REVIEW Lecture 15:

- Finite Volume Methods
  - Integral and conservative forms of the cons. laws
  - Introduction
  - Approximations needed and basic elements of a FV scheme
    - Grid generation ⇒ Time-Marching
    - 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

TODAY (Lecture 16): FINITE VOLUME METHODS

- Summary: Steps to step-up a FV scheme
- Examples: One Dimensional examples
  - Generic equations
  - Linear Convection (Sommerfeld eqn): convective fluxes
    - 2nd order in space, 4th order in space, links to CDS
  - Unsteady Diffusion equation: diffusive fluxes
    - Two approaches for 2nd 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

References and Reading Assignments

- Chapter 29.4 on “The control-volume approach for elliptic equations” of “Chapra and Canale, Numerical Methods for Engineers, 2014/2010/2006.”
- 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 I
Linear Convection (Sommerfeld) Eqn, Cont'd

- The resultant linear algebraic system is circulant tri-diagonal (for periodic BCs)

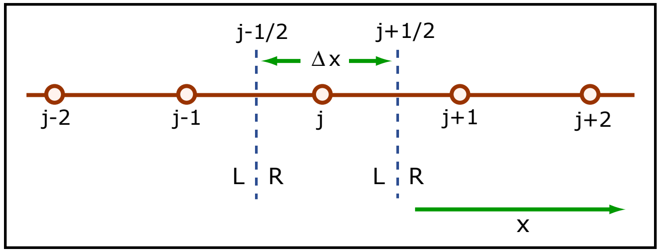
$$\frac{d\,\bar{\mathbf{\Phi}}}{dt} + \frac{c}{2\Delta x}\mathbf{B}_P(-1,0,1)\bar{\mathbf{\Phi}} = 0$$

- This is as the 2nd order CDS!, except that it is written in terms of cell averaged values instead of values at FD nodes/points
  - It is also 2nd order in space
  - Has same properties as classic CDS for $\frac{\partial \phi(x,t)}{\partial t} + \frac{\partial\, c\, \phi(x,t)}{\partial x} = 0$
    - Non-dissipative (check Fourier analysis or eigenvalues of $\mathbf{B}_P$ 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 $\Delta t, \Delta x$

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

- 1D exact integral equation still

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



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- Use 4th order accurate surface/volume integrals
  - Replace piecewise-constant approx. to $\phi(x)$ with piece-wise quadratic approx ($\xi = x - x_j$): $\phi(\xi) = a\xi^2 + b\xi + c$ (note ϕ defined over more than 1 cell)
  - 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:

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

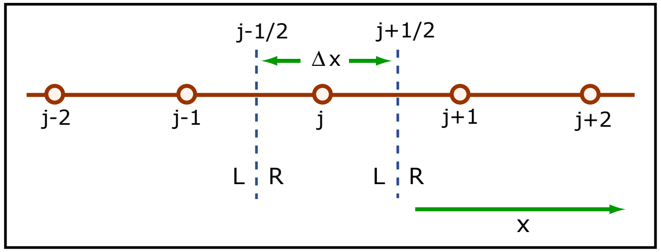
  - Next, we need to evaluate the values of $\phi(x)$ at the boundaries so as to compute the advective fluxes at these boundaries: $f^L_{j-1/2}\,,\ f^R_{j-1/2},\ f^L_{j+1/2}\,,\ f^R_{j+1/2}$

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

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

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

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



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

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

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

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

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

- For periodic domains: $$\frac{d\,\overline{\mathbf{\Phi}}}{dt} + \frac{c}{12\Delta x}\mathbf{B}_P(-1,-8,0,8,1)\,\overline{\mathbf{\Phi}} = 0$$

FIGURE 23.3
Centered finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

Centered Differences

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

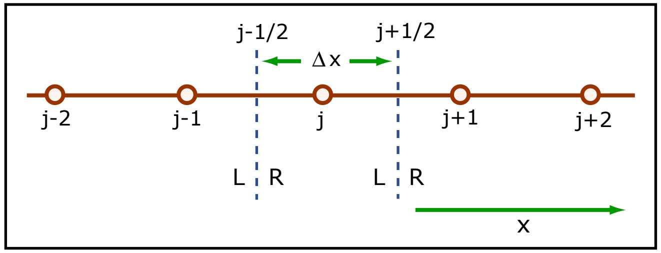
One-Dimensional Example III
2nd order approx. of diffusion equation:

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

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



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- Approximation of surface (flux) integral: Approach 1

  – Direct: we know that to second-order (from CDS and from $\bar{\phi}_j = \phi_j + O(\Delta x^2)$)

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

  – 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
2^{nd} 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.: $\phi(\xi) = a\xi^2 + b\xi + c \Rightarrow \frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial \xi} = 2a\xi + b$
    - 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

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

Similar for other integrals:

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

  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).

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

Similar for higher dimensions:

$$\phi(x,y) \equiv \mathcal{J}_{a_i}(x,y); \quad etc$$

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

- Boundary conditions:
  – Directly imposed for convective fluxes
  – One-sided 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 this approach 1
  - Symbolic evaluation:
    - To evaluate total surface fluxes (convective + diffusive),

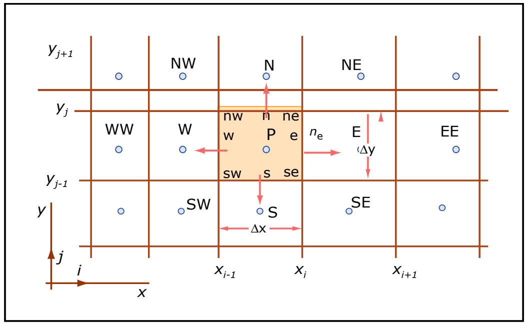
$$\int_S \vec{F}_\phi . \vec{n}\, dA = \int_S \underline{\rho\phi\,(\vec{v}.\vec{n})} dA + \int_S \underline{\vec{q}_\phi . \vec{n}}\, dA$$

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 $\bar{\phi}$

    - Similar for volume integrals
  - Next is interpolation:
    - Express the ϕ's as a function of nodal values. Numerous possibilities. We already saw some of the most common, provided again next.

Approx. of Surface/Volume Integrals: Classic symbolic formulas

(summary from Lecture 15)



Notation used for a Cartesian 2D and 3D grid.
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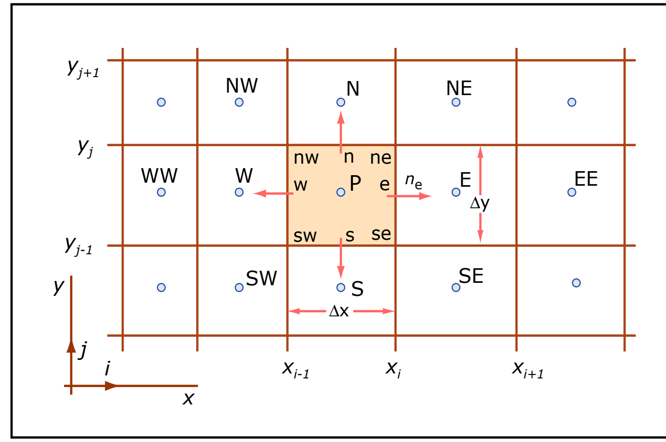
- Surface Integrals $F_e = \int_{S_e} f_\phi \, dA$
  - 2D problems (1D surface integrals)
    - Midpoint rule (2nd order): $F_e = \int_{S_e} f_\phi \, dA = \bar{f}_e S_e = f_e S_e + O(\Delta y^2) \approx f_e S_e$
    - Trapezoid rule (2nd order): $F_e = \int_{S_e} f_\phi \, dA \approx S_e \dfrac{(f_{ne} + f_{se})}{2} + O(\Delta y^2)$
    - 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: $S_\phi = \int_V s_\phi \, dV \,, \quad \bar{\Phi} = \dfrac{1}{V} \int_V \rho \phi dV$
  - 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): $S_P = \dfrac{\Delta x \, \Delta y}{36} [16 s_P + 4 s_s + 4 s_n + 4 s_w + 4 s_e + s_{se} + s_{sw} + s_{ne} + s_{nw}]$

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 Donor-cell.

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



Notation used for a Cartesian 2D and 3D grid.
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  - This approximation never yields oscillatory solutions (boundedness criterion), but it is numerically diffusive:
    - Taylor expansion about x_P: $\phi_e = \phi_P + (x_e - x_P)\left.\dfrac{\partial \phi}{\partial x}\right|_P + \dfrac{(x_e - x_P)^2}{2}\left.\dfrac{\partial^2 \phi}{\partial x^2}\right|_P + R_2$
    - UDS retains only first term: 1st order scheme in space

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

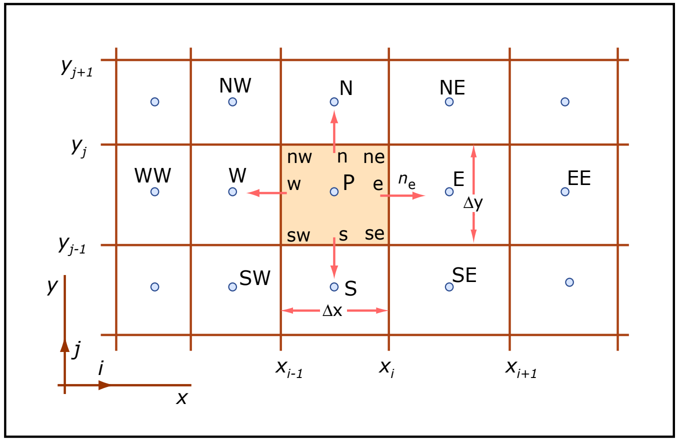
    - Leading truncation error is "diffusive", it has the form of a diffusive flux
    - The numerical diffusion is $\rho\left(\vec{v}.\vec{n}\right)_e \Delta x$ (has 2 components when flow is oblique to the grid)

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

- Linear Interpolation (CDS) for convective fluxes
  - 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.
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  - This approx. is 2nd order accurate (for convective fluxes):
    - Use Taylor exp. of ϕ_E about x_P to eliminate 1st derivative in Taylor exp. of ϕ_e (previous slide)

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

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

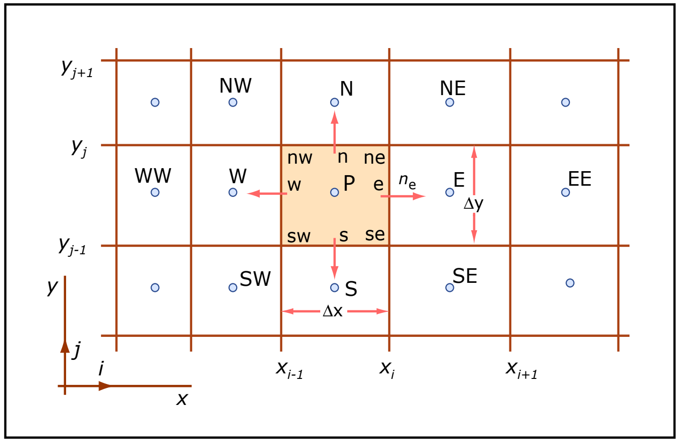
    - Truncation error is proportional to square of grid spacing, on uniform/non-uniform grids.
    - As all approximations of order higher than one, this scheme can provide oscillatory solutions
    - Corresponds to central differences, hence its CDS name (gives avg. if uniform grid spacing)

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

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

$$\phi = \phi_E \lambda + \phi_P (1-\lambda) \quad \Rightarrow \quad \left.\frac{\partial \phi}{\partial x}\right|_e \approx \frac{\phi_E - \phi_P}{x_E - x_P}$$

$$\lambda = \frac{x - x_P}{x_E - x_P}$$



Notation used for a Cartesian 2D and 3D grid.
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  - Taylor expansions of ϕ's around x_e, one obtains:

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

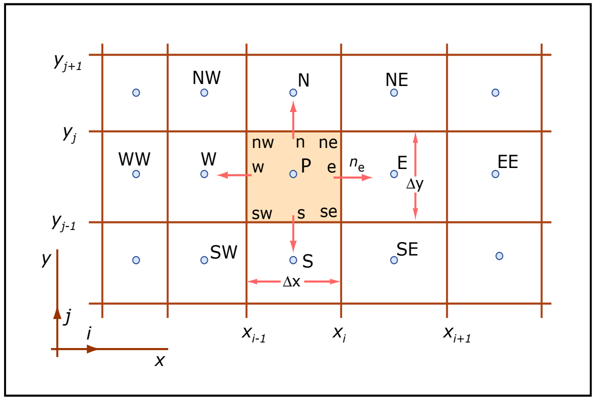
  - Approximation is 2nd order accurate if e is midway between P and E (e.g. uniform grid)
  - When the grid is non-uniform, the formal accuracy is 1st order, but error reduction when grid is refined is asymptotically 2nd order

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

- Quadratic Upwind Interpolation (QUICK), convective fluxes
  - 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.

    This gives:

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



Notation used for a Cartesian 2D and 3D grid.
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    where D, U and UU denote the downstream, first upstream and second upstream, 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 3rd order accurate on both uniform and non-uniform grids. For uniform grids:

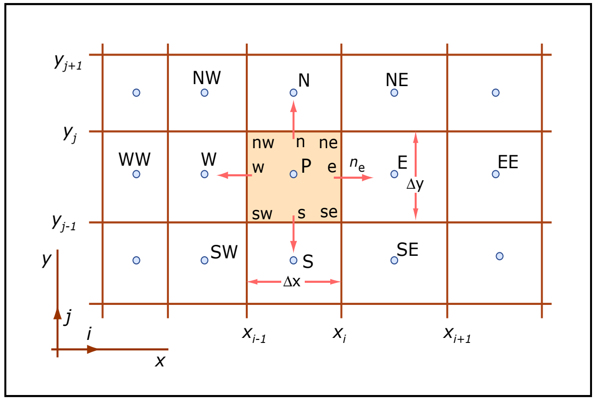
$$\phi_e = \frac{6}{8}\phi_U + \frac{3}{8}\phi_D - \frac{1}{8}\phi_{UU} - \frac{3\Delta x^3}{48}\left.\frac{\partial^3\phi}{\partial x^3}\right|_U + R_3$$

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



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

  – 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:

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

(Note: higher-order, approach 1 →≈ approach 2 !)

=> 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 (donor-cell & QUICK)

  – With $\phi(x)$, one can insert $\phi_e = \phi(x_e)$ in symbolic integral formula. For a uniform Cartesian grid:

    - Convective Fluxes: $$\phi_e = \frac{27\phi_P + 27\phi_E - 3\phi_W - 3\phi_{EE}}{48}$$ (similar formulas used for ϕ values at corners)

    - For Diffusive Fluxes (1st derivative):

$$\left.\frac{\partial \phi}{\partial x}\right|_e = a_1 + 2a_2 x + 3a_3 x^2 \quad \Rightarrow \quad \text{for a uniform Cartesian grid: } \left.\frac{\partial \phi}{\partial x}\right|_e = \frac{27\phi_E - 27\phi_P + \phi_W - \phi_{EE}}{24\,\Delta x}$$

  – This FV approximation often called a 4th-order CDS (linear poly. 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)

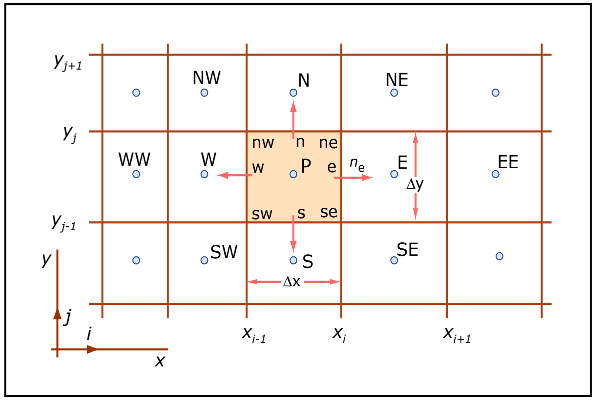
- Compact Higher Order Schemes
  - Polynomial of higher order lead too large computational molecules => use deferred-correction schemes and/or compact (Pade’) schemes
  - Ex. 1: obtain the coefficients of $\phi(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$ by fitting two values and two 1st derivatives at the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

2.29 Numerical Fluid Mechanics
Spring 2015