Parallel Algorithms and Adaptive Methods for Numerical Solution of the Multi-Dimensional Transport Equation

I.M.Belyakov, A.V.Alekseyev, V.V.Evdokimov, A.A.Nuzhdin, V.Yu.Rezchikov, R.M.Shagaliev*

*Russian Federal Nuclear Center - All-Russian Research Institute of Experimental Physics (RFNC-VNIIEF), 37 Mir Ave., Sarov, 607190, N.-Novgorod reg., Russia.

The paper considers parallelization methods and the problems of using adaptive grids in phase space to solve the multi-dimensional transport equation in kinetic multi-group approximation.

Introduction

Numerical simulation of multi- dimensional particle transport processes is one of the most difficult and labor-intensive (from viewpoint of computational burden) problems of applied mathematics.

It should be emphasized that the problem is especially hard to solve in general case, when the boundary-value problem for the transport equation is stated in regions of complex geometries and the equation is approximated using non-orthogonal spatial grids. To solve such problems numerically, implicit schemes in time variable are used, as a rule, and the system of grid equations in time steps is solved using the sweep method. This means the grid equations of transport in the grid cells are resolved, at a given time step, in the strict sequence order, with this sequence being different for various particle flight directions and varying with time. In other words, when solving the transport equation in transport approximation using multiprocessors, it is impossible to determine the topology of communications (the order of data exchanges) between PEs beforehand and this complicates, in principle, the task of development of efficient parallelization algorithms for transport problems.

In many problems of numerical simulation of transport a situation is possible, when there is a need to find a numerical solution of a higher accuracy within some sub-region of space and the sub-region moves in space with time. The wave front vicinity in the X-ray radiation transport problem is an example of such sub-region. In such cases, application of a more fine spatial grid for some sub-region of the computational region moving with time is required to find a numerical solution of a higher accuracy. The number of the reference grid cells contained in the sub-region mentioned above is significantly less, as a rule, than the total number of the reference grid cells. This provides a relative cost-efficiency of computations using such adaptable grids.

The paper presents results of application of some parallelization algorithms to solving the multidimensional time-dependent multi-group kinetic equation of transport using non-orthogonal spatial grids. The issues of using adaptive methods for the multidimensional transport equation with the application of refined grids in phase space are also considered.

Statement of Problem

The techniques are based on the kinetic model describing transport processes using the time-dependent multidimensional kinetic equation in its classic integro-differential form (Belyakov et al., 1999).

$$\partial/\partial t\left(N_i/v_i\right)+LN_i+\alpha_i N=F_i,\ F_i=\left(\beta_{ij}n_j^{(0)}+Q_i\right)/4\pi \qquad (1)$$

$$LN_i\equiv\frac{\partial}{r\partial r}\left(r\sqrt{1-\mu^2}\cdot\cos\varphi\cdot N_i\right)+\frac{\partial}{\partial z}\left(\mu N_i\right)+\frac{\partial}{\partial\Phi}\left(\frac{\sqrt{1-\mu^2}}{r}\cdot\sin\varphi\cdot N_i\right)-\frac{\partial}{\partial\varphi}\left(\frac{\sqrt{1-\mu^2}}{r}\cdot\sin\varphi\cdot N_i\right),$$

$$n_i^{(0)}=\int_{-1}^{1}d\mu\int_{0}^{2\pi}N_i\,d\varphi\ , \qquad (2)$$

where

r, z, Φ are cylindrical coordinates of a particle;. $\vec{\Omega}=\vec{\Omega}(\mu,\varphi)$ is a unit vector in the direction of a particle flight; $\mu=\cos\theta$, θ is the angle between vector $\vec{\Omega}$ and Z axis; φ is the angle between the vector $\vec{\Omega}$ projection onto the plane across point (r, z, Φ) normal to Z axis and the vector in this plane oriented from a point on Z axis to the given point (r, z, Φ); $-1<\mu<1$, $0<\varphi<2\pi$.

$\alpha_i=\alpha_i(t, r, z, \Phi)$; $\beta_{ij}=\beta_{ij}(t, r, z, \Phi)$ are particle collision and multiplication coefficients ;

$N_i=N_i(t, r, z, \Phi, \mu, \varphi)$ is a flux of particles flying in the direction μ, φ;

$Q_i=Q_i(t, r, z, \Phi)$ is an independent source of particles.

The system of equations (1) is solved in a phase space region

$$D=\{(r, z)\in L(\Phi),\ \Phi_1\le\Phi\le\Phi_2,\ -1\le\mu\le1,\ 0\le\varphi\le2\pi\}. \qquad (3)$$

L(Φ) is the cross section of the body of revolution by a plane across Z axis;

Φ_1, Φ_2 are the cross-sections bounding the solution region: Φ_1=const, Φ_2=const, $0\le\Phi_1\le\Phi_2\le2\pi$.

The boundary condition on the outer surface is given at $(\vec{\Omega}\cdot\vec{n})<0$ in the form

$$N_i(t, r, z, \Phi, \mu, \varphi)_{(r, z)\in\Gamma(\Phi)}=\psi_{1i}(t, r_\Gamma, z_\Gamma, \Phi, \mu, \varphi), \qquad (4)$$

where Γ=Γ(Φ) is generatrix of the body of revolution; $\vec{n}$ is the outer normal to surface of the body of revolution; $\psi_{1i}(t, r_\Gamma, z_\Gamma, \Phi, \mu, \varphi)$ is a given function.

The initial condition has the form:

$$N_i(t, r, z, \Phi, \mu, \varphi)|_{t=t0}=\psi_{2i}(t, r, z, \Phi, \mu, \varphi), \qquad (5)$$

where $\psi_{2i}(t, r, z, \Phi, \mu, \varphi)$ is a given function.

Approximation and solution methods

The transport equation approximation in time is built using an implicit two-layer difference scheme. The transport equation approximation in angular variables is built using the scheme of the method discrete ordinates.

The transport equation approximation in space is built with the finite difference method using regular spatial grids on the template that contains solutions at the centers of edges and at nodes of a cell.

At a time step, the system of equations is solved using the method of iterations in the right-hand part. For each iteration, the systems of grid equations with the specified right-hand parts are solved sequentially in particle flight directions. Explicit cost-effective sweep (point-to-point computation) algorithms are used to solve the system of grid equations with the specified right-hand part.

The extended template scheme (see Fig.1) has the following features:

- the scheme is conservative;
- it converges to the second-order solution of the transport equation using arbitrary non-orthogonal spatial grids;
- the requirement of diffusion maximum is met in optically dense media;
- DSn-scheme quadratures are used to approximate the transport equation in angular variables.

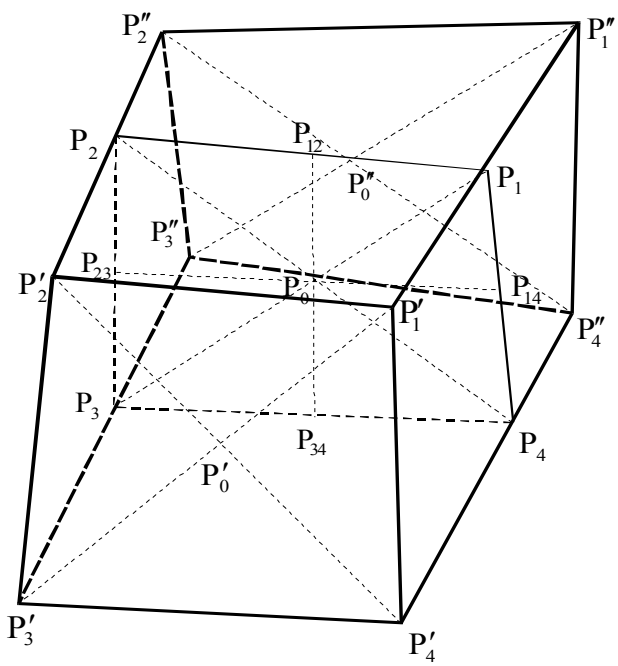


Figure 1. A space grid cell and the desired functions.

Parallel Techniques

Small-block parallelization algorithm for solving 2D and 3D problems using structured grids.

Parallelization in energy groups and neutron flight directions for solving 2D problems using structured and unstructured grids.

A pipelined algorithm of parallelization in layers and neutron flight directions to solve 3D problems using structured grids.

A combined algorithm of small-block parallelization and parallelization in energy groups to solve 2D and 3D problems using structured grids.

The algorithm of small-block parallelization is based on the idea of space decomposition of the original system's domains into sub-domains (Shagaliev et al., 2002). Decomposition into sub-domains (hereinafter called *para-domains*) to be processed on separate processors is performed in one space direction only, namely, either in columns of the spatial computational grid in use (1D decomposition), or in columns and rows (2D matrix decomposition).

The main ideas of the small-block parallelization algorithm with decomposition are, as follows (Shagaliev et al., 2003):

- spatial decomposition of a domain into para-domains;
- independent in angular variable solution of a system of grid equations;
- each para-domain, for a current direction, is resolved with the internal boundary conditions calculated during the previous iteration, this allows the solution accuracy to be preserved and doesn't increase the total number of iterations, as compared to the technique of sequential computations;
- interprocessor communications are performed simultaneously with calculations owing to the use of asynchronous transfer/receipt operations.

A single-domain spherically symmetric transport problem in one-group approximation was used as a test problem to study the efficiency of parallelization using the code for solving the 2D transport equation with matrix decomposition. A spatial grid consisted of 1200 rows and 1200 columns. The problem was solved with angular grid containing 6, 8, 12 and 14 intervals in μ in order to study the influence of the number of intervals in angular variable on the parallelization efficiency. There were 5 computational steps with 6 iterations in each step. The number of processors was selected so as to provide balanced computations, i.e. processors calculated the same number of points. Comparative results of these computations are shown in Fig.2.

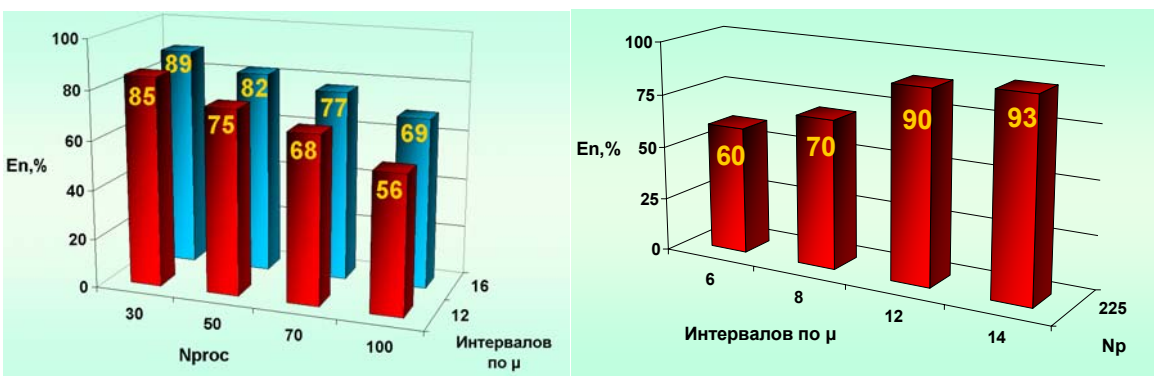


Figure 2. 1D and 2D decompositions for comparison.

Demands for the improved accuracy of multi-group transport computations determine the need in using a large number of intervals in energy variable (groups) for numerical simulation. The combined parallelization algorithm is a combination of parallelization in space and parallelization in energy variable.

When solving the multi-group transport equation, various intervals (ranges) in energy variable can be calculated independently on their own processors (groups of processors). Such approach allows using a large enough number of processors to solve the 2D transport equation with the acceptable efficiency preserved.

The model problem described below has been chosen for test computations. There is a single region in the form of a hemisphere. A grid has 80 rows uniformly distributed along the radius and 200 columns uniformly distributed in angle. The angular quadrature order is 12. The total number of particle flight directions is 96. The number of energy groups is 28.

The values of speedup and parallelization efficiency obtained as a result of numerical studies are given in Table 1. For each computation, the total number of processors, the number of para-domains during parallelization in space and the number of group-domains during parallelization in groups are given.

Table 1. The values of speedup (Sp) and parallelization efficiency (E).

Number of Processors	Number of Group-domains	Number of Para-domains	Sp	E (%)
7	7	1	5.5	78
25	1	25	25.4	102
28	28	1	12.3	44
100	1	100	66.2	66
100	4	25	74.9	75
200	1	200	92.7	46
200	4	50	111.7	56

The pipelined parallelization algorithm is used to solve 3D problems (Alekseyev and Shagaliev, 1993). The system is decomposed in layers.

Consider a problem with ~1000000 points in space (144 layers). The number of energy groups is 26, the number of dissipation anisotropy harmonics is 5. The angular quadrature order is 8, the total number of particle flight directions is 96.

Table 2. The parallelization efficiency (E) values.

Number of Processors	9	18	36	72	144
E (%)	92	85	81	78	76

The Main Ideas of the Adaptive Method

Consider application of grids adaptively refined in space, angular, and energy variables to solution of the multidimensional transport equation (Shagaliev, 2004).

Main ideas of the space-adaptive method

- Each cell of the reference spatial grid can be partitioned into smaller cells (adaptive cells) of an adaptive refined grid.
- An adaptively refined grid is constructed by uniformly partitioning in each space direction into 2^N spaces, where N is the adaptive grid level.

- When constructing a space-adaptive grid, the values of radiation temperature function in cells of the reference grid are examined. Each reference grid's cell is partitioned separately in rows and columns.
- The order of resolving space cells during the sweep method computations has to be determined on the reference grid. If a cell has an adaptive grid, the subsystem of equations corresponding to the transport equation approximation using the adaptive grid of this cell is solved.
- During reconstruction of the adaptive grid, re-interpolation of the grid values is performed by normalized conservative integration with weights.

The transport equation is solved in angular-variable cycles. The standard sweep method is used to solve the 2D transport equation in cycle arranged in the angular grid directions using the reference grid.

If the transport equation is solved using the adaptive spatial grid, the same sweep method is used, including computations inside reference cells.

Main ideas of the angular-adaptive algorithm

Consider the main ideas of the adaptive method for the transport equation approximation in angular variables:

The reference grid in angular variables is the main grid on which the transport equation is solved numerically at time steps. During the computation process, the reference grid doesn't enlarge, however, partition of separate intervals in angular variables μ and φ of the reference grid into smaller intervals is possible. Note that refinement is performed strictly within the reference grid intervals. In other words, availability of intervals in which points partially belong to one interval and partially to another interval in a finer angular grid of the adaptive method is not admissible.

An angular grid is refined only for the chosen set of spatial cells. In time-dependent computations elements of a given set are fixed, as a rule, at one time step, however, their modifications with transition to the next time step are possible. In various spatial cells partition into various quantities of smaller intervals in variables μ and φ of the reference grid is possible.

A set of spatial cells, in which the reference angular grid refinement to obtain finer intervals is required, is selected according to special criteria. The algorithms also determine the type of refinement, including the number of sub-intervals the corresponding interval of the reference angular grid is partitioned into. Here are some possible criteria:

- Analysis of gradients of the desired function in angular variables and use of the adaptive method at those space points and in those angular grid intervals, where the solution undergoes changes exceeding some specified values;
- Finding the heat wave front to use the adaptive method on this front (either on the heat wave front, or behind it);
- Application of the adaptive method at the specified number of near-boundary points (rows, columns), which number can vary with regard to specific features of the solution behavior in time.

The energy-adaptive algorithm

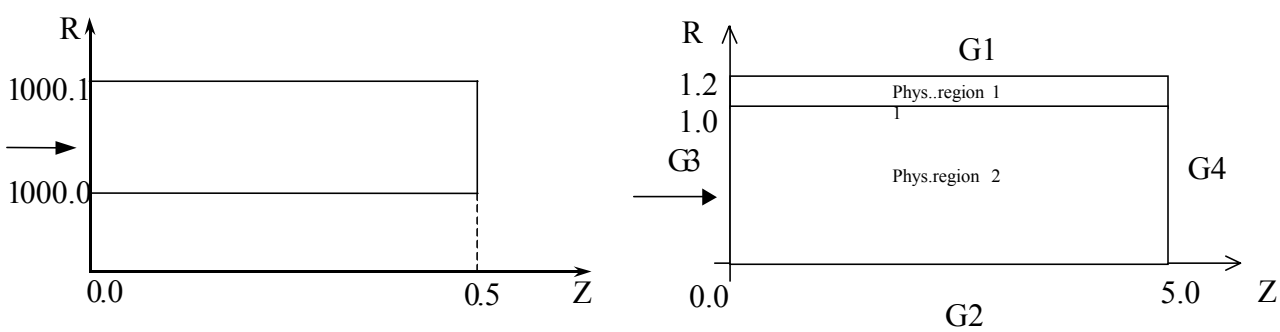
When approximating the transport equation using an energy-adaptive grid, the following problems have to be resolved:

- Development of criteria for and algorithms of partitioning a reference energy grid into smaller energy ranges (groups) at those space points and those ranges of the reference energy grid, where the solution in energy variable undergoes significant changes.
- Construction of approximation in energy variable to the transport equation using an adaptive grid.
- Generalization of the sweep method for numerically solving multi-group grid transport equations of the adaptive scheme.

In the phase of introduction of smaller energy ranges (groups) of the adaptive method (adaptive grid) inside one range of the reference grid factors and difference operators for equations describing energy (particles) transport in the adaptive grid spaces have to be specified. The following two points should be taken into account during computation of these factors and construction of difference operators. First, it is required to specify an approximate distribution of the desired solution over the groups of the adaptive grid introduced inside one space of the reference grid. In some cases the distribution law can be specified beforehand with regard to specific features of statement of one or another class of problems (balanced distribution of photon energies with Planck function, spectral distribution of other specified independent volume sources, spectral distribution of an incoming particle flux across the interface, etc.). Second, the requirement of conservativeness seems to be necessarily met, if factors and difference operators of the multi-group transport equations corresponding to the adaptive grid spaces are calculated. In other words, it is required that the total number of adsorbed particles (energy) in the adaptive grid spaces is absolutely equal to the number of adsorbed particles (energy) in the corresponding space of the reference grid. The other factors, as well as the introduced difference operators should meet the same requirement.

Problem Solution Examples

To verify the implemented space-adaptive algorithm and estimate its efficiency, numerical studies were carried out using a set of benchmarks. Table 3 gives the benchmark parameters.



a) **Figure 3.** The geometry of test problems b)

Table 3. The benchmark parameters

	Problem 1	Problem 2
Nature of problem	One-dimensional	Essentially two-dimensional

Geometric parameters	See Fig.3a	See Fig.3b
Boundary conditions	On the left boundary, there is an incoming radiation flux corresponding to $\varepsilon(0,\mu,t)=\dfrac{ct}{c+(cC_1\mu+1)}$, $\mu>0,\ C_1=-0.85903205...$ where $\varepsilon(z,\mu,t)$ is the radiation intensity multiplied by π.	On the left boundary: "mirror reflection" on the boundary section related to a dense casing; an incoming isotropic radiation flux corresponding to temperature T=1 on the boundary section related to the transparent region. On the upper boundary and on the right end: a zero incoming radiation flux.
Energy dependence on temperature	$E=2058*T^4$	$E=C_vT$, where $C_v=0.81$.
Absorption cross-section	$\chi_a=\dfrac{1}{2058*T^4}$	$\chi_a=\dfrac{A}{T^3}$, where *A*=50.89 in the 1st physical region; *A*=0.1374 in the 2nd physical region

Problem 1

A grid of 10 rows and 25 or 50 columns was used as a reference spatial grid for adaptive algorithm operation. Results of computations with the adaptive technique are practically the same as the results of computation using the fines spatial grid of 400 columns and the analytical solution. So, this fact confirms the adaptive algorithm adequacy.

Comparison between the running times shows that the adaptive computation with maximum refinement of the reference spatial grid (to obtain 8 cells) requires time by a factor of 6.2 less than the time required for this problem solution on the reference grid of 200 columns using the standard technique, with the results of the both computations being actually the same.

Problem 2

A grid of 10 rows (5 rows per region) and 50 columns (NR=10, NZ=50B) was chosen as a reference grid in space variables for computations using the adaptive algorithm. The level of adaptive refinement was chosen so as to provide maximum refinement corresponding to the grids in space variables with NR=40, NZ=200 and NR=80, NZ=400.

The solution obtained using the adaptive grid (NR=10, NZ=50) with maximum partition into 8 adaptive cells is close to that obtained using the finest spatial grid (NR=60, NZ=300), with the adaptive computation requiring less running time (by a factor of 4.8). In computations with a lower adaptability level (maximum partition into 4 adaptive cells in each direction), the grid of NR=10, NZ=50 provided the solution accuracy close to the accuracy of computation using the grid of NR=40, NZ=200 with significant run-time saving (by a factor of 8.9).

Problem 3

A cylindrical layer ($0 \le Z \le 4$; $100 \le R \le 103$) is considered. The reference spatial grid consists of 20 columns and 15 rows. Construction of adaptive grids of the 3rd or lower level (maximum partition into 8 cells in the both space directions) was permitted during computation. Fig.4 shows the problem geometry and the field of radiation temperatures on the space-adaptive grid.

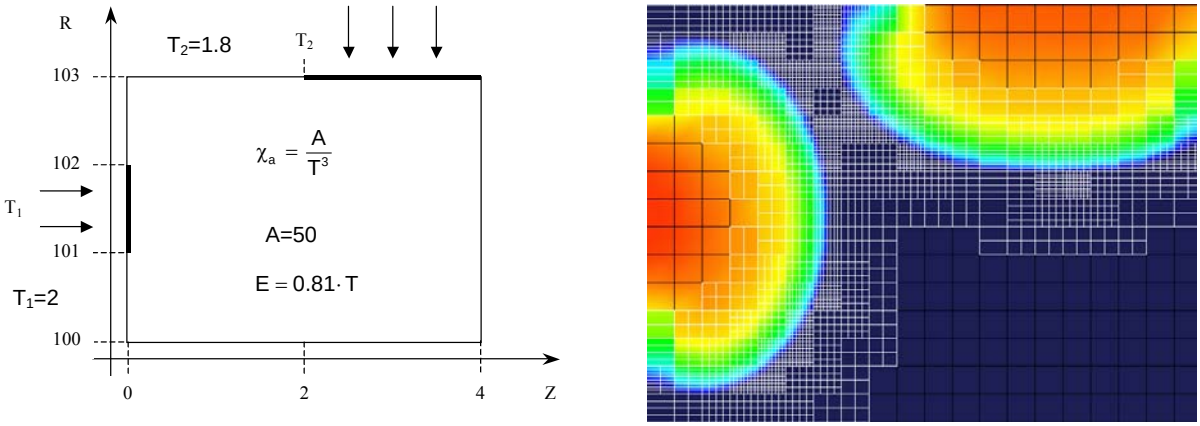


Figure 4. Statement of the problem and the radiation temperature field at an intermediate time.

The following two problems demonstrate the technique capabilities for inertial laser fusion computations using the multi-group transport equation describing the radiation transport process (Bel'kov et al., 2004).

ILLUMINATOR target's cylindrical channel

The problem considers the process of non-equilibrium radiation transport in multi-group kinetic approximation and gas dynamic motion of a substance.

Fig.5 shows a sketch of ILLUMINATOR target and the calculated substance temperature and radiation distributions in cylindrical channel at an intermediate time.

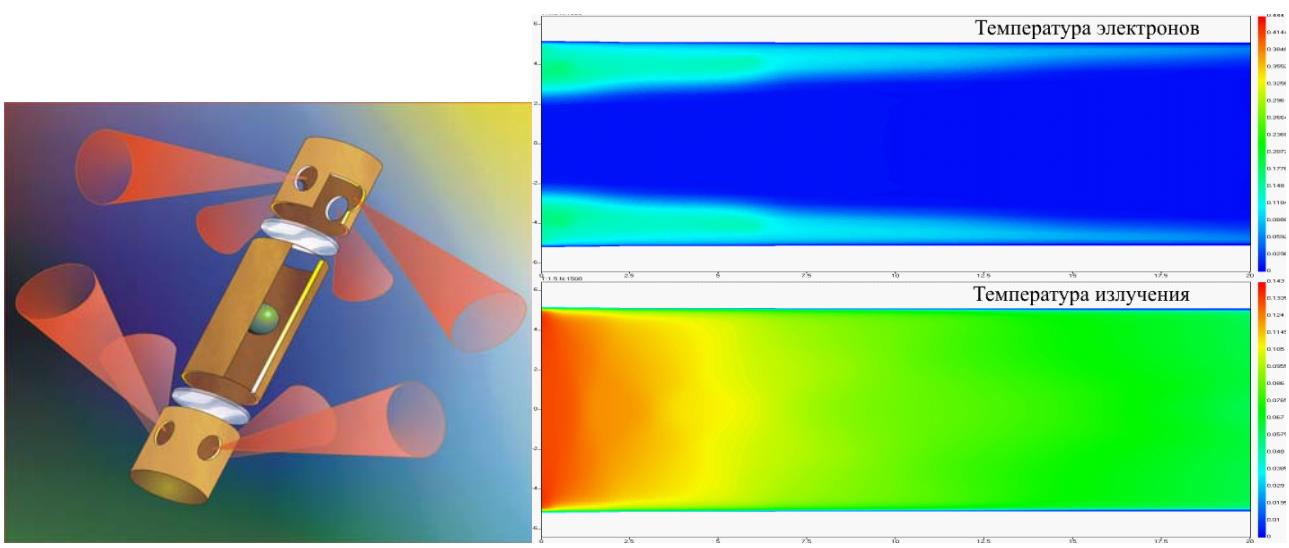


Figure 5. A target sketch and the space distributions of temperatures.

HOHLRAUM target. The problem considers the process of non-equilibrium radiation transport in multi-group kinetic approximation and gas dynamic motion of a substance.

Fig.6 shows a sketch of HOHLRAUM target.

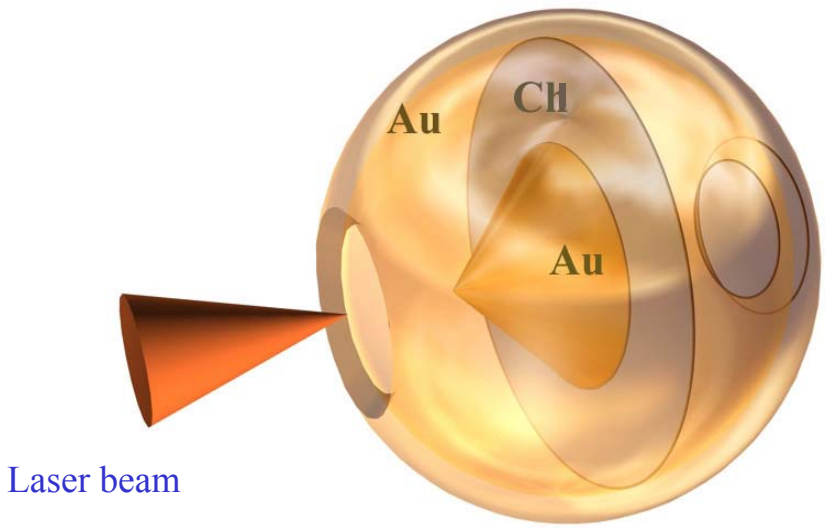


Figure 6. A sketch of HOHLRAUM target.

Fig.7 shows the distribution in space of the calculated values of the substance temperature and HOHLRAUM target radiation at an intermediate time.

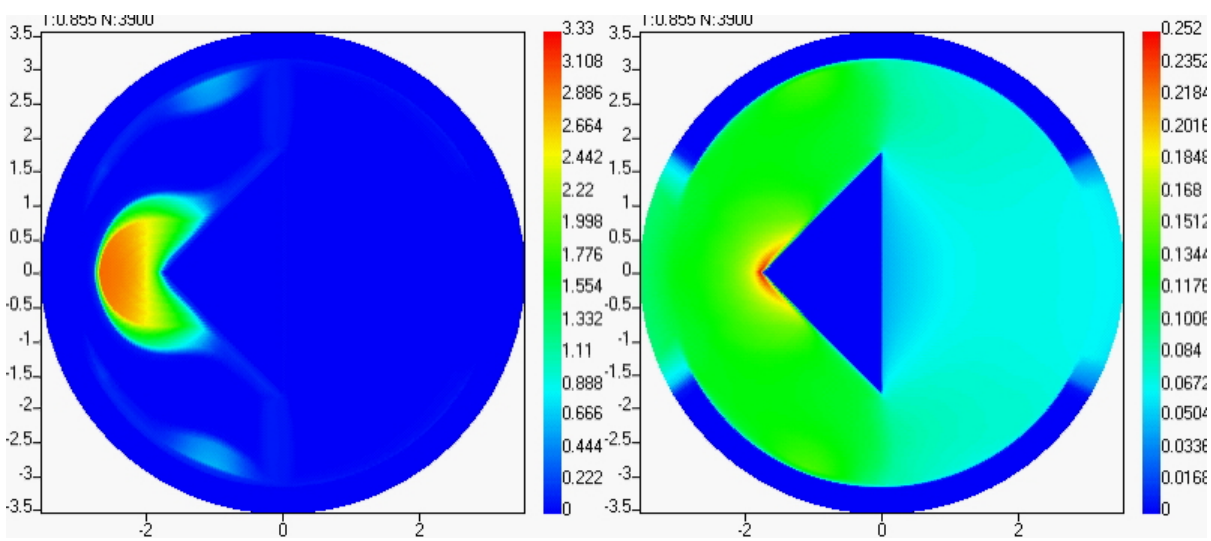


Figure 7. The distribution in space of the substance temperatures and radiation.

Conclusions

The paper describes the parallel algorithms and adaptive methods used to solve the kinetic multi-group transport equation. The results of numerical studies of the efficiency of parallelization algorithms and the space-adaptive method for solution of the multidimensional multi-group transport equation are presented. The main ideas of the developed methods adaptive in energy and angular variables of phase space to solve the transport equation are formulated. Use of these methods, separately and especially in combination, will allow multifold reduction of the time required for numerical simulations of the multidimensional multi-group transport equation.

Acknowledgements

The works have been carried out with financial support under

Contract 37713-000-02-35, Task Order 014 between Los Alamos National Laboratory of the U.S. University of California and RFNC-VNIIEF, Sarov;

Contract B526462 between Lawrence Livermore National Laboratory of the U.S. University of California and Sarov Laboratories, Sarov;

Contract B541415 between Lawrence Livermore National Laboratory of the U.S. University of California and Sarov Laboratories, Sarov.

References

Shagaliev R.M., Belyakov I.M., Alekseyev A.V., Evdokimov V.V., Zvenigorodskaya O.A., Moskvin A.N., Pleteneva N.P., Fedotova L.P., Shumilin V.A., Numerical Simulation and Techniques Used to Solve Multidimensional Particle and Energy Transport Problems in SATURN-3 Complex / VANT. Ser. Math. Model. Phys. Process. 1999. Issue 4. P. 20-26.

Alekseyev A.V., Shagaliev R.M., Nuzhdin A.A., The Method of Fine-Grain Parallelization of 2D and 3D Transport Problems Using Non-Orthogonal Grids // Works of RFNC-VNIIEF. Issue 3. Sarov. 2002. P. 96-109.

Alekseyev A.V., Shagaliev R.M., Parallelization Algorithms for Numerical Solution of the 3D Transport Equation Using SATURN Complex // VANT. Ser. Math. Model. Phys. Process. 1993. Issu 4. P. 3-7.

R. M. Shagaliev, I. M. Belyakov, A. V. Alekseyev, A. A. Nuzhdin, O. E. Vlasova, V. V. Evdokimov, V. Yu. Rezchikov, S. V. Subbot, Methods for Parallelization of Multigroup Transport Problem Solution for 2D and 3D Geometry. // Book of Abstracts. PCFD, May 13-15, 2003, Moscow, Russia. P. 269.

Shagaliev R.M., An Adaptive Method for Solving the Multidimensional Transport Equation Using Refined Grids in Phase Space // Works of RFNC-VNIIEF. 2004. Issue 8.

Belkov S.A., Belyakov I.M., Nuzhdina I.M., Vinokurov O.A., Computations of the Radiation Fields in “LABIRINT” Type Targets Under Conditions of Experiments on ISKRA-5 Facility/ Proceedings of the 31st Conference on Physics of Plasma of European Physical Community, London, 28 June-2 July, 2004, Volume 28G, P2.004.