Midterm Review

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Mechanical Engineering 692

Computational Fluid Dynamics

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Outline

- Differential equations of fluid dynamics
- Turbulence modeling
- Numerical analysis
  - Finite-differences and order of the error
  - Finite-volume approaches
- Finite-volume approaches for CFD
  - Convection, diffusion, source
  - Differencing approaches
  - Momentum and continuity: SIMPLE, *etc*.

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Common Variable Notation

- **Source = Outflow – Inflow + Storage**
- Different physical quantities, Φ: mass, momentum, energy, species K mass = $m^{(K)}$
- Per unit mass quantity $\phi = \Phi/m$
- Differential volume ΔV; $m = \rho\Delta V$
- In this differential volume, $\Phi = \rho\,\phi\,\Delta V$

Φ	m	mu	mv	mw	E + m**V**²/2	$m^{(K)}$
ϕ	1	u	v	w	e + **V**²/2	$W^{(K)}$

$W^{(K)} = m^{(k)}/m$ is mass (weight) fraction

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General Equation

- Look at general transport equation in same form as species transport equation

$$\underset{Transient}{c\left[\frac{\partial\rho\phi}{\partial t}\right.} + \underset{Convective}{\left.\frac{\partial\rho u_i\varphi}{\partial x_i}\right]} = \underset{Diffusive}{\frac{\partial}{\partial x_i}\Gamma^{(\varphi)}\frac{\partial\varphi}{\partial x_i}} + \underset{"Source"}{S^{(\varphi)}}$$

- c = 1 or c = heat capacity if $\phi = T$
- General transport coefficient, $\Gamma^{(\phi)}$ (*e.g.*, viscosity) has same dimensions as $x_i^2c\rho/t$ (for c = 1 this is mass/length/time)
  - For $\phi = T$, $\Gamma^{(\phi)}$ = thermal conductivity, k

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General Equation II

- This general equation applies to convervation of mass, momentum, energy and species
  - Will also be used for turbulence models
- Terms in "Source" are true source terms plus other terms that are not the pure second derivative terms
- Examine each equation to determine the contents of the "Source" term
  - Separate pressure gradient in momentum
- Source often zero for simple problems

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Momentum Equations

- General momentum equation shows pressure gradient explicitly

$$\frac{\partial\rho u_j}{\partial t} + \frac{\partial\rho u_i u_j}{\partial x_i} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\mu\frac{\partial u_j}{\partial x_i} + S_j^{**}$$

$$S_j^{**} = \frac{\partial}{\partial x_i}\mu\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] + \rho B_j$$

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Momentum Source Zero?

- We can show that S_j^{**} is zero for constant density (when $\Delta = 0$) and viscosity and no body force terms ($B_j = 0$)
  - For constant viscosity we have

$$\frac{\partial}{\partial x_i}\mu\frac{\partial u_i}{\partial x_j} = \mu\frac{\partial}{\partial x_i}\frac{\partial u_i}{\partial x_j} = \mu\frac{\partial}{\partial x_j}\frac{\partial u_i}{\partial x_i} = \mu\frac{\partial \Delta}{\partial x_j}$$

$$S_j^{**} = \frac{\partial \Delta}{\partial x_j} + \frac{\partial}{\partial x_j}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] + \rho B_j$$

  - This is zero for $\Delta = B_j = 0$

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Simplifications

- Constant property flows
  - Constant density ($\Delta = 0$)
  - Constant transport properties
  - Combination of both (can show $S^{(u_j)} = \rho B_j$)
- Low Mach number flows (no dissipation)
- Ideal gases $\beta_P = 1/T$ and $\kappa_T = 1/P$
- Boundary layer flows – predominant flow direction with no recirculation

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Turbulent Flows

No smoking in CSUN classrooms, but the smoke from a cigarette shows how laminar flows can transition into turbulent flows and the eddy nature of the turbulent flow structures

Turbulent pipe flow video

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Turbulence and Fluctuations

- Model flow variables in terms of main flow properties and fluctuations
  - Instantaneous value, ϕ
  - Fluctuation value ϕ'
  - Definition of mean value $\overline{\varphi} = \frac{1}{\Delta t}\int_0^{\Delta t} \varphi dt$
  - Basic result:

$$\varphi = \overline{\varphi} + \varphi'$$

  - Applied to velocity components sometimes use U_i for mean velocity component

$$u_i = \overline{u_i} + u_i' = U_i + u_i'$$

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Turbulence Models

- Cannot compute turbulence exactly except for simple flows
  - Need to use turbulence models
  - Based on combination of theory and empirical measurements
  - Many models available
    - No model correct for all flows
  - Basic approach is to model turbulent viscosity
    - Averages of turbulent fluctuation products are assumed to be proportional to mean gradients

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Average of a Product

- The mean of the product of two flow properties ϕ and ψ, written as $\overline{\psi\varphi}$, is the sum of two terms:
  - The product of the means of each individual term $\overline{\varphi}$ and $\overline{\psi}$
  - The mean of the product of the two fluctuation quantities $\overline{\varphi'\psi'}$ (correlation term)

$$\overline{\psi\varphi} = \overline{\varphi}\,\overline{\psi} + \overline{\varphi'\psi'}$$

  - Although $\overline{\varphi'}$ and $\overline{\psi'}$ are zero $\overline{\varphi'\psi'}$ is not zero
  - Derivation on next slide

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Reynolds-Average

- Reynolds average transport equation (including Navier Stokes, called RANS)
  - Start with general transport equation

$$c\left[\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_i \varphi}{\partial x_i}\right] = \frac{\partial}{\partial x_i}\Gamma^{(\varphi)}\frac{\partial \varphi}{\partial x_i} + S^{(\varphi)}$$

  - Look at steady-state, zero-source, constant properties

$$\frac{1}{\Delta t}\int_0^{\Delta t}\frac{\partial u_i \varphi}{\partial x_i}dt = \gamma^{(\varphi)}\frac{1}{\Delta t}\int_0^{\Delta t}\frac{\partial}{\partial x_i}\frac{\partial \varphi}{\partial x_i}dt \qquad \gamma^{(\phi)} = \frac{\Gamma^{(\phi)}}{\rho c}$$

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What is $\gamma^{(\phi)} = \Gamma^{(\phi)}/\rho c$?

- Recall definition of $\Gamma^{(\phi)}$ as general transport coefficient

ϕ	u	v	w	e	h	T	T
$\Gamma^{(\phi)}$	μ	μ	μ	k/c_v	k/c_p	k	k
c	1	1	1	1	1	c_v	c_p
$\gamma^{(\phi)}$	μ/ρ	μ/ρ	μ/ρ	$k/\rho c_v$	$k/\rho c_p$	$k/\rho c_v$	$k/\rho c_p$

- Dimensions for $\gamma^{(\phi)}$ are L^2/T
  - Kinematic viscosity, $\nu = \mu/\rho$
  - Thermal diffusivity $\alpha = k/\rho c_p$

k is thermal conductivity

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Reynolds Average II

- Use expression for average of a product to compute average of $u_i\phi$

$$\frac{\partial \overline{u_i \varphi}}{\partial x_i} = \frac{\partial\left(\overline{u_i}\,\overline{\varphi} + \overline{u_i'\varphi'}\right)}{\partial x_i} = \gamma^{(\varphi)}\frac{\partial}{\partial x_i}\frac{\partial \overline{\varphi}}{\partial x_i}$$

- Use Boussinesq approximation $\quad \overline{u_i'\varphi'} = -\gamma_t^{(\varphi)}\frac{\partial \overline{\varphi}}{\partial x_i}$

$$\frac{\partial \overline{u_i}\,\overline{\varphi}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\gamma_l^{(\varphi)}\frac{\partial \overline{\varphi}}{\partial x_i} + \gamma_t^{(\varphi)}\frac{\partial \overline{\varphi}}{\partial x_i}\right] = \frac{\partial}{\partial x_i}\left[\left(\gamma_l^{(\varphi)} + \gamma_t^{(\varphi)}\right)\frac{\partial \overline{\varphi}}{\partial x_i}\right]$$

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Turbulent Viscosity

- Arguments based on dimensional analysis
- Define characteristic velocity scale, $\mathfrak{v}$, and length scale, ℓ
- Consider kinematic viscosity, ν, with dimensions of L^2/T
- Dimensions of $\mathfrak{v}$ and ℓ and L/T and L
- Dimensionally correct choice for n is product of $\mathfrak{v}$ and ℓ or $\nu_T = C\,\mathfrak{v}\,\ell$

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Turbulence Modeling

- Reynolds averaging terms like $\rho u'\phi'$ modeled by a turbulent transport coefficient $\gamma_t^{(\phi)}$, *e.g.*, turbulent viscosity ν
- To use this approach we have to find ways to compute ν and the general $\gamma_t^{(\phi)}$
- Various turbulence models proposed
  - Some use simple concepts
  - Others require numerical solution of one or more partial differential equations (PDE)
    - PDEs have same form as other CFD equations

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k and ε

- Turbulence kinetic energy, k

$$k = \left(u_i'u_i'\right)/2 = \left(u'u' + v'v' + w'w'\right)/2$$

- Dissipation rate, ε, is rate of kinetic energy transfer from smallest eddies working against the viscous forces
- Defined in terms of deformation rates, e_{ij}

$$e_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \qquad \tau_{ij} = \mu e_{ij} + (\kappa - \frac{2}{3}\mu)\Delta\delta_{ij}$$

- Definition of ε is $\varepsilon = 2\nu\overline{e'_{ij}\,e'_{ij}}$

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Turbulence Models

- k-ε most common turbulence model for non-aerospace engineering applications
  - widely regarded as having many shortcomings in representing turbulence
  - most widely validated model
  - probably best choice for applications without strong directional effects or rotational flows
  - Renormalizable group and realizable k-ε models can give better results

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Turbulence Models II

- Spalart-Allmaras model developed especially for aerospace applications with wall-bounded flows
  - One equation model
- Relatively new model now seeing applications in areas other than its initial aerospace applications
  - Adverse pressure gradients
  - Turbomachinery

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Turbulence Models III

- Reynolds stress model has had success for flows with directional effects and rotational flows
  - Requires solution of seven partial differential equations to compute turbulent viscosity
  - Algebraic version has been used
- Other models available which may have better accuracy for limited range of flows

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Turbulence Models IV

- LES used for complex flows particularly transient and oscillating flows
- Not usually required for common engineering problems
- DES too expensive for practical flows
- Choice of turbulence model should be based on previous success of model in similar applications
- No one right model to choose

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Model Guidance

- Use model which has been used previously for your problem
  - Previous work at your organization or from literature research
- Consult user's manual for CFD code regarding increased computer time and memory use for more complex models
- Use default constants in model unless you have specific data to justify alternative values

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Model Guidance II

- Review material on turbulence models to see if they can handle unusual features of the flow you are modeling
  - Low Reynolds number (non-equilibrium) turbulence
  - High strain rates
  - Adverse pressure gradients
  - Rotating machinery
  - Compressible flows
  - Other complex flows

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Model Guidance III

- Whatever model you use, make sure that you have proper boundary conditions
  - Use special wall functions for non-equilibrium turbulence when laminar sublayer is not resolved
  - Use correct grid spacing for first node from wall for choice of wall functions or resolving laminar sublayer
    - Check this after calculations

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Numerical Analysis

- Finite-difference expressions
  - Forward, backward, central
  - Truncation error from Taylor series proportional to step-size, h, to n^{th} power is called n^{th} order error $\varepsilon = O(h^2)$
- Finite difference grids x_i, y_i, z_k, t_n with $u(x_i, y_i, z_k, t_n) = u^n_{ijk}$
- Used Taylor series to get expressions for derivatives on grids
- Greater error on non-uniform grids

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First Derivative Expressions

First order forward $f_i' = \dfrac{f_{i+1} - f_i}{h} + O(h)$

First order backward $f_i' = \dfrac{f_i - f_{i-1}}{h} + O(h)$

Second order central $f_i' = \dfrac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$

Second order forward $f_i' = \dfrac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} + O(h^2)$

Second order backward $f_i' = \dfrac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + O(h^2)$

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Other Expressions

Second derivative $f_i'' = \dfrac{f_{i+1} + f_{i-1} - 2f_i}{h^2} + O(h^2)$

Arithmetic mean $f_i = \dfrac{f_{i+1} + f_{i-1}}{2} + O(h^2)$

Uneven step sizes $h_{i+1} = x_{i+1} - x_i$; $r_i = h_{i+1}/h_i$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}} - \frac{f_i''}{2!}\frac{h_{i+1}^2 - h_i^2}{h_{i+1} + h_i} - \frac{f_i'''}{3!}\frac{h_{i+1}^3 + h_i^3}{h_{i+1} + h_i} + \ldots..$$

$$f_i'' = 2\frac{f_{i+1} + r_i f_{i-1} - (1 + r_i) f_i}{h_{i+1}^2 + h_{i+1}h_i} - \frac{f_i'''}{3}\frac{h_{i+1}^2 - h_i^2}{h_{i+1} + h_i} - \frac{f_i''''}{12}\frac{h_{i+1}^3 - h_i^3}{h_{i+1} + h_i} + \ldots.$$

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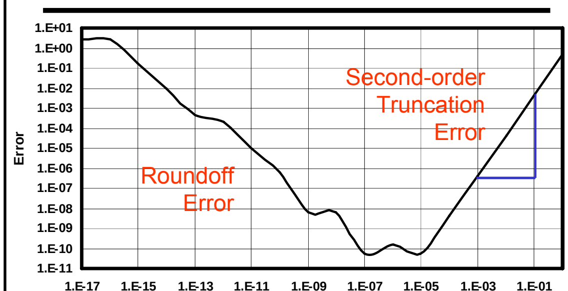
Truncation and Roundoff



Step Size $n = \dfrac{\log \frac{\varepsilon_2}{\varepsilon_1}}{\log \frac{h_2}{h_1}} = \dfrac{\log \frac{5x10^{-3}}{5x10^{-7}}}{\log 100} = 2$

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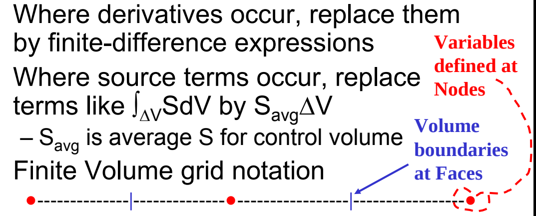
Finite-volume Approach

- Integrate PDE over a small volume
- Where derivatives occur, replace them by finite-difference expressions
- Where source terms occur, replace terms like $\int_{\Delta V} S dV$ by $S_{avg}\Delta V$
  - S_{avg} is average S for control volume
- Finite Volume grid notation



$x_W = x_{i-1}$ $x_w = x_{i-1/2}$ $x_P = x_i$ $x_e = x_{i+1/2}$ $x_E = x_{i+1}$

$\delta x_{WP} = x_P - x_W$, $\delta x_{wP} = x_P - x_w$, $\delta x_{Pe} = x_e - x_P$, $\delta x_{PE} = x_E - x_P$

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Finite Volume Method

- Consider 1D diffusion and source only

$$\frac{d}{dx}\Gamma\frac{d\varphi}{dx}+S=0 \qquad \int\left(\frac{d}{dx}\Gamma\frac{d\varphi}{dx}+S\right)dV=\int\left(\frac{d}{dx}\Gamma\frac{d\varphi}{dx}+S\right)Adx=0$$

- Integrate over finite-volume grid

$x_W = x_{i-1}$ $x_w = x_{i-1/2}$ $x_P = x_i$ $x_e = x_{i+1/2}$ $x_E = x_{i+1}$

$$A\int\frac{d}{dx}\Gamma\frac{d\varphi}{dx}dx+\int SdV=A\int_{x_w}^{x_e}d\left(\Gamma\frac{d\varphi}{dx}\right)+\bar{S}\Delta V=\left(\Gamma A\frac{d\varphi}{dx}\right)_e-\left(\Gamma A\frac{d\varphi}{dx}\right)_w+\bar{S}\Delta V=0$$

- Find Γ and $d\phi/dx$ at w and e faces
  - $\Gamma_e = (\Gamma_P + \Gamma_E)/2$ and $\Gamma_w = (\Gamma_W + \Gamma_P)/2$
  - $d\phi/dx|_e = (\phi_E - \phi_P)/\delta x$ $d\phi/dx|_w = (\phi_P - \phi_W)/\delta x$

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Finite Volume Method II

- Finite-volume result
  - Define $\bar{S}\Delta V = S_u + S_p\varphi_P$

$$a_E\varphi_E + a_W\varphi_W + S_u - a_P\varphi_P = 0$$

$$a_E = \frac{\Gamma_e A_e}{\delta x_{PE}} \quad a_W = \frac{\Gamma_w A_w}{\delta x_{WP}} \quad a_P = \frac{\Gamma_e A_e}{\delta x_{PE}} + \frac{\Gamma_w A_w}{\delta x_{WP}} - S_p = a_E + a_W - S_p$$

  - Write equations for all nodes in this one-dimensional problem
    - $a_{W,i}\phi_{i-1} - a_{p,i}\phi_i + a_{E,i}\phi_{i+1} = -S_{u,i}$
    - Apply this result for nodes from i = 1 to i = N – 1
    - Nodes i = 0 and i = N are boundary conditions

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Finite-Volume Example

- Example problem
  - Γ = 1 kg/m·s
  - A = 1 m^2
  - ΓA = 1 kg·m/s
  - δx = L/N with L = 1 m

$$a_E = a_W = \frac{\Gamma A}{\delta x} = \frac{\frac{1\,kg}{m\cdot s}\left(1\,m^2\right)}{\frac{1\,m}{N}} = N\frac{kg}{s}$$

  - Source terms: $S_u = 0$; $S_p = -10/N$ kg/s

$$a_P = a_E + a_W - S_p = \left(2N + \frac{10}{N}\right)\frac{kg}{s}$$

$$N\varphi_{i-1} - \left(2N + \frac{10}{N}\right)\varphi_i + N\varphi_{i+1} = 0 \quad\Rightarrow\quad \varphi_{i-1} - \left[2 + \frac{10}{N^2}\right]\varphi_i + \varphi_{i+1} = 0$$

  - Let ϕ_{left} = 2 at x = 0 and ϕ_{right} = 3 at x = L = 1

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Finite-Volume Example (N = 5)

- System of equations to solve

$$\begin{aligned}
-2.4\phi_1 + \phi_2 &= -2\\
\phi_1 - 2.4\phi_2 + \phi_3 &= 0\\
\phi_2 - 2.4\phi_3 + \phi_4 &= 0\\
\phi_3 - 2.4\phi_4 &= -3
\end{aligned}$$

- Matrix form

$$\begin{bmatrix}-2.4 & 1 & 0 & 0\\ 1 & -2.4 & 1 & 0\\ 0 & 1 & -2.4 & 1\\ 0 & 0 & 1 & -2.4\end{bmatrix}\begin{bmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{bmatrix}=\begin{bmatrix}-2\\ 0\\ 0\\ -3\end{bmatrix}$$

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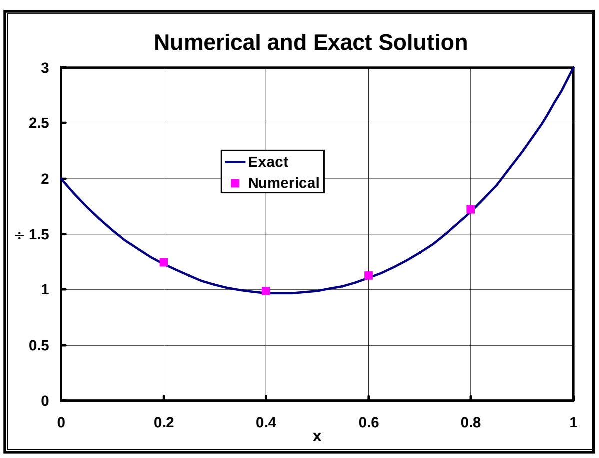

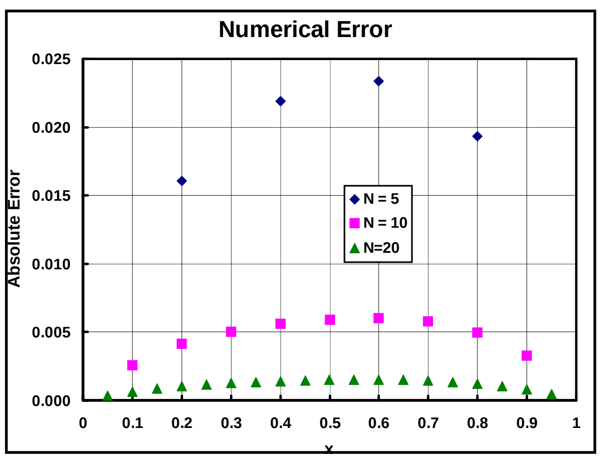

Error in Gradient

Exact d$\mathcal{H}$/dx at x = 0 is -5.54268				
	Second order		First Order	
	d$\mathcal{H}$/dx	Error	d$\mathcal{H}$/dx	Error
N = 5	-5.0175	0.5252	-3.7719	1.7708
N = 10	-5.3713	0.1713	-4.6014	0.9413
N = 20	-5.5024	0.0403	-5.0648	0.4779
Exact d$\mathcal{H}$/dx at x = L is 8.98450				
	Second order		First Order	
	d$\mathcal{H}$/dx	Error	d$\mathcal{H}$/dx	Error
N = 5	8.1181	0.8664	6.3976	2.5869
N = 10	8.7104	0.2741	7.5899	1.3946
N = 20	8.9184	0.0661	8.2704	0.7141

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Convection/Diffusion Algorithms

- Conservative schemes – conserve properties in finite difference equations
  - Requires exit flux from one face to be same as input flux in adjacent cell
- Transportive schemes – have correct balance between diffusion and convection
- Accuracy – need schemes that have a good truncation error

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Convection/Diffusion Algorithms II

- Limit on coefficient magnitude for iteration schemes (boundedness)
  - Absolute value of diagonal coefficient must be greater than the sum of absolute values of all other coefficients
    - For simple equations here $|a_P| \geq |a_E| + |a_W|$
  - Deferred correction separates coefficients into two parts
    - Adjustment leaves $|a_P| \geq |a_E| + |a_W|$
    - Places part removed from adjusted coefficients into source term

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Convection/Diffusion Terms

- Constant area result
  - Define F = ρu and D = Γ/δx

$$F_e\varphi_e - F_w\varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

- Different approaches for ϕ_e and ϕ_w
  - Central difference, upwind, hybrid, power-law, QUICK, TVD
  - All get relations among neighbor nodes
    - Three nodes for all but QUICK

$$a_W\varphi_W - a_P\varphi_P + a_E\varphi_E = 0$$

    - Special treatment for boundary nodes

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Example Problem

- Constant ρ, u, and Γ with $\phi = \phi_0$ at x = 0 and $\phi = \phi_L$ at x = L

$$\frac{d\rho u\varphi}{dx} = \frac{d}{dx}\Gamma\frac{d\varphi}{dx} \Rightarrow \frac{\rho u}{\Gamma}\frac{d\varphi}{dx} = \frac{d}{dx}\frac{d\varphi}{dx}$$

- Exact solution below with plot on next slide

$$\frac{\varphi(x) - \varphi_0}{\varphi_L - \varphi_0} = \frac{e^{\frac{\rho u x}{\Gamma}} - 1}{e^{\frac{\rho u L}{\Gamma}} - 1}$$

Pe = ρuL/Γ

Pe_{cell} = ρuδx/Γ = F/D

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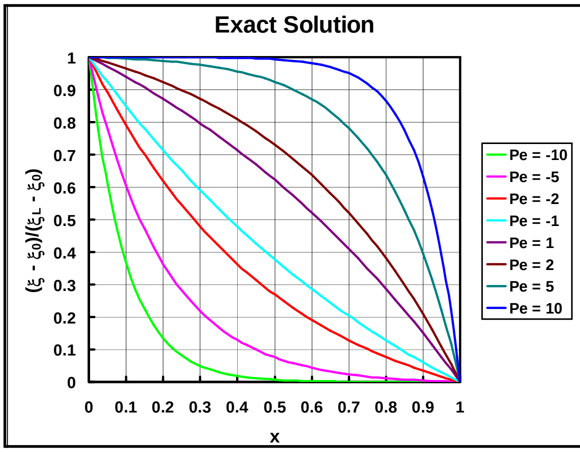

Central Difference

- Here δx, ρu and Γ are constants
  - $F_e = F_w = \rho u = F$ $D_e = D_w = \Gamma / \delta x = D$

$$a_W \varphi_W - a_P \varphi_P + a_E \varphi_E = \left(F + \frac{D}{2}\right)\varphi_W - 2F\varphi_P + \left(F - \frac{D}{2}\right)\varphi_E = 0$$

|-----•-----|-----•-----|-----•-----|-----•-----|-----•-----|-----•-----|
left 1 2 3 4 5 6 right

- Boundary conditions at x = 0 and x = L

$$-\left(\frac{F}{2} + 3D\right)\varphi_1 + \left(D - \frac{F}{2}\right)\varphi_2 = -(F + 2D)\varphi_{left}$$

$$\left(D + \frac{F}{2}\right)\varphi_{N-2} - \left(3D - \frac{F}{2}\right)\varphi_{N-1} = -(2D - F)\varphi_{right}$$

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Upwind Differences

|----------•----------|----------•----------|----------•----------|
W w P e E

- Computational formulas

$$a_W = D_w + \max(F_w, 0) \quad a_E = D_e + \max(-F_e, 0)$$
$$a_P = a_E + a_W + F_e - F_w$$

- Left boundary $a_W^* = 2D_w + \max(F_w, 0)$

$$-\left(a_E + a_W^* + F_e - F_w\right)\varphi_P + a_E \varphi_E = -a_W^* \varphi_{left}$$

- Right boundary $a_E^* = 2D_e + \max(-F_e, 0)$

$$a_W \varphi_W - \left(a_E^* + a_W + + F_e - F_w\right)\varphi_P = -a_E^* \varphi_{right}$$

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Hybrid Difference

- Computational Formulas

$$a_W = \max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right] \qquad a_E = \max\left[-F_e, \left(D_e + \frac{F_e}{2}\right), 0\right]$$

$$a_P = a_E + a_W + F_e - F_w$$

- Left boundary $a_W^* = \max[2D_w, (2D_w + F_w)]$

$$-\left(a_E + a_W^* + F_e - F_w\right)\varphi_P + a_E \varphi_E = -a_W^* \varphi_{left}$$

- Right boundary $a_E^* = \max[2D_e, (2D_e - F_e)]$

$$a_W \varphi_W - \left(a_E^* + a_W + F_e - F_w\right)\varphi_P = -a_E^* \varphi_{right}$$

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Power Law

- Computations $a_P = a_E + a_W + F_e - F_w$

$$a_W = D_w \max\left[0, \left(1 - |Pe_w|^5\right)\right] + \max[F_w, 0] \qquad Pe_w = F_w / D_w$$

$$a_E = D_e \max\left[0, \left(1 - |Pe_e|^5\right)\right] + \max[-F_e, 0] \qquad Pe_e = F_e / D_e$$

- Left boundary: get a^*_W with $D^*_w = 2D_w$

$$-\left(a_E + a_W^* + F_e - F_w\right)\varphi_P + a_E \varphi_E = -a_W^* \varphi_{left}$$

- Right boundary : get a^*_E with $D^*_e = 2D_e$

$$a_W \varphi_W - \left(a_E^* + a_W + F_e - F_w\right)\varphi_P = -a_E^* \varphi_{right}$$

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QUICK

- QUICK formulas for central node P involve five nodes instead of three

•-------|-------•-------|-------•-------|-------•-------|-------•
WW ww W w P e E ee EE

$$a_{WW}\varphi_{WW} + a_W \varphi_W - a_P \varphi_P + a_E \varphi_E + a_{EE}\varphi_{EE} = 0$$

$$a_W = D_w + \frac{6\alpha_w F_w + 3(1 - \alpha_w)F_w + \alpha_e F_e}{8} \qquad a_{WW} = -\frac{\alpha_w F_w}{8}$$

$$a_E = D_e - \frac{3\alpha_e F_e + 6(1 - \alpha_e)F_e + (1 - \alpha_w)F_w}{8} \qquad a_{EE} = \frac{(1 - \alpha_e)F_e}{8}$$

α_w = 1 if F_w > 0 and α_e = 1 if F_e > 0
α_w = 0 if F_w < 0 and α_e = 0 if F_e < 0

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QUICK II

- Boundary formulas (derivation in text)
  - Assume $F_e > 0$ and $F_w > 0$

First node from left	$a_W^* = \left(\frac{8}{3}D_w + \frac{1}{4}F_e + F_w\right)$ $a_E = \left(D_e + \frac{1}{3}D_w - \frac{3}{8}F_e\right)$ $-\left(a_E + a_W^* + F_e - F_w\right)\varphi_1 + a_E \varphi_2 = -a_W^* \varphi_{left}$
Second node from left	$a_{WW}^* = \frac{F_e}{4}$ $a_W = \left(D_w + \frac{7}{8}F_w + \frac{F_e}{8}\right)$ $a_E = D_e - \frac{3}{8}F_e$ $a_W \varphi_1 - \left(a_W + a_E + a_{WW}^* + F_e - F_w\right)\varphi_2 + a_E \varphi_3 = -a_{WW}^* \varphi_{left}$
Last node on right	$a_{WW} = \frac{F_w}{8}$ $a_W = \left(D_w + \frac{D_e}{3} + \frac{6F_w}{8}\right)$ $a_E^* = \frac{3}{8}D_e - F_e$ $a_{WW}\varphi_{N-3} + a_W \varphi_{N-2} - \left(a_{WW} + a_W + a_W^* + F_e - F_w\right)\varphi_{N-1} = -a_{WW}^* \varphi_N$

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Review TVD Algorithms

- Total Variation Diminishing schemes
  - Designed to maintain both accuracy and stability with no unphysical "wiggles"
  - Consider set of different differencing schemes for ϕ_e with positive u velocity
  - Work originated in transient gas dynamics
  - Later modifications to general CFD
  - Based on use of limiter functions that are applied to conventional formulas
  - Deferred correction required in iteration

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False Diffusion

- Upwind differencing causes errors similar to having a "diffusion" coefficient that is too large
- Causes smearing of results
- Especially noticeable in flows with sharp gradients and shock waves
- Effect is reduced if flow is aligned with grid (not always possible to do this)
- Different from artificial diffusion

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Review Navier-Stokes

- Continuity and momentum equations
- Apply previous work for general variable, ϕ, to finding u, v, and w
- Must consider nonlinearity (e.g., $u\phi$ can be uu, uv, or uw for momentum)
  - Use "outer iteration process"
    - Assume values for u, v, and w
    - Use these values to compute the convection/diffusion coefficients a_E, a_N, *etc*.
    - Use new u, v, w values to update a_E, a_N, *etc*.

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Navier-Stokes Approach

- Compressible flows
  - Solve continuity and momentum for three velocity components and density
  - Get pressure from equation of state
- Incompressible flows
  - Mach number is low
  - Density is a problem input, often related to temperature (may or may not be constant)
  - Solve continuity and momentum for three velocity components and pressure

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Incompressible Flows

- Mach number is low (< ~0.3)
- Density (e.g., $\rho = p/RT$) may depend on mean, but not local pressure
- Can have equations like $\rho = \rho_0(1 + \beta T)$ for where $\beta = -(1/\rho)(\partial\rho/\partial T)_P$
- Density may be constant, but need not be for incompressible flows
  - Furnace flows a good example of this
- Basic idea is that density does not depend on local pressure

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Steady 2D Problem

- Continuity and momentun equations
  - Have x and y direction convection-diffusion
  - Now have source term and pressure gradient

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

$$\frac{\partial \rho uu}{\partial x} + \frac{\partial \rho vu}{\partial y} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}\mu\frac{\partial u}{\partial x} + \frac{\partial}{\partial y}\mu\frac{\partial u}{\partial y} + S^{(u)}$$

$$\frac{\partial \rho uv}{\partial x} + \frac{\partial \rho vv}{\partial y} = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial x}\mu\frac{\partial v}{\partial x} + \frac{\partial}{\partial y}\mu\frac{\partial v}{\partial y} + S^{(v)}$$

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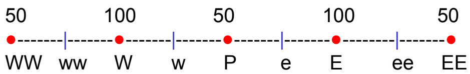
Problem with Pressure

- Consider the x momentum equation for the u velocity component at point P



- Second-order expression for pressure gradient at P $\left.\frac{\partial p}{\partial x}\right|_P = \frac{p_E - p_W}{2\delta x}$
- With this expression the velocity at P is not affected by the pressure at P
  - Also a checkerboard pattern of pressure would compute as zero pressure gradient

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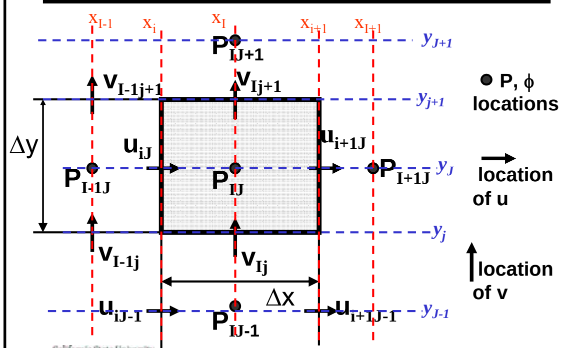
Staggered Grid



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Finite Volume Equations

- Extend previous results for one dimension to two dimensions
- Can use any of the difference methods discussed for convection and diffusion
  - Have four faces, n, e, s, w, in 2D
  - Apply same relations to get coefficients a_N, a_S, a_E, and a_W, using F = ρu and D = Γ/δ for each face
  - As before $a_P = (a_N + a_S + a_E + a_W + \Delta F)$
    - Here $\Delta F = (F_n - F_s) + (F_e - F_w)$

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Finite Volume Equations II

- Integration of pressure terms

$$\left(\int_{\Delta V} \frac{\partial p}{\partial x} dV\right)_{iJ} \approx \frac{p_{IJ} - p_{I-1J}}{x_I - x_{I-1}}(x_I - x_{I-1})A_{iJ}$$
$$= (p_{IJ} - p_{I-1J})A_{iJ} = (p_{IJ} - p_{I-1J})(y_{j+1} - y_j)\Delta z$$

$$\left(\int_{\Delta V} \frac{\partial p}{\partial y} dV\right)_{Ij} \approx \frac{p_{IJ} - p_{IJ-1}}{y_J - y_{J-1}}(y_J - y_{J-1})A_{Ij}$$
$$= (p_{IJ} - p_{IJ-1})A_{Ij} = (p_{IJ} - p_{I-1J})(x_{i+1} - x_i)\Delta z$$

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Finite Volume Equations III

- Have similar equations for u and v
- b represents integrated source term
- Note that a_K coefficients vary from node to node and are different for u and v

$$a_N u_{iJ+1} + a_S u_{iJ-1} + a_E u_{i+1J} + a_W u_{i-1J} - a_P u_{iJ}$$
$$a_{N_{iJ}}^{(u)} u_{iJ+1} \quad = (p_{IJ} - p_{I-1J})A_{iJ} + b_{iJ}^{(u)}$$

$$a_N v_{Ij+1} + a_S v_{iJ-1} + a_E v_{I+1j} + a_W v_{I-1j} - a_P v_{Ij}$$
$$a_{N_{Ij}}^{(v)} v_{Ij+1} \quad = (p_{IJ} - p_{IJ-1})A_{Ij} + b_{Ij}^{(v)}$$

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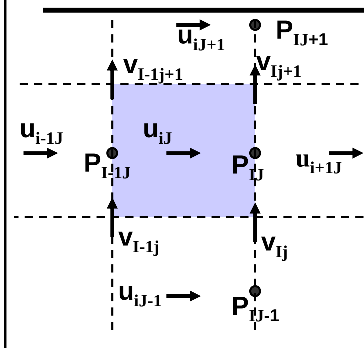
Control Volume for u (e face)



equations for e face at IJ

$$F_e = \frac{F_{i+1J} + F_{iJ}}{2} = \frac{1}{2}\left[\left(\frac{\rho_{IJ} + \rho_{I+1J}}{2}\right)u_{i+1J} + \left(\frac{\rho_{I-1J} + \rho_{IJ}}{2}\right)u_{iJ}\right]$$

$$D_e = \frac{\Gamma_{IJ}}{x_{i+1} - x_i}$$

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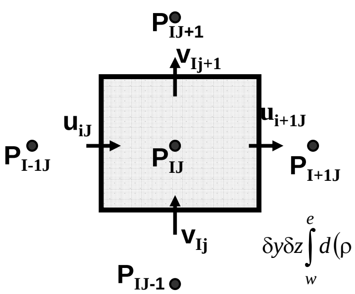
Integrated Continuity Equation



$$\int_{\Delta V}\left(\frac{\partial \rho u}{\partial x}+\frac{\partial \rho v}{\partial y}\right)dV=0$$

$$\int_{\Delta V}\frac{\partial \rho u}{\partial x}dxdydz+$$

$$\int_{\Delta V}\frac{\partial \rho v}{\partial y}dxdydz=0$$

$$\delta y\delta z\int_{w}^{e}d(\rho u)+\delta x\delta z\int_{s}^{n}d(\rho v)=0$$

$$\delta y\delta z\left[(\rho u)_e-(\rho u)_w\right]+\delta x\delta z\left[(\rho v)_n-(\rho v)_s\right]=0$$

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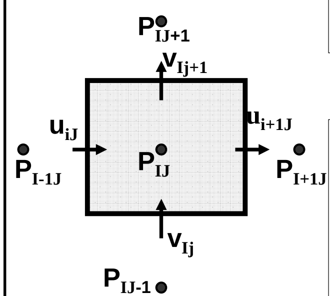
Integrated Continuity Equation II



$$\delta y\delta z\left[(\rho u)_e-(\rho u)_w\right]+\delta x\delta z\left[(\rho v)_n-(\rho v)_s\right]=0$$

$$\left[(\rho uA)_{i+1J}-(\rho uA)_{iJ}\right]+\left[(\rho vA)_{Ij+1}-(\rho vA)_{Ij}\right]=0$$

$$\frac{\rho_{I+1J}+\rho_{IJ}}{2}(uA)_{i+1J}-\frac{\rho_{IJ}+\rho_{I-1J}}{2}(uA)_{iJ}+\frac{\rho_{IJ+1}+\rho_{IJ}}{2}(vA)_{Ij+1}-\frac{\rho_{IJ}+\rho_{IJ-1}}{2}(vA)_{Ij}=0$$

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SIMPLE

- Solves for pressures and velocities
  - Start with guessed pressures, p*
  - Solve momentum equations for u* and v* based on p* pressures
  - Get correction pressure equation by substituting finite-volume equations for u and v into finite-volume continuity
  - Work with correction terms p = p + p’

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p’ Equation Terms

$$b_{IJ}^{'}=\frac{\rho_{I+1J}+\rho_{IJ}}{2}A_{i+1J}u_{i+1J}^{*}-\frac{\rho_{IJ}+\rho_{I-1J}}{2}A_{iJ}u_{iJ}^{*}+\frac{\rho_{IJ+1}+\rho_{IJ}}{2}A_{Ij+1}v_{Ij+1}^{*}-\frac{\rho_{IJ}+\rho_{IJ-1}}{2}A_{Ij}v_{Ij}^{*}$$

$$a_{I+1J}=\frac{\rho_{I+1J}+\rho_{IJ}}{2}A_{i+1J}d_{i+1J}\qquad d_{i+1J}=\frac{A_{i+1J}}{a_{i+1J}}$$

$$a_{I-1J}=\frac{\rho_{IJ}+\rho_{I-1J}}{2}A_{iJ}d_{iJ}\qquad d_{iJ}=\frac{A_{iJ}}{a_{iJ}}$$

$$a_{IJ+1}=\frac{\rho_{IJ+1}+\rho_{IJ}}{2}A_{Ij+1}d_{Ij+1}\qquad d_{Ij+1}=\frac{A_{Ij+1}}{a_{Ij+1}}$$

$$a_{IJ-1}=\frac{\rho_{IJ}+\rho_{IJ-1}}{2}A_{Ij}d_{Ij}\qquad d_{Ij}=\frac{A_{Ij}}{a_{Ij}}$$

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SIMPLE Equation for p’

$$a_{IJ}=a_{I+1J}+a_{I-1J}+a_{IJ+1}+a_{IJ-1}$$

$$a_{I+1J}p_{I+1J}^{'}+a_{I-1J}p_{I-1J}^{'}+a_{IJ+1}p_{IJ+1}^{'}+a_{IJ-1}p_{IJ+1}^{'}-a_{IJ}p_{IJ}^{'}=b_{IJ}^{'}$$

- Like other equations, p’ relates values at a central node to values at the four nearest neighbors
- Similar solution algorithms

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Using Corrections

- Use of p = p* + p’ can lead to divergence
  - Use underrelaxation: p = p* + α_pp’, where α_p is the underrelaxation factor (0 < α_p < 1)
- Similar underrelaxation factors (between 0 and 1) for velocity correction

$$u_{iJ}=u_{iJ}^{*}+\alpha_u\left(p_{I-1J}^{'}-p_{IJ}^{'}\right)d_{iJ}$$

$$v_{Ij}=v_{Ij}^{*}+\alpha_v\left(p_{IJ-1}^{'}-p_{IJ}^{'}\right)d_{Ij}$$

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SIMPLE Algorithm

0. Start with initial guesses for p*, u*, v*
1. Start iterations
2. Compute coefficients in finite volume equations for momentum and pressure
3. Do an iteration on u* and v* equations
4. Get p' source term
5. Do an iteration on p' equation
6. Use p' to correct p*, u*, and v
7. Check convergence; if not converged return to step 1

Variations on Simple

- SIMPLEC
  - SIMPLE Consistent
  - Small correction to p' equation
- SIMPLER
  - SIMPLE Revised
  - Has two correction equations
- PISO
  - Pressure Implicit with Splitting of Operators
  - With two correction equations, originally intended for transient problems

SIMPLEC

- Almost the same as SIMPLE except for a small correction to the d terms
- Rationale: reduce the effect of neglecting the neighboring correction velocities in SIMPLE

$$d_{iJ} = \frac{A_{iJ}}{a_{iJ}} \quad \Rightarrow \quad d_{iJ} = \frac{A_{iJ}}{a_{iJ} - \sum a_{nb}}$$

$$d_{Ij} = \frac{A_{Ij}}{a_{Ij}} \quad \Rightarrow \quad d_{Ij} = \frac{A_{Ij}}{a_{Ij} - \sum a_{nb}}$$

SIMPLER Algorithm

0. Start with initial guesses for p*, u*, v*
1. Start iterations
2. Compute coefficients in finite volume equations for momentum and pressure
3. Compute u-hat and v-hat terms
4. Do an iteration on pressure
5. With p just found iterate momentum
6. Compute source terms for p'
7. Do an iteration on p' equation
8. Use p' to correct u* and v* only
9. Check convergence; if not converged return to step 1

PISO Algorithm

0. Start with initial guesses for p*, u*, v*
1. Start iterations
2. Compute coefficients in finite volume equations for momentum and pressure
3. Iterate momentum equations to update u* and v* using p* for pressure
4. Form and iterate equations for p'
5. Use p' to get u** and v**
6. Form and iterate equations for p"
7. Use p" to get second corrections on pressure and velocities
8. Check convergence; if not converged return to step 1

Comparison of Methods

- Each method solves the momentum equations for u and v plus some one or two other equations
  - Chorin's original 1967 approach solves for u, v, p, and velocity correction
  - SIMPLE, SIMPLEC solve for u, v, and p'
  - SIMPLER solves u, v, p, and p' as a velocity correction only
  - PISO solves for u, v, p', p" where both p' and p" correct both pressure and velocity

Which Is Better?

- SIMPLE is still used in commercial CFD codes and gets good solutions
- Other methods, although solving an extra equation can take less time
- Hard to distinguish between others
- PISO good when other properties not linked to momentum equtions
- PISO also good for transient problems
- Different relaxation factors in each

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Midterm Exam

- Open book and notes
- Homework solutions not allowed
- Problems similar to homework
  - No problems from first homework assignment
  - Turbulence relationships
  - Forming and solving finite-volume equations

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