Computational Uncertainty Principle: Meaning and Implication

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Naturally you will recall the uncertainty principle of quantum mechanics when you meet the concept of computational uncertainty principle. In fact, they have similar form, but they have different connotation. The former reveals the relation between two kinds of uncertainty due to the imperfection of numerical method itself and the finiteness of machine precision in numerical differential equations. The later reflects the relation between two kinds of uncertainty in the position and momentum measurement of a quantum particle in quantum mechanics. After hard work for some years, on the basis of large numerical experiments and strictly mathematical analysis, the related study group, Institute of Atmospheric Physics (IAP), Chinese Academy of Sciences (CAS), obtained new achievements, found two universal relations, and presented the computational uncertainty principle. The principle not only gives a great challenge to the reliability of long-time numerical integration for nonlinear differential equations, but also has significance for numerical differential equations. The achievements in this aspect are evaluated as creative work in the national key laboratory assessment in 2000, and are placed in the creative achievement list of CAS.

1. Computational uncertainty principle

Numerical results and theoretical analysis show that there is an inverse variation between method error (i.e., discretization error) and round-off error against stepsize, and thus a computational uncertainty principle similar to the well-known Heisenberg uncertainty relation of quantum mechanics is led. The explicitly mathematical expressions of the principle are as follows

$$\Delta e + \Delta r \geq C \,, \tag{1}$$

$$\Delta e \cdot \Delta r \geq \hbar \,, \tag{2}$$

where Δe represents a measure of uncertainty due to the imperfection of numerical method itself, $\tilde{r}$ a measure of uncertainty due to the inherent inaccuracy of digital computers, C and $\hbar$ are positive numbers dependent on differential equations while the machine precision is finite. Specifically, if the discretization error and the round-off error are treated as two "adjoint variables", the computational uncertainty principle reveals that the smaller one of them, the greater will be the other adjoint variable. In other words, there are two basic limitations in numerical integration under finite machine precision: on one hand, there is an upper bound limitation for the magnitude of stepsize due to the stability condition of numerical method, on the other hand, there must be another limitation of upper bound for the number of integration steps because of the limitations of finite accuracy due to computing on actual machines. The two aspects are contradiction with each other, with the result that they have to complement each other, leading the computational uncertainty principle.

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Owing to the inherent relationship between the two uncertainties due to numerical method and computer respectively, it naturally causes a limitation in the width of interval of effectively numerical solution. This is just the root cause of the inexorable existence of maximally effective computation time (MECT) and optimal stepsize (OS). Therefore, once the precision of calculation machine used is given, the best degree of accuracy which can be achieved for the numerical solution obtained by a numerical method is determined entirely. That is to say, if one fixes on the error tolerance $\delta > 0$ (i.e., the numerical solutions which are less than the tolerance are acceptable), there is surely MECT T, so that the numerical solutions in the interval [0, T] satisfy the requirement of the tolerance and present the exact solutions in the interval very well, and that the exact solutions beyond the interval can not be determined by numerical method. Thus, the computational uncertainty principle gives a certain limitation to the computational capacity of numerical method under the inherent property of finite machine precision.

2. Two universal relations

Numerical results and theoretical analysis also show that there are two universal relations which are dependent on the machine precision and the order of numerical method and are independent of types of differential equations, initial values and numerical schemes. The relations are

$$l = \frac{\mathrm{H}_1}{\mathrm{H}_2} = 10^{\frac{\Delta n}{p+0.5}}, \tag{3}$$

$$k = \frac{C(\mathrm{T}_2)}{C(\mathrm{T}_1)} = l^p, \tag{4}$$

where H_1 and H_2 are the OSs of the same *k*-step numerical method of order p in two machine precision γ_1 and γ_2 with n_1 and n_2 significant digits respectively ($\gamma_1 = 5\times 10^{-n_1}$, $\gamma_2 = 5\times 10^{-n_2}$, $n_1 \le n_2$), $C(\mathrm{T}_1)$ and $C(\mathrm{T}_2)$ are the MECT functions under two machine precision respectively, $\Delta n = n_2 - n_1$. From the relation (4) it results immediately that

$$\Delta\mathrm{T} = \hat{C}\cdot p\ln l, \tag{5}$$

where $\Delta\mathrm{T} = \mathrm{T}_2 - \mathrm{T}_1$, $\hat{C}$ is a positive number, T_1 and T_2 are the MECTs under two machine precision respectively.

The two relations have significance and practical value. They reveal the intrinsic relationships between two OSs and between two MECTs under any two machine precision. According to the two relations, OS and MECT can be determined under any machine precision provided that OS and MECT under certain machine precision are known.

3. Optimal integration method of step-by-step adjustment

We always hope to achieve optimal numerical integration while we design numerical model. Here the optimum means computational accuracy; that is, the optimal numerical integration is that a numerical method carries out calculation with its best accuracy that can be achieved. Given differential equations and numerical method, spatial-temporal resolution and machine precision are main parameters to determine the best accuracy of the method. Based on the computational uncertainty principle, we present an optimal integration method of step-by-step adjustment. The flow diagram of the method is shown in the Fig. 1. Numerical experiments verify that the step-by-step adjustment method is an effective method for achieving optimal numerical integration. It can be expected that the method will has extensive applications in practice.

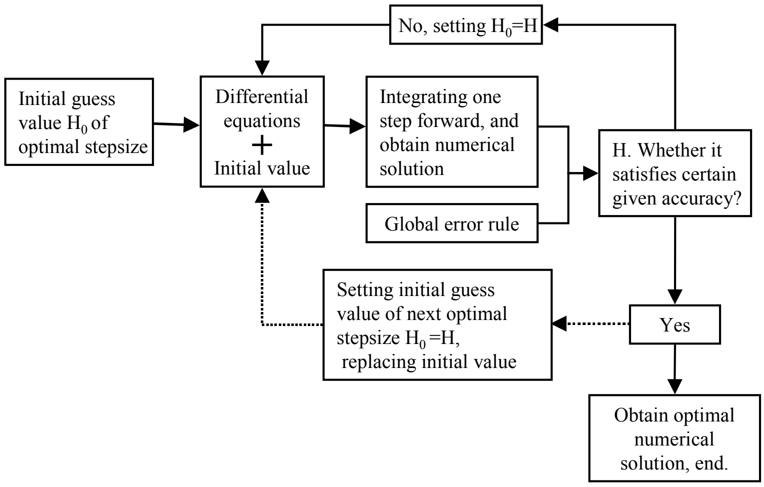

Figure 1. Flow diagram of the step-by-step adjustment optimal integration method.

4. Implications

(1) In practice, the computational uncertainty principle points out that there is a limit to the ability of effective simulation of computer. The existence of this limit is inherent and is independent of the objects simulated (more precisely except a zero measure set). The size of the limit, however, usually depends on the objects simulated. (2) Using the computational uncertainty principle we make simulations to the best. The computational uncertainty principle on the one hand points out the limit of simulation ability, and on the other hand, points out an optimal relation. The optimal relation gives the way to come up the best ability of simulation. (3) Developing the computers with higher precision is a way to enhance the ability of effective computation. At present for the various numerical methods in differential equations, all their kernels are the recurrent processes step by step. There is surely MECT for this class of methods, and the integration results beyond the time will be invalid, and so the long-time behavior of system can not be properly analyzed. According to the computational uncertainty principle, as long as machine precision is added, MECT can be extended, and thus the ability of effective computation is raised. (4) The accumulated effect and long-time influence of error should be paid great attention. In fact, the problem becomes more outstanding because mainframe computer and supercomputer can carry out variously large calculations.

In a word, we are up against the change of idea from the idealization of infinite precision to the reality of finite precision. In the course of the change it is an important problem to be solved urgently how to break through the computational uncertainty principle and to raise the ability of long time numerical integration.

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