Miscellaneous Topics and Review for Final Exam

Larry Caretto
Mechanical Engineering 692

Computational Fluid Dynamics

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Outline

- Student presentation schedule
- Improving accuracy
- Other topics
  - Reacting flows
  - Two-phase flows
  - Heat transfer including radiation and conjugate heat transfer
  - Moving grids
  - Free surface flows
- Review for final

Student Projects Schedule

- Schedule is 8-9 minutes per student
  - Includes time for questions and time for setup
  - Bring any presentations on memory sticks
  - Can submit your presentation and wirtten report electronically
- Seven students per night
  - Volunteers for Monday or draw names from hat
  - Same for who goes first each night
- Each student rates each speaker

Improving Accuracy

- Two kinds of decisions programmers and users
- Programmers can decide order of error to provide and models to use for approximate phenomena
- Users can control mesh size and quality, set convergence criteria for iteration errors
- Users can also check for blunders

Convergence Criteria

- Seek balance between accuracy and computer time
  - We have seen that accurate solutions of the finite difference equations are no help if the truncation error has been reached
  - Typical choice is to use residuals that are 10^{-3} to 10^{-4} of the original residuals
  - Using change from iteration to iteration is less effective because these changes are small for a fine grid

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Ensuring Convergence

- Some problems are inherently transient and will not reach a steady state
- Monitor important physical variables with iterations to ensure that the iteration-to-iteration change is less than the desired accuracy
- In principle the errors should decrease with iterations, but this does not always occur in complex flows

Some Convergence Checks

- Examine results after convergence at a loose tolerance
- Set more stringent convergence error
- Compare differences in results to ensure no significant changes
- Examine effects on overall properties of interest (lift coefficient, wall heat transfer)
  - Can create dynamic plots of these to view during execution

Truncation Error

- Determine this by refining the grid
- Use two or three grids with different spacing differing by a factor of two
  - Once an appropriate grid size has been determined for one problem, it can be used for other problems with similar geometry
  - Factor of two difference is rule of thumb, but small changes in grid size may not have much effect
- Solution should be grid independent

Truncation Error II

- Three grids where grid density is increased by a factor of r (r ≈ 1.2 to 2)
  - ϕ_h is solution on grid with average step h
  - Estimate order of method, p, from top equation
  - Use Richardson extrapolation given by second equation to get final result

$$p = \frac{\log\left(\frac{\left|\phi_{rh} - \phi_{r^2h}\right|}{\left|\phi_h - \phi_{rh}\right|}\right)}{\log r}$$

$$\phi_{final} = \frac{\phi_h - \phi_{rh}}{r^p - 1}$$

Other Truncation Checks

- Plot results *versus* 1/N where N is the number of grid nodes and extrapolate to 1/N = 0
- Can use equations below to estimate errors on different grid sizes using Richardson extrapolation
- Roach recommends multiplying these error estimated by a safety factor (conservative safety factor is 3)

$$E_h = \frac{\phi_h - \phi_{rh}}{r^p - 1} \qquad E_{rh} = r^p \frac{\phi_h - \phi_{rh}}{r^p - 1}$$

Model Errors

- Models for turbulence, reacting flows, two-phase flow, etc. may have assumptions that are not met
- Review advice on selecting turbulence models, wall functions, parameters in turbulence models in lecture on turbulence
- Variation of physical properties (density, viscosity, *etc*.) could be important for large temperature variation

Reducing Errors

- Try to compare modeled results with experimental data for problem similar to yours
- Look at use of code for similar problems with analytical solution
- Use common sense tests
  - Compare results to similar problems and look for values that seem too high or low
- Have someone else check the results for possible errors

Global Conservation Checks

- Check to see that overall mass, momentum and energy are conserved
- Mass in = mass out
- Momentum out = momentum in + net forces
  - Net forces include wall shear, pressure and buoyancy
- Energy in = energy out + heat added
- Good balances do not assure correct results, but bad balances are a problem

Steady-state Checks

- Have solutions really converged to a steady state for a steady-state problem
- Sometimes you can get low residuals while the parameter you are really interested in is changing
- Get dynamic plots of important parameters *versus* iterations to better show attainment of steady state
  - Can always examine final results with different convergence criteria

Grids

- The most significant factor affecting accuracy, that users control, is the grid
- For complex geometry it is not only the grid spacing, but also the configuration of the grid that matters
- Ideally each control volume would be a square or an equilateral triangle
  - In three-dimensions a cube or a tetrahedron with four equal sides

Grid Accuracy

- Ideal control volumes are both “orthogonal” and equal-sided
  - Orthogonality means that lines between control volume centers are perpendicular to the control volume sides
  - Reduces errors in using difference expressions for gradient terms
  - Equal-sided avoids aspect ratios significantly different from 1:1 that affect convergence
- Use grid quality checks in code

Grid Recommendations

- Cluster nodes in regions of sharp changes
  - shear layers, separated regions, shock waves, boundary layers, and mixing zones
  - boundary layer must have fine mesh for accurate computation of wall shear stress and heat transfer
  - turbulent flows should have wall spacing that gives appropriate values of y+

Grid Recommendations II

- Use adaptive grid procedures if available (as in Fluent)
- Keep grid changes smooth
  - Avoid sharp changes in grid spacing between adjacent cells. Use expansion coefficients no greater than 1.3
- Cell angles and aspect ratios
  - Avoid highly skewed cells and large aspect ratios.

Grid Recommendations III

- Match mesh design to expected flow patterns
- Better accuracy if flow follows mesh lines
- Not always possible to achieve for complex flows
- Can use in refining meshes based on initial solutions

Simplifying Assumptions

- Estimate validity of simplifying assumptions
  - Two-dimensional instead of three-dimensional flows
  - Laminar flows for transition Reynolds numbers
  - Ignoring different species or different phases in a mixture
  - Assuming steady state for flows that are periodic
  - Assuming incompressible flow

Verification and Validation

- Verification examines the possible sources of error in solving the CFD problem and tries to quantify the errors in the CFD solution
- Validation seeks comparison with experimental data to show that code has modeled the process correctly
- Validation also assesses errors in input data and their effect on results

Special Applications

- Flows with chemical reactions
- Turbulent reacting flows (combustion)
- Multiphase flows (particles in air, bubbles in boiling fluids)
- Heat transfer
  - Conjugate heat transfer: analysis of both fluid and wall heat transfer
  - Radiation heat transfer
- Moving grids
- Free surface flows

Reacting Flows

- Have chemical reaction rate as source term in species balance equation
- Reaction rates found by empirical equations or by detailed mechanisms
  - Described detailed steps in going from reactants to products via intermediates
  - Example, reaction of H_2 + O_2 to produce water involves species like OH, H, O, and HO_2 with 20 to 50 individual reactions
  - CHEMKIN commercial tool for chemical kinetics

Chemical Reactions II

- Have to solve partial differential equation for each species in mechanism
- Can get some species by element conservation
- Simple models use a single variable to assess progress of overall reaction

$$\frac{\partial \rho W^{(K)}}{\partial t} + \frac{\partial \rho u_i W^{(K)}}{\partial x_i} = \frac{\partial}{\partial x_i} \rho D_{K,mix} \frac{\partial_i W^{(K)}}{\partial x_i} + s^{(K)}$$

Turbulent Reacting Flows

- Important for range of practical combustion problems in aerospace and terrestrial applications
- Many models available typically based on two extremes: reaction limited and mixing limited
- Cases where reactants are premixed versus where they enter reaction zone unmixed

Turbulent Reacting Flows II

- Flame front models are mixing limited models that assume once reactants mix they burn
- More complex models use probability density functions (PDF) for reactants
- Other models use laminar flamlets to include chemical kinetics
- Such models are computationally intensive but address important enginering problems

Two-Phase Flows

- Many engineering problems
  - Liquid or solid particles in a gas flow
  - Gas bubbles in a liquid (vaporization)
  - Liquid and powder sprays
  - Fluidized beds
  - Flow through porous media
- The different phases can transfer momentum, energy and species
  - In equilibrium models the properties of both phases are the same

Two-phase Flows II

- For non-equilibrium models we need drag laws for momentum transfer, and interphase heat and mass transfer relationships which are usually empirical
- Have complex problems such as pulverized coal combustion where coal particles have surface reactions and transfer volatile materials to gas phase

Heat Transfer

- In multispecies flows can have cross effects known as thermal diffusion, and diffusion thermo
- Radiation heat transfer does not fit the usual general transport equation
  - Approximate models for radiation use directional radiation fluxes I in plus x and J in minus x direction
  - Solve equations for I and J which are then used in energy equation source term

Conjugate Heat Transfer

- Simultaneous solution of energy transfer in fluid and adjacent solid
- Solve conduction heat transfer problem in solid with appropriate boundary conditions for solid
- At fluid-solid interface the heat flux computed for each phase must match

Moving Grids

- Used for rotating machinerhy, piston engines and free surface flows such as wave motion
- Derive basic equations with boundary velocity, $\mathbf{v}_b$, to give relative velocity, $\mathbf{v} - \mathbf{v}_b$ in transport equations
- Problem in ensuring conservation
  - Use space conservation law for moving velocity, $\mathbf{v}_b$

$$\frac{d}{dt}\int_{\Omega} d\Omega - \int_{S} \mathbf{v}_b \cdot \mathbf{n} dS = 0$$

Free Surface Flows

- Adds problem of finding interface to previous problem of moving grid
- Have boundary conditions at the interface of the two fluids
  - Must account for surface tension
- Different types of methods
  - Interface tracking methods
  - Interface capturing methods
    - Marker and cell (MAC) and volume of fluid (VOF) methods

Finite Elements

- Entirely different approach from that used in class
- Somewhat similar to finite-volume
  - Some authors claim that it is equivalent to a FEM known as collocation
- Representing variables over an element by an interpolation function
  - Interpolation data are element whose coordinate values are known, but whose flow variables are unknown

Finite Elements II

- Typically use a method of weighted residuals to satisfy approximate differential equation (with interpolated values) in an approximate sense
- Approach known as Galerkin’s method
  - For CFD a variant known as Petrov-Galerkin is used
- Some commercial codes use FEM
  - Adapted from FEM solutions of other equations for stress, heat transfer, etc.

CFD Conclusion

- Quote from Oran and Boris, *Numerical Simulation of Reactive Flow*, Elsevier, 1987, p 572.

Maintain a healthy skepticism. Nothing works until it is well tested, and probably not even then.

Final Exam

- Monday, May 10
- From 8 to 10 pm in this room
- Final will be open book and notes
- Problems will be similar to homework and midterm problems
  - Remote possibility of asking essay question or review of brief article
  - Also remote possibility of definition questions, e.g. what are wall functions?

Outline for Review

- Go over course outline
- Mention important points about each topic
- Discuss the items that are likely to be included in the final exam
- No final exam questions have been formulated yet

Equations of Fluid Dynamics

- Be familiar with applying these equations including the general transport equation and simplifications for constant properties
- Will not have any questions like those on first homework set that deal with manipulations of the equations
- Equations are used in various algorithms that will appear in questions

Turbulence

- Models needed for turbulent flows
- Nature of turbulence
- Reynolds-average Navier-Stokes (RNS)
- Mixing length theory
- Models using one differential equation
- Two-equation models, especially k–ε
- Reynolds stress models
- Large-eddy simulation (LES)
- Direct numerical simulation (DNS)

Turbulence on the Final

- This is one area where there may be an essay type question such as discuss the various turbulence models that can be used and explain the pros and cons of the different models.
- You should understand how models are used and the role of wall functions in getting boundary conditions
    - Grid width near the wall depends on the turbulence structure – $y^+ \approx 30$

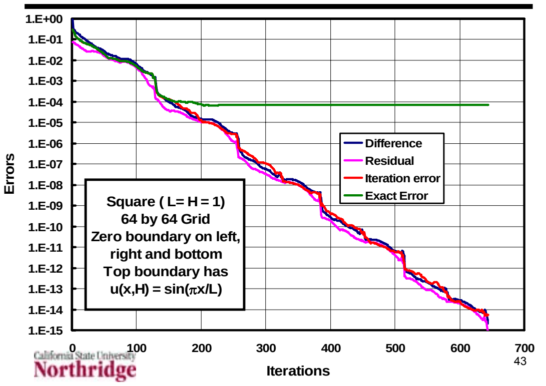
Numerical Analysis

- Be familiar with both finite-difference and finite-volume approaches
- May be questions like second question on midterm on using finite-difference or finite-volume expressions for data or functions
- Understand truncation error and roundoff error
- Uniform and nonuniform grid sizes

Solving Algebraic Equations

- Be able to apply common iterative techniques such as Gauss-Seidel and SOR
- Understand difference between actual iteration error (unknown) and computable error estimates
- Understand difference between error in solving equations by iteration and truncation error (see next slide)

Effects of Iterations on Laplace Equation Errors



Square (L= H = 1)
64 by 64 Grid
Zero boundary on left, right and bottom
Top boundary has
u(x,H) = sin(πx/L)

Numerical Analysis of PDEs

- Analysis by finite-difference and finite-volume methods
- Construct grid in one to three space dimensions and time
- Explicit and implicit approaches
- Obtain algebraic equations to be solved for values of flow variables at set of points (nodes) in the flow field
- Apply appropriate boundary conditions at nodes on boundaries

Stability Considerations

- Keeping iterations stable
- Absolute *vs*. conditional stability
- Mainly a problem for explicit methods
- Some implicit methods may remain stable, but give incorrect results
- von Neumann stability analysis
  - Finite difference equation as error equation
  - Substitute Fourier components
  - Solve for growth factor

General Transport Equations

- Understand both central and upwind difference approaches
  - Different coefficients used to relate values at a central node to those of nearest neighbors
- Be able to use other equations that may be given to you
  - Finding coefficients from data on a grid
  - Setting coefficients into the iteration process

Incompressible Navier Stokes

- Density constant or given by equation that does not involve local pressure
- Solve momentum equations for velocity components at guessed pressure
- Combine continuity momentum to get difference equation for pressure
- Inner and outer iterations
- Linearizing coefficients
- Understand overall process for final

Correction Procedures

- Start with initial conditions on u, v, p
- Iterate on the momentum equations for fixed p to get the new u and v values
- Compute u* and v* with p*
- Compute mass sources and pressure equation coefficients
- Iterate pressure equation to get new p
- Correct velocities with new pressure gradient terms

Correction Methods

- Origin with Chorin (1967)
- Patankar and Spalding developed SIMPLE
- Later improvements to SIMPLE include SIMPEC, SIMPLER, and PISO
  - Relaxation factors required for SIMPLE not so critical for PISO or SIMPLER
- Common algorithms in current commercial CFD codes

Transportive Property

- Solution to $\partial u/\partial t + c\partial \phi/\partial x$ is $\phi(x,t) = f(x - ct)$ where $f(\xi)$ is the initial condition for ϕ
- Discontinuities in the initial conditions are propagated in the solution
- Algorithms that do this can resolve shocks properly
- Difficult to construct algorithm that can resolve shock without dispersion or dissipation errors
- TVD methods try to do this

Final Exam Navier Stokes

- No clear idea of specific questions to ask at this time
- Place less emphasis on number crunching on any potential final exam problem
- Understand following items
  - The overall calculation cycle
  - The individual equations used in the cycle
  - The importance of relaxation factors