Reliable Engineering Computing Using Interval Analysis

High performance computing can be used not only for greater computational speed, but also for improved, even guaranteed, reliability. The focus of this research is on the development and application of strategies for reliable engineering computing. In many applications of interest in engineering, it is necessary to deal with nonlinear models of complex physical phenomena, on scales ranging from the macroscopic to the molecular. Frequently these are problems that require solving a nonlinear equation system and/or finding the global optimum of a nonconvex function. Thus, the reliability with which these computations can be done is often an important issue. For example, if there are multiple solutions to the model, have all been located? If there are multiple local optima, has the global optimum been found? The goal is to develop the tools needed to resolve these issues with mathematical and computational certainty, thus providing a degree of problem-solving reliability not available when using standard methods. Some application areas of current interest include parameter estimation, nonlinear dynamics, ecosystem modeling and molecular modeling.

Objective function in Trefethen Challenge Problem

This surface, with thousands of local minima, is characteristic of potential energy surfaces that arise in modeling molecular conformations. The global minimum is easily and deterministically found using interval methods. For application to larger problems, see Y. Lin and M. A. Stadtherr, J. Computational Chemistry, 26, 1413 (2005).

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