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UNCERTAINTY MANAGEMENT IN SCIENTIFIC NUMERICAL COMPUTATION

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Abstract. The uncertainty in scientific computing has induced serious accidents and disasters. New proposals are presented toward an uncertainty inference or management in scientific numerical computing. The first important point is to share the knowledge on uncertainty with other researchers. Sharing known uncertainties contributes to the uncertainty management. In addition, for specific problems, one can prepare multiple programs with different rounding methods and / or with different precisions, and can compare the results among the programs generated for the specific problems. If differences appear among the results, it suggests that the specific program may have some uncertainty problems, and has a lack of the precision or a lack of the digit number. This second method provides a simple and effective inference method of the uncertainty. Uncertainty comes from various sources from physical and mathematical model errors, unknown input data, numerical model errors, insufficient numerical precision, floating point precision, programming errors, data processing errors, visualization errors, etc., as well as human errors. Another uncertainty comes from the discretization step size of Δt or Δx in numerical computations. The discretization step size of Δt or Δx must be selected appropriately in numerical computations in order to describe short waves or fast phenomena concerned to the target problems. This uncertainty would be also reduced by multiple program computations with the different size of Δt and Δx to find out the appropriate step size under keeping numerical stabilities. These uncertainty reduction mechanisms are proposed in this paper.

Key words. scientific computing, uncertainty, validation, verification, computer assisted science, PSE (problem Solving Environment), uncertainty quantification.

1. Introduction

Scientific numerical computing has become a powerful and key method to study scientific issues, to develop and design new products, to discover new physics in science and to provide a perspective for decision making, together with theoretical and experimental methods. For example, global warming problems have been discussed and studied based on computer simulation predictions on temperature increase, sea level elevation, human population, economical trend, energy resource consumption, etc. [1]. Computer simulations have also contributed to scientific discoveries, innovations and new findings. In physics, chemistry and other disciplines, mathematical equations including PDEs (partial differential equations) are employed to model phenomena concerned. The mathematical equations might be discretized so that the equations can be treated and solved on computers. In computer simulation, then numerical data are obtained and analyzed on physical quantities of interests (QOI). Not always but frequently QOI is visualized.

On one hand, numerical computations and simulations are always under threats of uncertainty, that includes model errors, numerical errors, bugs, data analysis errors, etc. In 2009 Air France447 met blocking of all the Pitot tubes by which airplanes measure their speed [2]. The Pitot tube holes were blocked by the condensed super cooled moisture. That means that the speed of the airplane becomes low, and

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the computers started to speed the airplane up. The three pilots could not find the reason for the acceleration. Finally at the steep attack angle the airplane stalled and was crashed in the ocean. All 228 people were killed by the accident. In this disaster, the input data was wrong from the Pitot tubes to the computers. Another accident happened at the Gulf war in 1991, and a missile killed unpredictably 28 people [3]. This accident came from an insufficient software precision.

On the other hand, PSE (Problem Solving Environment) studies have been explored intensively to support users of software and hardware for problem solving. PSE studies were started in 1970s to provide initially a higher-level programming language rather than Fortran, etc. in scientific computations. PSE is defined as follows: A system that provides all the computational facilities necessary to solve a target class of problems. It uses the language of the target class and users need not have specialized knowledge of the underlying hardware or software by John Rice [4]. PSE provides integrated human-friendly innovative computational services and facilities to enrich science and our society. In the PSE concept, human concentrates on target problems themselves, and a part of problem solving process, which can be performed mechanically, is performed by computers or machines or software.

So far, many PSEs have been developed and have contributed to solve problems: program generation support PSE [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15], job execution support PSE on cloud or grid [16, 17], an education support PSE [18], etc. Though computer simulation is a powerful tool to solve and study scientific problems, powerful computer simulations are always facing to the threat of uncertainty. The threat of the uncertainty does not always appear but cannot be ignored [19]. Uncertainty in scientific computing could be managed by PSEs [20].

Toward the uncertainty management in scientific computing, we will discuss the origin and characteristics of the uncertainty and present proposals based on the PSE concept in this paper. In this paper three methods are presented toward the reduction of uncertainty: uncertainty knowledge sharing, implication of the precision or digit number required, and selection of the appropriate discretization step size.

2. Origin of Uncertainty in Scientific Numerical Computation

The uncertainty in computer simulation has a wide variety. Below is the summary of the origin of uncertainty:

- Physical model error or uncertainty, including unknown physics.
- Mathematical model error.
- Computing model error including computing algorithm error, discretization errors, etc.
- Numerical error, including errors in floating-point computations and rounding error. Numerical stability is also essential to obtain reasonable results.
- Input data uncertainty, including unknown input data and boundary conditions.
- Output data processing error, including visualization error.
- Measurement error, when computations are cooperated with measurement equipments.
- Human errors.

From real physical phenomena, physical model is constructed to find out which physics is concerned. In this process, some physics involved could be missed, and it may lead to uncertainty to describe the real phenomena. From physical model, mathematical model is derived. Mathematical model does not always present