ParCFD’2020
32nd International Conference on Parallel Computational Fluid Dynamics
May 11-13 2020, Nice FRANCE

AN EXPLICIT SCHEME FOR RADIATIVE HEAT CONDUCTION ON HIGH-PERFORMANCE COMPUTING SYSTEMS

BORIS N. CHETVERUSHKIN, OLGA G. OLKHOVSKAYA, VLADIMIR A. GASILOV AND ILYA P. TSYGVINTSEV

Keldysh Institute of Applied Mathematics (Russian Academy of Sciences) 125047 Moscow, RUSSIA
e-mail: olkhovsk@gmail.com, web page: https://keldysh.ru/index.en.shtml

Key words: radiative thermal conductivity, hyperbolic model of heat conduction, explicit difference scheme.

Summary. We consider an algorithm for solving problems related to the process of radiative heat conduction, which is well adapted to the architecture of systems with extra-massive parallelism. The technique is based on including a term with a small parameter of the second time derivative. The computation results using the new scheme on detailed spatial meshes and their comparison with the classical radiative heat conduction model are presented.

1 INTRODUCTION

Radiative heat conduction describes the process of heat transfer via radiation in optically thick media[1], which is typical of high-temperature gas-dynamic processes. This model is applied in astrophysics, dense laser plasma technologies[2], thermonuclear fusion[3], etc.

The divergence of heat flux due to radiation $\overline{W}$ is described as

$$div\overline{W} = div\frac{16\sigma T^3 l(T,\rho)}{3}grad\,T$$

T is the temperature, σ is the Stefan-Boltzmann constant, l is the Rosseland mean free path of the photon. Assuming that the heat capacity coefficient is constant, and the motion of the medium is neglected, we obtain the parabolic equation of radiative heat conduction:

$$C_v\frac{\partial T}{\partial t} = div\frac{16\sigma T^3 l}{3}grad\,T + Q \tag{1}$$

Q is the given heat source, and C_v is the heat capacity.

2 HYPERBOLIC MODEL FOR THE RADIATIVE HEAT CONDUCTION

One can use both explicit and implicit difference schemes to solve this equation. Implicit schemes offer an advantage of absolute stability, but they drastically lose the efficiency of parallel processing when using a large number of processors (cores). This problem is crucial for advanced computing systems with GPU accelerators. Explicit schemes do not reduce parallel efficiency, but they suffer a very strict limitation of the allowable time step[4]

$$\Delta t \lesssim \frac{h^2}{2\tilde{l}}, \text{ where } \quad \tilde{l} = \frac{16\sigma T^3 l(T,\rho)}{3} \tag{2}$$

Therefore explicit schemes are impractical for detailed spatial meshes essentially using parallel computations. As concerns radiative heat conduction, the time step Δt is further restricted because of a strong increase in the heat conductivity coefficient $\tilde{l}$ in eq. (2) with increasing temperature. The possible way out of this seeming deadlock situation is the use of the hyperbolic model of thermal conduction which has already been used for fast processes[5]:

$$C_v \frac{\partial T}{\partial t} + \varepsilon \frac{\partial^2 T}{\partial t^2} = div\, \tilde{l}\, grad\, T + Q \tag{3}$$

As appears from physical considerations, the solutions of equations (1) and (3) will differ slightly, if the following condition is satisfied:

$\left[\varepsilon \frac{\partial^2 T}{\partial t^2}\right] \ll \left[C_v \frac{\partial T}{\partial t}\right]$, i.e. $\frac{\varepsilon}{C_v} \ll t_{proc}$, where t_{proc} is the characteristic time of the process.

The idea of reducing parabolic equations to a hyperbolic form arose from an analogy with the quasi-gas-dynamic system[6], which is a hyperbolic system, differing from the Navier-Stokes equations by the terms of the second order of smallness in relation to the Knudsen number $O(Kn^2)$. A theoretical analysis of the solution of the linear analogue of the equation (3) and its comparison with the solution of the linear analogue of the equation (1) was carried out in [7,8]. The conservation laws for a hyperbolic equation of type (3) were formulated in [9].

3 EXPLICIT SCHEMES FOR THE HYPERBOLIC HEAT EQUATION

We choose the small parameter ε to be a value proportional to the ratio of the spatial size of the mesh cell h to the characteristic rate of the process V: $\varepsilon < h / V$.

Such a choice provides the required accuracy of the solution of the equation (3) and its proximity to the solution of the parabolic equation (1). The theoretical estimates[10] showed that it makes possible to solve equation (3) using an explicit scheme with an acceptable time step:

$$\Delta t \le a \cdot h^{3/2} \tag{4}$$

The restriction (4) is more reasonable than the condition (2). The advantages of condition (4) are especially evident on detailed spatial meshes, allowing a real possibility of using explicit schemes for parallel computing. However, even milder stability condition similar to the Courant condition was observed in the presented computational experiments: $\Delta t \le a \cdot h$.

We apply a three-layer difference scheme for solving the hyperbolic equation (3). With a constant Δt, the approximation of time derivatives is as follows:

$$\frac{\partial T}{\partial t} \to \frac{T_i^{j+1} - T_i^{j-1}}{2\Delta t} \quad \text{and} \quad \varepsilon \frac{\partial^2 T}{\partial t^2} \to \varepsilon \frac{T_i^{j+1} - 2T_i^j + T_i^{j-1}}{\Delta t^2} \tag{5}$$

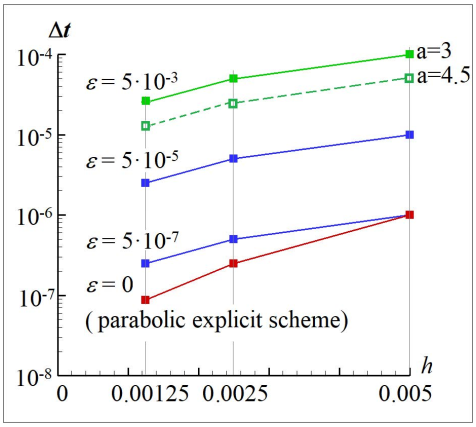
(j–1), j, and (j+1) are successive time layers. The spatial derivatives are approximated in the point i at the central time layer $t = t^j$, as well as the coefficient $\tilde{l}$ depending on the known temperature T^j. Thus the temperature values T^{j+1} on the layer (j+1) are computed using the already known values T^j and T^{j-1}. This scheme provides $O(\Delta t^2)$ order of convergence.

4 NUMERICAL RESULTS

The aim of the numerical tests was the stability study of the explicit scheme (5) for the hyperbolic heat equation (3), and comparison of hyperbolic (3) and parabolic (1) solutions.

A model problem was examined: $\frac{\partial T}{\partial t} + \varepsilon \frac{\partial^2 T}{\partial t^2} = \mathrm{div}\left(k_0\, T^{\alpha} \mathrm{grad} T\right)$; $\alpha = 3$; $\alpha = 4.5$; $k_0 = 1$.

3D numerical solution on a regular mesh 100^3 with the same time step using an implicit two-layer scheme for the parabolic equation (1) and that using the explicit tree-layer scheme (5) for the hyperbolic model (3), $\varepsilon = 5 \cdot 10^{-3}$, differ in norm C by less than 1%. The difference decreases with the mesh refinement. 1D results on a regular mesh (1000 points) differ by the 5th digit only.



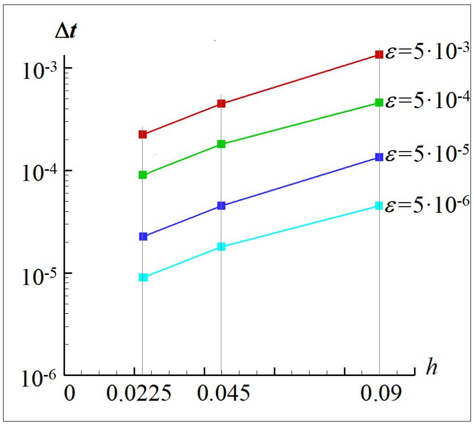


Fig. 1 – Stability condition for the explicit scheme: left – 1D , right – 3D.

Figure 1 (left) shows the dependence of the maximum permissible time integration step Δt on the spatial mesh step h. We found the stability condition $\Delta t \le a_1 h$ for the scheme (5) with a_1 depending on ε and α, and $\Delta t \le a_2 h^2$ for the parabolic equation (1) using an explicit two-layer scheme. Figure 1 (right) presents the results of 3D numerical experiments on rectangular meshes. Similar results were also obtained on tetrahedral meshes.

Explicit schemes are well fitted to the architecture of HPC systems, including multi-level parallelism using MPI/OpenMP/Cuda for CPU-GPU clusters. We have already accumulated a wealth of experience in spatial approximation of the term $div\, \tilde{l}\, grad\, T$ on various kinds of unstructured spatial meshes and octree meshes with adaptive mesh refinement. In these cases an implicit scheme deals with a distributed sparse matrix for the appropriate system of linear algebraic equations. An iteration procedure requires additional data exchanges, and its convergence may not be always evident. Therefore the above explicit scheme is preferable, especially for numerical study of fine structures and/or fast processes.

5 APPLICATION TO CFD: SIMULATION OF LASER TARGET COMPRESSION

One of the prominent areas to use the above approach is the radiative hydrodynamic simulations of DT target in the indirectly driven inertial confinement fusion scheme[3]. We investigated the influence of physical and numerical instabilities on the resulting target dynamics in a simplified approximation (one temperature – one fluid hydrodynamics with two-term equation of state[2]). The radiative heat conduction emulated the target irradiation. We used a power-law dependency $l\left(T,\rho\right)=C_1T^{C_2}\rho^{-C_3}$ for the photon mean free path, and the experimental temperature dynamics[3] *T(t)* was applied at the boundary.

Preliminary 1D simulations using lagrangian code in spherical geometry have shown a good agreement of the target dynamics with the experimental shadowgraphs. We have used completely implicit full conservative numerical scheme for these simulations and expected that iteration convergence rate and timestep would be the similar in 3D Cartesian setting with the same cell size. However, in 3D we met a number of difficulties related to the thermal conduction: usage of implicit scheme with a reasonable step Δt led to a very slow convergence rate even on relatively meager grid 256^3. Explicit scheme, on the other hand, while being computationally saving on one time step, required too low Δt value to fulfill stability restrictions. The hyperbolic model allowed overcoming these difficulties.

6 CONCLUSIONS

The hyperbolic model of thermal conductivity with the second time derivative coefficient being a small parameter ε is a useful tool for numerical simulation of radiative heat transfer. The optimal ε value was defined that provides both the proximity to the classical parabolic solution, as well as a noticeable computational effectiveness when using explicit schemes. These advantages are especially pronounced in comparison with the parabolic model when the use of detailed spatial meshes is supported by HPC systems with hybrid architecture.

The work was supported by Russian Foundation for Basic Research, project 18-01-00587a.

REFERENCES

[1] Ya. B. Zel'dovich and Yu. P. Raizer *Physics of Shock Waves and High Temperature Hydrodynamic Phenomena* Dover, New York, 2002.
[2] A. I. Lebo and I. G. Lebo *Physica Scripta*. 2010. V. 142, P. 014024
[3] B. Nayak and S. V. G. Menon *Laser and Particle Beams* (2012) 30(04), P. 517–523.
[4] A. A. Samarskii *The Theory of Difference Schemes* CRC Press, 2001
[5] V. E. Golant, A. P. Zhilinsky and I. E. Sakharov *Fundamentals of Plasma Physics* John Wiley & Sons, New York, 1980
[6] B. N. Chetverushkin *Kinetic Schemes and Quasi-Gas Dynamic System of Equations* CIMNE Barcelona, 2008
[7] S. I. Repin and B. N. Chetverushkin *Doklady Mathematics* 2013. V. 88. N. 1. P. 417-420.
[8] E. E. Myshetskaya and V. F. Tishkin *Comp. Mathem. and Math. Physics* 2015. V. 55. N. 8. P. 1270-1275.
[9] M. D. Surnachev, V. F. Tishkin and B. N. Chetverushkin *Diff. Equations* 2016. V. 52. N. 7. P. 817-823.
[10] B. N. Chetverushkin and A. V. Gulin *Doklady Mathematics* 2012. V. 86. N. 2. P. 681-683.