ON NUMERICAL SIMULATION IN FLUID DYNAMICS

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This paper discusses some questions of numerical simulation of experiments in physics and fluid dynamics problems.

I. Recently the problems in magnetohydrodynamics, radiative fluid dynamics, plasma flow in strong electric fields, etc. have become of considerable interest along with the classical issues of continuum mechanics, i.e. the problems of the elasticity theory, gas dynamics or flow around a body.

The formulation of many such problems that demands intensive applying the numerical methods has originated with plasma physics. As a rule, the mathematical models in plasma physics are nonlinear. In general, two limiting cases most widely used can be emphasized:

a) a model of dense plasma - equations of radiative magneto-gas-dynamics (RMGD);

b) a model of collisionless plasma in the Vlasov equation approximation.

At present the problem of controlled thermonuclear fusion (CTR) should be considered as most urgent in plasma physics. A number of approaches to solving this problem has been proposed (stationary Tokamak-type installations, fast plasma heating and compressing in inertial pulse systems by a laser pulse or relativistic electron beam, etc.).

The CTR problem is closely associated with problems of utilizing the thermonuclear energy released, so the problem of constructing an effective reactor is in prospect.

2. Currently a numerical experiment (NE) is the basis for comprehensive theoretical investigations of problems in fluid mechanics [I] . The NE enables us not only to explain some known experimental facts or confirm the theoretical concepts but, in some cases, to predict new physical effects. A new physical phenomenon, the T-layer effect, discovered through the NE may be an example [2] . The main point is that under certain conditions a self-maintained,

high-temperature, electro-conductive gas layer forms and develops during the magneto-hydrodynamic plasma motion. The conditions of the T-layer formation predicted by theoretical investigation permitted to reveal the effect later in laboratory experiments. The NE may be considered as a sequence of a number of the following stages:

I) choice of a physical approach and mathematical formulation of a problem (choice of a mathematical model); as a rule the equations describing the mathematical model express the conservation laws (for mass, energy, momentum, charge, etc.) and are the partial differential equations of mathematical physics;

2) development of a computational algorithm;

3) algorithm programming;

4) computing;

5) analysis of computational results; comparison with experimental and theoretical results; revision and correction of the mathematical model; improvement of the calculation technique.

The typical features of NE are as follows:

I) Within the mathematical model chosen, a number of runs (not one) is computed in the required interval of the parameters involved.

2) The mathematical model may be repeatedly varied.

In fact, one may speak of a new approach to performing the theoretical investigations on the basis of NE, which provides a proper connection between the mathematical model and a physical experiment through computing.

3) The multi-variant nature of computations in NE imposes strict requirements on the computational algorithms and corresponding software as well. While the same problem is being solved, the form of non-linearity or equations type may vary, discontinuities may arise, interact and dissipate, domain geometry and topology may change, and so on.

3. The numerical methods should have a sufficient resolution, i.e. accuracy for an admissible amount of computations, to describe correctly the main characteristics of complex, nonlinear processes.

In discretizing the continuum problems, i.e. changing differential equations by the difference ones, the natural requirement is that the discrete model obtained should reflect the basic properties of continuum correctly. In particular, the conservation of mass, momentum and total energy is such a property (these laws hold on the grid for conservative difference schemes [I] , [3]) as well as the balance equations for internal and kinetic energies, electromagnetic field energy, etc. The difference schemes with such properties we shall call the completely conservative schemes (CCS) [4] . CCS have proved to be highly effective and permitted to obtain the solutions sufficiently accurate for the MHD - and RMGD-problems in both cases of low and high temperature plasmas.

A heuristic approach to obtaining CCS, proposed by Popov and Samarskii (I969), allowed to construct CCS for other problems too, e.g. the Landau kinetic equation.

4. At present an integro-interpolation method, i.e. a balance method [3] , as well as projection and variational methods are used for obtaining CCS of the desired quality for the classical equations of mathematical physics.

In case of arbitrary dimension the variational method has proved to be effective for obtaining CCS for the MHD-problems [5] . The hydrodynamic equations result from a variational principle similar to that of least action in classical mechanics. For example, let us consider the liquid volume Ω of an ideally conductive adiabatic plasma, moving in the $x-y$ plane. In Lagrangian coordinates (α,β) the volume Ω corresponds to the domain $G(\alpha,\beta)$. The Lagrangian $L(t)$ of the volume Ω is taken as the integral in $G(\alpha,\beta)$ of the expression proportional to $(u^2+v^2)/2-\varepsilon-|H|^2/8\pi\rho$,where ε is the internal energy, $(u^2+v^2)/2$ is the kinetic energy, $|H|^2/8\pi\rho$ is the magnetic field energy per unit mass, ρ is the density. The integral of action $S=\int_{t_0}^{t_1}L(t)\,dt$ is varied with taking into account the additional constraints, i.e. equations of continuity and freezing-in of magnetic field. By setting the first variation δS equal to zero we obtain the Euler equation. Note that the energy and momentum conservation results from the absence of an explicit dependence of the Lagrangian and constraint equations upon time and coordinates.

The CCS are obtained in a similar way. The Lagrangian and constraint equations are approximated on the grid $\omega_h\{\alpha_i,\beta_j\}$. Varying the integral of action with the constraint equations taken into account gives us a system of differential-difference equations. After replacing the derivatives in t by the difference relations and introducing an artificial dissipation we obtain the homogeneous CCS of the first- and second-order approximation in t (the schemes of run-through computations). The above approach permitted to obtain CCS for the MHD-equations in arbitrary cirvilinear coordinates with heat conductivity, magnetic field diffusion and other factors involved, and to apply them to solving a number of physical problems [6] ,

5. Taking into account the radiation transfer, i.e. the transformation of MHD-problems into the RMGD ones, requires additional efforts for constructing and implementing the CCS.

Let us consider a technique proposed by Goldin and Chetverushkin [8] for solving the non-stationary problems (including two-dimensional ones) of radiative gas dynamics. The radiation transfer is considered in the multi-group diffusion approximation.

Solving the set of corresponding RMGD-equations is performed in three steps: I) solving the proper gasdynamic equations, 2) solving the transport and diffusion equations, and 3) obtaining the temperature from the combined solution of the energy and diffusion equations.

We now dwell on difficulties arising when the radiation is involved, i.e. the second and third steps. Due to the complex structure of absorption coefficients the general number of diffision equations is rather great. Solving the non-linear difference diffusion equations on each step in time is quite a problem that requires applying the specific iterational methods. In a number of cases the most simple explicit scheme for solving the combined diffusion and energy equations requires a very small time step to provide the stability of computations. While the technique having been developed the difficulties were overcome. The diffusion approximation used in the problems of radiative gas dynamics describes correctly the radiative contribution in the energy equations. In the numerical implementation the direct use of transport equation for determining the radiation field may cause an undesirable effect, "the beam effect" (it arises in case when the zone generating, in general, the radiation is small as compared with the whole region under investigation).

Recently a technique has been developed to compute the radiation transfer equations with the use of Vladimirov's self-adjoint equations and the above effect eliminated.

6. The verified methods for solving the gasdynamics problems being available, the hydrodynamic approximation can be used to solve other physical problems [9] . In nonlinear optics and plasma physics, of great interest are the problems on wave field dynamics, energy localization in the vicinity of a certain point (for example, light self-focusing in a nonlinear medium, collapse of Langmuir waves). For an amplitude of electric field in plasma, the nonlinear Schrödinger-type equation

$$2i\frac{\partial E}{\partial t}+\frac{1}{r^{\nu}}\frac{\partial}{\partial r}\left(r^{\nu}\frac{\partial E}{\partial r}\right)+|E|^{2}E=0$$
$$0<r<R\ ,\quad t>0\ ,\quad \nu=0,1$$

is reduced to the "gasdynamic" equations

$$\frac{\partial \rho}{\partial t}+\frac{1}{r^{\nu}}\frac{\partial}{\partial r}\left(r^{\nu}\rho v\right)=0,\quad \frac{\partial v}{\partial t}+v\frac{\partial v}{\partial r}+\frac{1}{\rho}\frac{\partial P}{\partial r}+g=0$$

where $\rho=|E|^{2}$ has the sense of density, and the "state" equation has the form

$$P=-\frac{1}{4}\rho^{2}\left[\frac{1}{\rho r^{\nu}}\frac{\partial}{\partial r}\left(\frac{r^{\nu}}{\rho}\frac{\partial \rho}{\partial r}+1\right)\right],$$
$$E=\rho^{1/2}e^{i\psi},\quad v=\frac{\partial \psi}{\partial r}\ ,\quad g=g\left(\rho,\frac{\partial \rho}{\partial r}\right).$$

By introducing the energy Lagrangian coordinate $\ell=\int_0^r \rho r^{\nu}dr$ the set of equations obtained may be solved using the known schemes on the Lagrangian grid.

The implementation of the above approach made it possible to investigate the dynamics of self-focusing in a cubic medium as well as successfully construct the computational algorithms for Langmuir turbulence.

7. Let us discuss particularly such important questions as the "physical attributes" of a numerical experiment, the thermodynamic properties of a medium.

The RMGD-equations describe some macroscopic phenomena in a moving medium. In fact, primary are the microscopic motions of particles (electrons, ions, atoms and photons) in the field created by the external sources and other particles. Averaging the microscopic motions yields the coefficients of RMGD-equations, i.e. thermodynamic funotions, electric conductivity and other properties of the matter. It is evident that the best gasdynamic calculation procedures do not give the correct solution to a physical problem if they contain incorrect properties of the matter. Finding the properties of the matter is a complex individual problem.

In solving the RMGD-problems one has to know the properties of various substances: hydrogen, inert gases, water and metal vapors, products of coal and oil combustion, etc. In the processes of interest for physicists, most various conditions develop, temperatures from the room to stellar ones and densities from those of gases to those of solids. Most of these conditions are so different from the room ones that the direct experimental determination of the matter properties seems to be impossible. On the other hand, the simplified models similar to that for an ideal gas, which are commonly treated in the theoretical physics, often cannot be used under those conditions. Therefore, we have to develop new physical approximations to determine the matter properties of interest.

To provide this part of our gasdynamic computations it was necessary to construct the mathematical description of continuum (in this connection we had to solve a number of most complex problems in quantum mechanics) and to develop the proper computational algorithms. At present quantum, exchange and oscillation (envelope) corrections to the Tomas-Fermi model have been obtained at arbitrary temperatures for chemical elements and arbitrary compounds. The computational algorithms have been developed and calculations of the above corrections performed. This work is carried out under the direction of N.N. Kalitkin.

To obtain the coefficients of electrical conductivity and electron heat conductivity a semi-classical model of electron transfer was constructed, involving the most essential quantum effects [IO] . Now the methods have been developed (under the direction of A.Ph. Nikifforov and V.V. Uvarov) to calculate the photon free paths in a high-temperature plasma of any complex composition with not only the inverse bremsstrahlung and photoeffect taken into account but the line absorption as well. One can conceive a complexity of this problem by noting that solving the Hartry-Fok equation for multi-electron atoms is a part of it.

The tables for the equations of states, conductivity, electron heat conductivity and photon (and other particles) free paths being available, numerical computations are in good quantitative agreement with physical experiments in many complex problems of plasma physics.

8. The CCS developed for the MHD- and RMGD-problems permitted to carry out NEs for investigating a number of problems in plasma physics and radiative gas dynamics. We restrict ourselves by listing some problems with brief comments supplied.

I) The investigation of pulsed radiating discharges in inert gases [II] .

The RMGD-model coupled with an electric circuit was chosen. The accurate treatment of the physical properties of substances involved and the proper description of the electric circuit with the photon transport taken into account allow to solve the $\mathfrak{Z}$ -pinch and inverse $\mathfrak{Z}$ -pinch problems with detailed quantitative agreement between the experimental and computed values of total current, Joule heat released, location of shock and boundaries of emitting regions in discharge etc. The spectral effects were found to be of major importance in heat transfer, and the luminosity boundary observed corresponds to the ionization front, and so on.

2) The T-layer stability. The T-layer was shown to be stable with respect to two-dimensional disturbances. The investigation was performed by means of CCS for the MHD-problems [I2] .

3) The study of compressing and heating a thermonuclear target by a laser pulse [I3] . The stability of compression was investigated with respect to the disturbances of initial target form and laser pulse [7] .

4) The investigation of the Rayleigh-Taylor instability.

5) The problems of laser "pumping" and searching for periodic solutions I4 .

Here we speak mainly of two-dimensional problems of gas dynamics and MHD. Among the people engaged in gas- and aerodynamics the complexity of a problem is usually defined by the number of dimensions.

However in the plasma physics problems, such as compressing a thermonuclear target by laser pulse or electron beam and burning in a target, the basic difficulties are in comprising various physical effects. Since the question of mathematical model choice is not clear it is necessary to consider different approaches to describing the same physical effect which implies comparing a few mathematical models. In conducting the numerical experiment we stick to the following principle:

a) taking into account all physical effects in "one-dimensional" approximation (e.g., under the assumption of spherical or cylindrical symmetry);

b) considering the influence of two- or three-dimension on the physical process under investigation.

In some cases it is expedient to carry out an one-dimensional physical experiment to compare it with an one-dimensional NE.

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