$ (similar formulas used for values at corners)
    - For Diffusive Fluxes (1st derivative):

$$\left.\frac{\partial \phi}{\partial x}\right|_e = a_1 + a_2 x + a_3 x^2 \quad \Rightarrow \quad \text{for a uniform Cartesian grid: } \left.\frac{\partial \phi}{\partial x}\right|_e = \frac{27\phi_E - 27\phi_P + \phi_W - \phi_{EE}}{24\,\Delta x}$$

  - This FV approximation is often called a 4th-order CDS (linear FV interpol. was 2nd-order CDS)
  - Polynomials of higher-degree or of multi-dimensions can be used, as well as cubic splines (to ensure continuity of first two derivatives at the boundaries). This increases the cost.

Interpolations and Differentiations

(to obtain fluxes "$F_e = f(\phi_e)$" as a function of cell-average values)

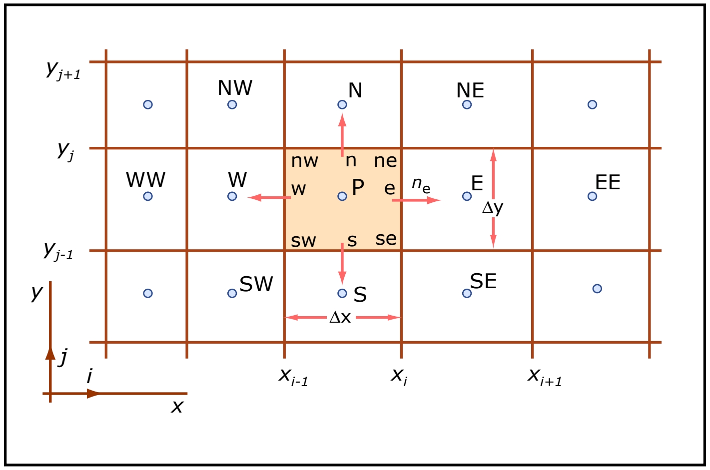
- Compact Higher Order Schemes
  - Polynomial of higher order lead too large computational molecules => use deferred-correction schemes and/or compact (Pade') schemes
  - Ex. 1: obtain the coefficients of $\phi(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$ fitting two values and two 1st derivatives at the two nodes on either side of the cell face by
    - 4th order scheme: $\phi_e = \frac{\phi_P + \phi_E}{2} + \frac{\Delta x}{8}\left(\left.\frac{\partial \phi}{\partial x}\right|_P - \left.\frac{\partial \phi}{\partial x}\right|_E\right) + O(\Delta x^4)$
    - Use CDS to approximate derivatives. Result retains the fourth order:

$$\phi_e = \frac{\phi_P + \phi_E}{2} + \frac{\phi_P + \phi_E - \phi_W - \phi_{EE}}{16} + O(\Delta x^4)$$

  - Ex. 2: use a parabola, fit the values on either side of the cell face and the derivative on the upstream side (equivalent to the QUICK scheme, 3rd order)

$$\phi_e = \frac{3}{4}\phi_U + \frac{1}{4}\phi_D + \frac{\Delta x}{4}\left.\frac{\partial \phi}{\partial x}\right|_U$$

  - Similar schemes are obtained for derivatives (diffusive fluxes), see Ferziger and Peric (2002)



Notation used for a Cartesian 2D and 3D grid.
Image by MIT OpenCourseWare

- Other Schemes: more complex and difficult to program
  - Large number of approximations used for convective fluxes: Linear Upwind Scheme, Skew Upwind schemes, Hybrid. Blending schemes to eliminate oscillations at higher order.

Methods for Unsteady Problems – Time Marching Methods
ODEs – Initial Value Problems (IVPs)

- Major difference with spatial dimensions: Time advances in a single direction
  - FD schemes: discrete values evolved in time
  - FV schemes: discrete integrals evolved in time
- After discretizing the spatial derivatives (or the integrals for finite volumes), we obtained a (coupled) system of (nonlinear) ODEs, for example:

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

- Hence, methods used to integrate ODEs can be directly used for the time integration of spatially discretized PDEs
  - We already utilized several time-integration schemes with FD schemes. Others are developed next.
  - For IVPs, methods can be developed with a single eqn.: $\frac{d\phi}{dt} = f(\phi, t)$; with $\phi(t_0) = \phi_0$
  - Note: solving steady (elliptic) problems by iterations is similar to solving time-evolving problems. Both problems thus have analogous solution schemes.

2.29 Numerical Fluid Mechanics
Fall 2011