Quality and trust of CFD analyses

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1. Model uncertainties

Experimental observations ↔ Analytical solution of the governing equations

Because we solve the wrong equations.

- Turbulent models.
- Is it really a steady flow?
- Equation of state.
  (Is it an really an ideal gas?)
- Non-newtonian characteristics.
- Simplification of chemical reactions.

Aims of comparing our results …

I. **Debugging:**
Are the governing equation correctly approximated and solved?
Do the results converge towards the analytic solution?
Does the order of convergence meet the formal order?
Results can be compared with analytic solutions or to more exact numerical solutions.

II. **Validation:**
Are the model equations correct?
Are the boundary conditions appropriate?
Results must be compared with measured data.

III. **Calibration:**
Tuning of some important model parameter on the basis of measured data.
The calibrated model is hoped to be able to predict tendencies, therefore it is useful in engineering optimization or for exploring the dynamics of the process.

2. Discretization error

Analytical solution of the governing equations ↔ Exact solution of the discretized equations

- Can be reducer by refinement of the numerical resolution.
- Order of convergence can be predicted on the basis of the magnitude of terms omitted from the Taylor series when deriving the solution.
- Ideally, the discretization error of a first order scheme is proportional to the numerical resolution and it is proportional to the square of the numerical resolution for second order schemes.
- It can come from spatial and from temporal discretization.
- Sometimes - depending on mesh quality, on cell Reynolds number (when upwinding is used) and on boundary layer mesh - the numerical solution does not meet the formal order of convergence.
- Order of convergence need to be measured by systematic mesh refinement.

Errors and uncertainties

Exact ↔ Approximate

- **Error**:
  The reason is known. It comes from intentional approximations. Can be reduced by increased computational effort or with more elaborated numerical methods.
- **Uncertainties**:
  Its magnitude cannot be estimated, because the reason is not described in mathematical terms. Cannot be reduced by increased computational effort.

Error estimation and extrapolation to the grid-independent solution

- The refinement need to be substantial, e.g. interval halving: number of cells are increased by a factor of 8. The necessary minimum increase in linear resolution is about 1.5, which leads to a factor of 3.4 increase in the number of cells.
- At least consecutive refinements are necessary (Φ_{4h} is already "fine enough"):
  Course mesh: Φ_{4h},
  Practical mesh: Φ_{2h},
  Fine mesh: Φ_h.
- Refinement must be uniform, and the grid quality (skewnes, aspect ratio…) must be preserved.
- Attention! Low of the wall can be violated due to the refinement, which is another important source of modeling error.
  Grid independent solution can be estimated by using Richardson extrapolation:

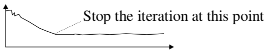
$$\varepsilon_h \cong \frac{\Phi_h - \Phi_{2h}}{r^p - 1}, \qquad p = \log\left(\frac{\Phi_{2h} - \Phi_{4h}}{\Phi_h - \Phi_{2h}}\right)$$

- Φ can be an integral property or field variable, in the later case we can monitor the error distribution as well.
- E.g. the error of a first order scheme on the finer mesh can be estimated by the difference between the solutions obtained on the fine and coarse grids if linear interval halving (r=2) is used.

3. Iteration error

Converged solution ↔ Partially converged solution

- Does it converge at all? If not:
  1. is it a grid problem;
  2. contradicting boundary conditions;
  3. the applied turbulent model does not stabilize the solution > try running it in unsteady mode (URANS).
- Monitor the residuals! Iteration error is proportional to the residuals (excepting for the very beginning of the iteration process.) The initial error is limited too, therefore a factor of 10^{-3} reduction in the error usually acceptable from practical point of view.
- When the solution seems to be converged the underrelaxation factors can be increased for checking convergence.
- We can start the iteration from another initial state.
- There are some slowly converging properties e.g. wall friction and drag force. We can monitor the convergence of these properties too.
- Iteration error cannot be reduced below the truncation error:



Geometrical uncertainties

- The real geometry differs from the original design. (production aspect e.g. manufacturing were taken into account);
- Even little details can have great fluid mechanical significance:
  - tip clearance in axial fans;
  - wall roughness caused by welding.
- When the geometry has a fine geometrical structure porous zone models are often used. Parameterization of such zones can have an impact on the solution. > Flow micro structure can be analyzed via micro-modeling.
- Geometry can be deformed under working conditions due to mechanical load (e.g. tent roofs). Fluid-structure interaction is one of the cutting edge modeling issues.
  FLUENT – ABACUS / CFX – ANSYS

4. Truncation error

Solution with infinitely precise numbers ↔ Solution with finitely precise numbers

- Default precision in FLUENT is 4 bytes (some 7 digits), and we can use double precision too.
- Some flows are known to be sensitive for precision of storage:
  - low Re turbulent models;
  - natural convection with small temperature difference;
  - radiation heat transfer;
  - mixture model with low concentrations;
  - massive hydrostatic (equilibrium) pressure gradients.

Uncertainties of boundary conditions

- In most cases only the flow rate is known, but the simulation requires profiles for magnitude and direction.
- Inlet profiles for turbulent quantities are usually not known. ε cannot be measured either.
- We can carry out sensitivity studies by perturbing the boundary conditions.
- The increase in geometrical extent of the domain reduces boundary dependence of the most important part of the flow. Dependence on upstream BC is larger than dose of downstream BC. (E.g. a box should be added from outside to the building when modeling natural convection through a door.)
- Atmospheric flow calculations are very sensitive for the inlet profiles for turbulent quantities. ε profiles being far from the equilibrium can cause an abrupt change in the velocity profile. (We can run e.g. a 2D pre-calculation for the inlet profiles.)
- Large Eddy Simulation is very sensitive for boundary conditions. Realistic (turbulent like) fluctuation must be added to the time averaged inlet velocity profile.

5. Application uncertainties

Because we are working with the wrong data.

- Geometrical uncertainties;
- Uncertainties of boundary conditions;
- Uncertainties of material properties.

Uncertainties in fluid properties

Only two examples:

- Atmospheric pressure and temperature:
  p: 900 – 1050 kPa → 15 %
  T: 253 – 313 K → 22 %
- Kinematical viscosity of water between 100 and 20 °C:
  $0.25 * 10^{-6} \dots 1 * 10^{-6}$ m^2/s → 400 %

Summary

1. Model uncertainties
2. Discretization error
3. Iteration error
4. Truncation error
5. Application uncertainties
   - Geometry
   - Boundary conditions
   - Fluid properties
6. User errors
7. Software errors