

7 Best practice guidelines

Computational fluid dynamics does not provide an exact solution to all problems, but is in many cases a reliable tool that can provide useful results when it is employed by an experienced user. An inexperienced user, on the other hand, may obtain very nice graphs that are very far from being a prediction of the stated problem. Some of the problems arise from the many default settings in commercial CFD codes, since the user may obtain results without knowing what the code is doing by accepting settings that are not appropriate for the specific problem. The user must make an active decision regarding each setting due to the fact that many problems can arise from a user failing to understand what the proper settings should be. This chapter provides some guidelines that can help a new user to avoid the most common mistakes. Many more recommendations selected by experienced CFD users can be found in the ‘Best Practice Guidelines’ for single-phase flows [20] and for dispersed multiphase flows [21] by the European Research Community on Flow Turbulence and Combustion (ERCOFTAC).

A CFD simulation contains both errors and uncertainties. An *error* is defined as a recognizable deficiency that is not due to a lack of knowledge, whereas an *uncertainty* is a potential deficiency that is due to a lack of knowledge.

Poor simulation results may arise for many different reasons; the user may make mistakes in formulating the problem to solve or in formulating the geometry and meshing. Numerical errors may occur due to lack of convergence and a poor choice of discretization methods. The models for turbulence, reactions and multiphase flow are not exact descriptions of the real world, and poor results may be introduced by not selecting the best model for the specific case. In the end, the robustness and reliability of the simulations should be analysed by sensitivity analysis, verification, validation and calibration.

In general, it is good practice to study the obtained simulation results critically. CFD is not (yet) at the stage at which it can be treated as a black box. Simulation results should be verified with experimental findings, fluid-mechanics theory and, sometimes, instinct. It may also help to understand the limitations of the CFD model if a simulation is performed for a case regarding which the results are known, prior to exploring new ground with the model. Some common errors and recommendations for best practice are given in this chapter.

7.1 Application uncertainty

Many problems in CFD simulations arise from inaccurately stated problems. The actual problem that is being solved is not always straightforward. It is seldom possible to select the right settings from the beginning. The properties of the flow are not all known in advance. The flow can be laminar or turbulent, or laminar in some regions and turbulent in other regions. The local hold-up in multiphase flow and the local Damköhler number in reacting systems can affect the choice of model. The flow within the system may also affect the flow at the inlet and the outlet. These are just a few of the possibilities.

7.1.1 Geometry and grid design

A number of general guidelines can be given.

- Make sure that the CAD geometry is complete for the flow simulation. The CAD drawing should be kept as simple as possible, but it must not be simpler than that. All details smaller than the computational cells can in most cases be removed, but small details on the surface can sometimes be important for the flow, e.g. a welded joint may induce flow separation.
- Symmetric boundary conditions restrict the solution to a symmetric solution, and no transport is allowed across the symmetry plane, e.g. bubble columns and fluidized beds are poorly described by 2D simulations.
- When the inflow and outflow are not known exactly, they should be put far from the region of interest.
- With constant-pressure outflow, specify the direction of the outflow (e.g. normal to the plane) to minimize the pressure difference across the surface.
- Use pressure outflow for multiple outflow boundaries.
- Avoid having non-orthogonal cells close to the boundaries. The angle between the grid lines and the boundary should be close to 90° . Use body-fitted grids when the grid cannot be aligned with the surface.
- Avoid the use of highly skewed cells. The angles should be kept between 40° and 140° . The maximum skewness should be <0.95 and the average below 0.33. The aspect ratio should be below 5, but may be up to 10 inside the boundary layer.
- The squish index describes how the cell faces are oriented, where 0 is a perfect cell and the upper limit is 1. The recommendation is that the maximum squish index should be below 0.99.
- Perform a grid check to avoid problems due to incorrect connectivity. This can often be done in the mesh-generator software.

7.2 Numerical uncertainty

7.2.1 Convergence

Poor convergence is the most common numerical reason for poor results. Residuals are defined differently in various programs, and monitoring the residual is in most cases not sufficient to verify that a converged solution has been reached. Convergence problems

for steady-state simulations may also indicate that a steady solution does not exist. The residual should always be combined with other measures of convergence. Keep in mind that a converged solution is not always a correct one.

- Use different convergence criteria for different variables. Concentration may need a lower residual than velocity.
- Monitor integral quantities of solution-sensitive variables.
- Make global balances for mass, momentum and energy.
- Monitor the solution at specific important points.
- Test for steady state by switching to a transient solver.
- Plot the residual to evaluate whether the solution is poor in some regions of the computational domain.

7.2.2 Enhancing convergence

There are many different methods by which to enhance convergence.

- Use more robust numerical schemes, e.g. initially employ first-order upwind, changing to a higher order for the final iterations.
- Reduce the under-relaxation or CFL number initially.
- Examine the local residual. The convergence problem might be localized to one small region. Use grid adaptation to refine or coarsen the mesh in areas where it is needed. Using a fine grid throughout may diminish the convergence rate.
- Solve steady-state problems transiently.
- Try different initial guesses, e.g. obtain an initial guess from a short transient simulation or obtain an initial guess from a steady-state simulation.
- Solve for only a few variables at a time, e.g. solve for the flow field first and keep the velocities constant whilst solving concentration and chemical reactions. Finally solve for all variables.
- Use the coupled solver for high-speed compressible flows, highly coupled flows with strong body forces or flows being solved on very fine meshes. Keep in mind that the coupled solver requires 1.5–2 times more memory than needed by a segregated solver.

7.2.3 Numerical errors

The numerical error is the difference between the exact solution and the numerical solution.

- Avoid the use of first-order schemes. First order can be used initially when you have convergence problems, but will always lead to problems with numerical diffusion.
- Estimate the discretization error by showing that the solution is independent of the mesh density.
- Use node-based gradients with unstructured tetrahedral meshes.
- If possible, compare the solutions with different orders of accuracy.

- Perform refinement or coarsening of the computational mesh. Ideally, the solution should become less dependent on the mesh as it is refined. If the results reveal a strong dependence on the computational mesh spacing, further refinement is required.

7.2.4 Temporal discretization

The choice of time step depends on the flow features being studied. Large-eddy simulation requires very short time steps to resolve the turbulent eddies. Some of the turbulent structures can also be resolved with RANS models, i.e. unsteady RANS or URANS, but usually the time step is much larger than the turbulence timescales and only the transient behaviour of the mean flow is resolved.

- Start with a short time step, i.e. a low CLF number that can increase with time.
- The time step should be selected so that fewer than 20 iterations are needed in each time step with an implicit solver.
- Make sure that the solution has converged for each iteration for implicit schemes.
- For temporal accuracy, a second-order-accurate discretization scheme is recommended, such as Crank–Nicolson or second-order backward Euler.

7.3 Turbulence modelling

Only DNS is an exact formulation of the Navier–Stokes equations. All other turbulence models contain model approximations. Table 4.4 contains a comparison of turbulence models.

- Test different turbulence models. The cost of running a second model starting from a converged solution is usually not high. Different values of the model constants that are recommended for specific kinds of flows should also be tested.
- Transition between turbulent and laminar flow is very difficult to simulate for all models. Simulations involving transition must be verified with experimental data.
- Be aware of the limitations of the specific model, e.g. the k – ε model will suppress swirl in a flow and the absence of swirl in a k – ε model does not certify that swirl would not appear with another turbulence model.
- Many physical phenomena are not captured by turbulence models and require understanding from the user. Examples include, but are not limited to, transition, separation, unsteady boundary layers and low-Reynolds-number turbulence.

7.3.1 Boundary conditions

- The exact inlet conditions for the turbulence properties are usually not known exactly. The value of k/ε times the average velocity gives an order-of-magnitude estimation of how far into the system the settings at the inlet will survive.
- Exact inlet conditions for LES are not possible. Modern CFD programs can generate simple turbulent eddies at the inlet, but the inlet should be far from the area of

interest in order to allow a proper statistical distribution of eddies to develop. Periodic boundary conditions should be used when possible, but may introduce unphysical correlations. As always, it is important to verify the obtained solution critically.

- For RANS models, the lower level of y^+ should typically be between 20 and 30 at the walls. Some commercial CFD programs can be made to accept lower y^+ levels by adjusting the appropriate model. (Check the manual for actual values.) The upper limit of y^+ is usually in the range 80–100.
- LES models require additional treatment at no-slip walls.
- For low- Re turbulence models the first grid should be at $y^+ < 4$, preferably at $y^+ \approx 1$ with 5–10 mesh points below $y^+ = 20$.
- Standard wall functions are not recommended for flow with a negative pressure gradient, e.g. with flow separation at the wall.

7.4 Reactions

- Check the Damköhler number. Slow chemical reactions with $Da \ll 1$ are straightforward. Very fast, mixing-controlled, isothermal chemical reactions with $Da \gg 1$ can be modelled rather accurately. Most other conditions with $Da \approx 1$ and reactions that lead to heat formation and changes in density will give uncertain results.
- Very low residuals as a convergence criterion for concentration are often required, and monitoring integral quantities for mass balances or steady local concentrations usually provides more reliable indicators than low residuals.

7.5 Multiphase modelling

Generally speaking, multiphase flows are more challenging than single-phase flows, and errors in multiphase flow simulations are typically larger than those in single-phase simulations. These errors may have a number of different origins.

- **Not knowing the most important physical mechanisms.** Because of the wide variety of multiphase flow types, there is not one ‘generic’ model for multiphase flows. Before attempting to model a multiphase flow system, it is very important to understand the physical mechanisms occurring in the flow system. This includes understanding the most important forces and mechanisms in the flow and the properties of the fluid(s) and/or solids, as well as a good estimate of the length scales and timescales of the physical processes. Only with this knowledge can appropriate models be selected and their shortcomings in a simulation estimated.
- **Closure models.** Most errors in multiphase flow simulations arise from shortcomings of the closure models employed. Most closure models are empirically determined, which makes them applicable, strictly speaking, only under conditions similar to those for the data they are built from. Analytical closure models are developed for ‘ideal’ conditions, which are hardly ever met in reality. Using closure models for

conditions or regimes different from those to which they are applicable may be asking for trouble.

- **Timescale and length-scale separation.** In the derivation of turbulence models, a separation between the timescales and length scales of the ‘large’ eddies carrying the energy and the scale(s) at which energy is dissipated is assumed. Similar assumptions are required in order to derive governing and closure models for multiphase flows. For instance, many closure models require the particles to be smaller than the large-scale flow structures in a flow.
- **Choice of model and governing equations.** It is important to understand the implications and assumptions of each multiphase model, and under what conditions it may be employed. For instance, in the derivation of the Euler–Euler or two-fluid model, the pressure gradient over large interfaces, which is important in separated-flow situations, is neglected. This means that such a model will not capture the dynamics of free surfaces very accurately.
- **Numerical errors.** Many numerical errors potentially arising in single-phase calculations may also arise in multiphase flow calculations. Therefore, it is important to check the best-practice guidelines for single-phase flow computations. However, there may be additional problems. Many of the ideas employed in solving multiphase flows arise from single-phase flows, leading to slow convergence, or, worse, an erroneous result.

To minimize the potential problems occurring when performing multiphase flow simulations, the following checklist may be employed,

1. If possible, start the simulation with a single-phase flow situation resembling the system. This simulation can be optimized in terms of grid size, time step, etc. by using the best-practice guidelines for single-phase flow.
2. Determine the regime of the multiphase flow in terms of dimensionless parameters (Re , We , St , ...). This enables the choice of suitable closure models and may give insight into the expected flow situation.
3. Make an estimate of the forces acting on bubbles, particles or droplets and under which conditions these forces will occur.
4. Make a suitable selection of the turbulence model and decide which terms (and coupling to the dispersed phase) are important.
5. If possible, start with a geometry, flow properties and dispersed-phase properties similar to those of a system of which you know the behaviour or for which experimental data are available. This creates confidence in the models employed.
6. If there is a large size distribution of the dispersed phase, a multi-fluid approach might be required for the dispersed phase. This allows the use of a range of size classes, which can be monitored separately. Size distributions can have a big effect on the flow.
7. First-order-accurate models, such as the VOF model and the surface-tension models, require a very fine mesh – in these cases a relatively mesh-independent solution is very important.

8. Make sure that iterations are well converged. Many popular commercial CFD solvers will start with a new time step when a specified maximum number of iterations is reached, regardless of convergence criteria. This may be detrimental in terms of the quality of results obtained.

7.6 Sensitivity analysis

There are many choices that are uncertain, and sensitivity analysis is one way to examine the effect of the specific choice. It is good practice to start from a converged solution and change all uncertain settings in the model.

7.7 Verification, validation and calibration

Verification is a procedure to ensure that the program solves the equations correctly. Validation is done to test how accurately the model represents reality, and calibration is often used to adjust the simulation to known experimental data in order to study parameter sensitivity ('what if') in the design process.