

Institute of Theoretical and Mathematical Physics



Russian Federal Nuclear Center -

VNIIEF

Numerical Simulation Methods Used at VNIIEF for Multidimensional Radiation and Particle Transport Problems

R.M. Shagaliev

RFNC-VNIIEF, 607190, Sarov, Nizhni Novgorod region

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Abstract

- **Numerical simulation of multidimensional particle transport problems falls into the category of the most complex and labor-intensive application problems.**
- **The paper reviews the numerical simulation methods used at RFNC-VNIIEF for various categories of multidimensional transport problems (linear and nonlinear, time-dependent and time-independent, etc.). It briefly describes, in particular, some specific features of application of the methods, such as Monte Carlo method and the method of angular coefficients (view factors), and gives a detailed analysis of deterministic grid methods. Special emphasis is put on the issues concerning nonlinear multidimensional time-dependent linked problems, where many other physical processes are considered along with the transport process.**



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**Monte Carlo method for numerical solution of transport problems
(Zhitnik A.K. et al, 1999), (Kochubey Yu.B. et al, 2000),
(Donskoy E.N. et al, 1993)**

Solvable problems:

- **Linear particle transport problems (transport of neutrons and photons, calculation of critical parameters K_{eff} and λ , calculations of protection against gamma-neutron radiation, calculation of nuclear radiation safety of containers for transportation and storage of spent nuclear fuel, etc.).**
- **Transport of charged particles**
- **Solution of linked problems with consideration of other physical processes along with transport processes.**



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Specific features of numerical methods and algorithms in use

To provide simulation of physical processes to a rather high accuracy and high efficiency of computations, the following methods have been implemented in Monte Carlo codes :

- Method of maximum cross-sections for simulation of trajectories that ensures the same speedup both with spectral constants and group constants.
- Consideration of thermal motions of medium nuclei during simulation of trajectories on cold cross-sections of a material (Ivanov N.V. et al, 2003). This allows avoiding computations of cross-sections at given temperatures.
- Method of accidental collisions during simulation of electron trajectories, in which Fokker-Planck approximation is used to describe collisions with small transfers of energy and momentum (Donskoy E.N. et al, 1993).
- The developed model for accounting generation of annihilation and bremsstrahlung photons that allows sufficiently accurate description of their distribution without simulation of electron and positron trajectories.



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- **The code has been parallelized based on MPI library of interprocessor communications. The algorithms in use demonstrate a high parallelization efficiency on a large enough number of processors.**
- **Another area of Monte Carlo method application to transport problems is the development of simulation algorithms for grid geometries. The developed algorithms allow using arbitrarily structured grid geometries and the simulation efficiency is actually independent of cell sizes of the grid in use.**



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Computations of radiation transport in vacuum using the method of view factors
(Babayev Yu.N. et al, 1978), (Zel'dovich Ya.B. et al, 1966), (Dementiev
Yu.A. et al, 1984), (Babayev Yu.N. et al, 1995), (Bazin A.A et al., 1998),
(Dementiev Yu.A. et al, 1983)

Solvable problems:

- Engineering heat problems.
- Linked problems of X-ray transport in optically transparent regions with taking account of a number of other physical processes (laser thermonuclear fusion problems, etc.)
- In such regions, the integral radiation transport equation obtained in assumption of no radiation/medium interactions is solved.

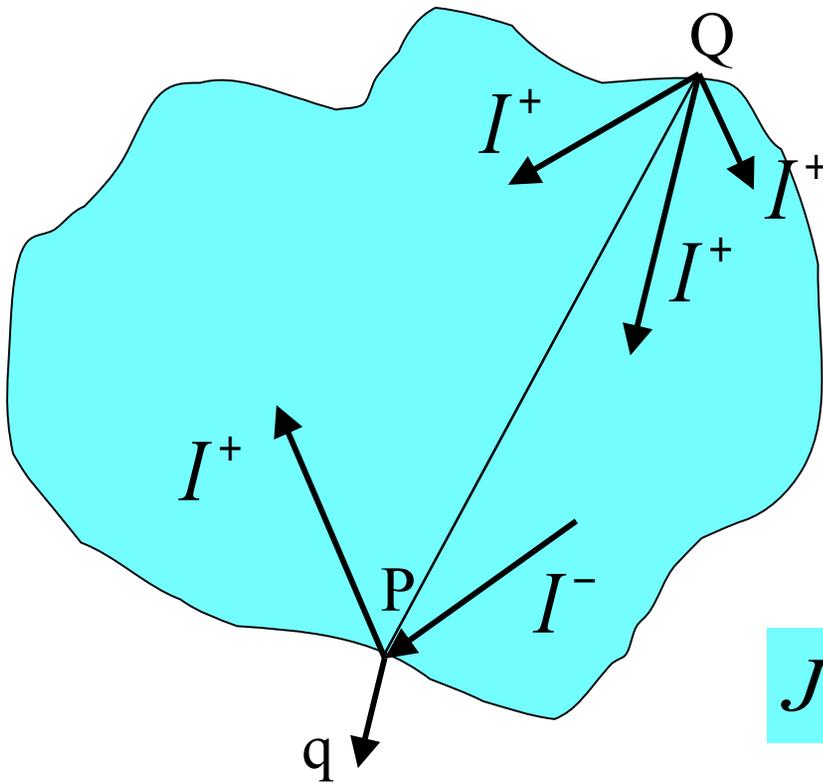
Equation of radiation transport in vacuum

$$J^-(P, t) = \int_{Q \in S(P)} J^+(Q, t - \frac{\rho_{PQ}}{c}) \frac{\mu_P \mu_Q}{\pi \rho_{PQ}^2} dS_Q$$

$$J^\pm(P, t) = \int_{2\pi} I(P, \bar{\Omega}, t) \mu_P d\Omega$$

$$\mu_P = \text{Cos}(\bar{n}_P, P\bar{Q})$$

$$\mu_Q = \text{Cos}(\bar{n}_Q, Q\bar{P})$$



$$J^-(P, t) - J^+(P, t) = q(P, t, T)$$



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Numerical approximation

$$\int_{S_i} J^-(P, t) dS = S_i J_i^- = \sum_{j=1}^N \iint_{S_i S_j} J^+(Q, t - \frac{\rho_{PQ}}{c}) \frac{\mu_P \mu_Q}{\rho_{PQ}^2} dS_Q dS_P,$$

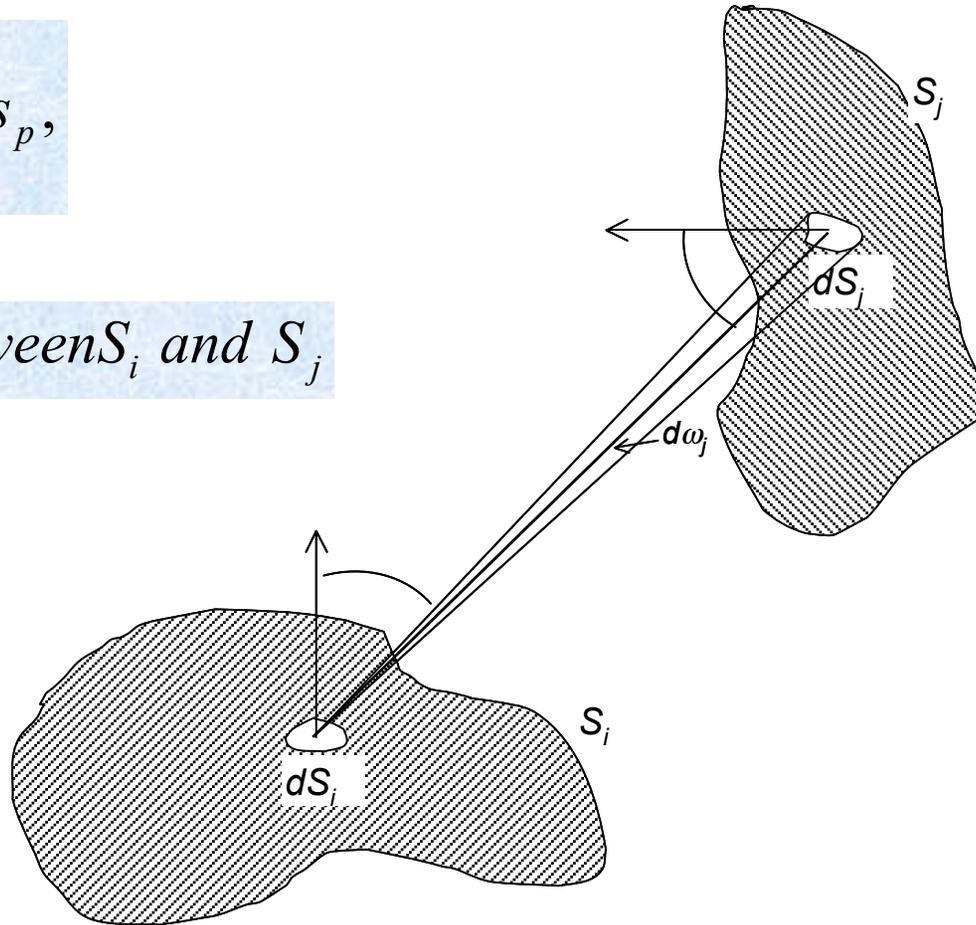
$$J_i^-(t) = \sum_{j=1}^N a_{ij} J_j^+ \left(t - \frac{\rho_{ij}}{c} \right), \quad i = 1, \dots, N$$

$$J_i^-(t) - J_i^+(t) = q(t), \quad i = 1, \dots, N$$

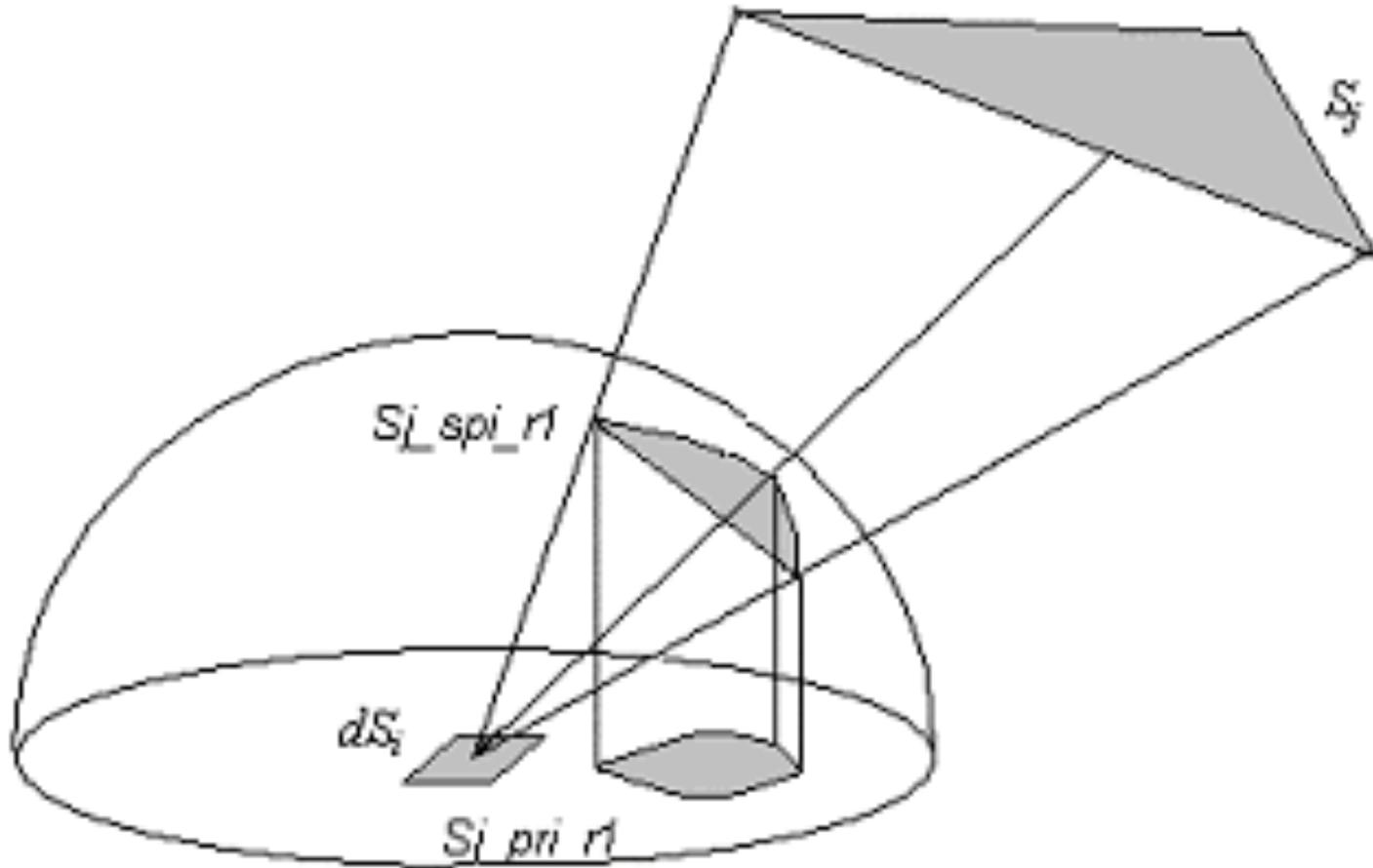
Determination of view factor

$$a_{ij} = \frac{1}{S_i} \iint_{S_i S_j} H_{ij} \frac{\mu_p \mu_q}{\pi \rho_{PQ}^2} ds_q ds_p,$$

H_{ij} – account of shading between S_i and S_j



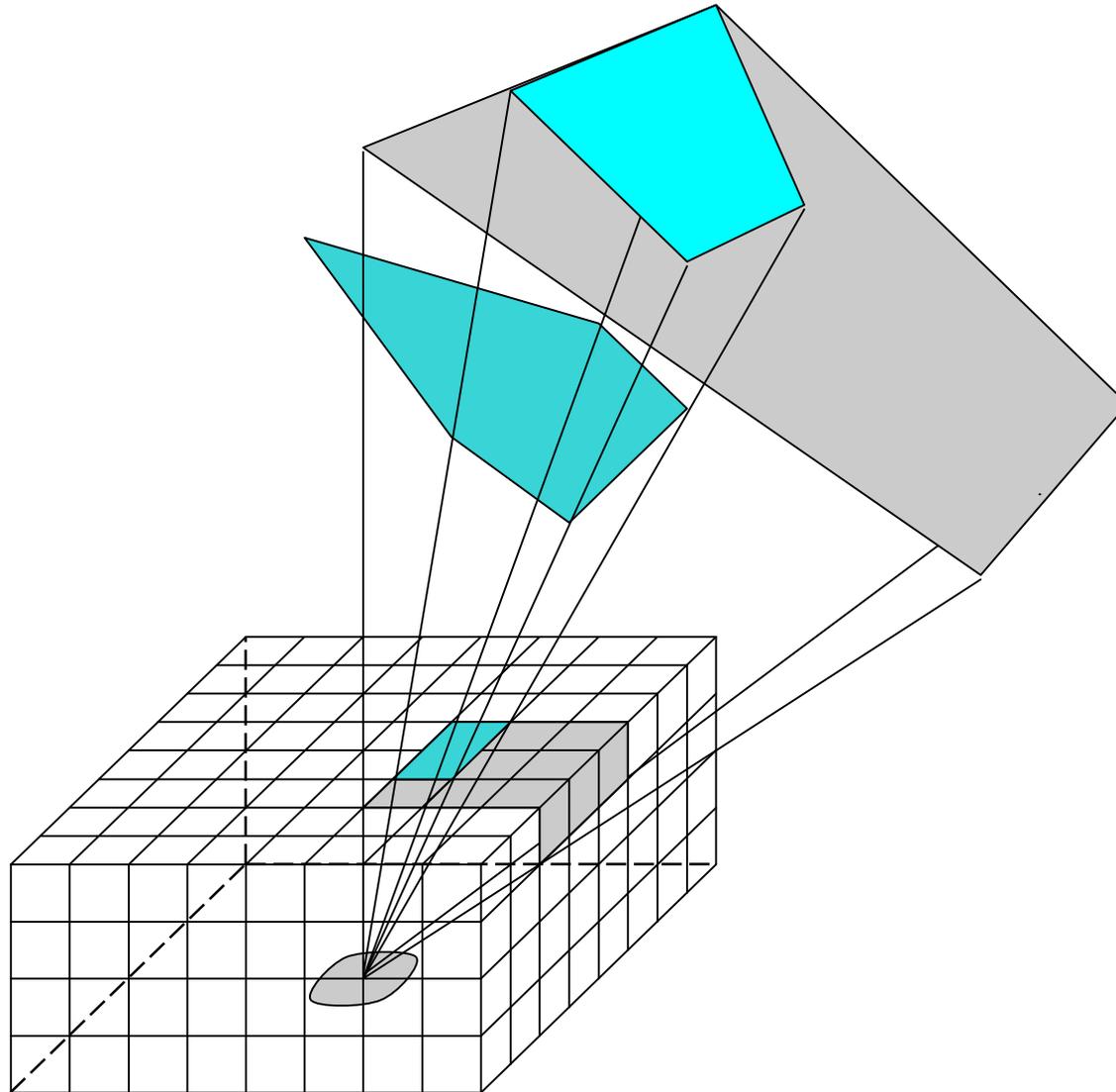
“Hemisphere” method





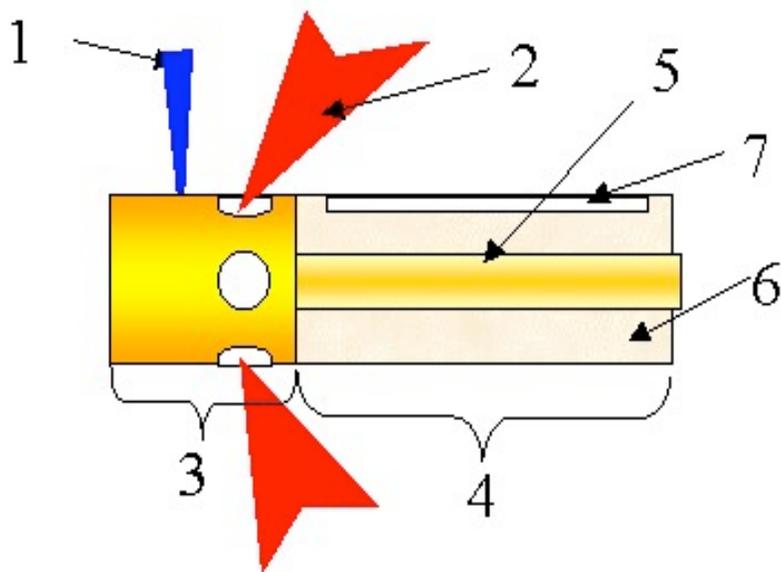
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“Hemicube” method



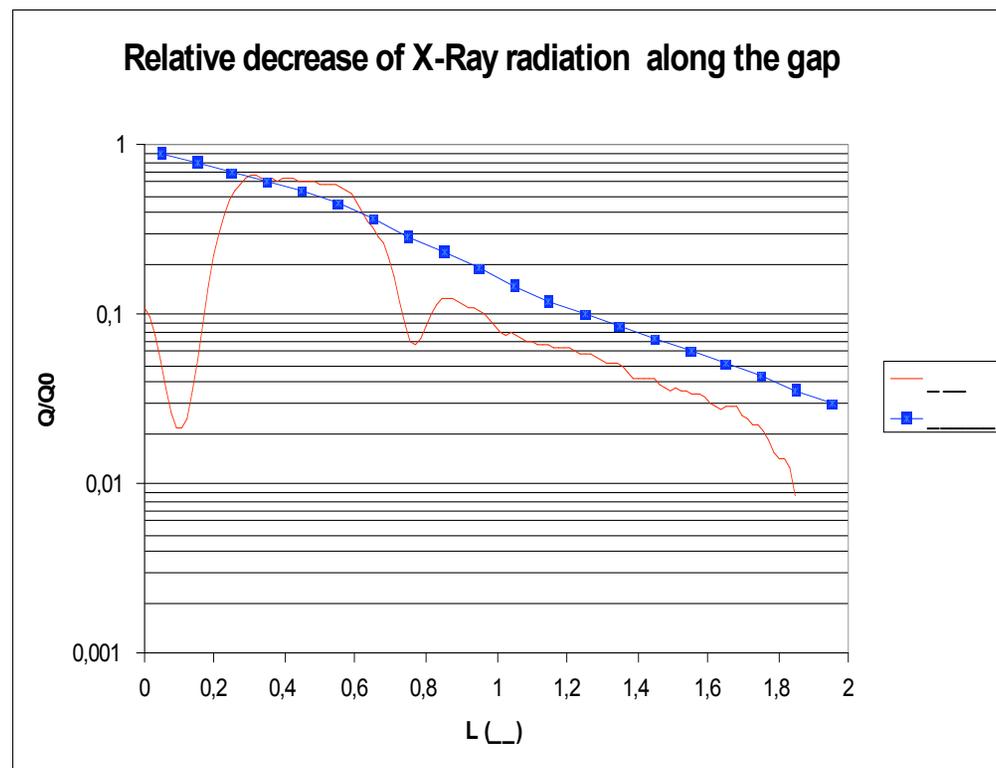
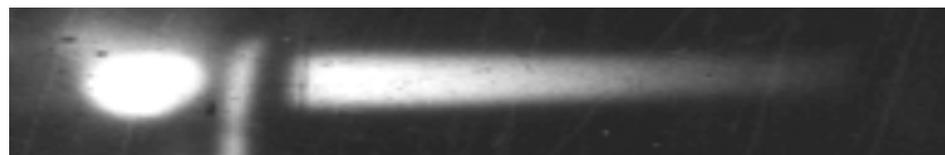
X-Ray radiation propagation through the gap in laser facility «Iskra-5»

Diagram of a target



- 1 - holder, 2 – laser beams,
- 3 – “illuminator”,
- 4 – external cylinder (Au),
- 5 – internal cylinder (Au),
- 6 - gap, 7 – diagnostic slot

X-Ray photograph



X-Ray radiation flow around the sphere in the channel

X-Ray photograph

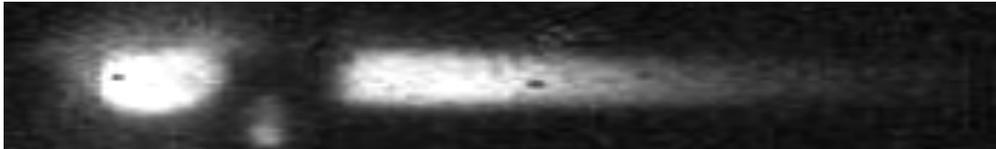
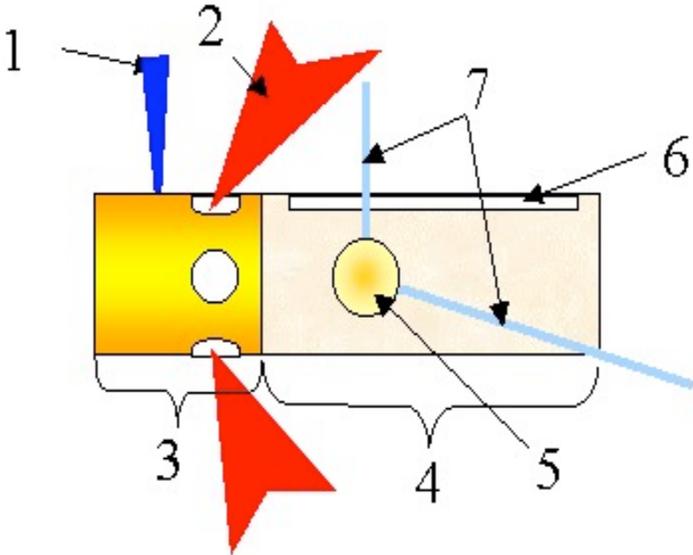
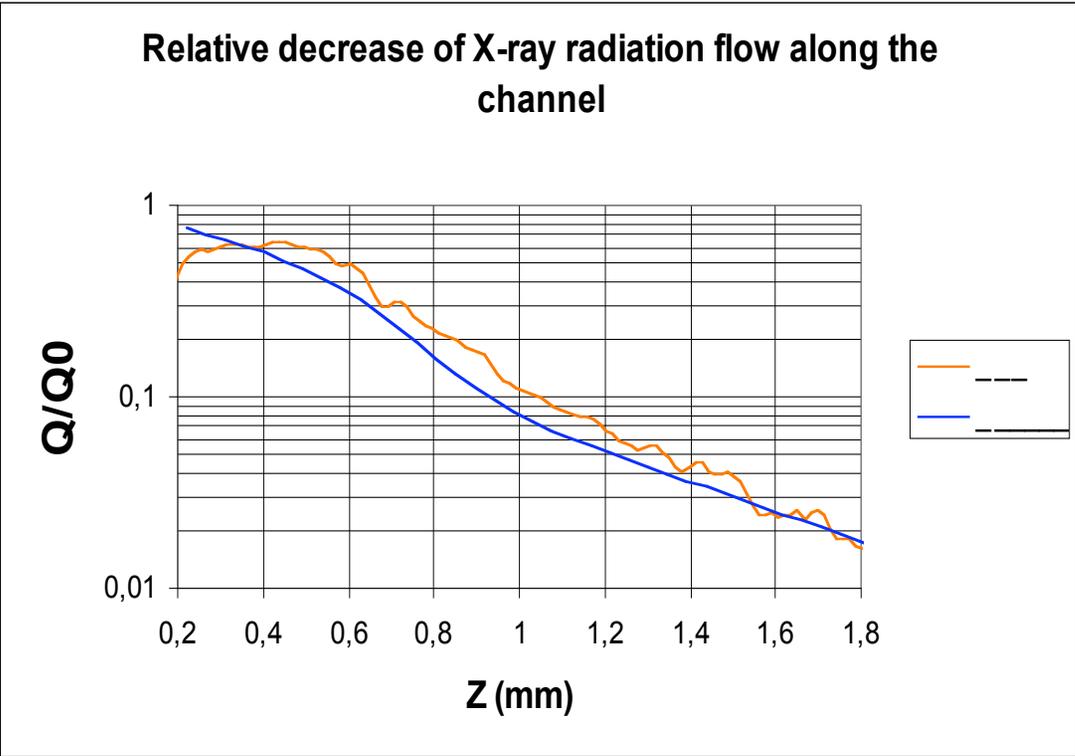


Diagram of a target



- 1 - holder,
- 2 – laser beams,
- 3 – “illuminator”,
- 4 – X-Ray propagation channel,
- 5 – obstacle (Au),
- 6 – diagnostic slot





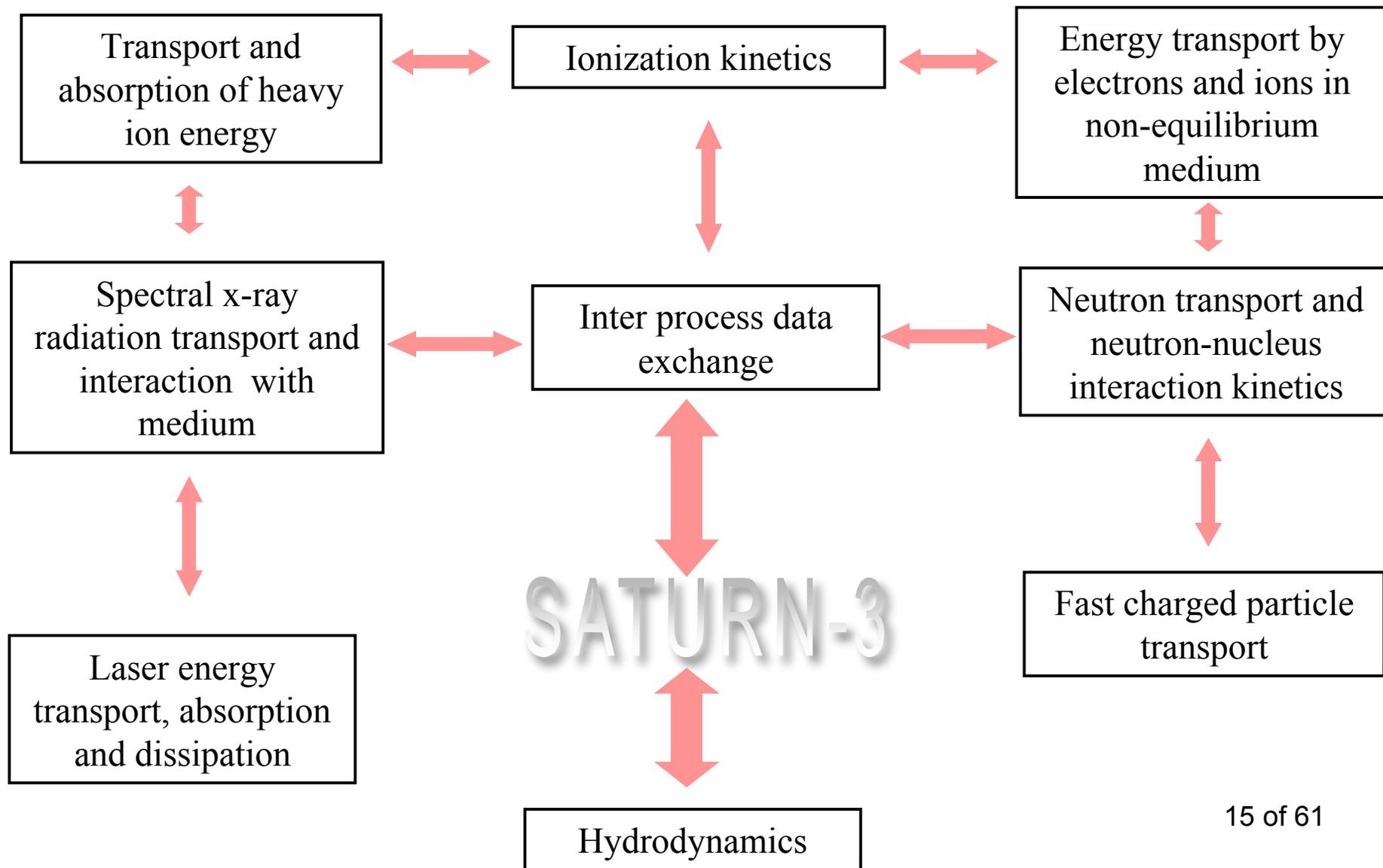
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Numerical solution of multidimensional transport problems using the methods of finite differences and finite elements



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Accountable physical processes



2D and 3D neutron transport problems in group approximation

The system of group neutron transport equations in cylindrical coordinate system:

$$\frac{\partial}{\partial t} \left(\frac{N_i}{v_i} \right) + LN_i + \alpha_i N_i = F_i$$

$$F_i = \left(\sum_{j=1}^{i-1} \beta_{ij} n_j^0 + Q_i \right) / 4\pi$$

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

$$n_i^0 = \int_{-1}^1 d\mu \int_0^{2\pi} N_i d\varphi; i = 1, 2, \dots, i-1$$

$V = V(r, z, \hat{O}, t)$ – velocity;

$\alpha = \alpha(r, z, \hat{O}, t)$ – collision factor;

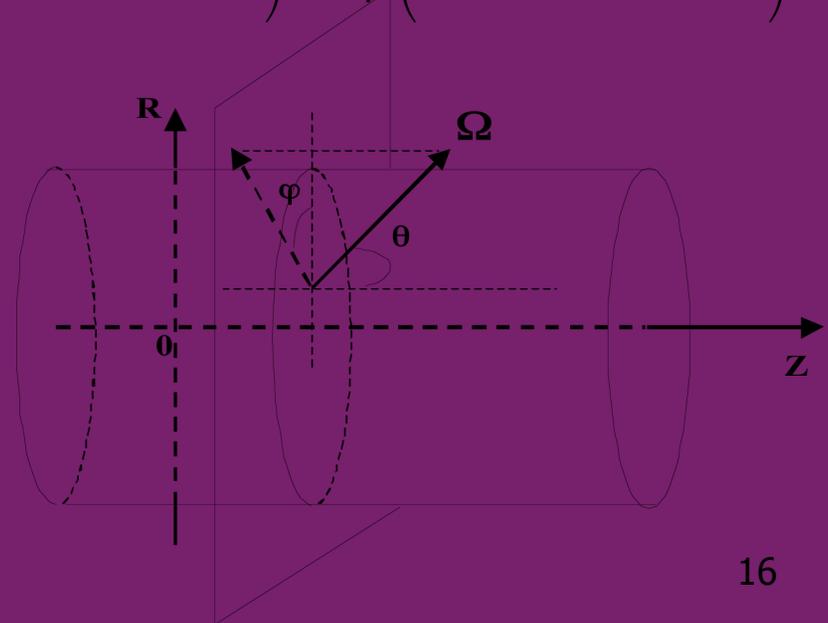
$\beta = \beta(r, z, \hat{O}, t)$ – particle multiplication constant;

$Q = Q(r, z, \hat{O}, t)$ – independent source of particles;

$\bar{\Omega} = \bar{\Omega}(\theta, \varphi)$

$N = N(r, z, \hat{O}, t, \theta, \varphi)$ – flux of neutrons at point (r, z, \hat{O}, t) flying in a given direction;

$\mu = \cos \Theta$ ($-1 < \mu < 1, 0 < \varphi < 2\pi$).



2D time-dependent problems of radiation and material energy transport in group approximation

The system of group radiation transport equations written in cylindrical coordinate system:

$$\frac{1}{c} \frac{\partial \varepsilon_i}{\partial t} + L \varepsilon_i + \chi_{\cdot i} \varepsilon_i = \frac{\chi_{ai}}{2\pi} \varepsilon_{ip} + \sum_{j=1}^{i1} a_{ij} \chi_{sj} \varepsilon_j^{(0)}$$

where the transport operator is

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

Energy equation:

$$\frac{1}{\rho} \frac{\partial E_e}{\partial t} = \sum_{i=1}^{i1} \chi_{ni} \varepsilon_i^{(0)} \Delta \omega_i - \sum_{i=1}^{i1} \chi_{ai} \varepsilon_{ip} \Delta \omega_i - \sum_{i=1}^{i1} \sum_{j=1}^{i1} a_{ij} \chi_{sj} \varepsilon_j^{(0)} \Delta \omega_i$$

$\varepsilon_i = \varepsilon_i(r, z, \mu, \varphi, \omega_i, t)$ radiation rate function

ω_i mean energy of photon in group

$\Delta \omega_i$ - width of interval in energy variable;

$T = T(r, z)$ medium temperature

ρ - medium density;

$E_e = E_e(\rho, T_e)$ internal energy

a_{ij} - coefficients describing energy exchange during Compton scattering.

$\chi_{ai} = \chi_{ai}(\rho, T_e, \omega_i)$ Absorption cross section

$\chi_{si} = \chi_{si}(\rho, T_e, \omega_i)$ scattering cross section

$\chi_{\cdot i} = \chi_{ai} + \chi_{si}$ total cross section

$\varepsilon_{ip} = \varepsilon_{ip}(T_e, \omega_i)$ Planck function

$\hat{a}_j^{(0)} = \int_{-1}^1 \int_0^{2\pi} \hat{a}_j d\mu d\varphi$

$Q_i = Q_i(r, z, \omega_i)$ independent source



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Some assumptions underlying the numerical methods used to solve transport problems:

1. The transport equation is approximated in time using the implicit two-point difference scheme.
2. The transport equation approximation in space is constructed using non-orthogonal spatial grids, namely:
 - Regular non-orthogonal grids of convex quadrangles;
 - Irregular non-orthogonal grids of arbitrarily shaped convex polygons.

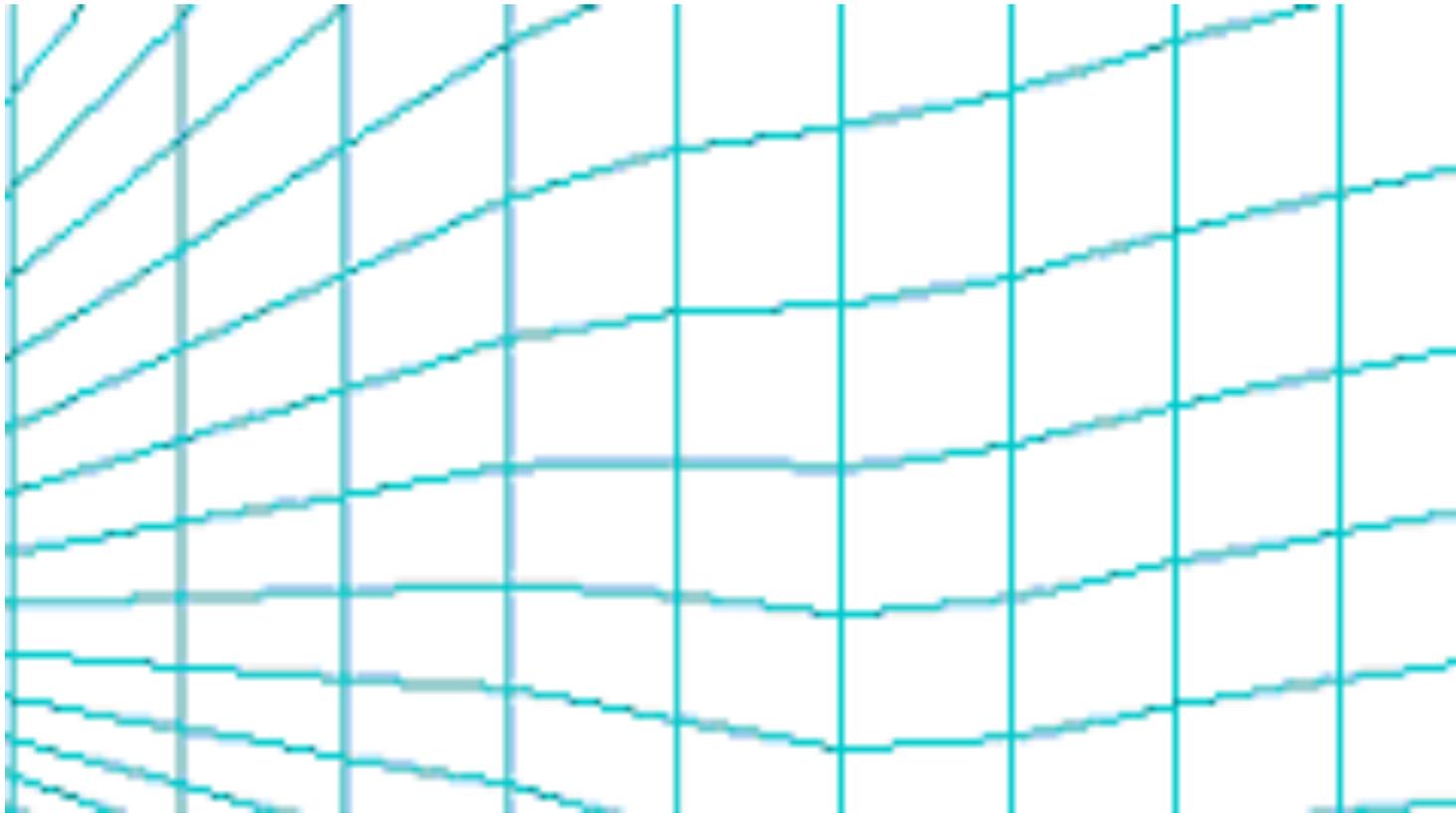
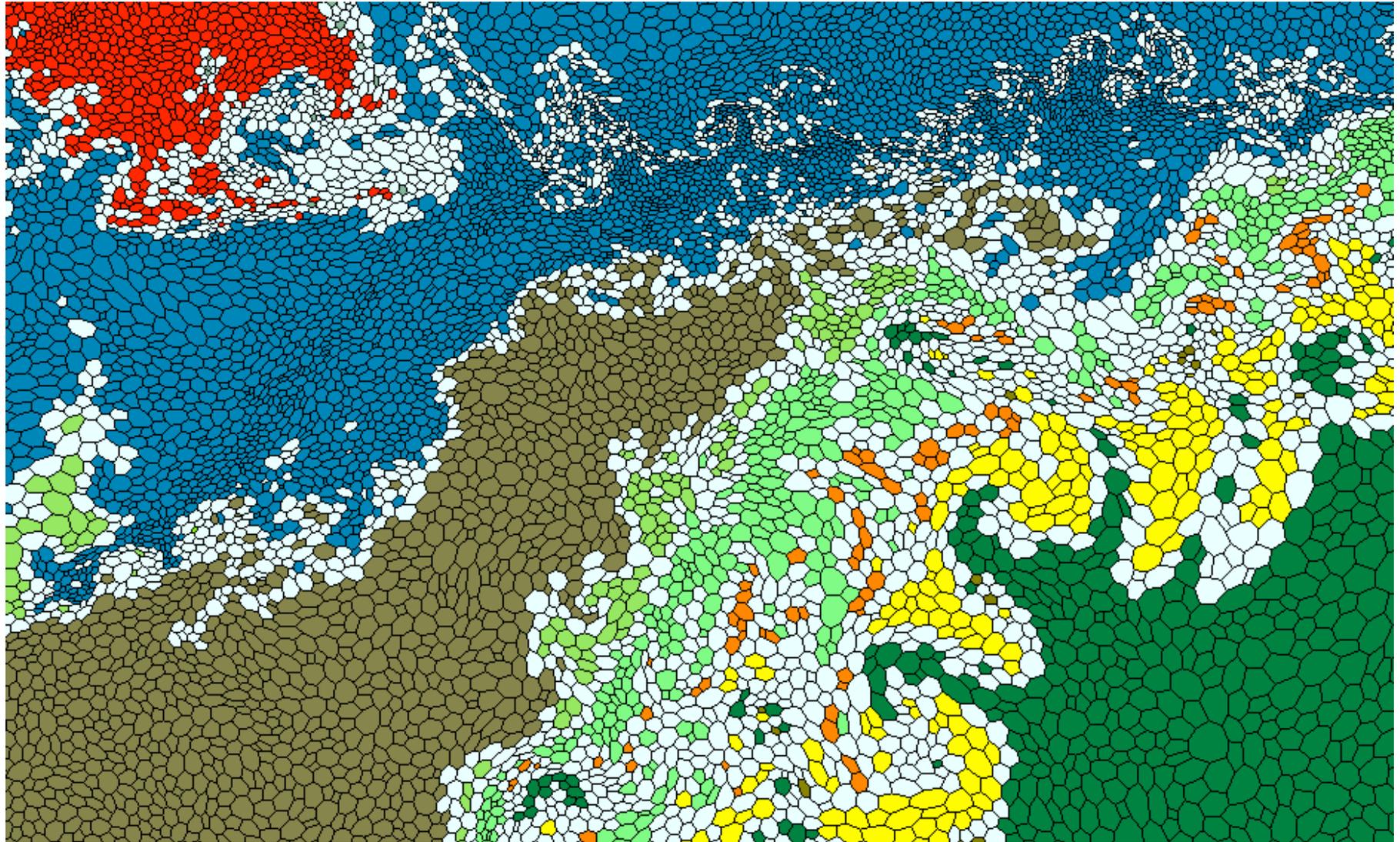


Fig.1. A structured quadrangular (regular) grid



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Using irregular non-orthogonal grids of arbitrary-shape convex polygons





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The grids mentioned above were used to construct a number of conservative finite difference schemes:

- **the extended-template scheme (Pleteneva N.P. et al, 1989), (Moskvin A.N. et al, 2005);**
- **the scheme with introduction of closing relations based on moment equations;**
- **the scheme based on the use of adaptively refined grids in phase space (Shagaliev R.M, 2004), (Shagaliev R.M. et al, 2004);**
- **schemes of the discrete-ordinates method type are used for the transport equation discretization in angular variables.**



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The schemes above have the following common features: with the use of non-orthogonal grids they preserve important features of DS_n – schemes, such as the transport equation approximation within a single phase space cell and, consequently, a possibility to resolve systems of grid equations using sweep (point-to-point) method of computations (Troshchiyev V.E., 1976).

Nevertheless, they differ from each other in the accuracy of approximation using essentially non-orthogonal grids, in monotone behavior of the grid solution and some other features.



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4. The numerical solution to the system of grid transport equations with the known right-hand side can be found using the sweep method (point-to-points computations) (Troshchiyev V.E, 1976) and modification to this method oriented to a multiple-group case (Fedotova L.P. et al, 1991).



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- 3. The method of source iterations is used to solve the system of multiple-group grid transport equations numerically. The following methods are used to accelerate the iterative process convergence:**
- **FCA method for the category of time-independent linear multiple-group problems of calculating the critical parameter K_{eff} (Evdokimov V.V. et al, 1994), (Evdokimov et al, 1996), (Moskvin A.N. et al, 1996);**
 - **KM method for the category of time-dependent nonlinear multiple-group problems of radiation transport (Fedotova L.P. et al, 1991).**



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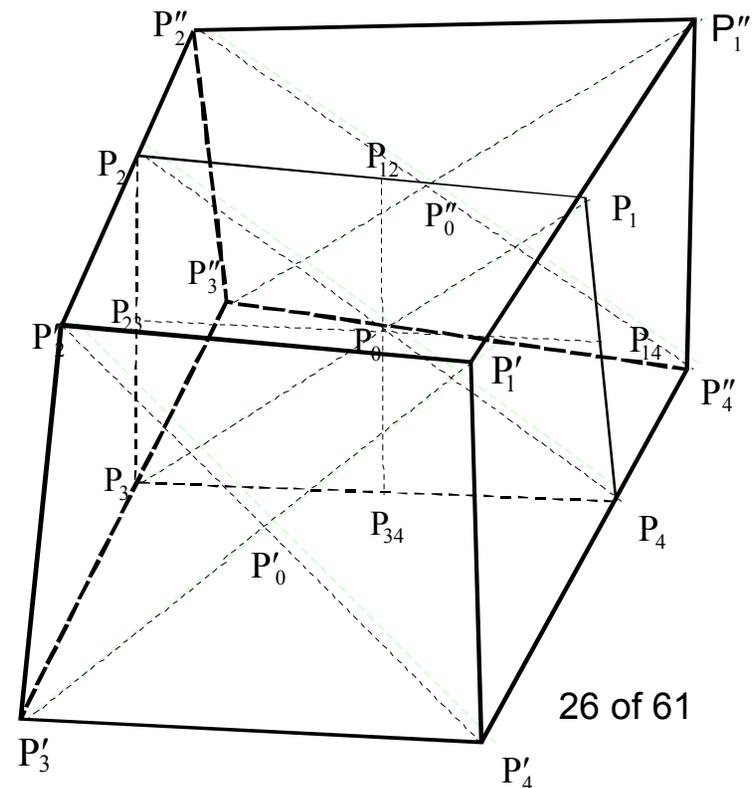
**Finite-difference schemes
used to approximate 2D
transport equations using
non-orthogonal space grids**

Multiple-group transport equation approximation

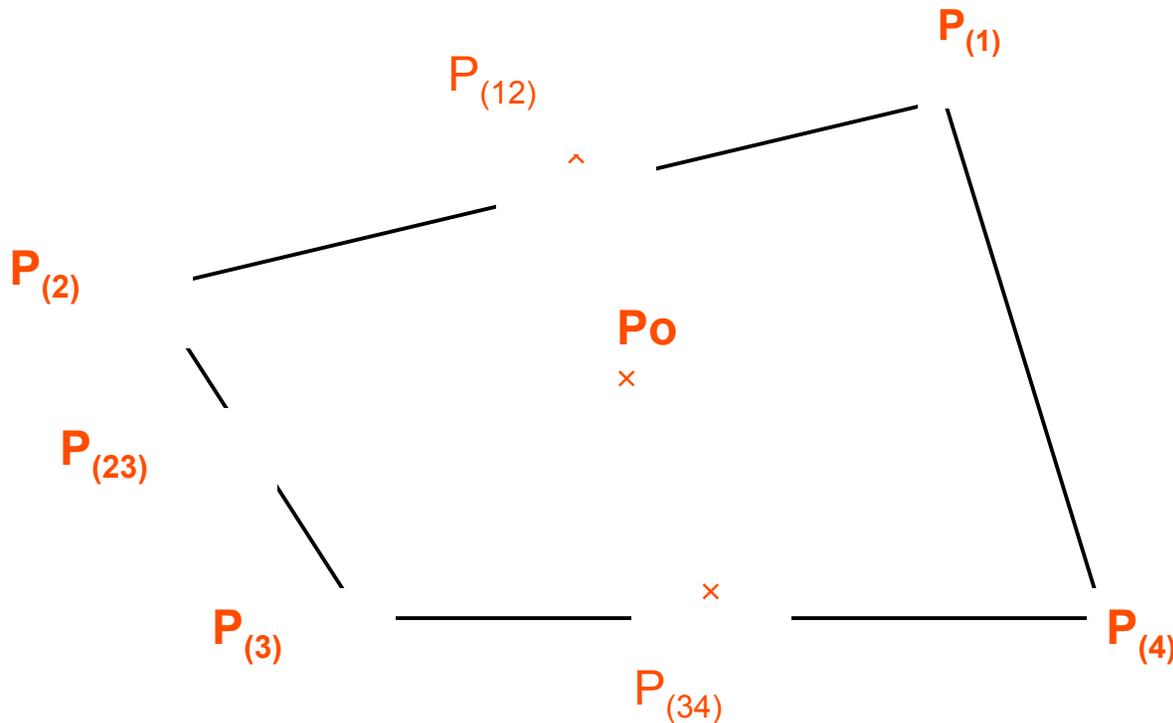
- in time: implicit scheme with weighting multipliers;
- in angular variables: method of discrete ordinates (S_n -quadratures);
- in space: using the extended template for non-orthogonal space grids

The extended template scheme features:

- the scheme is conservative;
- convergence to the transport equation solution with the second order of accuracy using non-orthogonal space grids;
- the scheme complies with the diffusion limit condition in optically dense media;
- it uses DS_n -method quadratures to approximate the transport in angular variables.



The scheme is built using the grid function values in a cell, on sides and at vertexes of a quadrangular cell .



$l = 1, 2$ The system of grid equations includes the following:

$$\Delta V_{(P_0, l+1)} = \frac{\Delta t}{2} \left[\sum_{l=1}^L R_{P_0, l+1}^{(l+1)} \frac{N_{P_0}^{n+1}}{P(l+1)} - R_{P_0, l}^{(l)} \frac{N_{P_0}^n}{P(l)} \right] \cos \varphi_q,$$

1. Grid equations for particle balance in the grid cells:

$$R_q = \Delta S_{P_0} \cdot \frac{N_{P_0}^{n+1} \cdot V_{P_0} \cdot \mu_m \cdot \Delta \varphi_q - F_{P_0}}{\Delta \varphi_q}, \quad R_{q-1} = \Delta S_{P_0} \cdot \frac{\sqrt{1 - \mu_m^2} \sin \varphi_q}{\Delta \varphi_q}$$

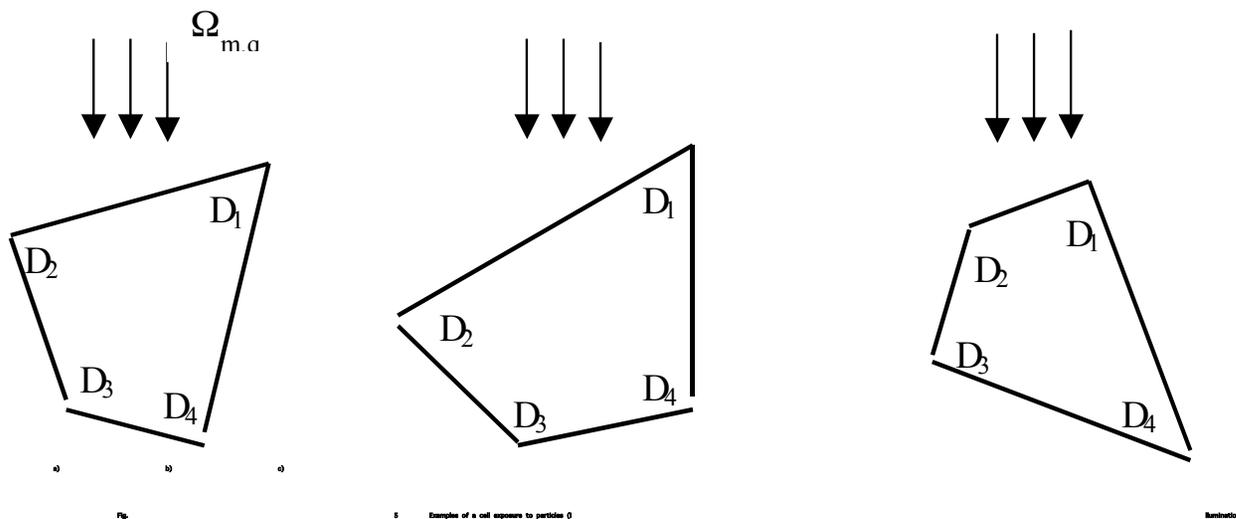
w h e r e

2. Additional correlations in time variable and angular variable φ

$$N_{P_0}^{n+1} = \gamma N_{P_0}^{n+1} + (1 - \gamma) N_{P_0}^n, \quad 0.5 \leq \gamma \leq 1$$

$$N_{P_0} = \eta N_q + (1 - \eta) N_{q-1}, \quad 0.5 \leq \eta \leq 1$$

3. Additional space relations between the values of the desired function in a cell, on sides and at nodes of a cell. The number of relations in the scheme considered depends on the number of illuminated (exposed to particles) quadrangular cell's sides. Here the following three variants shown below in Fig.5 are possible depending on the values of $\mu_m, \varphi_{q,m}$



The following additional correlations correspond to the three illumination

vertices in the extended

template scheme:

$$a) \quad N_{P(2,3)} = \delta N_{P3} + (1 - \delta) N_P,$$

$$N_{P(3,4)} = 0.5(N_{P3} + N_{P4}),$$

$$N_{P(4,1)} = \delta N_{P4} + (1 - \delta) N_{P1}$$

$$b) \quad N_{P6} = 0.5(3\delta - 1)N_{P3} + 0.5(1 - \delta)(N_{P5} + N_{P2} + N_{P4})$$

$$c) \quad N_{P0} = \delta N_{P(3,4)} + (1 - \delta) N_{P(1,2)}$$

$$N_{P0} = \delta N_{P3} + (1 - \delta) N_{\bar{P}}$$

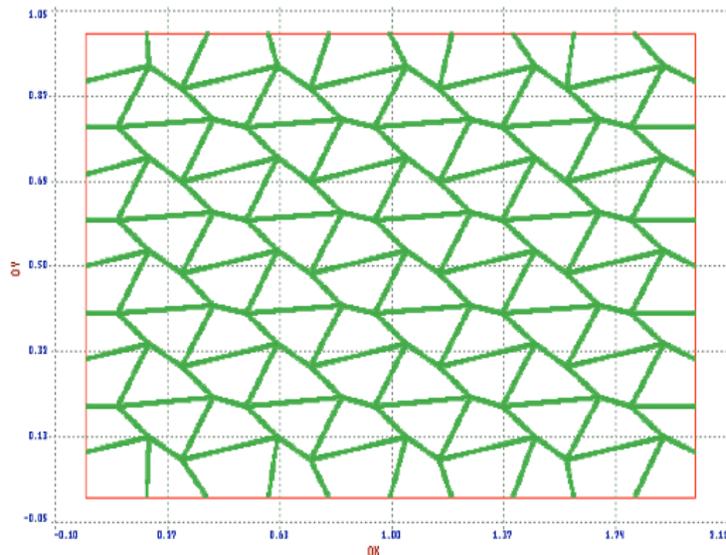
$$N_{P0} = \delta N_{P4} + (1 - \delta) N_{\bar{P}}$$



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2D test problem

One-group time-independent transport equation specified in a cylinder with dimensions $0 < R < 1$, $0 < Z < 2$. Full cross-section α and multiplication coefficient β are $\alpha=1.34$ and $\beta=2.25$, respectively. The boundary condition is a zero incoming flow.



Computations were made using an angular grid with 24 particle flight directions. The problem statement provides for finding the values of the critical parameter λ . The exact value of this parameter found by convergence computations is $\lambda=0.1474$. The table below gives computation results for the problem obtained using Schemes 1 and 2. There were two variants of computations using Scheme 1, they differed in the transport equation approximation in angular variable φ . Namely, in the first variant the standard approximation of the discrete ordinate method was used (Scheme I in the table – DS_n), and in the second one approximation using some modified scheme was used (Scheme 1 in the table – MDS_n).

Table 1. The values of parameter in computations using scheme 1 and scheme 2 for various spatial grids.

Grid		h	h/2	h/4	h/8
Size of cells (h=0.1cm)					
Rectangular	Sch.1 (DS _n)	0.1471177	0.1473767	0.1474143	0.1474012
	Sch.1 (MDS _n)	0.1627532	0.1522199	0.1487623	0.1477563
	Sch.2 (DS _n)	0.162753	0.15222	0.148762	0.147756
Non-orthogonal	Sch.1 (DS _n)	0.1462831	0.1472815	0.1473650	0.147415
	Sch.1 (MDS _n)	0.1618866	0.1521236	0.1487131	0.147795
	Sch.2 (DS _n)	0.161205	0.152042	0.148793	0.147811

The scheme with introduction of closing relations based on the moment equations

During such scheme construction the solution inside a grid cell is represented in the form of bilinear decomposition in space variable and in angular variable φ :

$$N(\tau, \eta, \varphi', \mu) \approx N_0 + \frac{\tau}{2} N_\tau + \frac{\eta}{2} N_\eta + \frac{\varphi'}{2} N_{\varphi'} + \frac{\tau \eta}{4} N_{\tau\eta} + \frac{\tau \varphi'}{4} N_{\tau\varphi'} + \frac{\eta \varphi'}{4} N_{\eta\varphi'}$$

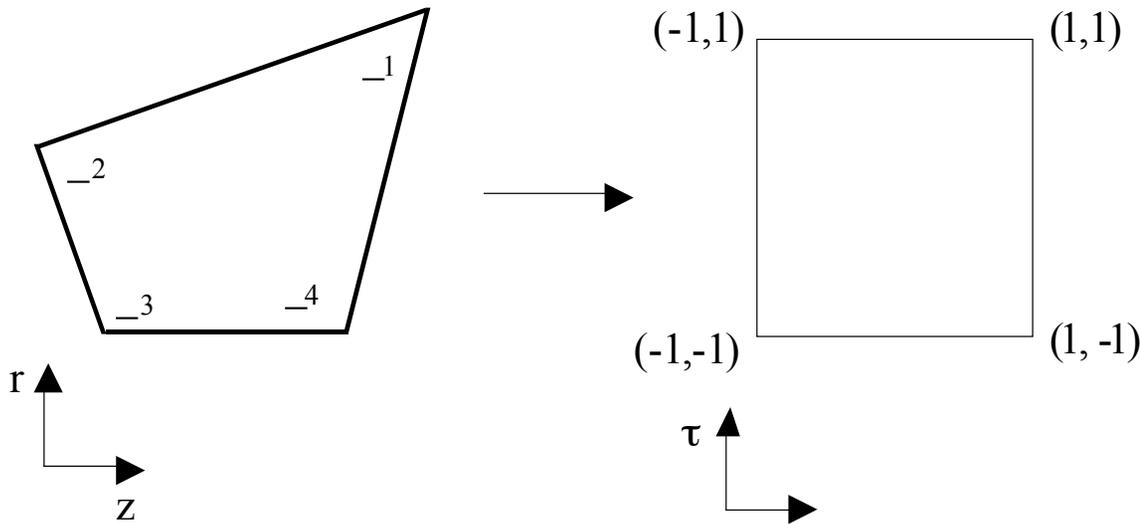
where

$$\varphi' = \frac{\varphi}{\Delta\varphi_{q-1/2}},$$

η, τ

are the coordinates of a point of space inside a cell during bilinear

transformation of a quadrangle into a unit square (Fig.7).





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The balance equations for particles in space grid cells and the corresponding moment equations are used to find the unknown coefficients of the expansion in series.

- 1. Moment difference equation in angular variable φ .**
- 2. Moment difference equations in space variables. Similarly to the case described above, the simplified expansion in series containing only the dependences on space bilinear variables is used to construct such equation:**

$$\frac{\partial}{\partial \eta} (B(\eta)N) + \frac{\partial}{\partial \tau} (A(\tau)N) + J(\tau, \eta) \rho \alpha N = J(\tau, \eta) \rho F$$

Statement of the test problem.

The linear time-independent particle transport problem (1)-(3) is considered in axially symmetric region $\{0 \leq R \leq 1, 0 \leq Z \leq 2\}$. The source and the equation coefficients are taken as $Q=1, \alpha=1, \beta=1$. The incoming flow equal to zero is specified for the boundaries parallel to R-axis (on the bases of cylinder) and the boundary condition “mirror reflection” is specified for the boundary parallel to Z-axis.

A series of computations was carried out using grids concentrating in angular and spatial variables: $[10 \times 10, DS_6]$; $[20 \times 20, DS_{12}]$; $[40 \times 40, DS_{24}]$.

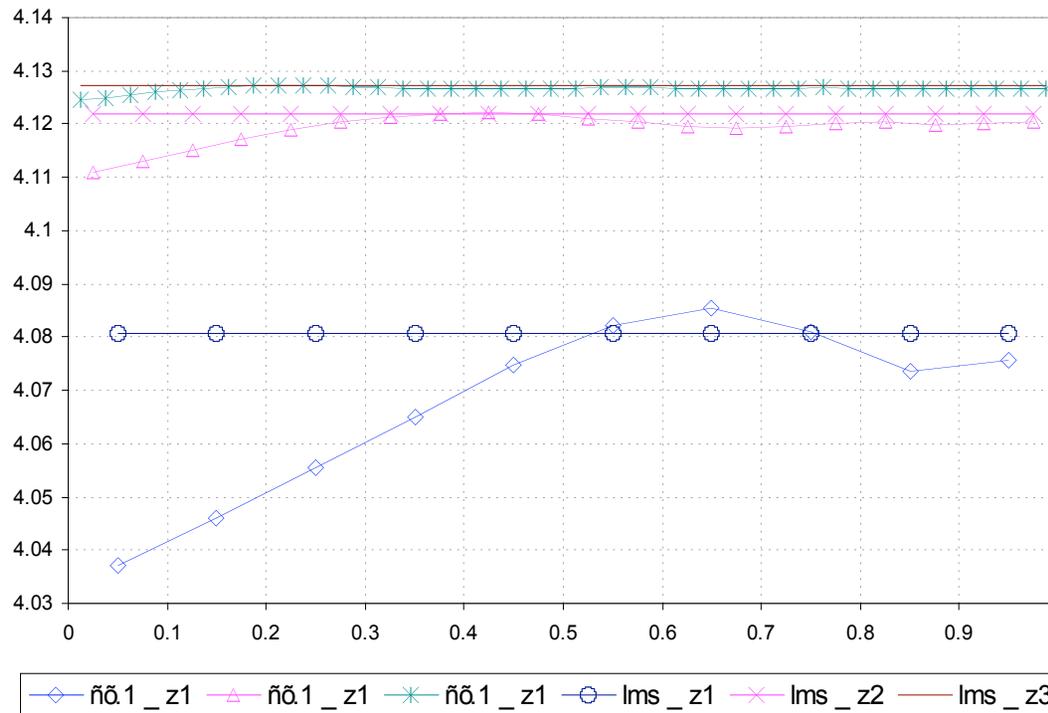


Fig.8. The profile of solution along the central column

The adaptive method of refined grids in phase space

The idea of the method is that in phase space, where the problem solution is to be found, some region (which is not a simply connected one, in general) is separated, where the original grid cells are refined to obtain cells of smaller sizes. (Shagaliev, 2004), (Shagaliev et al., 2004). Such refinement of the grid cells can be made in space variables, angular variables and energy variable.

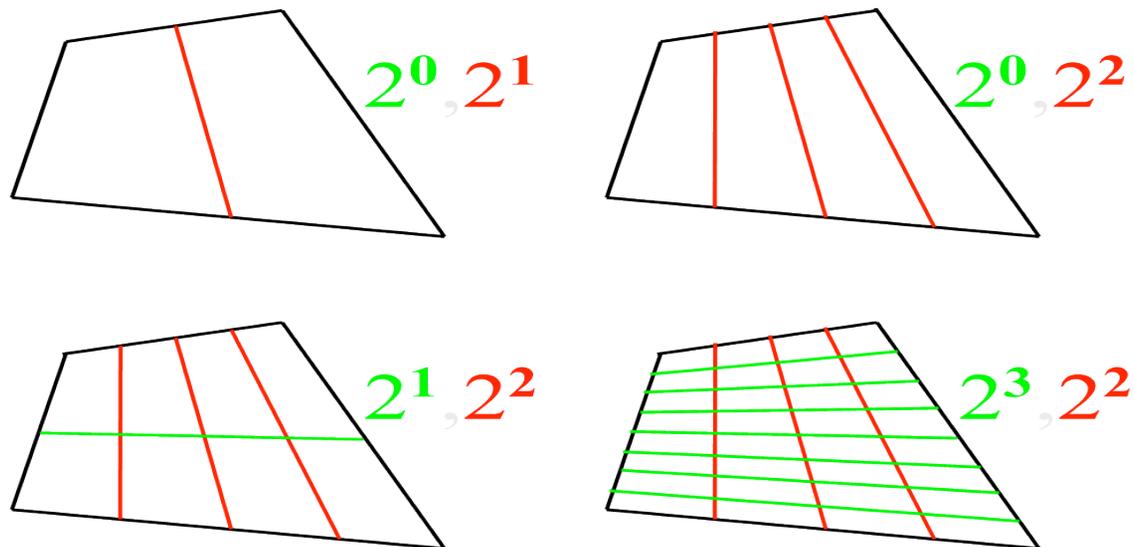


Fig. 9. Examples of refinement in space variables



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The transport equation approximation on non-orthogonal spatial grids using the adaptively refined grids entails the problem of preservation of the principal properties of the scheme used for finding the numerical solution to the transport equation on the reference grid, such as the transport equation approximation within a single computational cell, conservatism of the scheme, a possibility to solve the grid transport equation with the point-to-point computation algorithm, a possibility to use acceleration algorithms, and some others. An important feature of the developed adaptive method of refined grids is that it ensures the solution to the above problem.

**Benchmark problem. A rectangular region in 2D axially symmetric geometry is considered. The region is presented in Fig. 10. The computational domain is composed of two physical regions: Region 1 is a dense casing $\{0 \leq Z \leq 5; 1 \leq R \leq 1.2\}$;
Region 2 is a transparent region $\{0 \leq Z \leq 5; 0 \leq R \leq 1\}$, $E = 0.81 T$, $\chi_a = A/T^3$, where $A = 50.89$ in region 1 and $A = 0.1374$ in region 2.**

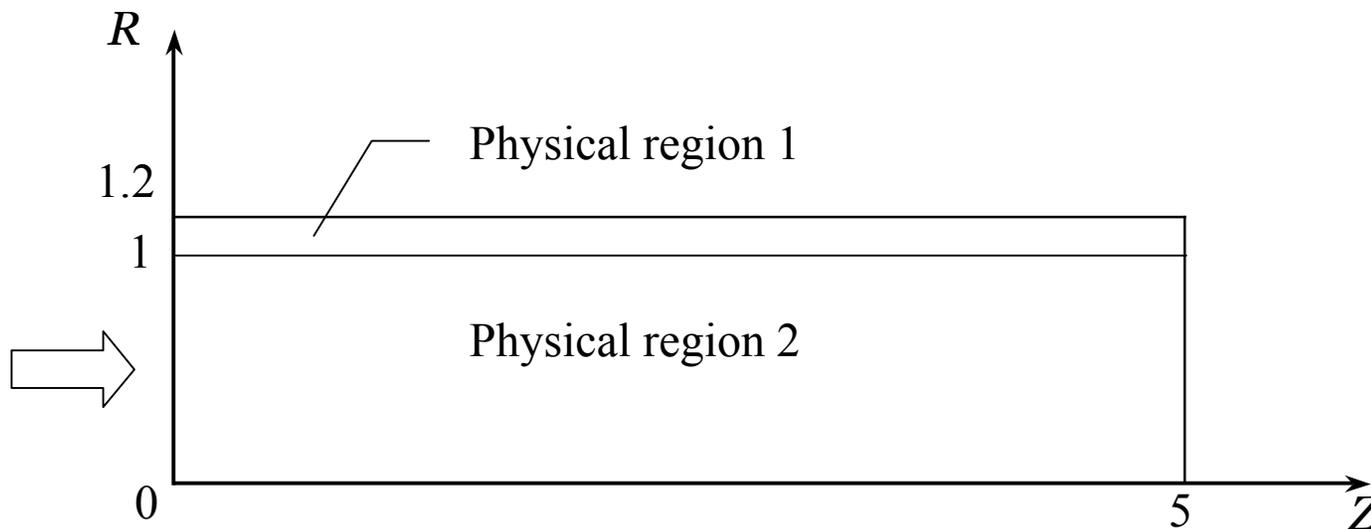
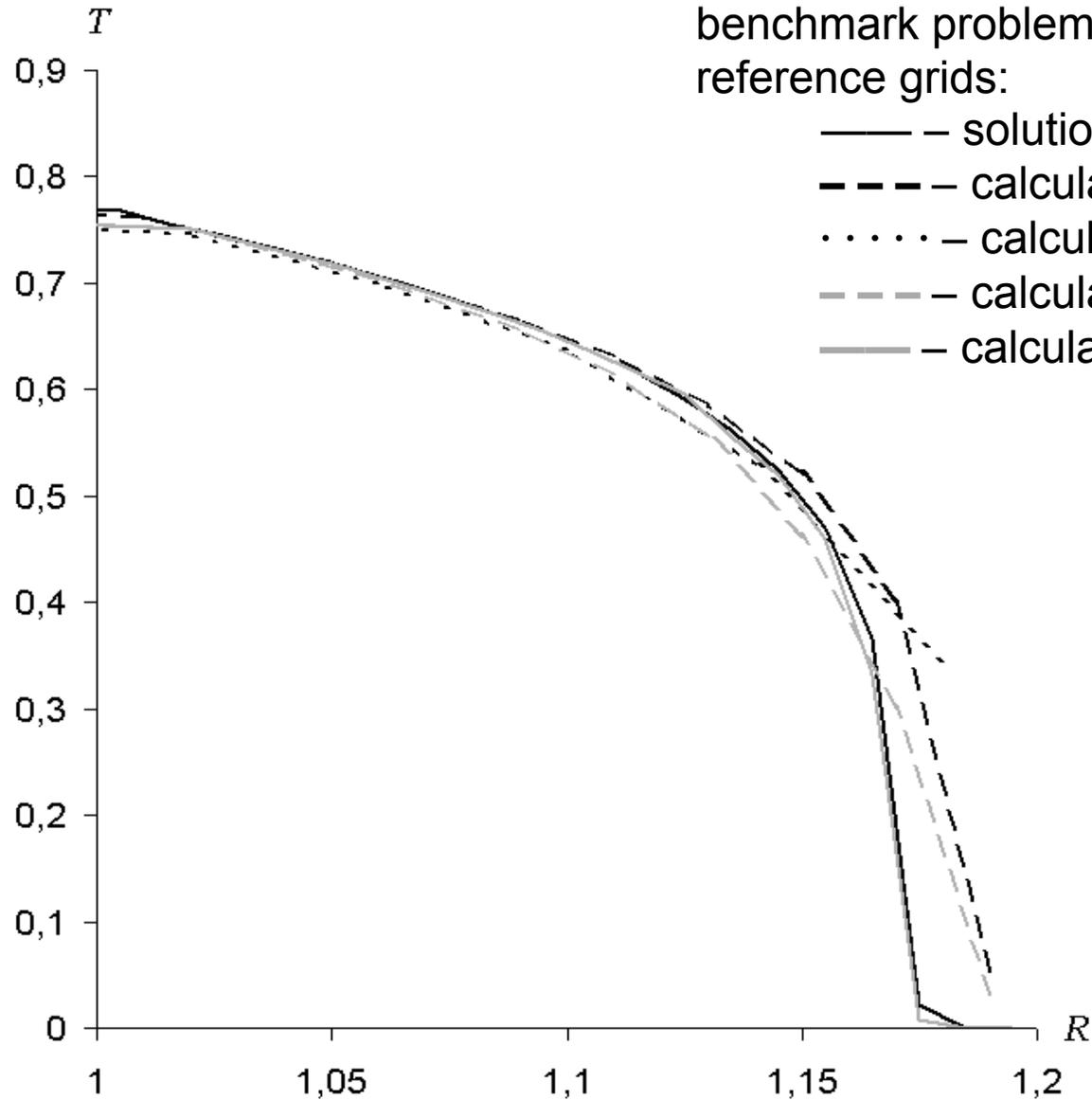


Fig. 10. The system geometry in the 2D benchmark problem

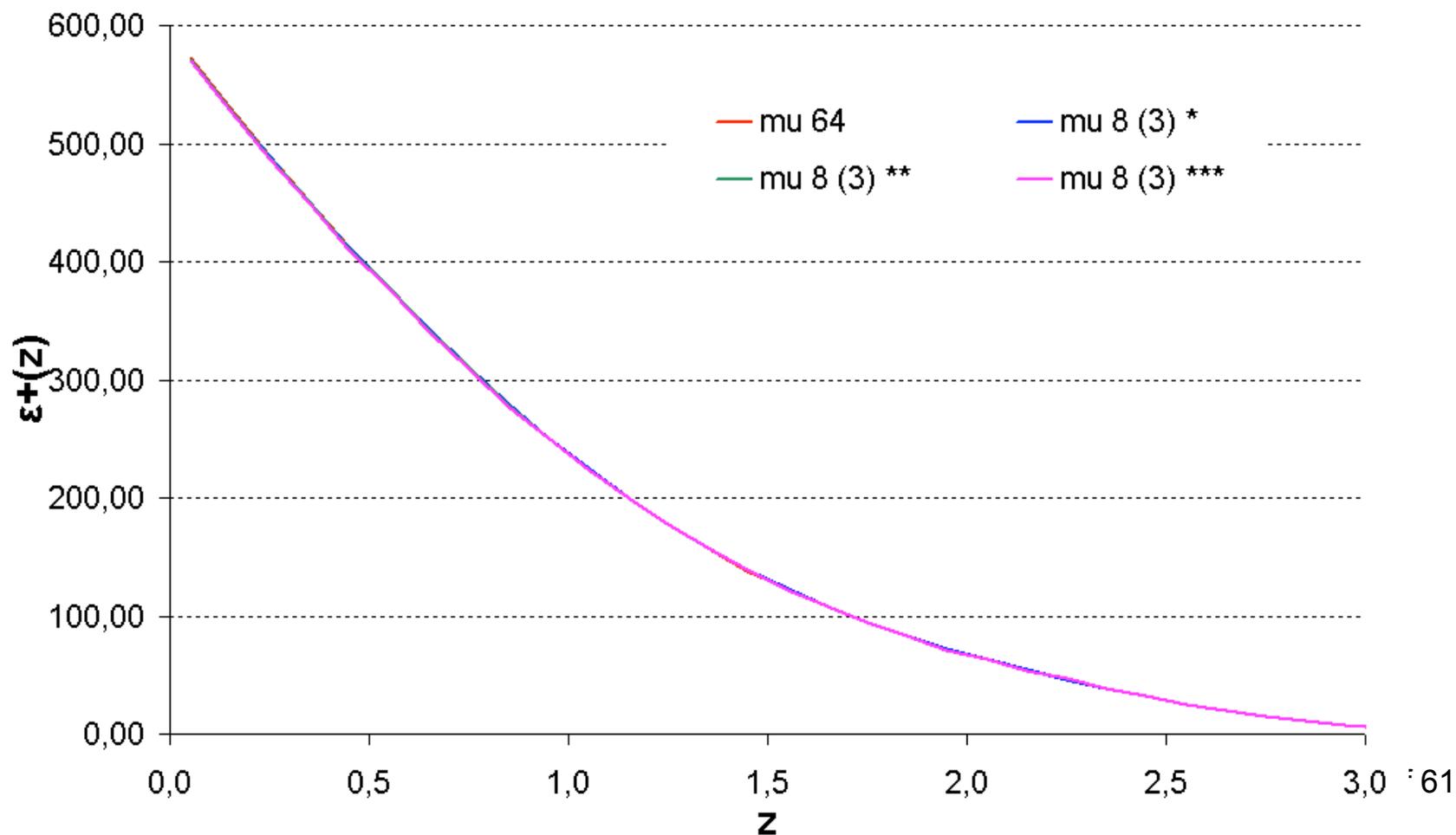
Fig. 11. Material temperature profile along line $Z = 2$ at time 0.01 in the 2D benchmark problem for different reference grids:





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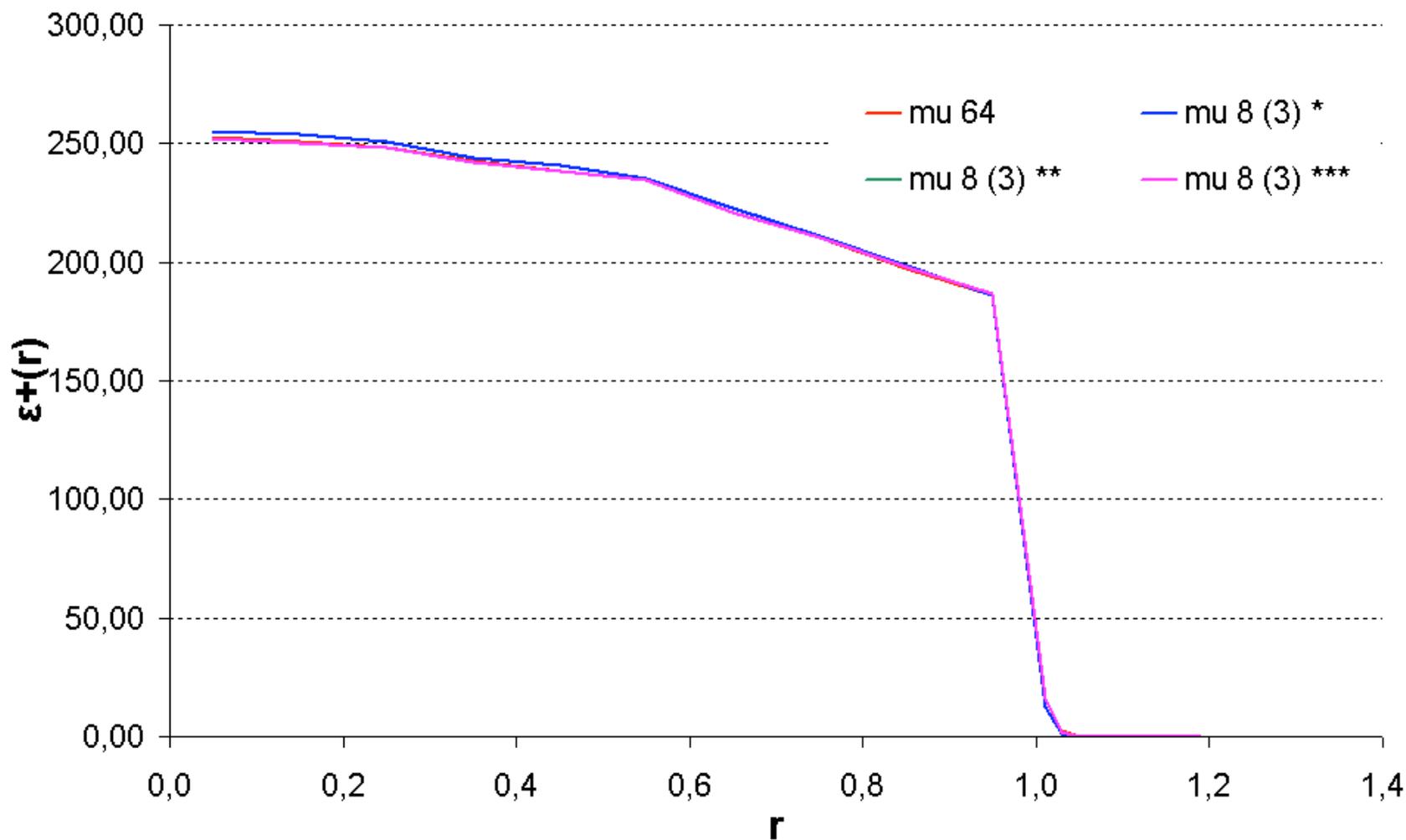
The flow density bottom-to-top distribution along
boundary $r=1.0$ for various options of the adaptive grid
construction





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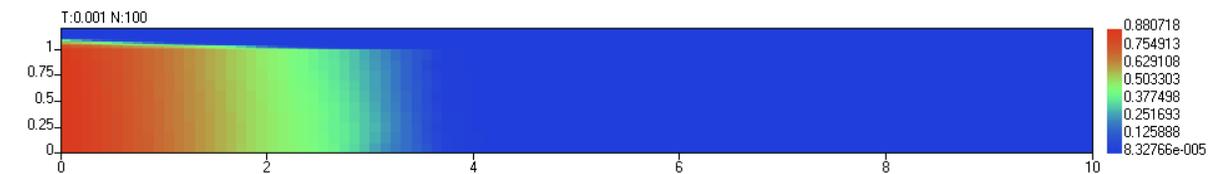
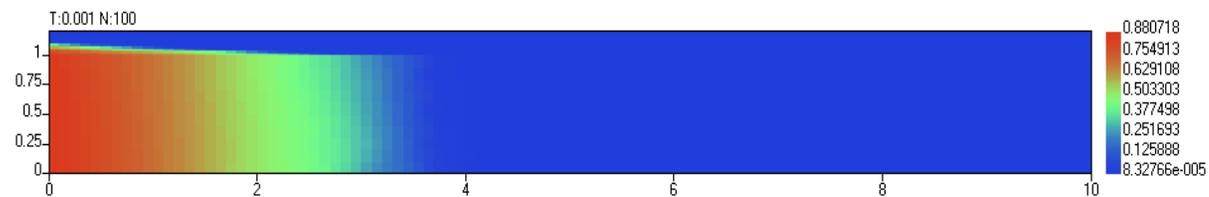
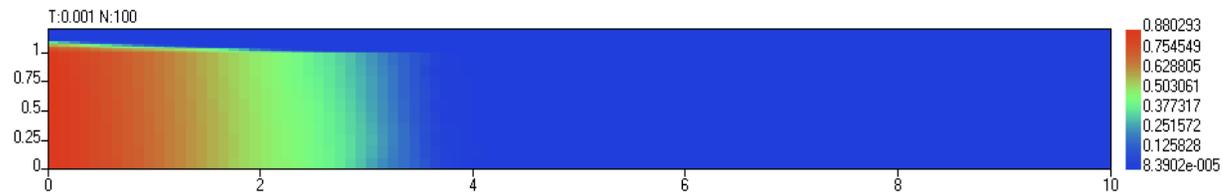
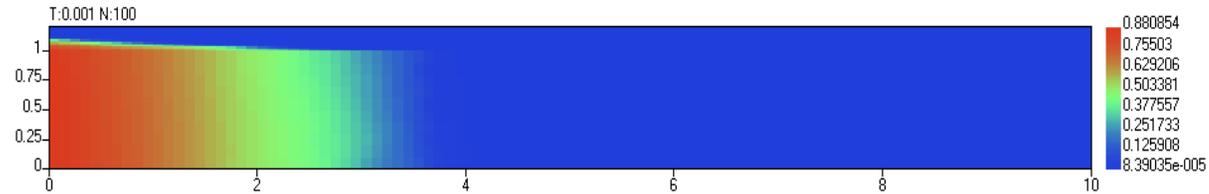
The flow density distribution from left to right along boundary $z=2.0$ for various options of the adaptive grid construction





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The radiation temperature distribution in computations





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Algorithms for iterative process convergence acceleration in complex SATURN

Finding the numerical solutions to various application problem classes requires methods for acceleration

of convergence of iterations in source (in the right-hand side of the transport equation) to ensure the computation efficiency.

For computations on linear time-independent problems of critical parameter calculation we have developed and are successfully using a flow consistent acceleration method (FCA method).

The brief description of the method and some results of its numerical studies are presented below.

FCA method (Flow Consistent Method)

$$\left\{ \begin{array}{l} P_k^+ = \iint_{(\bar{\Omega}, \bar{n}_k) \succ 0} (\bar{\Omega}, \bar{n}_k) N_k d\Omega \\ P_k^- = - \iint_{(\bar{\Omega}, \bar{n}_k) \prec 0} (\bar{\Omega}, \bar{n}_k) N_k d\Omega \end{array} \right. , \quad W_k = P_k^+ - P_k^- , \quad n^{(0)} = \iint_{\Omega} N d\Omega$$

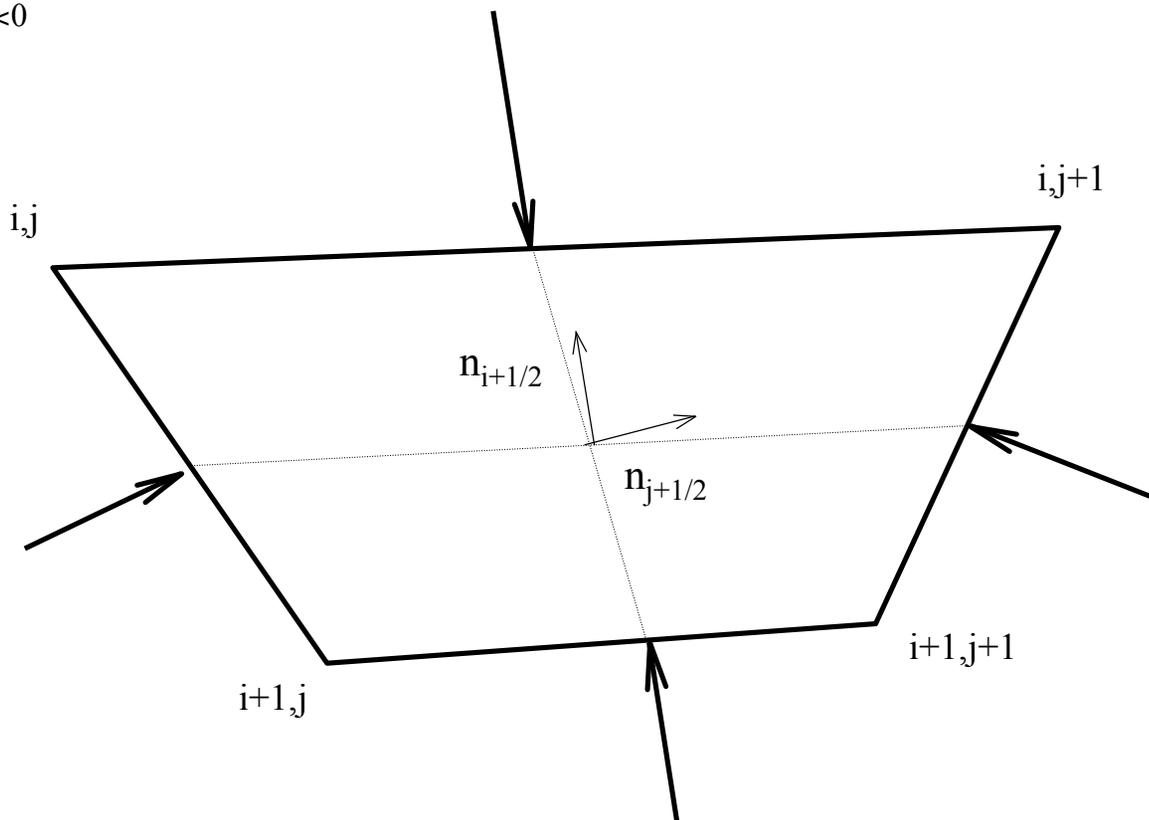


Fig. 13. The spatial grid cell

The FCA method is constructed using the integral moment equations, namely, the equations for zero and first moments of function N of the solution to the initial transport equation that include the compensating sources of the simple iteration.

$$\tilde{L}N^{S+1} + \tilde{\alpha}N^{S+1} = (\beta n^{(0)S} + Q) \frac{1}{4\pi}$$

$$\sum_{k \in (i, j, l)} (SL_k W_k - SL_{k+1} W_{k+1}) + (\alpha - \beta) n^{(0)} = (Q + F)$$

$$D_{k+1/2} \left[(P_{k+1}^+ + P_{k+1}^-) - (P_k^+ + P_k^-) \right] + \alpha \cdot m \cdot W_{k+1/2} = F W_{k+1/2}, \text{ where } k \in (i, j, l)$$

$$\begin{cases} P_k^+ = \iint_{(\bar{\Omega}, \bar{n}_k) > 0} (\bar{\Omega}, \bar{n}_k) N_k d\Omega \\ P_k^- = - \iint_{(\bar{\Omega}, \bar{n}_k) < 0} (\bar{\Omega}, \bar{n}_k) N_k d\Omega \end{cases} \quad W_k = P_k^+ - P_k^-, \text{ where } k \in (i, j, l, i+1/2, j+1/2, l+1/2)$$

$$\begin{cases} P_{k+1/2}^+ = (\delta \cdot P_k^+ + (1 - \delta) P_{k+1}^+) + F \delta_k^+ \\ P_{k+1/2}^- = (\delta \cdot P_{k+1}^- + (1 - \delta) P_k^-) + F \delta_k^- \end{cases} \quad , \text{ where } k \in (i, j, l)$$



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Numerical studies of the FCA method for the iterative process convergence acceleration

Region $\{0 < x < 1.5, 0 < y < 1.5, 0 < z < 1.5\}$

	β	2D		3D	
		N/A	FCA	N/A	FCA
10.	9.	81	7	116	12
10.	9.9	331	7	300	13
10.	9.99	463	7	361	13
10.	10.	482	7	370	13

Results of the computations for reactor SNR-300

Method	Number of iterations
Kellog method	143
Direct method	141
Method of inverse iteration	112
Method of inverse iteration + FCA	20



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Results of the computations for the RBMK reactor channel

Method	Number of iterations
Kellog method	229
Direct method	412
Source iteration method	555
Source iteration method + FCA	42
Source iteration method + FCA + Chebyshev method	24

Homogeneous sphere R=10

$\alpha=\beta$	Number of iterations		
	SI	DSA method	FCA method
1.	221	8	6
2.	597	8	6
4.	1627	9	6
8.	3927	8	6
12.	6003	12	6
16.	7658	24	9

The KM method is a two-step iterative method.

$$\frac{1}{v_i} \frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} + L \varepsilon_i^{n+\gamma} + \alpha_i \varepsilon_i^{n+\gamma} = \frac{1}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \varepsilon_j^{(0)n+\gamma},$$

$$\varepsilon_i^{n+\gamma} = \gamma \varepsilon_i^{n+1} + (1 - \gamma) \varepsilon_i^n, \quad i = 1, 2, \dots, NI$$

$$\varepsilon^{(0)} = \int_{-1}^1 \int_0^{2\pi} \varepsilon(r, z, \mu, \varphi, t) d\mu d\varphi \approx 2\pi \varepsilon, \quad \frac{1}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \varepsilon_j^{(0)n+\gamma} \approx \sum_{j=1}^{NI} \beta_{ij} \varepsilon_j^{n+\gamma}.$$

At step 2 of the KM method (corrector), the correction equation system of the following form is solved:

$$\frac{1}{v_i} \frac{\Delta \varepsilon_i^{n+1}}{\Delta t} + L \Delta \varepsilon_i^{n+\gamma} + \alpha_i \Delta \varepsilon_i^{n+\gamma} - \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{n+\gamma} = \frac{1}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{(0)n+\gamma},$$

$$\Delta \varepsilon_i^{s+1} = \varepsilon_i^{s+1} - \varepsilon_i^{s+\frac{1}{2}}, \quad \Delta \varepsilon_i^{n+\gamma} = \gamma \Delta \varepsilon_i^{n+1},$$

$$\Delta \varepsilon_i^{(0)} = \varepsilon_i^{(0)s+\frac{1}{2}} - \varepsilon_i^{(0)s}, \quad i = 1, 2, \dots, NI$$



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Mention some features of the group correction equations of KM-method step 2:

- 1. The KM method is a conservative iterative method, with the two major laws of conservation characteristic of the transport equation, i.e. the law of conservation relative to the particle transport and that relative to the medium-radiation energy exchange, being simultaneously satisfied at each iterative process step.**
- 2. The KM-method step 2 group equations are of the same form as the original group transport equations, which allows the same difference methods as those for the governing equations to be used for their grid approximation.**
- 3. The cost-efficient “point-to-point computation” method can be extended to the numerical solution of the KM-method step 2 correction difference group equation system.**

KM3 method

I step: predictor – like in the KM method

II step: corrector – iterative:

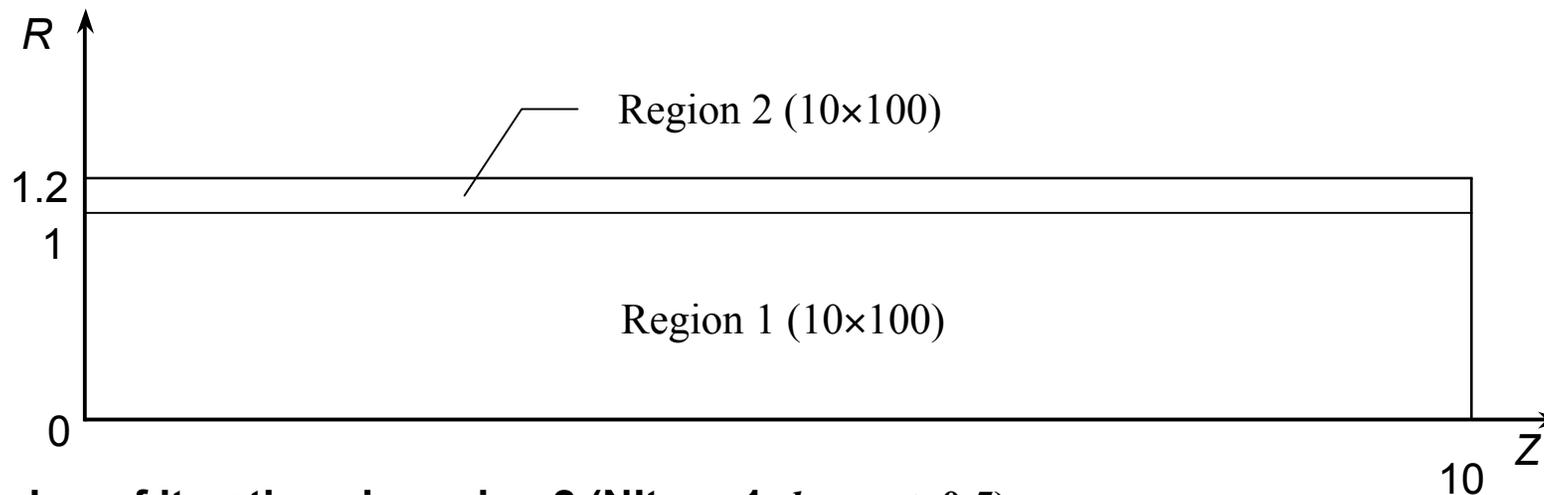
$$\begin{aligned} \frac{1}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1(0)n+\gamma} &= \frac{l_i}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1(0)n+\gamma} + \frac{1-l_i}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1(0)n+\gamma} \approx \\ &\approx l_i \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1n+\gamma} + \frac{1-l_i}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1(0)n+\gamma}, \quad 0 < l_i \leq 1, \end{aligned}$$

$$\begin{aligned} \frac{1}{v_i} \frac{\Delta \varepsilon_i^{s+1, v+\frac{1}{2}n+1}}{\Delta t} + L \Delta \varepsilon_i^{s+1, v+\frac{1}{2}n+\gamma} + \alpha_i \Delta \varepsilon_i^{s+1, v+\frac{1}{2}n+\gamma} - l_i \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1, v+\frac{1}{2}n+\gamma} &= (1-l_i) \frac{1}{2\pi} \times \\ &\times \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1, v(0)n+\gamma} + \frac{1}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+\frac{1}{2}, v+\frac{1}{2}n+\gamma}, \quad \Delta \varepsilon_i^{s+1, v+\frac{1}{2}} = \varepsilon_i^{s+1, v+\frac{1}{2}} - \varepsilon_i^{s+1, v} \end{aligned}$$

$$\begin{aligned} \frac{1}{v_i} \frac{\Delta^2 \varepsilon_i^{s+1, v+1n+1}}{\Delta t} + L \Delta^2 \varepsilon_i^{s+1, v+1n+\gamma} + \alpha_i \Delta^2 \varepsilon_i^{s+1, v+1n+\gamma} - \sum_{j=1}^{NI} \beta_{ij} \Delta^2 \varepsilon_j^{s+1, v+1n+\gamma} &= (1-l) \frac{1}{2\pi} \times \\ &\times \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+1, v+\frac{1}{2}(0)n+\gamma} - (1-l) \frac{1}{2\pi} \sum_{j=1}^{NI} \beta_{ij} \Delta \varepsilon_j^{s+\frac{1}{2}, v+\frac{1}{2}n+\gamma}, \quad \Delta^2 \varepsilon_i^{s+1, v+1} = \Delta \varepsilon_i^{s+1, v+1} - \Delta \varepsilon_i^{s+1, v+\frac{1}{2}} \end{aligned}$$

Numerical studies of the KM3 method

Benchmark problem «Tube»:



The number of iterations in region 2 ($N_{iter}_v=1, l=const=0.5$)

Step No.	sec			sec			sec		
	SI	KM	KM3	SI	KM	KM3	SI	KM	KM3
1	19108	14	14	28696	26	26	26454	35	35
5	3332	24	20	6363	121	88	7960	238	174
10	1559	27	20	8477	101	75	9146	179	135
<i>t, sec</i>	<i>2880</i>	<i>61</i>	<i>47</i>	<i>7020</i>	<i>233</i>	<i>184</i>	<i>8580</i>	<i>435</i>	<i>347</i>



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Techniques and algorithms for parallelizing 2D and 3D problems



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Parallel techniques

The development of highly efficient algorithms for parallelization of the problem class under discussion is an involved methodological problem. There are a number of objective reasons for this, among which the following should be primarily mentioned.

1. As it is known, implicit schemes are mainly used to find the numerical solution to the transport problem, hence, spatial grid cell computations should be performed in some strictly determined sequence. When using non-orthogonal spatial time-varying grids, the sequence of the cell computation may be different at different time steps. In other words, in parallelization of this problem class in space variables it is very hard, in contrast to the problems solved using explicit numerical methods, to ensure a simultaneous uniform loading of all the processor elements used.
2. In numerical solution of nonlinear transport equations the costs of the transport equation coefficient computations are significantly different at various space points, this leads to an additional disbalance of the parallel computations.
3. In numerical solution of the problem class under discussion a number of other physical processes must be simulated along with the transport process in separate sub-regions, this also significantly influences the parallel computation balance.

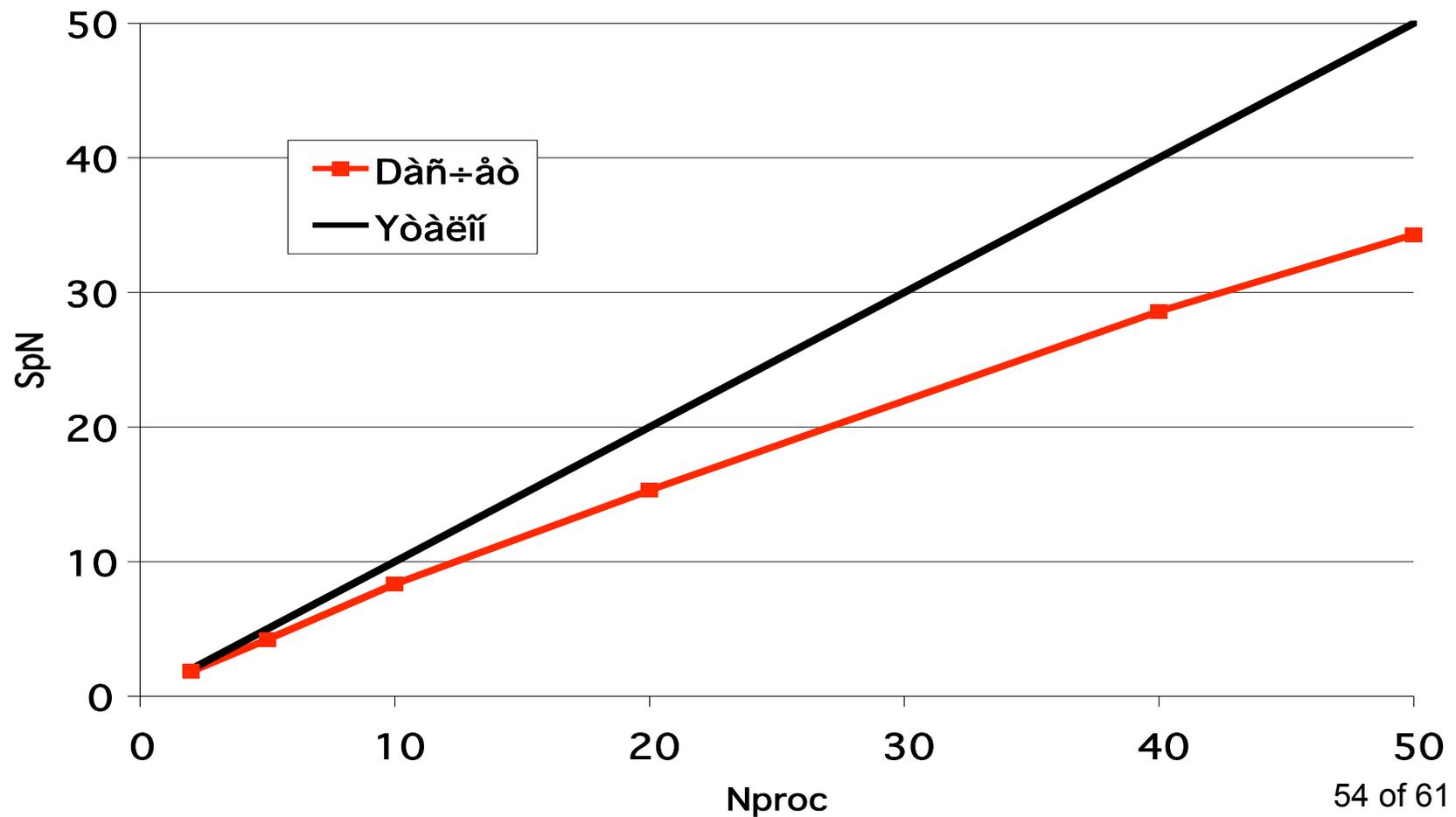


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As it was already mentioned above, numerical simulation of many various categories of multidimensional time-dependent transport problems leads to a heavy computational burden. We developed effective methods of fine-grain parallelization oriented to a general case of using non-orthogonal spatial grids to the problems above in 2D and 3D space approximations on multiprocessor systems (Alekseyev et al., 2001) (Alekseyev et al., 1993) (Alekseyev et al., 1996).

These parallelization algorithms are to be presented at the conference in a separate report. Here, I only demonstrate their efficiency by the example of one 3D test problem. The problem parameters are: 8 energy groups, 96 particle flight directions (S_8), 250000 three-dimensional spatial cells. The efficiency is estimated using the method of increase. The problem size remains unchanged on each processor.

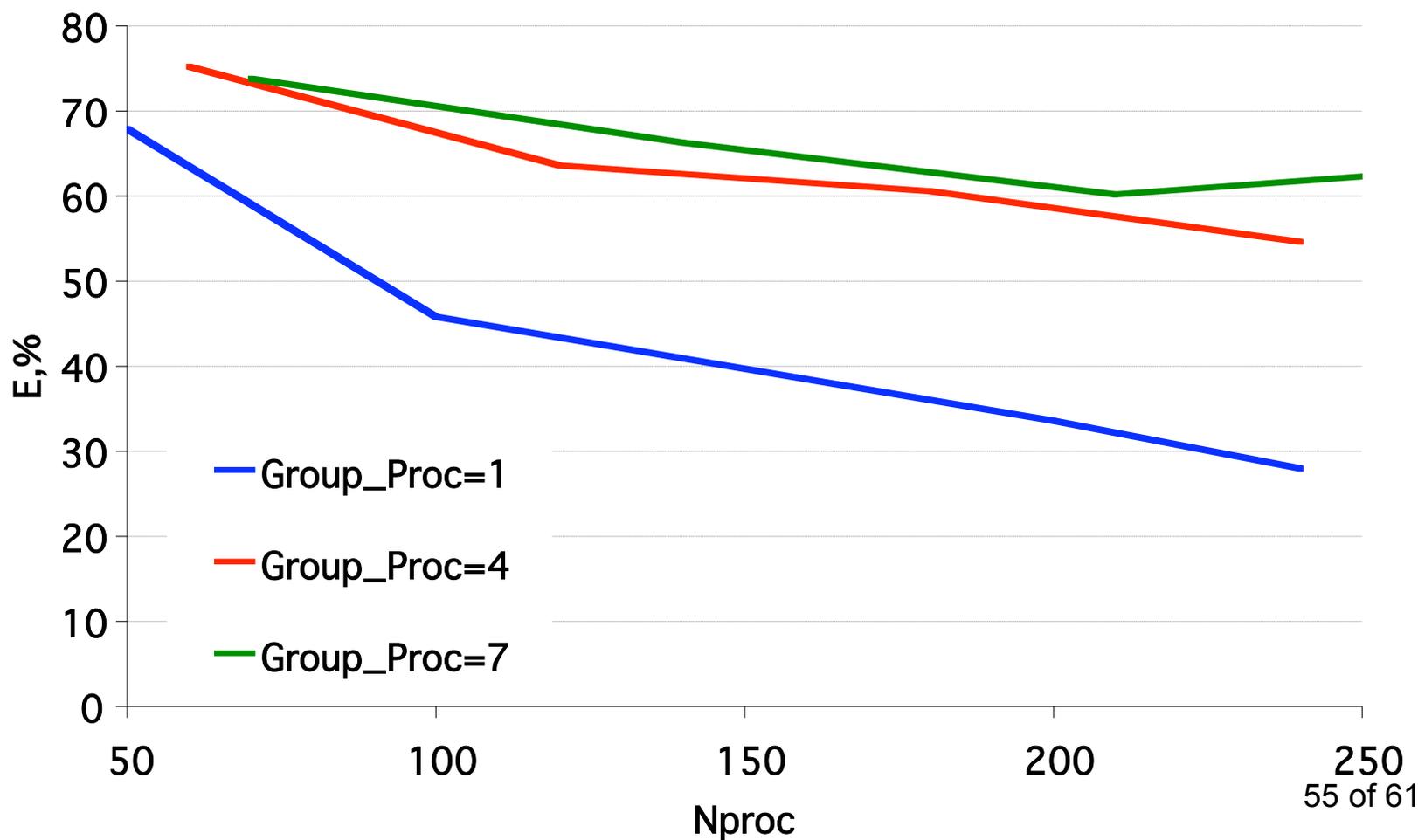
The speedup versus the number of processors





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The efficiency of the combined parallelization algorithm for solving the 2D benchmark (28 groups, 96 particle flight directions, 250000 spatial cells).





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Some examples of computations for 2D application problems

The above-discussed numerical methods and algorithms are extensively used at present for computation of various application problems in multidimensional geometries.

To demonstrate the capabilities of the methods developed, below are some results of the computations for 2D coupled time-dependent problems that describe experiments on laser facility ISKRA-5 .

- **Three-temperature hydrodynamics**

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \text{grad}(P + Q) \quad \frac{d\mathbf{z}}{dt} = \mathbf{u} \quad \frac{d\rho}{dt} = -\rho \cdot \text{div } \mathbf{u}$$

$$\frac{dE_f}{dt} = -P_f \frac{d\left(\frac{1}{\rho}\right)}{dt}, \quad \frac{dE_e}{dt} = -P_e \frac{d\left(\frac{1}{\rho}\right)}{dt}, \quad \frac{dE_i}{dt} = -(P_i + Q) \frac{d\left(\frac{1}{\rho}\right)}{dt}$$

- **Multi-group spectral radiation transport**

$$\frac{\partial U_{\nu}}{\partial t} + \text{div} \frac{c}{3\chi_{\nu}^{abs}} \text{grad} U_{\nu} = j_{\nu} - c\chi_{\nu}^{abs} U_{\nu} \quad \rho \frac{dE_e}{dt} = c \sum_{\nu} \left(\chi_{\nu}^{abs} U_{\nu} - j_{\nu} / c \right)$$

- **Energy transfer by electrons and ions**

$$\frac{\partial E_e}{\partial t} = -\frac{1}{\rho} \text{div}(\chi_e \cdot \text{grad} T_e) \quad \frac{\partial E_i}{\partial t} = -\frac{1}{\rho} \text{div}(\chi_i \cdot \text{grad} T_i)$$

- **Energy exchange between ions and electrons**

$$\frac{dE_e}{dt} = A(T_i - T_e) \quad \frac{dE_i}{dt} = -A(T_i - T_e)$$

- **Alpha particle energy transfer in space in the multi-group diffusion approximation**

- **Thermonuclear reaction kinetics**

- **Ionization and recombination kinetics**

- **Laser energy import into target**

Numerical simulation of experiments on laser facility ISKRA -5

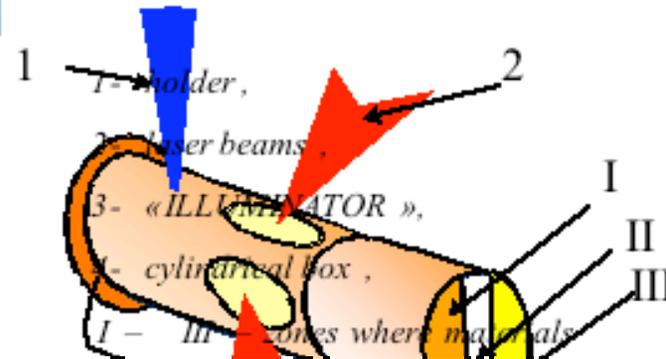
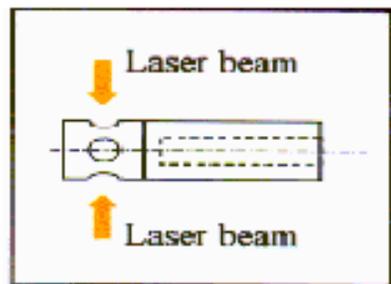
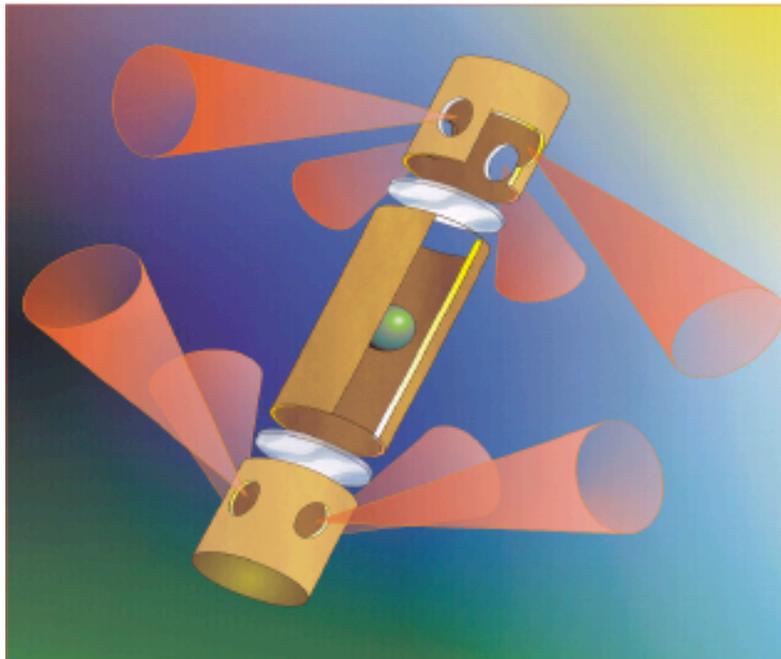
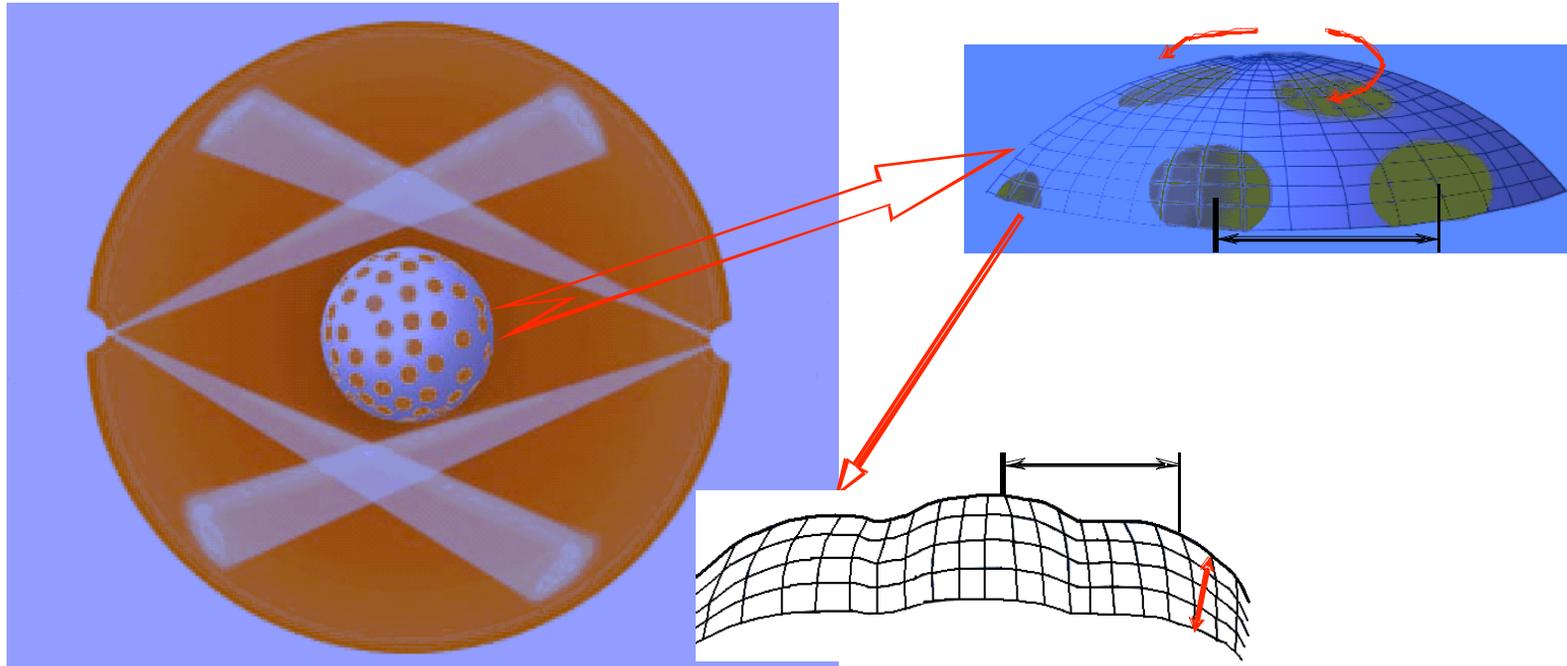


Fig. 16 presents the “illuminator” target



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Simulations of multibeam-laser irradiated target dynamics



Minimum number of points on the target surface	$250 \times 250 \sim 6 \cdot 10^4$
Minimum number of points in radius	200
Minimum number of groups in photon energy and
.....	$2 \cdot 10^3$
Total number of arithmetic operations over all points that are required for computation of one timestep	$4.4 \cdot 10^{14}$
Number of timesteps	10^4
Required performance of the super-computer for computation of the thermonuclear target implosion stage	$\frac{4\pi R_0^2}{\lambda} \frac{N}{\theta} \rightarrow \sqrt{\frac{4\pi R_0^2}{\lambda} \frac{N}{\theta}} \approx \sqrt{\frac{4\pi \cdot 250^2 \mu m}{0.35 \mu m} \frac{10^4}{0.1}} \approx 20 \sqrt{10^4} \approx 20 \cdot 10^2 = 2000$ (cost 100-100 h per computation) int s
Required performance of the super-computer for full-scale computations of laser thermonuclear facility dynamics	> 100 Tflops



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Spherical chamber of ISKRA-5 facility

