

Computational Fluid Dynamics, still a field where various kinds of mathematical researches are expected

AISO, Hideaki

Information Technology Center, JAXA (Japan Aerospace Exploration Agency)

Jindaiji-Higashi 7-44-1 Chofu TOKYO 185-8522 JAPAN.

Dedicated to Professor Yukio Matsumoto on the occasion of his 60th birthday with deep thanks for the mathematical training and education given by the professor. The author works in a research area far from the area where the education was given but feels the basic training given there is useful still now.

Introduction

Recently we often hear the words like Numerical Analysis, Numerical method, Numerical Calculation or Numerical Computation, Numerical Simulation, Computational Science and so on. The progress of computer hardware technology during the last few decades is very fast and eminent. For example, in some research institutes it is not so difficult for people to use computers of T(Tera)FLOPS class. TFLOPS means that the computer executes 10^{12} times basic floating operation, *i.e.* addition, reduction, multiplication, or division, per second. The large computing power has realized the idea to solve the partial differential equations (PDE's) numerically, exactly speaking, to obtain an approximate solution by calculating a discretized model of the original PDE.

Computational Fluid Dynamics, which is often called CFD in abbreviation, is one of the examples.

Seeing the situation above, people may think that so called numerical methodology including CFD has realized a great progress. Of course it is not wrong. But from the viewpoint of mathematics or mathematical manner of thinking, there are still many problems left open. Some of them are not only important from the practical viewpoint but also interesting from the theoretical viewpoint. Here we would like to show a few example of such problems.

1 Framework of Numerical Computation for PDE's

Before entering the main discussion, let us review the framework of numerical computation to solve PDE's numerically.

1. Modeling a phenomenon into PDE. (Real Phenomenon \Rightarrow PDE=Continuous Model)

In the practical field of engineering, physics etc., such numerical computation is done to analyze phenomena in physics, biology, economics etc. Therefore, one has to establish a governing equation to describe the phenomenon of one's interest.

2. Modeling PDE into discretized equations. (Continuous Model \Rightarrow Discrete Model)

Everyone knows that the computers can never solve the continuous model of PDE. One always needs some discretization of the PDE. Several methods of discretization are used; finite difference method, finite volume method, finite element method, boundary element

method, etc. The discrete model is called “scheme”. Of course large part of error in numerical computation is from the discretization. The “truncation error” is one of them.

3. Execution of Computation by Computer (Discrete Model \Rightarrow Result of Calculation=Raw Numerical Data)

It is expected that the discrete model obtained at the previous step is exactly solved by the computer as we do manual calculations using pencil and paper. But the present computers can not do it. The computers recognize real numbers by finite binary bits representation and so called “quantumization error” or “round off error” is inevitable. When the discrete model has some instability against numerical noise, or when one tries to capture some singular phenomenon that occurs in the original continuous model, the problem can not be neglected.

4. Understanding the Result. (Raw Numerical Data \Rightarrow Understanding)

It is a little bit outside of mathematics or applied mathematics even if we understand them in a rather wide sense. But it is very important how to understand the result from the raw data of computation that are just a huge list of numbers. Computer graphics technology is one of the tools for the purpose.

It is well known that the PDE’s obtained at the step 1 are often subjects of mathematics. They are rather classical problems in mathematics. But almost all the problems occurring at the step 2 should be discussed in the manner of mathematics also. While the “convergence” or “stability” of discrete model is a popular problem, there are many other problems to be discussed mathematically. It is also noted that analysis of the behavior of discrete model is essential to resolve some of the problems we encounter at the step 3.

Now let us focus ourselves into CFD especially finite difference or finite volume method to solve the compressible Euler equations numerically. We note that almost all the governing equations for fluid motion including the well known Euler equations and Navier-Stokes equations are still open in the sense of existence and uniqueness of solution. The mathematical discussion in the field of CFD is naturally suffering from the situation, because we do not have enough information on the property of exact solution with which discrete models should be consistent.

2 Nonlinear Hyperbolic Conservation Laws and Numerical Computation

There are various equations describing the motion of fluid. Among them the most classical examples may be four; Euler/Navier-Stokes equations for compressible/incompressible fluid.

We here concentrate ourselves into the compressible Euler equations. The compressible Euler equations describe the motion of compressible fluid (gas) with no dissipation from viscosity taken into account. The one dimensional compressible Euler equations are;

$$\begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix}_t + \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(e + p) \end{bmatrix}_x = 0, \quad (1)$$

where ρ , u , p and e are the density, velocity, pressure and total energy per unit volume, respectively. The set of equations represents a typical example of nonlinear hyperbolic conservation laws, which are generally written in the form of

$$U_t + F(U)_x = 0. \quad (2)$$

We need an initial condition like $U(x, 0) = U_0(x)$. Sometimes we also include a boundary condition.

Roughly speaking, basic property of solution to nonlinear hyperbolic conservation laws are the following.

1. Even if the initial condition is smooth enough, the temporally global existence of smooth solution is not guaranteed. The concept of weak solution is introduced to allow singularity such as shock discontinuity in the solution and to establish the existence of solution.
2. The uniqueness of solution is lost once the weak solution is allowed. Infinitely many distinct weak solutions may exist. To choose a solution that is physically relevant or to establish a framework to discuss the uniqueness of solution we introduce some additional condition called “entropy condition”.
3. The existence and uniqueness of solution is still open in the system’s case (U is a vector), especially in the compressible Euler equations.

Related with the situation above, the difficulty of numerical computation is explained as follows.

1. A simple discussion based on the order of truncation error in discrete models is useless for designing the discrete models because the smoothness of solution can not be assumed. It is not easy to satisfy the two requirements somehow contradictive, to capture the singularity like shock without instability or numerical dispersion and to realize better resolution where the solution is smooth.
2. Even if a discrete model is consistent with weak solutions, it is only guaranteed that the numerical computation captures one of the weak solutions. It is required that the discrete model has some consistency with the entropy condition to guarantee that the numerical computation captures the physically relevant solution.
3. Various schemes have been developed to obtain high resolution result. But mathematical tools to guarantee the convergence of scheme or to estimate the quality of scheme is not yet enough. It is required that mathematics gives such tools.

3 Scalar Conservation Laws.

Because the mathematical tools are not yet enough to handle the system’s case, the (one dimensional) scalar conservation law

$$u_t + f(u)_x = 0 \quad (3)$$

is still used for theoretical analysis or design of discrete model. We assume that the flux function f is strictly convex, *i.e.* $\inf f'' > 0$. In fact the scalar case is enough to show some essential part

of theory. Numerical schemes or concepts obtained in the scalar case is usually extended to the system's case that is more practical, but the extension is still heuristic in almost all the cases.

Some basic property of solution to nonlinear hyperbolic conservation law is observed even in the simple scalar case. We solve (3) with the initial condition

$$u(x, 0) = u_0(x). \quad (4)$$

Theorem 1 *Even if the initial condition (4) is smooth, a temporally global smooth solution to the initial value problem (3)-(4) does not always exist.*

It is easily proved by the following observation. Let us assume a smooth function $u = u(x, t)$ is a solution to (3)-(4). The curves $x = x(t)$ in x, t -space determined by

$$\frac{dx}{dt} = f'(u(x, t)) \quad (5)$$

are called characteristics. Along with each of characteristics u takes a constant value because

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} \frac{dx}{dt} = u_t + f'(u)u_x = u_t + f(u)_x = 0, \quad (6)$$

which implies that all the characteristics are lines. Then we easily observe that two characteristics starting at $(x_0, 0)$ and $(x_1, 0)$, $x_0 < x_1$ intersects each other if $f'(u_0(x_0)) > f'(u_0(x_1))$. It contradicts the assumption that a smooth solution exists. This completes the proof.

Therefore, we employ the concept of weak solution.

Definition 1 *If $u = u(x, t)$ satisfies the equation*

$$\int_0^\infty \int_{-\infty}^\infty \{u(x, t)\phi_t(x, t) + f(u(x, t))\phi_x(x, t)\} dx dt + \int_{-\infty}^\infty u_0(x)\phi(x, 0)dx = 0 \quad (7)$$

with an arbitrary C^∞ -function $\phi(x, t)$, $(x, t) \in (-\infty, \infty) \times [0, \infty)$ with compact support, $u = u(x, t)$ is said to be a weak solution to the initial value problem (3)-(4)

But we may have infinitely many weak solutions. Then we impose an additional condition called entropy condition to choose a physically relevant solution.

Definition 2 *A weak solution $u = u(x, t)$ is said to satisfy the entropy condition if the inequality*

$$U(u)_t + F(u)_x \leq 0 \quad (8)$$

is satisfied in the sense of distribution, where (U, F) is an arbitrary pair of a convex function U and another function F satisfying $F' = U' f'$.

Theorem 2 *A weak solution satisfying the entropy condition exists and it is unique.*

It is proved in [2], see also [5, 8]. [5] is the first work to prove the existence and uniqueness of solution to the scalar conservation law, but a different form of entropy condition is used. The unique solution is called entropy solution.

The numerical computation for the problem (3)-(4) is not so straightforward. A difference approximation like

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{f(u_{i+1}^n) - f(u_{i-1}^n)}{2\Delta x} = 0, \quad (9)$$

is easily imagined, where u_i^n approximates $u(i\Delta x, n\Delta t)$. But it does not work at all even in a very simple case of linear flux function $f(u) = u$.

In fact, it was impossible to solve the nonlinear hyperbolic conservation laws numerically until the discovery of Lax-Friedrichs scheme [3] (see also [4, 8])

$$\frac{u_i^{n+1} - \frac{u_{i+1}^n + u_{i-1}^n}{2}}{\Delta t} + \frac{f(u_{i+1}^n) - f(u_{i-1}^n)}{2\Delta x} = 0. \quad (10)$$

There is a story that the discovery was made in the Manhattan project during WW2. The numerical solution given by (10) converges to the entropy solution, while the definition of convergence is not given exactly because of the short of space. Briefly, the convergence is discussed in L^1_{loc} -topology. The proof is given in [5]. In fact Lax-Friedrichs scheme is an essential tool to prove the existence of entropy solution in [5].

Almost all the practical numerical schemes of difference approximation to the problem (3)-(4) are written in the form

$$u_i^{n+1} = u_i^n - \frac{1}{2} \frac{\Delta t}{\Delta x} \{f(u_{i+1}^n) - f(u_{i-1}^n)\} + \frac{1}{2} \frac{\Delta t}{\Delta x} \left\{ a_{i+\frac{1}{2}}^n (u_{i+1}^n - u_i^n) - a_{i-\frac{1}{2}}^n (u_i^n - u_{i-1}^n) \right\} \quad (11)$$

For example, $a_{i+\frac{1}{2}}^n \equiv \frac{\Delta x}{\Delta t}$ gives Lax-Friedrichs scheme. The behavior of scheme depends on the numerical viscosity coefficients $\{a_{i+\frac{1}{2}}^n\}$. For the stability of numerical computation we need larger numerical viscosity coefficients but it makes the computation more dissipative and deteriorates the resolution. For better resolution especially around shock discontinuity, we need to decrease the coefficients but there is a risk that numerical solution becomes unstable or converges to a fake solution (a weak solution not satisfying the entropy condition).

Various schemes were proposed after [3] (for example, see a textbook [4]) and “what is the optimal numerical viscosity coefficient?” had been a question for a long time. An answer is given by [1].

Theorem 3 Fix the ratio $\frac{\Delta t}{\Delta x}$ so that $\frac{\Delta t}{\Delta x} \cdot \sup |f'| \leq 1$ is satisfied. Let ϵ be an arbitrary positive real number less than $\frac{\Delta x}{\Delta t}$. If each coefficient $a_{i+\frac{1}{2}}^n$ satisfies

$$\max \left\{ \left| \frac{f(u_{i+1}^n) - f(u_i^n)}{u_{i+1}^n - u_i^n} \right|, \epsilon \cdot \operatorname{sgn}(u_{i+1}^n - u_i^n) \right\} \leq a_{i+\frac{1}{2}}^n \leq \frac{\Delta x}{\Delta t}, \quad (12)$$

the numerical solution given by (11) converges to the entropy solution to the problem (3)-(4).

The result is the optimal when the range of coefficient $a_{i+\frac{1}{2}}^n$ is described in terms of u_i^n, u_{i+1}^n .

In some sense the theorem gives some direction to design numerical schemes. But it is not yet enough for computation of high resolution. After 1980's various high resolution schemes are proposed and only a small class of them are mathematically proved to converge to the entropy solution, while they are well tested through numerical experiments. Some more mathematical criteria are still required.

4 A Stability Problem of Discrete Model

We are concerned with the two dimensional compressible Euler equations.

$$U_t + F(U)_x + G(U)_y = 0, \quad (13)$$

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, \quad F(U) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(e + p) \end{bmatrix}, \quad G(U) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(e + p) \end{bmatrix}$$

For the numerical computation we prepare the computation nodes $(i\Delta x, j\Delta y)$, i and j are integers, to each of which an approximate value $U_{i,j}^n$ is assigned at every discretized time $t = t^n = n\Delta t$, in x, y -space.

We calculate a progressing planar shock wave. The initial condition is given by

$$U(x, y, 0) = \begin{cases} U_-, & x < 0, \\ U_+, & x > 0, \end{cases} \quad (14)$$

where U_- and U_+ are the states of both sides of shock wave satisfying the Rankine-Hugoniot condition

$$F(U_+) - F(U_-) = s(U_+ - U_-). \quad (15)$$

with some shock speed (propagation speed of shock) s . Then the solution to the problem (13)-(14) is

$$U(x, y, t) = U_0(x - st, y). \quad (16)$$

The problem is rather simple. But the numerical computation is not so easy. When a scheme of small dissipation or high resolution is used, we may have a strange instability around the shock wave.

The following is recognized through numerical experiments

1. It is impossible to find any factor triggering the instability from the equation of discrete models (schemes). In fact, if Δx and Δy are taken to be 1 of integer-type representation in the computer, the instability is never observed. Therefore it is clear that some round off error triggers the instability.
2. Once the instability occurs, it seems to grow in the exponential order. It implies that the phenomenon is not just an accumulation of round off error that is assumed quasi-stochastic. It is natural to understand that some machinery in schemes works to amplify the noise from the round off error.

An interesting fact about the instability is that the phenomenon had not been recognized as one of essential problems coming from the numerical schemes' property. until Quirk published [6] in 1994 although the phenomenon was already observed by many people even in 1970's. (It seemed to be understood just as a "computer error" problem.) After [6] some researches are made for the instability. While it is easily found that some additional numerical dissipation prevents the computation from the instability, the first works where the machinery of instability is discussed are those by Moschetta et al. For example, see [7].

We also made some theoretical analysis and numerical verification in JAXA. The result shows the machinery of instability rather clearly. It also implies that, when the nonlinear problems include linearly degenerate fields, the treatment of linearly degenerate fields may be more difficult than that of nonlinear fields in numerical computation as well as in theoretical analysis of PDE, while it has been believed that numerical computation for linearly degenerate fields is not so difficult because well developed computational methods for linear problems are applied.

Another question, while it is very basic, naturally arises; “Directionality of Computational Mesh (or Computational Grid, Computation Coordinate)”. The original PDE has no directionality, but we introduce some mesh, which has directionality, for numerical computation. It is very easily seen that, if we replace the initial condition (14) by

$$U(x, y, 0) = \begin{cases} U(\theta)_-, & x \cos \theta + y \sin \theta < 0 \\ U(\theta)_+, & x \cos \theta + y \sin \theta > 0, \end{cases} \quad U(\theta)_\pm = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta & 0 \\ 0 & \sin \theta & \cos \theta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} U_\pm, \quad (17)$$

where θ is an arbitrary angle, then the solution to the problem is

$$U(x, y, t) = U_0(x - st \cos \theta, y - st \sin \theta). \quad (18)$$

The situation does not change at all except the rotation of angle θ . But the numerical computation is not so simple. Unless $\theta = \frac{n\pi}{2}$, n is an integer, the resolution of shock is deteriorated by smearing or the loss of monotonicity and not so ideal as that in the case $\theta = \frac{n\pi}{2}$.

In practical computations we try to avoid the “directionality” problem by fitting computational mesh to the flow aspect. The convergence would give the consistency of scheme, while it is not yet given in fact. Of course we need some more progress in research on the exact solution to original PDE. (The existence and uniqueness problem is still open.)

But some more qualitative or quantitative consistency discussion is required to measure the quality of numerical computation because the real numerical computation is always conducted with finite values of discretization increments Δx , Δy and Δt etc. and the result obtained is never a converged one.

The structure of computational mesh is introduced so that numerical computation could be conducted. It is rather artificial but inevitable. Therefore the property of discrete model that is derived from the mesh but is not inherited from the original PDE should be discussed more seriously in some mathematical manner. The mesh problem seems to become more important when the computation tries to capture so called singular phenomena in real physics like local erosion of rocket nozzle. But such discussion has not been done so much because of the lack of mathematical tools. It is now expected that geometry and topology might give some new idea.

5 Concluding Remarks

The author tries to explain a few mathematical topics in CFD research, being afraid that they might be so primitive for the topologists and geometrists. But it is the author’s pleasure if some part of topics interests the people.

Finally let us have a little general statement. The education and training of mathematics give a rather general framework of thinking. It seems useful even outside of mathematics research. Let us see an example. National Aerospace Laboratory, which is now merged with other organizations and reorganized as JAXA, sometimes organized small research projects of validation of numerical computation for aircraft together with heavy industries and universities. Twenty years ago the validation of computation means just the comparison with the experiments and it was believed that the improvement of reliability of numerical computation is to arrange the computation so that it could give a result as near to the experimental result as possible. After the progress of computation technology, such a simple idea as above does not work any more. We classify or categorize many pieces of problems found into basic elements that belong to one of the steps 1-4 mentioned in the beginning of article or the steps (model setting, measurement etc.) in experimental procedures carefully, and then discuss each element precisely. People trained in the field of mathematics would be suitable to organize this kind of work because unbiased classification or categorization of problems using an appropriate logic is one of important bases of mathematics. It would be also important that such usefulness of mathematics (or mathematicians?) should be known in the society, although the idea is less popular in Japan compared with some other countries.

References

- [1] H. Aiso. Admissibility of difference approximation for scalar conservation laws. *Hiroshima Math. J.*, 23(1):15–61, 1993.
- [2] S. N. Kružkov. First-order quasilinear equations with several space variables. *Math. USSR-Sb.*, 10:217–273, 1970.
- [3] P. D. Lax. Weak solution of nonlinear hyperbolic equations and their numerical computation. *Comm. Pure Appl. Math.*, 7:159–193, 1954.
- [4] Randall J. LeVeque. *Numerical Methods for Conservation Laws*. Birkhauser-Verlag, Basel, 1990. ISBN 3-7643-2464-3.
- [5] O. Oleĭnik. Discontinuous solutions of nonlinear differential equations. *Uspekhi Mat. Nauk.(N.S.)*, 12:3–73, 1957. English transl. in *Amer. Math. Soc. Transl., Ser. 2, vol. 26*, 95–172.
- [6] J. Quirk. A contribution to the great Riemann solver debate. *International Journal for Numerical Methods in Fluids*, 18:555–574, 1994.
- [7] J.-Ch. Robinet, J. Gressier, G. Casalis, and J.-M. Moschetta. Shock Wave Instability and Carbuncle Phenomenon: same intrinsic origin? . *J. Fluid Mechanics*, 417:237–263, 2000.
- [8] J. Smoller. *Shock waves and reaction-diffusion equations*. Springer-Verlag, NewYork, 1982.