

Part III

Solution verification

Solution verification is an important aspect of ensuring that a given simulation of a mathematical model is sufficiently accurate for the intended use. It relies on the use of consistent and convergent numerical algorithms as well as mistake-free codes; the two key items addressed in Part II of this book. If code verification studies have not been conducted, then even the most rigorous solution verification activities are not sufficient since there is no guarantee that the simulations will converge to the exact solution to the mathematical model. Just as code verification is a necessary prelude to solution verification, meaningful model validation assessments (Part IV) cannot be conducted until solution verification has been completed.

The main focus of solution verification is the estimation of the numerical errors that occur when a mathematical model is discretized and solved on a digital computer. While some of the strategies employed will be similar to those used for code verification, there is an important difference. In solution verification, the exact solution to the mathematical model is not known, and thus the numerical errors must now be estimated and not simply evaluated. In some cases, when these numerical errors can be estimated with a high degree of confidence, then they can be removed from the numerical solution (a process similar to that used for well-characterized bias errors in an experiment). More often, however, the numerical errors are estimated with significantly less certainty, and thus they will be classified as numerical uncertainties.

Numerical errors can arise in scientific computing due to computer round-off, statistical sampling, iteration, and discretization. The first three sources are discussed in Chapter 7. Discretization error, discussed in detail in Chapter 8, is often the largest numerical error source and also the most difficult to estimate. For complex scientific computing problems (e.g., those involving nonlinearities, geometric complexity, multi-physics, multiple scales), generating an appropriate mesh to resolve the physics before any solutions are computed is often inadequate. Chapter 9 discusses approaches to solution adaptation wherein either the mesh or the numerical algorithm itself is modified during the solution process in order to reliably control the discretization error. In our opinion, solution adaptation is required for reliable numerical error estimates in complex scientific computing applications.