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Minimizing Error in Scientific Numerical Computation

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Abstract: **The error in scientific computing has induced serious accidents and disasters. New proposal are presented toward an error reduction mechanism or management in scientific numerical computing. The first important point is to share the knowledge of error with other researchers. Sharing known error contributes to the error reduction or management. In addition, for specific problems, one can prepare multiple programs with different rounding methods and or different precisions, and can compare the results among the programs generated for a specific problem. If differences appear among the results, it suggests the specific problem may have some error problem. The second method provides a simple and effective inference method of the error. Error come from various sources, from physics and mathematical model error, insufficient numerical precision, floating point precision, programming error, data processing error, visualization errors, as well as human errors. Another type of error comes from the discretization step size of Δt or Δx in numerical computation, the discretization step size of Δx or Δt must be selected appropriately in numerical computations in order to describe short waves phenomena concerned to the target programs. This error 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. In this paper we proposed these error reduction mechanisms.**

Keywords: **Error, Scientific Numerical computation, Verification, Error quantification and Problem Solving Environment (PSE).**

1. INTRODUCTION

Scientific numerical computing has became a powerful and key method to study scientific issues, to develop and design new products, to discover new physics in science and technology and to provide a perspective for decision making, together with theoretical and experimental methods . for example, global worming problem have been discussed and studies based on computer simulation predictions, economical trend, energy resources 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 equation) are employed to model phenomena concerned. The mathematical equations might be discretized so that the equation can be treated and solve on computers. In computer simulation, the numerical data are obtained and analyzed on physical quantities of interest which is not always, but frequently visualized.

On one hand numerical computations and simulations are always under treats of error, that includes model errors, numerical error bugs, data analysis errors, etc. in 2009 Air France 447 meet blocking of all the pilot tubes by which air planes measure their speed [2]. The pilot tube hole were blocked by the condensed super cooled moisture. That means the speed of the air-plane becomes low, and the computer started to speed the air-plane up. The three pilots could not find the reason for the acceleration. Finally as the steep attacked angle the air-plane stalled and was crashed in the ocean. All the 228 people were killed in the accident. In this disaster the impute data was wrong from the pilot tubes to the computers. Another accident happened at the gulf war in 1991, where a missile killed about 28 people [3]. This accident came from the insufficient software precision.

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On the other hand, PSE (Problems 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 define as, A system that provides all the computational facilities necessary to solve a target class of problems. It uses the language of a target class and users, need not have specialized knowledge of the underlying hardware or software [4].

PSE provides integrated human friendly innovative computational services and facilities to enrich science and our society. In PSE concept, human concentrates on target problems themselves and a part of problem solving process, which can be performed mechanically, is performed by computer or machines or software.

So far many PSE, have developed and have contribute to solving problems. Program generation support PSE [5-15], job execution support PSE on cloud or grid [16-17] , an educational 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 error. This threat of the error does not always appear but cannot be ignored [19]. Error in scientific computing could be managed or reduced by PSEs [20].

Toward the error reduction in scientific computing, we will discuss the origin and characteristics of the error and present proposals base on the PSE concept in this paper.

2. ORIGIN OF ERROR IN SCIENTIFIC NUMERICAL COMPUTATION

There are wide variety of error in computer simulation, below is the summary of the origin of error.

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

From real physical phenomena, physical model is constructed to find out which physical is concerned. In this process, some physic, involved could be missed, and it may lead to error to describe the real phenomena. From physical model, mathematical model is derived. Mathematical model does not always present the real world. Sometime exact equations are not known, or some perturbation is ignored, which may be essentially important in the phenomena. The mathematical model may often include PDEs which should be discretized to be solved on computers. In the discretization, well known numerical instabilities may appear. In the computing program the numerical stability condition must be always fulfilled during a whole computation. If the stability condition is violated during computation, the numerical result does not meet the validity. The floating point error is another issue in computer simulation, because recently long computing time on super computers becomes common to obtain meaningful results. A first digit number is used in computers to describe real number and to perform arithmetic operations. This induces the floating point error, including rounding errors and truncation errors. For the computation input data and boundary data should be prepare. Some time the input data is measured and in this case the measurement itself may have some errors. It is difficult to find the exact input data which may induce another source of errors. We may approximate the input data after or during computations. We also perform scientific visualization. In the visualization processes we could find some error depending on the visualization method, precision and so on [21]. Some time hidden important structures or features could not be found in the simple visualization, or a surface position may not be exact.

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Human errors also share the contribution to error with other issues discussed above. When software gives a wrong result for users it may course some difficulties, error and accidents, depending on target problems. The validation and verification mechanism is essentially important as useful software. This was pointed out by Rice et al [22]. Standardization and bench mark problems in each field may help to perform the validation and verification. In addition, error reduction must be addressed insensibly in order to avoid serious accidents and disasters in our society. PSE is one of the candidates to manage the errors in a relatively easy way [20].

3. TOWARD ERROR MINIMIZATION

Errors verification and validity in scientific computation have been recently studies intensively [19,20,]. On the other hand, each error has its own origin, and has very different characteristic with one another, as we have discussed above. Just one solution might be insufficient to manage all the errors. This consideration suggests to us multiple solutions in the various directions of the error characteristics. One promising way is to develop a PSE for the error management [20]. A PSE for sharing error knowledge. The PSE propose in this paper should have multiple solutions, eg the PSE for minimization of error should have known solutions including self validating method, program reliability test function, floating-point error control as well as mechanical program generation assistant function [4,5,……….15]. each known solution is not yet perfect and is still under study. PSE for mechanical program generation are also not almighty, but work for a specific limited area, eg FEM (Finite Element Method), PSEs for PDEs base problems by FDM (Finite Deference Method), etc. However, some part of the error could be already covered or managed by the present PSE research results. In addition the sharing function of known error and their solution is significantly important to avoid accident, so that one can find what kind of error could happen and what solutions are. PSEs is good at working for sharing the error.

For the error knowledge sharing, we have proposed one mechanism in a PSE, called PSE park [20] which is a PSE for PSE. PSE Park is a Meta PSE system or frame word enabling us to construct PSEs easily. in the near future, many uses may start to do simulations as their hobbies, for a better lifestyle, etc. PSE Park is a framework to enable the construction of PSE by combining those existing function and function that are newly developed. In PSE park users can select cores which are components for a PSE, and connect them to build up a new PSE. A new function against the error in scientific computing is also implemented. When uses register core, that is a function composing a PSE, PSE park request the user to impute information for the error relating to the function. Eg an applicable range of the method employed or the parameters specified in the core, etc. this new function of PSE park enhances to share the information or knowledge about the error, and it may contribute to reduce the error risk. This idea could contribute also to reduce human errors, human is not always perfect. We cannot always avoid human errors. The knowledge sharing function in PSE can also contribute to share knowledge.

3.1. Implication of error based on different rounding method; One of the error sources is the rounding error the four rounding methods are rounding to the nearest even, rounding upward, rounding downward and rounding toward zero. Not always but in many cases, computation results by vulnerable or sensitive computation are strongly influenced by rounding methods. Here we call software containing error sensitive software. So we would presume that computational results from the sensitive software may be influenced by the rounding methods.

Application of the method:

The error introduced by attempting to represent a number using a finite string of digits is a form of round-off error called representation error. Here are some examples of representation error in decimal representations:

Notation	Representation	Approximation	Error
1/7	0.142 85714	0.142 857	0.000 000 14
ln 2	0.693 147 180 559 945 309 41...	0.693 147	0.000 000 180 559 945 309 41...
$\log_{10} 2$	0.301 029 995 663 981 195 21...	0.3010	0.000 029 995 663 981 195 21...
$\sqrt[3]{2}$	1.259 921 049 894 873 164 76...	1.25992	0.000 001 049 894 873 164 76...
$\sqrt{2}$	1.414 213 562 373 095 048 80...	1.41421	0.000 003 562 373 095 048 80...
e	2.718 281 828 459 045 235 36...	2.718 281 828 459 045	0.000 000 000 000 000 235 36...
π	3.141 592 653 589 793 238 46...	3.141 592 653 589 793	0.000 000 000 000 000 238 46...

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Increasing the number of digits allowed in a representation reduces the magnitude of possible round-off errors,

Numerical stability is affected by the number of the significant digits the machine keeps on, if we use a machine that keeps on the first four floating-point digits, a good example on loss of significance is given by these two equivalent functions

$$f(x) = x\left(\sqrt{x+1} - \sqrt{x}\right) \text{ and } g(x) = \frac{x}{\sqrt{x+1} + \sqrt{x}}.$$

If we compare the results of

$$f(500) = 500\left(\sqrt{501} - \sqrt{500}\right) = 500\,(22.3830 - 22.3607) = 500(0.0223) = 11.1500$$

and

$$g(500) = \frac{500}{\sqrt{501} + \sqrt{500}} = \frac{500}{22.3830 + 22.3607} = \frac{500}{44.7437} = 11.1748$$

by looking to the two results above, we realize that the true value for the result is 11.174755…. which is exactly g(500) = 11.11748 after rounding the result to 4 decimal digit, which has a huge effect on the results, even though both functions are equivalent; to show that they are equivalent simply we need to start by f(x) and end with g(x). To minimize this one should use the suitable formula of the two function each time one evaluate either f(x) or g(x) the choice dependent on the parity of (x).

3.2. Discretization Step Size Control under Numerical Stability Condition:

One of other uncertainties comes from the discretization step size, which is the time step Δt or the special step size Δx. Even for a fixed value of Δx one could obtain a numerical result; when Δx is too large to represent a special distribution,short wavelength waves cannot be represented precisely. The insufficient discretization step size would result in one kind of numerical uncertainty. When the time step Δt is too large, short time scale phenomena cannot be expressed exactly. The insufficient Δt orΔx leads another kind of uncertainty in numerical computations. In order to reduce the uncertainty coming from the insufficiently large Δt or Δt, one should use sufficiently small value for Δt or Δx. The problem is what the sufficiently small Δt or Δt is. Reasonable Δt or Δx cannot be obtained a priori. We also cannot go to the infinitesimally small values of Δt or Δx for a reasonable computation time. In addition, numerical stability conditions must be fulfilled during the computation. For example, a simple diffusion equation $\frac{\partial f}{\partial t} = \frac{\partial 2f}{\partial x2}$ would be discretized explicitly as follows: $f_i^{n+1} = f_i^n + (\Delta t/\Delta x^2)(f^n_{i+1} - 2f^n_i + f_i^{n+1})$.

The superscript shows the time index, and the subscript shows the spatial index. In this discretization explicit method the stability condition is Δt=(Δx)2<1=2. When Δtor Δx is reduced, the stability condition must be always fulfilled during the computations.

Table 1. Show relative difference among the numerical results for the diffusion problem, in which the discretization step size is changed under the stability condition t=(Δx)2<1=2. When the sufficiently small Δt are Δx selected, the numerical results do not change much. Then one can assume the corresponding Δt and Δx are sufficiently small to describe the short waves and fast phenomena. In a PSE framework, this uncertainty management procedure can be easily implemented: when a numerical program is generated by hand or by a program generation PSE, the programmer or scientists would include the numerical stability for the program which must be fulfilled during the computation.

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Table 1. Change in the numerical results depend on the discritization step size, condition for the program

Δx	Δt	Relative differences
$1/2\Delta x$	$1/4\Delta t$	1.11×10^{-2}
$1/4\Delta x$	$1/16\Delta t$	4.45×10^{-3}
$1/8\Delta x$	$1/64\Delta t$	2.06×10^{-3}

The PSE could submit several job for the specific problem with the different Δt and Δx together. After getting the numerical results, the users compare the results and find the appropriate Δ t and Δx for the problem. This error management method is also general for numerical computations to find out the appropriate Δt and Δx for specific problems.

4. CONCLUSIONS

In this paper we have discussed the origin of Error in computing sciences first. Then we stressed three important issue and proposals: the first important point is to share the knowledge on the error with other researchers and engineers. Sharing the previous or known error with others contributes to the error management. Probably this is the essentially important and realistic solution for the error management. The second is that PSEs can provide a reliable tool to manage the error to avoid future accidents and disasters originated from the error. For specific problems, the PSE provides multiple programs with different precisions or with different rounding methods, and then we can compare the results among the programs generated for the specific problems. If some differences appear among the results by the multiple programs generated by the PSE, it suggests that the specific program may have some error problems. The third proposal is to supply the information for the appropriate discretization step sizes of Δt and Δx. When Δt and Δx are sufficiently small, the numerical results do not depend on the size of Δt and Δx. When the differences appear among the numerical data from the programs using the different Δt and Δx and the differences are visible, it suggests the users or scientists to reduce Δt and Δx to obtain the accurate results. These three approaches and proposals are realistic and rather general toward the error reduction.

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