The Technique for Solving the 2D Transport Equation Using Irregular Polygonal Grids

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A conservative finite difference scheme for polygonal spatial grids has been constructed to solve the 2D transport equation. The difference scheme is constructed in two phases. During the first phase temporary values of the unknown function in a computational cell are to be found by approximately solving the transport equation along characteristics. During the second phase the balance equation is used to find the correction factor and all the obtained values of the unknown function are multiplied by this factor. There have been developed cost-efficient algorithms implementing the sweep method using spatial grids which components are polygons of arbitrary shapes. The technique serviceability is demonstrated using the results of numerical simulations.

Introduction

Construction of difference schemes to solve the 2D transport equation using irregular spatial grids is of great interest, because the use of such grids for problems of complex geometries provides an efficient space grid.

The paper by Troshchiyev (1976) gives the formulated approach to construction of conservative difference approximations to the 2D transport equation using polygonal spatial grids. The important feature of this approach is that the resultant difference operator of transport is triangular, if all computational grid cells are convex.

The paper by Troshchiyev and Shumilin (1986) describes the conservative difference scheme for solving the 2D transport equation using irregular spatial grids consisting of convex quadrangles with grid values introduced at the centers of cells and on their edges. To close the system of grid equations, additional correlations are used, which provide either the first, or the second order of approximation depending on the number of illuminated sides of cells. The scheme has been successfully used for many years to solve a wide range of application problems.

Basing on the results of works (Troshchiyev, 1976) and (Troshchiyev and Shumilin, 1986), Shagaliev and Pleteneva (1989) proposed the extended template scheme, in which the grid values of the desired functions are determined simultaneously at nodes, on edges and at the centers of the grid cells. Additional correlations in space variables are introduced using the resultant template and provide the second order of approximation with any variant of illumination of sides of a quadrangular cell. The scheme has been generalized to a case of arbitrary convex polygons.

The given paper describes the construction of the conservative finite difference scheme using polygonal spatial grids to solve the 2D transport equation. The grid values are introduced at the centers of cells and on their edges, while supplementary values are introduces at nodes of cells. The difference scheme is built in two phases. During the first phase temporary values of the unknown function in a computational cell are determined by finding an approximate solution to the transport equation along characteristics. During the second phase the correction factor is determined from the balance equation and all the obtained values of the unknown function are multiplied by this factor. Similarly to the works described in papers (Troshchiyev and Shumilin, 1986) and (Shagaliev and Pleteneva, 1989), the system of grid equations for convex cells is triangular and, hence, allows implementation of the sweep method for any illumination direction. For non-convex cells, special algorithms have been developed with emphasis put on their cost-efficiency. The technique serviceability is demonstrated by the presented results of numerical computations.

Statement of Problem

Consider a time-dependent 2D kinetic equation of particle transport in axial-symmetry geometry in multigroup approximation. In cylindrical system of coordinates and with the divergent form of writing the equation looks like

$$\frac{\partial}{dt}\left(\frac{N_i}{\upsilon_i}\right) + L N_i + \alpha\, N_i = F_i\,, \tag{1}$$

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

$$F_i(z,r) = \frac{1}{2\pi}\left(\sum_{j=1}^{i1}\beta_{ij}\cdot n_j^{(o)} + Q_i\right), \qquad n_j^{(o)} = \int_{-1}^{1} d\mu \int_0^{\pi} N_i\, d\varphi\,,$$

where **i** is the energy group number; ***r***, ***z*** are cylindrical coordinates of a particle; $\vec{\Omega}(\mu,\varphi)$ is a unit vector in the direction of a particle flight; $\mu = \cos\theta$, θ and φ are the polar and azymuthal angles ($-1 \le \mu \le 1,\ 0 \le \varphi \le \pi$); $\alpha_i(t,r,z)$, $\beta_{ij}(t,r,z)$ are particle absorption and multiplication factors; $\upsilon_i(t,r,z)$ is velocity; $N_i(t,r,z,\mu,\varphi)$ is a flux of particles flying in the direction $\vec{\Omega}$; $Q_i(t,r,z)$ is an independent source of particles.

An input flux of particles is specified on the outer surface at $(\vec{\Omega}\cdot\vec{n}) < 0$, where $\vec{n}$ is the external normal.

The equation system (1) is solved iteratively in the integral of collisions. For simplicity, we'll further consider the equation for one group with the known right-hand side (indexes of the iteration and group numbers are omitted).

Approximation in Angular Variables and Time

The way of constructing the angular and time approximations is similar to that described in the papers (Troshchiyev and Shumilin, 1986) and (Yelesin et al., 1972).

The time derivative in Eq.1 is approximated in the following manner:

$$\frac{\partial}{\partial t}\left(\frac{N}{\upsilon}\right)=\frac{\Phi^{n+1}-\Phi^{n}}{\Delta t^{n+1}}, \tag{2}$$

where $\Phi\left(t,r,z,\mu,\varphi\right)=\dfrac{N}{\upsilon}$, $\Delta t^{n+1}=t^{n+1}-t^{n}$.

It is assumed, when approximating in time, that all quantities depending on ***r*** and ***z*** are specified at time $t^{n+\gamma}=(1-\gamma)\cdot t^{n}+\gamma\cdot t^{n+1}$, $(0.5\le\gamma\le 1)$.

The additional time correlation is inequality of the form

$$\frac{N^{n+\gamma}}{\upsilon}=\gamma\cdot\Phi^{n+1}+(1-\gamma)\cdot\Phi^{n}. \tag{3}$$

For variable φ, the following additional correlation is used:

$$N_{m,\,q-1}=\eta\,N_{m,q}+(1-\eta)\,N_{m,q-1},\ (0.5\le\eta\le 1) \tag{4}$$

.

With regard to Eqs.2-4, Eq.1 within the ranges $\left(\varphi_{q-1},\ \varphi_{q}\right)$ and with the specified value of μ_m is approximated by the following difference equation:

$$\begin{aligned}&\frac{\partial}{r\cdot\partial r}\left(r\cdot\sqrt{1-\mu_m^2}\cdot\cos\hat{\varphi}_q\cdot N^{n+\gamma}_{m,q-\frac{1}{2}}\right)+\frac{\partial}{\partial z}\left(\mu_m\cdot N^{n+\gamma}_{m,q-\frac{1}{2}}\right)-\\&-\frac{1}{r}\cdot\sqrt{1-\mu_m^2}\cdot\sin\varphi_q\cdot\frac{N^{n+\gamma}_{m,q}}{\Delta\varphi_q}+\frac{1}{r}\cdot\sqrt{1-\mu_m^2}\cdot\sin\varphi_{q-1}\cdot\frac{N^{n+\gamma}_{m,q-1}}{\Delta\varphi_q}+\\&+\left(\alpha+\frac{1}{\upsilon\gamma\Delta t}\right)\cdot\Delta\mathrm{V}\cdot N^{n+\gamma}_{m,q-\frac{1}{2}}=\Delta\mathrm{V}\left(F^{n+\gamma}+\frac{\Phi^{n}(r,z,\mu,\varphi)}{\gamma\Delta t}\right),\\&m=1,2,\dots,\hat{m},\quad q=1,2,\dots,\hat{q}_m,\end{aligned} \tag{5}$$

.

where $\Delta\varphi_q = \varphi_{q-1} - \varphi_q$, $\cos\bar{\varphi}_q = \dfrac{1}{\varphi_q - \varphi_{q-1}} \cdot \int\limits_{\varphi_{q-1}}^{\varphi_q} \cos\varphi \; d\varphi = \dfrac{\sin\varphi_q - \sin\varphi_{q-1}}{\varphi_q - \varphi_{q-1}}$.

Approximation is Space

A region of space is covered with polygons. Introduce the grid values of function $N(t,r,z,\mu,\varphi)$ on edges, $N_{(\kappa,\,\kappa+1)}$ and at the centers of polygons, N_0. To construct the finite difference scheme, use the integro-interpolation method (Samarsky, 1977) and the method of additional correlations (Troshchiyev and Shumilin, 1986), (Yelesin et al., 1972).

Multiply Eq.5 by the phase volume component $r\,dr\,dz\,d\varphi$ and perform integration in a computational cell having the shape of a prism with a polygonal cell in its base (Fig.1).

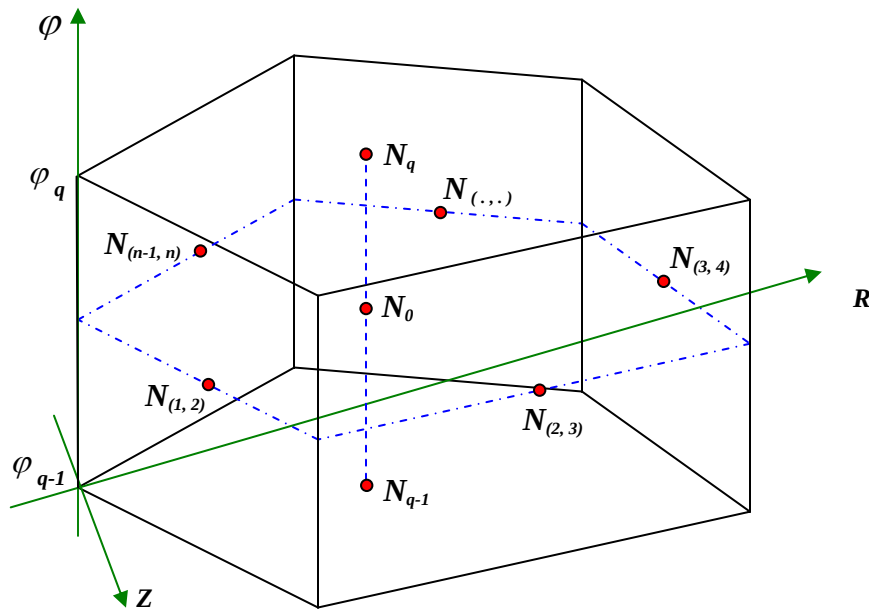


Figure 1. Example of a computational cell with the grid values of function $N(t,r,z,\mu,\varphi)$.

Use Gauss-Ostrogradsky formulation for integration on edges and then the "mean value" theorem and obtain

$$\sum_{k=1}^{\tilde{k}} \chi_k \cdot N_{(k,k+1)} + N_q \cdot \chi_q - N_{q-1} \cdot \chi_{q-1} + \left(\alpha + \frac{1}{\upsilon\gamma\Delta t}\right) \cdot \Delta V \cdot N_0 = \Delta V \cdot \left(F + \frac{N^n}{\upsilon\gamma\Delta t}\right). \quad (6)$$

Here, $\tilde{k}$ is the number of sides of a polygon, $N_{(k,k+1)}$ ($N_{(\tilde{k},\tilde{k}+1)} \equiv N_{(\tilde{k},1)}$) are the values of function $N(t,r,z,\mu,\varphi)$ on lateral faces of the prism; N_q and N_{q-1} are the

values of function $N(t,r,z,\mu,\varphi)$ on the lower and upper bases of the prism; N_0 is the value of function $N(t,r,z,\mu,\varphi)$ at the central point;

$$\chi'_k = \mu_m\left(r_{k+1} - r_k\right) - \sqrt{1-\mu_m^2}\cos\bar{\varphi}_q\left(z_{k+1} - z_k\right),$$

$$\chi_k = \frac{r_k + r_{k+1}}{2}\cdot\chi'_k, \quad r_{\tilde{k}+1} \equiv r_1\,,\ z_{\tilde{k}+1} \equiv z_1 \tag{7}$$

$$\chi_{q-1} = \frac{\sqrt{1-\mu_m^2}\cdot\sin\varphi_{q-1}\cdot dS}{\varphi_{q-1} - \varphi_q} \quad \chi_q = \frac{\sqrt{1-\mu_m^2}\cdot\sin\varphi_q\cdot dS}{\varphi_{q-1} - \varphi_q}$$

where $dS = \iint dz\,dr$ is the computational cell area in plane RZ; $\Delta V = \iint r\,dz\,dr$ is the cell volume component.

Construction of additional correlations in space variables is an important phase of scheme construction on polygonal grids. It is required that with any direction μ_m and $\bar{\varphi}_{q,m}$, i.e. with any illumination variant, these correlations lead to a non-degenerate system of grid equations and at the same time provide a possibility to approximate the corresponding algebraic identities to the second order (or close to the second order) of accuracy.

The difference scheme is built in two phases. During the first phase temporary values of the unknown function on the "non-illuminated" contour of a polygon and at its central point is to be determined by finding an approximate solution to the transport equation along characteristics. During the second phase the correction factor is to be found from the particle balance equation (Eq.6) in a cell and all the obtained values of the function are to be multiplied by this factor.

Consider an example. Fig.2 shows a convex polygonal cell.

For the specified direction $\vec{\Omega}$, the values of function $N_{(i,i+1)}$ on the corresponding sides $i = \overline{1, j-1}$ are the known values in space variables.

It is required to find

- the values of function N_0 at the cell center;
- the values of function $N_{(i,i+1)}$ on its sides $i = \overline{j,n}$.

To close the system of equations in the given cell for the given direction, use (n-(j-1))+1 additional correlations in space.

Let the solution at the center of the cell be a normal value of function N on all lateral sides:

$$N_0 = \frac{1}{n}\cdot\sum_{i=1}^{n} N_{(i,i+1)}, \text{ n is the number of sides of the polygon} \tag{8}$$

We obtain the rest (n-(j-1)) additional correlations using the following assumptions. The solution along characteristics of the desired function at the centers of non-illuminated[1] sides can be written in the form

$$N_{(k,k+1)} = \left(1 + d \cdot \ell_{(k,k+1)}\right) N^{P}{}_{(k,k+1)} \qquad \left(j \le k \le n\right), \tag{9}$$

where

d is the linear particle multiplication (adsorption) factor along the characteristic; $\ell_{(k,k+1)}$ is the distance from the center of the non-illuminated side (k,k+1) to its projection onto the illuminated contour of the polygon; $N^{P}{}_{(k,k+1)}$ is the value of the function projection onto the illuminated[2] contour of the polygon that can be obtained by linear interpolation of the corresponding node values of the side, to which the projection falls. For this purpose, on the illuminated contour of the polygon introduce the values of function $N\left(t,r,z,\mu,\varphi\right)$ at nodes of the cell to our template.

Construction of projections can be represented in the form shown in Fig.3.

The «illuminated» side, which the projection from the center of the "non-illuminated" side falls onto, can be efficiently determined with regard to factors χ' from Eq.7.

As for calculation of parameter $\ell_{(k,k+1)}$, note the following. Instead of a real length that can be calculated, for example, using the square root function, it is possible to use an increment along one of the coordinate axis.

Thus, the above-mentioned possibilities significantly reduce the labor-intensity of computations using this scheme.

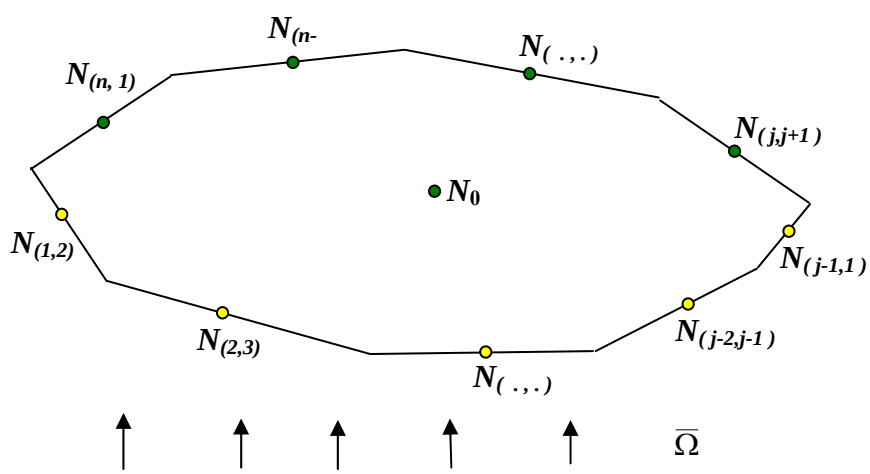


Figure 2. Example of a convex n-gon.

[1] Sides for which the requirement of $\chi_k > 0$ is met.

[2] Sides for which the requirement of $\chi_k < 0$ is met.

Substitute Eq.8 and Eq.9 into Eq.6 and obtain the equation for calculation of parameter d for the cell of interest:

$$d \cdot \left\{ \sum_{\chi > 0} \ell_{(k,k+1)} \cdot N^{P}{}_{(k,k+1)} \cdot \chi_k + \frac{1}{n} \left(\sum_{\chi > 0} \ell_{(k,k+1)} \cdot N^{P}{}_{(k,k+1)} \right) \cdot \left(\frac{\chi_q}{\eta} + \left(\alpha + \frac{1}{\upsilon \gamma \Delta t} \right) \cdot \Delta \mathrm{V} \right) \right\} =$$

$$= \Delta \mathrm{V} \cdot \left(F + \frac{N^n}{\upsilon \gamma \Delta t} \right) - \sum_{\chi < 0} N_{(k,k+1)} \cdot \chi_k - \sum_{\chi > 0} N^{P}{}_{(k,k+1)} \cdot \chi_k - \left(\frac{\chi_q}{\eta} + \left(\alpha + \frac{1}{\upsilon \gamma \Delta t} \right) \cdot \Delta \mathrm{V} \right) \cdot \qquad (10)$$

$$\cdot \left(\frac{1}{n} \sum_{\chi < 0} N_{(k,k+1)} + \frac{1}{n} \sum_{\chi > 0} N^{P}{}_{(k,k+1)} \right) - N_{q-1} \left(\frac{\chi_q \cdot (1 - \eta)}{\eta} - \chi_{q-1} \right)$$

where $\sum_{\chi > 0}$ is the sum over all non-illuminated sides; $\sum_{\chi < 0}$ is the sum over all illuminated sides; n is the number of sides of a polygon.

Upon calculation of the value of parameter d, use Eq.9 to find all the desired values of the function at the centers of "non-illuminated" sides and then use Eq.8 to find the function values at the central point of the polygonal cell.

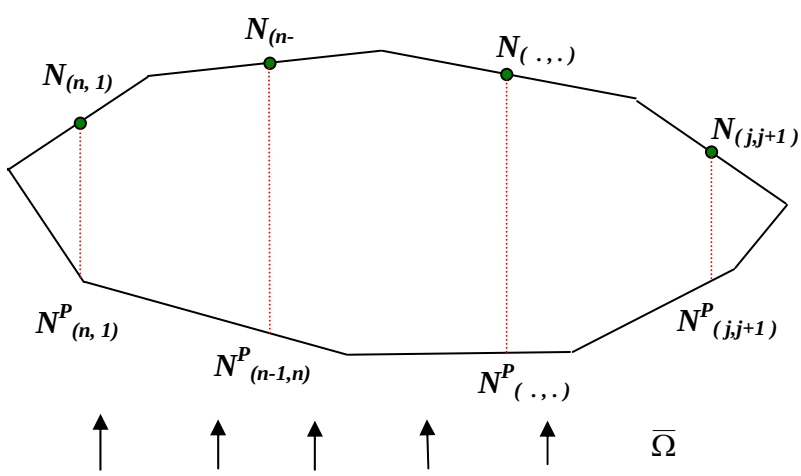


Figure 3. Example of projections onto mid points of "non-illuminated" sides of a cell.

We focus on the issues of construction of efficient algorithms for transformation of matrix of the algebraic equation system resultant from replacement of the differential equation in polygons by the difference equation into the triangular one (the so-called algorithms of regulating polygons in a region).

Troshchiyev (1976) proved a feasibility of regulating convex polygons. In general, both convex and non-convex polygons can be the components of the spatial grid considered by this paper authors.

Let a region contain several non-convex polygons. Find local sub-regions consisting of a non-convex polygon and its neighboring polygons. If we remove non-convex polygons from such sub-regions, for example, by geometric reconstructions, we can bring

the system of interest to the conditions of the theorem proved by Troshchiyev (1976) (Fig.4).

Hence, if for each of the sub-regions with non-convex polygons (see Fig.5) we offer special regulating algorithms, the problem, as a whole, can be solved.

Now consider issues of cost-efficiency of the regulating algorithms.

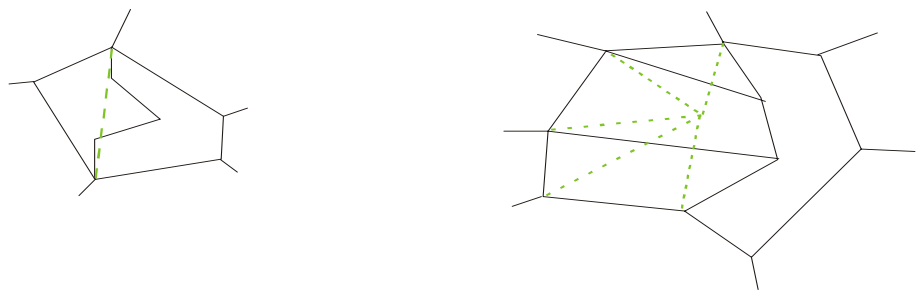


Figure 4. Example of algorithms avoiding non-convex polygons

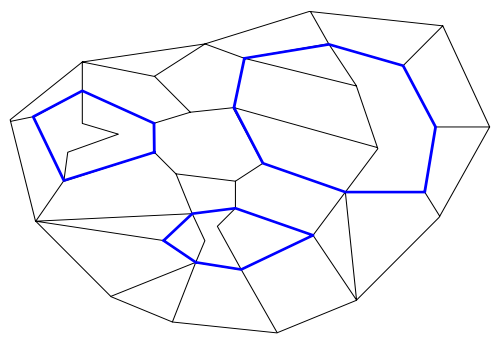


Figure 5. Example of identification of local sub-regions with non-convex cells.

Remember that for the chosen particle flight direction the transport equation can be solved numerically for those polygons, which have, at a current time, the known values of function $N(t,r,z,\mu,\varphi)$ on each of the illuminated sides. One can see that the procedure of finding the resolvable polygons can significantly increase the problem run-time.

For irregular grids, a special polygon-regulating algorithm has been developed. Data on cells having at least one illuminated side (edge) is entered into a stack; when a cell has been resolved, its data is removed from this stack. A particular cell checking for resolvability is reduced to this cell checking for equality to zero of one parameter. The proposed regulating algorithm is quite efficient and virtually doesn't increase the total computation costs.

Examples of Computations

Problem 1. Consider a cylinder with parameters $0 \le r \le 1$, $0 \le z \le 2$, $\alpha = 1.34$, $\beta = 2.25$, $\rho = 1$, $Q = 0$. It is required to determine the eigenvalues of parameter λ, which is a constant of particle variation in time (Troshchiyev and Shumilin, 1986).

To solve the problem, spatial grids of two types were used: a rectangular grid and a spatial grid consisting of regular hexagons.

Computations were carried out using refined spatial grids. The angular grids were varied to solve this problem. Computations were carried out with 6 (i.e. 24 particle flight directions), 12 (84 particle flight directions), 24 (312 particle flight directions), and 48 (1200 particle flight directions) intervals in variable μ.

Tables 1-2 give the values of parameter λ depending on angular and space quadrangular grids in use.

Let the values obtained for computation using a rectangular grid be the exact value of λ_T for the specified number of intervals in variable μ:

$\lambda_T = \lambda_n + ah^2$, where h is a linear size of a computational cell.

We have $\lambda_T^6 = 0.164755$, $\lambda_T^{12} = 0.152714$, $\lambda_T^{24} = 0.148885$, $\lambda_T^{48} = 0.147787$.

Table 3 gives the values of errors $\lambda_T - \lambda$ for all computations.

Table 1. The values of parameter λ in computations using rectangular spatial grids.

Grid	Number of intervals in variable μ	Size of cells in r			
		h=0.1 cm	h/2	h/4	h/8
Rectangular	6	0.162753	0.164256	0.164631	0.164724
	12	0.150734	0.15222	0.15259	0.152683
	24	0.146903	0.148393	0.148762	0.148854
	48	0.145817	0.147295	0.147664	0.147756

Table 2. The values of parameter λ in computations using hexagonal spatial grids.

Grid	Number of intervals in variable μ	Size of cells in r (cm)			
		ℓ=0.1	ℓ=0.07	ℓ=0.035	ℓ=0.0175
Hexagonal	6	0.16219	0.16407	0.16464	0.164835
	12	0.150546	0.152302	0.152821	0.15292
	24	0.146242	0.147957	0.148874	0.149012
	48	0.14480	0.145054	0.146106	0.147558

Table 3. The obtained computational errors.

Grid	Number of intervals in μ	Errors			
		$\lambda_T-\lambda_h$	$\lambda_T-\lambda_{h/2}$	$\lambda_T-\lambda_{h/4}$	$\lambda_T-\lambda_{h/8}$
Rectangular	6	0.002007	0.000504	0.000129	3.6E-05
	12	0.001976	0.00049	0.00012	2.7E-05
	24	0.001987	0.000497	0.000128	3.6E-05
	48	0.001973	0.000495	0.000126	3.4E-05
		$\lambda_T-\lambda_{l=0.1}$	$\lambda_T-\lambda_{l=0.07}$	$\lambda_T-\lambda_{l=0.035}$	$\lambda_T-\lambda_{l=0.0175}$
Hexagonal	6	0.00257	0.00069	0.00012	-7.5E-05
	12	0.002164	0.000408	-0.00011	-0.00021
	24	0.002648	0.000933	1.6E-05	-0.00012
	48	0.00299	0.002736	0.001684	0.000232

As one can see from Table 3 above, computations using rectangular grids provide convergence of at least the second order in space variables. Results of computations using hexagonal grids are close in accuracy to the results of computations using rectangular grids.

Fig.6 shows graphical representation of parameter λ for computations in angular and space variables.

Problem 2. The task is to calculate the values of parameter k_{eff} in four-group approximation (Buckel et al.,1977).

Consider a horizontal section of the upper 3D half-reactor SNR-300 (Fig. 7). Materials: 1,2 – fissionable materials, 3 - reflector, 5,6 –control rods.

Five spatial grids (Fg.8) of various kinds were used to solve the problem.

All computations were carried out with 6 intervals in variable μ (24 directions of particle flights). Table 4 gives the results of these computations.

As one can see from the Table 4 data, convergence in space variables has been achieved (the spatial grid used in computations was irregular). The results of computations by our code are in good agreement with the results presented in the paper (Buckel et al., 1977).

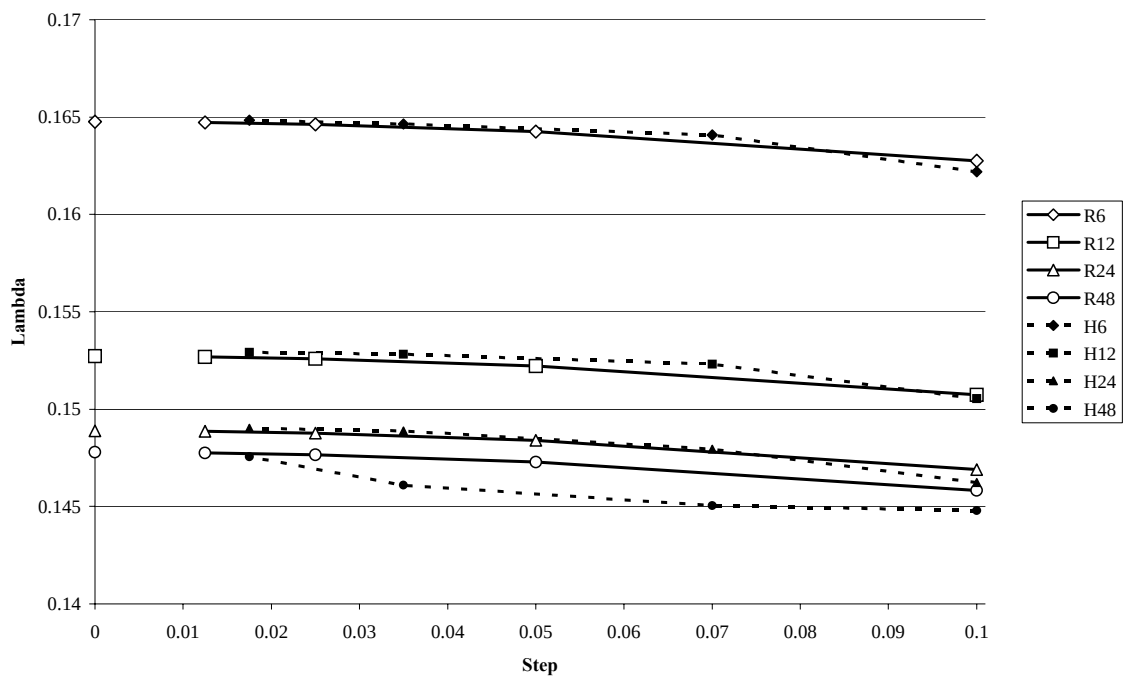


Figure 6. The curves of parameter λ for computations in angular and space variables.

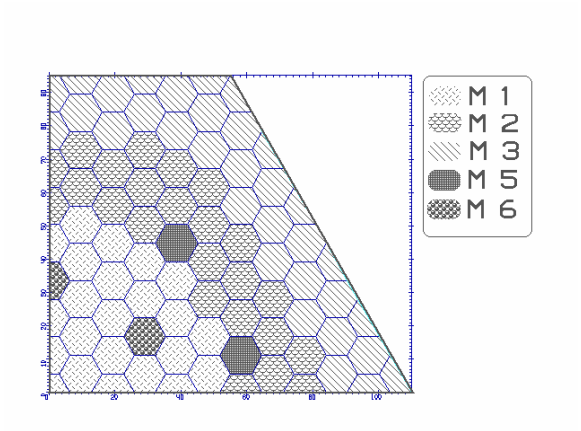
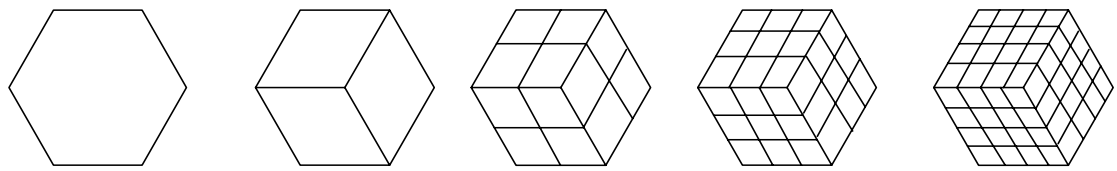


Figure 7. The problem 2 geometry.



a) hexagonal grid b) grid L_3 c) grid L_{12} d) grid L_{27} e) grid L_{48}

Figure 8. Components of space grids used to solve problem 2.

Table 4. The values of parameter k_{eff}.

Grid	**$k_{эфф}$**
Hexagonal	1.13035
L_3	1.13171
L_{12}	1.13337
L_{27}	1.13362
L_{48}	1.13368

Conclusion

The practice of computations with the techniques of the transport equation simulation using polygonal spatial grids demonstrated a high efficiency of these algorithms. This is especially true for problems of complex geometries having local small-scale sub-regions, where application of polygonal cells allows efficient grid construction.

Acknowledgements

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