Accuracy and reliability in scientific computing

Abstrak

Numerical software is used to test scientific theories, design airplanes and bridges, operate manufacturing lines, control power plants and refineries, analyze financial derivatives, identify genomes, and provide the understanding necessary to derive and analyze cancer treatments. Because of the high stakes involved, it is essential that results computed using software be accurate, reliable, and robust. Unfortunately, developing accurate and reliable scientific software is notoriously difficult. This book investigates some of the difficulties related to scientific computing and provides insight into how to overcome them and obtain dependable results. The tools to assess existing scientific applications are described, and a variety of techniques that can improve the accuracy and reliability of newly developed applications is discussed. Accuracy and Reliability in Scientific Computing can be considered a handbook for improving the quality of scientific computing. It will help computer scientists address the problems that affect software in general as well as the particular challenges of numerical computation: approximations occurring at all levels, continuous functions replaced by discretized versions, infinite processes replaced by finite ones, and real numbers replaced by finite precision numbers. Divided into three parts, it starts by illustrating some of the difficulties in producing robust and reliable scientific software. Well-known cases of failure are reviewed and the what and why of numerical computations are considered. The second section describes diagnostic tools that can be used to assess the accuracy and reliability of existing scientific applications. In the last section, the authors describe a variety of techniques that can be employed to improve the accuracy and reliability of newly developed scientific applications. The authors of the individual chapters are international experts, many of them members of the IFIP Working Group on Numerical Software.