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COMPUTER SCIENCE

Modeling of Radiative Heat Conduction on High-Performance Computing Systems

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Abstract—For problems related to radiative heat conduction, an algorithm is proposed that is well adapted to the architecture of systems with extramassive parallelism. According to the underlying method, a term with a small parameter multiplying the second time derivative is included in the model describing the process. Examples of numerical results obtained using this model on detailed spatial meshes are given, and their comparison with results based on the classical radiative heat conduction model are presented.

Keywords: radiative heat conduction, hyperbolic model of heat conduction, explicit difference scheme

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1. HYPERBOLIC MODEL FOR DESCRIBING RADIATIVE HEAT CONDUCTION

Radiative heat conduction describes heat transfer with the help of radiation in optically thick media [1, 2]. This model is used to describe phenomena in astrophysics [3], in some engineering problems related to dense laser plasmas [4], and in processes associated with thermonuclear fusion [5].

According to this model, the divergence of the heat flux $\bar{W}$ caused by radiation is described in the form

$$\operatorname{div}\bar{W} = \operatorname{div}\frac{16\sigma T^3 l(T,\rho)}{3}\operatorname{grad}T, \tag{1}$$

where T is the temperature, σ is the Stefan–Boltzmann constant, and $l(T, \rho)$ is the Rosseland mean free path. In turn, l is defined as

$$l(T,\rho) = \frac{\int_0^\infty l_\nu(\nu,T,\rho)\frac{dU_{\nu p}}{dT}d\nu}{\int \frac{dU_{\nu p}}{dT}d\nu}, \tag{2}$$

where ν is the photon frequency, $l_\nu(\nu, T, \rho)$ is the free path of a photon of frequency ν, and $U_{\nu p}$ is the spectral radiation intensity of an absolutely black body given by

$$U_{\nu p} = \frac{2\pi h\nu^3}{c^2}\times\frac{1}{e^{\frac{h\nu}{kT}}-1}; \tag{3}$$

here, h is Planck's constant and k is the Boltzmann constant.

Finally, assuming that the heat capacity is a constant and neglecting the motion of the medium, the evolution of temperature is described by the parabolic equation of radiative heat conduction

$$C_\nu\frac{\partial T}{\partial t} = \operatorname{div}\frac{16\sigma T^3 l}{3}\operatorname{grad}T + Q, \tag{4}$$

where Q is a given source of heat and C_ν is the heat capacity.

This equation can be solved using explicit or implicit difference schemes. Implicit schemes are absolutely stable, but become inefficient under parallelization with a large number of solvers (processors, cores). This problem is especially challenging for promising computer systems using graphics processing units as accelerators.

Explicit schemes do not lose efficiency when numerous processors are used in parallel, but impose a severe restriction on the admissible time step [6], namely,

$$\Delta t \le \frac{h^2}{2\tilde{l}}, \tag{5}$$

where

$$\tilde{l} = \frac{16\sigma T^3 l(T,\rho)}{3}. \tag{6}$$

It is hardly possible to use explicit schemes on fine spatial meshes, for which, in fact, systems with extramassive parallelism are required. The situation is aggravated by the fact that the coefficient $\tilde{l}$ grows strongly with increasing temperature, which is typical for high-temperature gasdynamic processes. As can be

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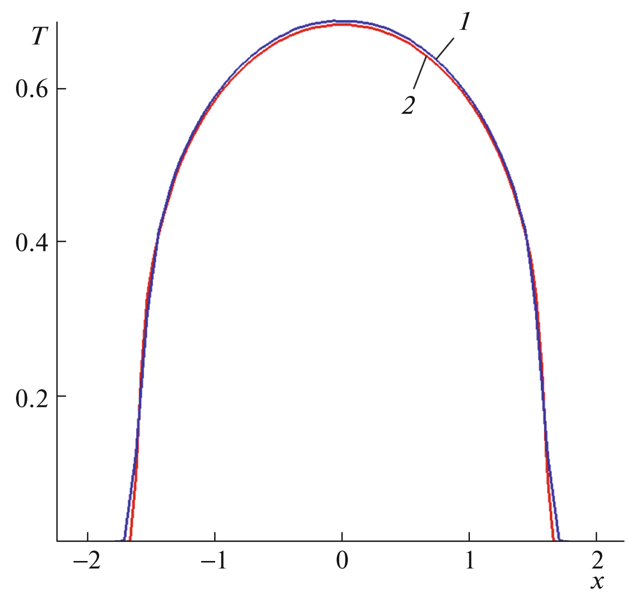

Fig. 1. Numerical results for the test problem of a cooling ball.

seen from (5), this imposes further restrictions on the admissible time step size Δt.

A way out of this seemingly deadlock situation relies on the hyperbolic heat conduction model:

$$C_v \frac{\partial T}{\partial t} + \varepsilon \frac{\partial^2 T}{\partial t^2} = \operatorname{div} \tilde{l} \operatorname{grad} T + Q, \tag{7}$$

which has previously been used to describe rapid processes [7].

Relying on physical considerations, we can see that the solutions of Eqs. (4) and (7) will differ little if

$$\left[\varepsilon \frac{\partial^2 T}{\partial t^2}\right] \ll \left[C_v \frac{\partial T}{\partial t}\right], \tag{8}$$

i.e.,

$$\frac{\varepsilon}{C_v} / t_{\text{proc}} \ll 1, \tag{9}$$

where t_{proc} is the characteristic time of the process.

Let us discuss the properties of the solution to Eq. (7) in more detail. The idea of reducing parabolic equations to a hyperbolic one was underlain by the analogy with the quasi-gasdynamic system, which is a hyperbolic system that differs from the Navier–Stokes equations in the small second-order terms in the Knudsen number ($O(Kn^2)$) [8].

This model admits the use of algorithms that are well adaptable to the architecture of high-performance computing systems. In [9, 10] the solution to the linear analogue of Eq. (7) was theoretically analyzed and compared with the solution to the linear analogue of Eq. (4). The formulation of conservation laws for a hyperbolic equation of type (7) was discussed in [11].

2. EXPLICIT SCHEMES FOR SOLVING THE HYPERBOLIC HEAT CONDUCTION EQUATION

In this work, Eq. (7) was solved numerically using explicit schemes. Below, we discuss the choice of a small parameter ε for this equation and compare its solution with that of its parabolic counterpart (4) for various values of the radiative thermal conductivity $\tilde{l}$.

As a small parameter ε, we use a quantity proportional to the ratio of the spatial mesh size h to the characteristic speed V of the process:

$$\varepsilon < \frac{h}{V}. \tag{10}$$

This choice of ε ensures the necessary accuracy of the solution of Eq. (7) and its proximity to the solution of parabolic equation (4). On the other hand, this choice of ε makes it possible to compute Eq. (7) by applying an explicit scheme with an acceptable (as shown by theoretical estimates [12]) time step size Δt such that

$$\Delta t \le k h^{3/2}. \tag{11}$$

The Δt-constraint (11) is more acceptable than condition (5). The advantages of (11) are especially pronounced on fine spatial meshes, providing the opportunity of using explicit schemes in massive parallel computations. However, it should be noted that some of the numerical experiments presented in this work were characterized by a milder Courant-type stability condition, namely,

$$\Delta t \le a \cdot h. \tag{12}$$

The hyperbolic equation (7) was solved using a three-level difference scheme relating the solutions at the time levels $j-1$, j, and $j+1$. For a constant Δt, the time derivatives were approximated as

$$\frac{T_i^{j+1} - T_i^{j-1}}{2\Delta t} \quad \text{and} \quad \varepsilon \frac{T_i^{j+1} - 2T_i^j + T_i^{j-1}}{\Delta t^2}. \tag{13}$$

The spatial derivatives were approximated at the central time level $t = t^j$.

The temperature values T^{j+1} at the level $j+1$ were determined using known temperature values T^j and T^{j+1}. The coefficient $\tilde{l}$ was determined from the known temperature value T^j. It should be noted that the strong nonlinear dependence of $\tilde{l}$ on temperature imposes additional constraints on Δt, but they are determined by the accuracy of the numerical solution, rather than by stability.

3. NUMERICAL EXAMPLES

The main goal of the conducted numerical experiment was to experimentally analyze the stability of the explicit three-level scheme for solving the hyperbolic heat equation (7), and to compare its solutions with

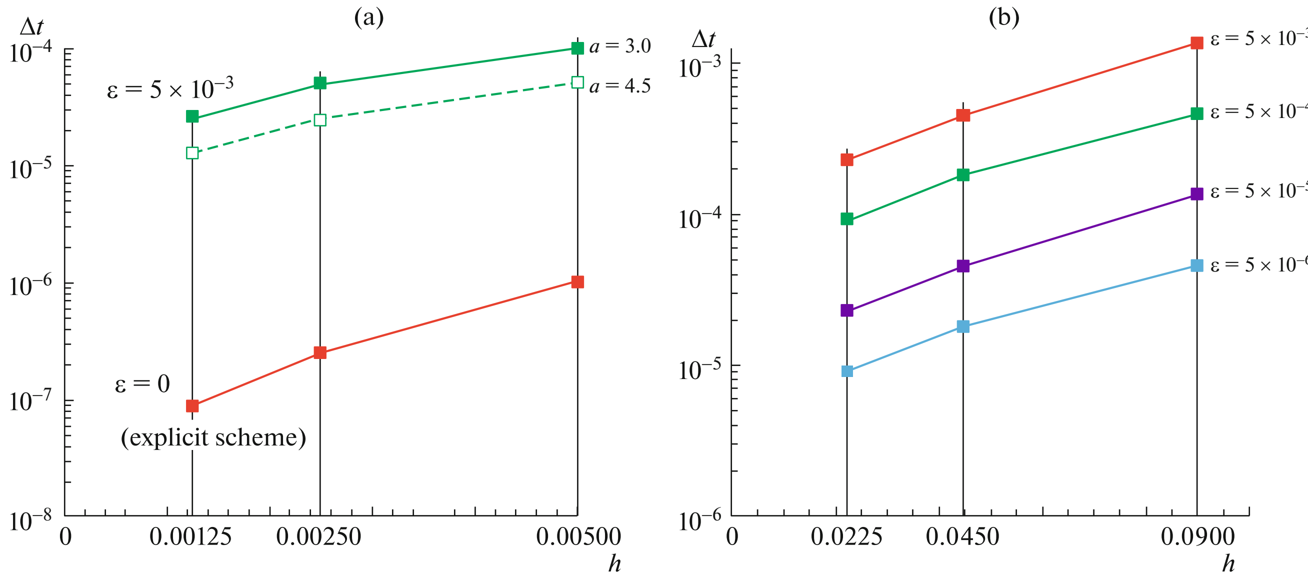

Fig. 2. Stability of explicit schemes: (a) 1D computations and (b) 3D computations.

those of the parabolic equation (4). The basic computations were performed for the one-dimensional (1D) formulation, which provides more opportunities for mesh refinement. Computations were also performed in the two- and three-dimensional (2D and 3D) formulations. The computations were conducted with various values of the nonlinear radiative thermal conductivity.

The test problem

$$\frac{\partial T}{\partial t} + \varepsilon \frac{\partial^2 T}{\partial t^2} = \operatorname{div}(k_0 T^{\alpha} \operatorname{grad} T)$$

was considered in the computational domain

$$-2.25 \le x \le 2.25;$$

$$-2.25 \le y \le 2.25; \quad -2.25 \le z \le 2.25;$$

with initial conditions

$$T(r,0) = \begin{cases} 2, & -1 \le r \le 1 \\ 0,01, & r > 1; \end{cases}$$

$\alpha = 3$; $k_0 = 1$; and the computation time $t_{\max} = 1$.

Figure 1 shows the numerical solutions produced by (*1*) a two-level implicit scheme for parabolic equation (4) and (*2*) the three-level scheme for hyperbolic model (7) at $\varepsilon = 5 \times 10^{-3}$ in 3D-computations performed on a regular grid consisting of 100 cells in one coordinate ($h = 4.5 \times 10^{-2}$) with the identical time step $\Delta t = 4.5 \times 10^{-4}$. The resulting solutions differ within 1% in the C norm. Under mesh refinement, this difference is further reduced. The results of 1D-computations on a regular grid consisting of 1000 cells in coordinate ($h = 4.5 \times 10^{-3}$, $\Delta t = 10^{-4}$) differ at most in the fifth decimal.

Figure 2 presents the maximum admissible time step Δt as a function of the spatial mesh size h. For the three-level scheme (7), we have $\Delta t_{\max} \le a_1 h$, where a_1 is a constant depending on the parameter ε. Similar computations were performed for $\alpha = 4.5$. In this case, the constant a_1 was approximately half as large (dashed curve in the plot). The lower curve in Fig. 2a corresponds to the explicit two-level scheme as applied to the parabolic equation (4). In this case, the stability condition has the form $\Delta t_{\max} \le a_2 h^2$. The numerical results produced in the 3D case are displayed in Fig. 2b. Similar results were obtained on tetrahedral meshes.

Since explicit schemes are well adaptable to the architecture of multiprocessor systems, issues associated with parallel implementation were not addressed in this study. The approximation of the term $\operatorname{div} \tilde{l} \operatorname{grad} T$ on various unstructured meshes was not considered either. In the future, we intend to use previously developed techniques for spatial approximation.

CONCLUSIONS

The hyperbolic heat conduction model (7) with a small parameter ε multiplying the highest time derivative yields results that are similar to those based on the classical parabolic model (4). It seems that an optimal choice of ε is given by (10). As a result, on the one hand, the closeness of the solutions of the parabolic and hyperbolic models is ensured and, on the other hand, the computational costs are reduced noticeably in the case of explicit schemes.

With the use of explicit schemes, the hyperbolic model exhibits noticeable advantages. As compared with parabolic model (4), they are especially pronounced on fine spatial meshes, whose application became possible with the creation of ultrahigh-performance computing systems.

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