Institute of Theoretical and Mathematical Physics

Russian Federal Nuclear Center - **VNIIEF**

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

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Setting up the transport problem

$$\frac{\partial}{\partial t}\left(\frac{\varepsilon_i}{v_i}\right) + L\varepsilon_i + \alpha_i\varepsilon_i = F_i; \quad F_i^N = \left(\sum_{j=1}^{i1}\beta_{ij}n_j^0 + Q_i\right)\Big/4\pi;\; F_i^\varepsilon = \frac{\chi_{ai}}{4\pi}\varepsilon_{ip} + \frac{\chi_{si}}{4\pi}n_i^{(0)} + \frac{Q_i}{4\pi};$$

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

$$n_i^0 = \int_{-1}^{1}d\mu\int_0^{2\pi}\varepsilon_i d\varphi; \qquad i = 1, 2, \ldots, i1 \qquad \frac{\partial E}{\partial t} = \sum_{i=1}^{i1}\chi_{\text{ài}}\cdot\varepsilon_i^{(0)}\Delta\omega_i - \sum_{i=1}^{i1}\chi_{ai}\,\varepsilon_{ip}\,\Delta\omega_i$$

r, z, Φ - cylindrical coordinates, i - the number of the energy interval (group),

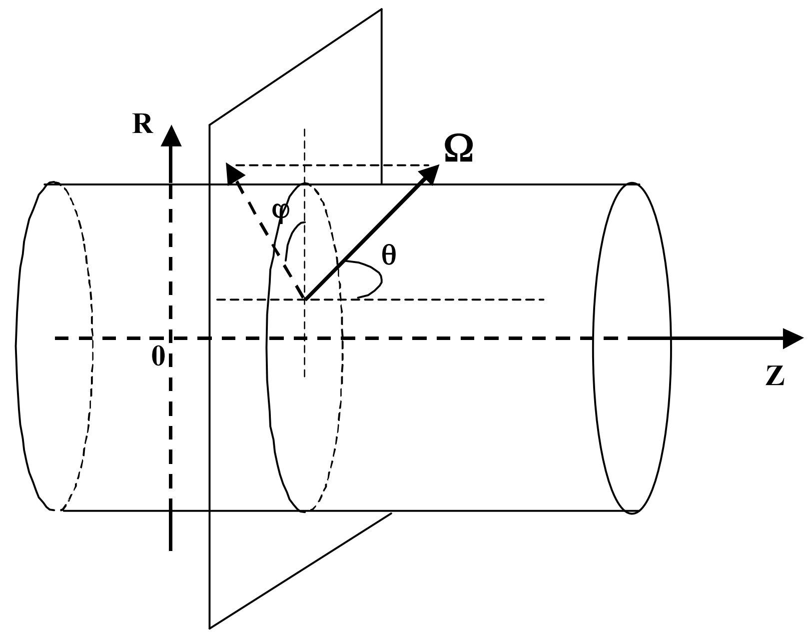
$\varepsilon_i = N_i(r,z,\Phi,t,\mu,\varphi,v_i)$ - the flux of neutrons or $\varepsilon_i(r,z,\mu,\varphi,\omega_i,t)$ - radiation intensity function (desired function), of group i at point (r,z,Φ,t) that fly in direction, $\mu=\cos\theta$, $-1 < \mu < 1$, $0 < \varphi < 2\pi$;

$\varepsilon_i = \omega_i$ - average energy of photons in group i,

$\Delta\omega_i$ - width of the interval in energy variable ω_i ,

T=T(r,z) - medium temperature, E=E(T) - internal energy,

$\varepsilon_{ip} = \varepsilon_{ip}(T, \omega_i)$ - Plank function



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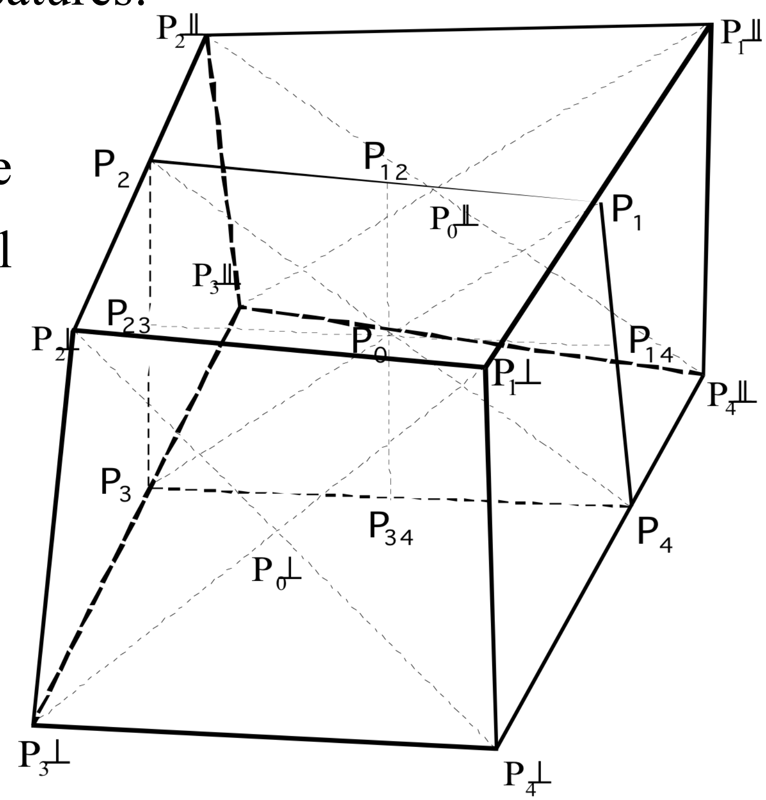
Approximation to the transport equation

• approximation in time is built using an implicit two-layer difference scheme;

• approximation in angular variables is built using the scheme of the method discrete ordinates;

• 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. The extended template scheme 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.



Methods

- Method of iterations in the right-hand part.
- Explicit cost-effective sweep (point-to-point computation) algorithms.
- Parallel Techniques.
- Adaptive Method in space, angular, and energy variables.

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.

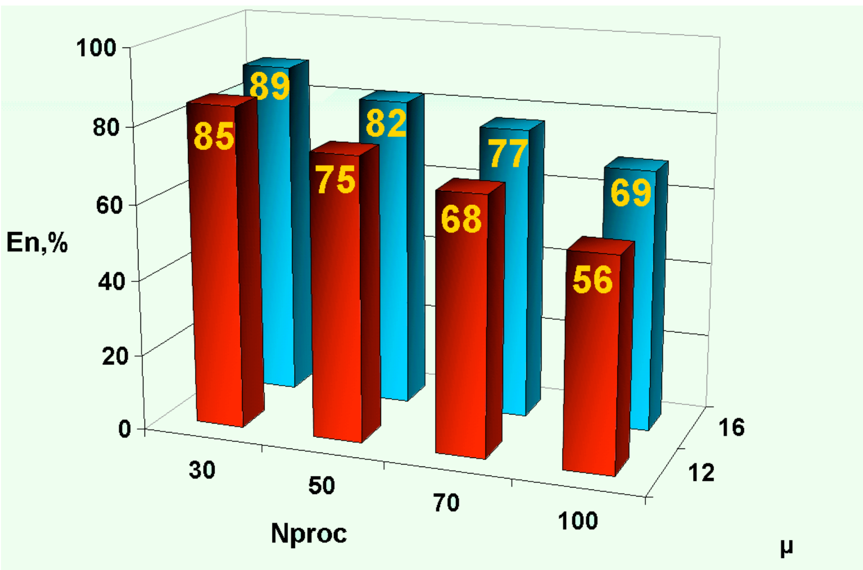
A pipelined algorithm of parallelization in layers and neutron flight directions to solve 3D problems using structured grids.

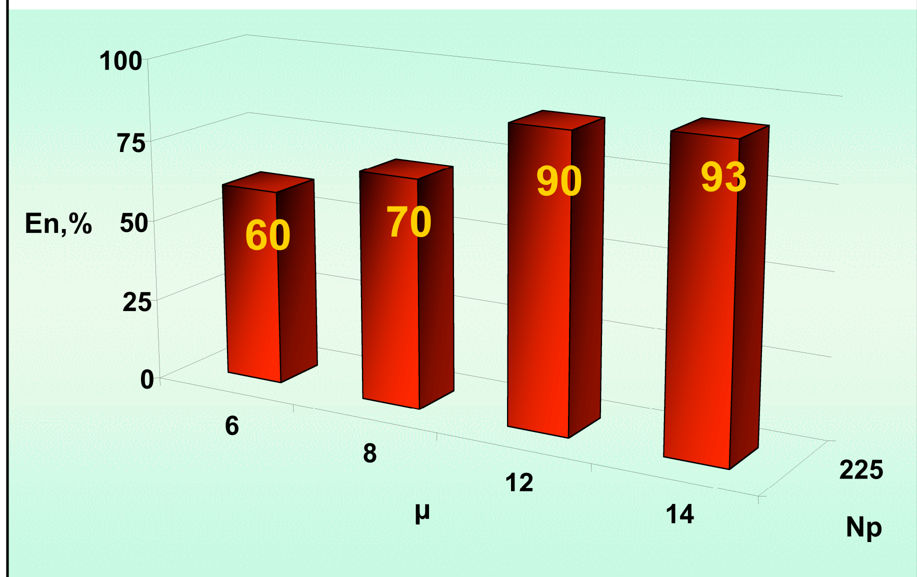
A combined algorithm of small-block parallelization and parallelization in energy groups to solve 2D and 3D problems using structured grids.

The main ideas of the small-block parallelization algorithm

- 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

Efficiency of the small-block parallelization algorithm





1D decomposition	2D decomposition

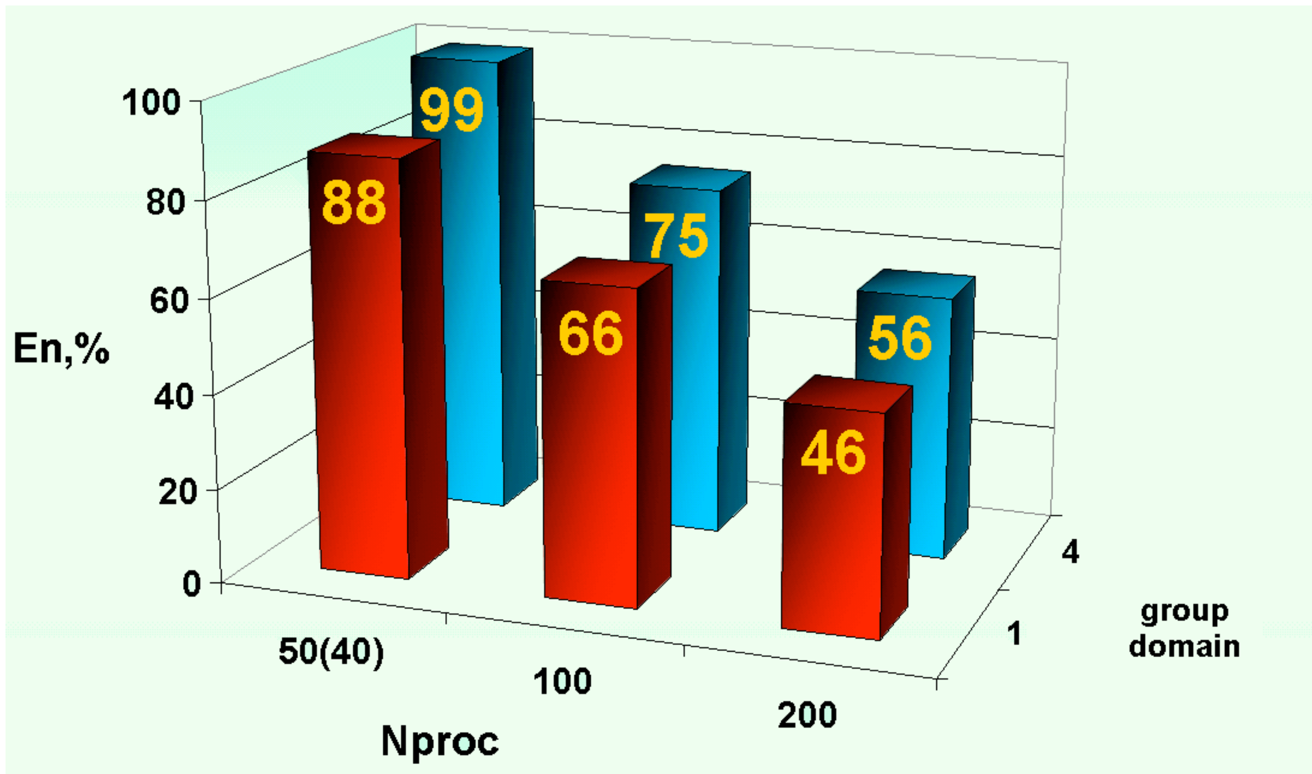
2D test. A single-domain spherically symmetric transport problem in one-group approximation.

A spatial grid consisted of 1200 rows and 1200 columns.

Combined parallelization algorithm

Hemi-spherical space-domain model problem had been selected as a test one: 80 rows were homogenously distributed at the radius, 200 columns were homogenously distributed at the angle.

The order of the angle quadrature was 12, in total there were 96 directions of the particles motion. Number of energy groups was 28



1D decomposition

Combined parallelization algorithm

2D decomposition

Number of Processors	Number of Group-domains	Number of Para-domains	E, % 8 groups	E, % 28 groups
1	1	1	**100**	**100**
50	1	50	**83**	**80**
75	1	75	**79**	**76**
100	1	100	**72**	**71**
100	4	25	**84**	**81**
150	1	150	**69**	**66**
200	1	200	**63**	**62**
200	4	50	**76**	**77**

Pipeline type parallelization method for numerical solution of 3D transport equation

Time diagram of the transport equation solution with parallelization (N_Φ=6, N_μ=2, N_φ=3)

Step	Processor 1			Processor 2			Processor 3		
	μ	φ	Φ	μ	φ	Φ	μ	φ	Φ
1	1	1	1	-	-	-	-	-	-
2	1	1	2	-	-	-	-	-	-
3	1	2	1	1	1	3	-	-	-
4	1	2	2	1	1	4	-	-	-
5	1	3	1	1	2	3	1	1	5
6	1	3	2	1	2	4	1	1	6
7	2	1	1	1	3	3	1	2	5
8	2	1	2	1	3	4	1	2	6
9	2	2	1	2	1	3	1	3	5
10	2	2	2	2	1	4	1	3	6
11	2	3	1	2	2	3	2	1	5
12	2	3	2	2	2	4	2	1	6
13	-	-	-	2	3	3	2	2	5
14	-	-	-	2	3	4	2	2	6
15	-	-	-	-	-	-	2	3	5
16	-	-	-	-	-	-	2	3	6

26 energy groups;
96 flight directions (S_8);
~1000000 3D space cells (144 layers).

Npr	9	18	36	72	144
E_N, %	92	85	81	78	76

Adaptive Method

- ✓AM-S scheme (spatial variables)
- ✓AM-A scheme (angular variables)
- ✓AM-E scheme (energy variable)

Main ideas

Each cell of the reference spatial grid can be partitioned into smaller cells of an adaptive refined grid (adaptive cells).

An adaptive refined grid is generated by partitioning into 2^N equal ranges in each direction, where N is the adaptive grid level.

Separate intervals in angular variable μ of the reference grid can be partitioned into smaller ones. The number of the subintervals in the reference interval of the grid in μ should be 2^N, N is the adaptivity order.

The angular grid is refined only for the selected set of spatial cells. In different spatial grids fragmentation to different numbers of smaller intervals in variable μ of the reference angular grid is admitted.

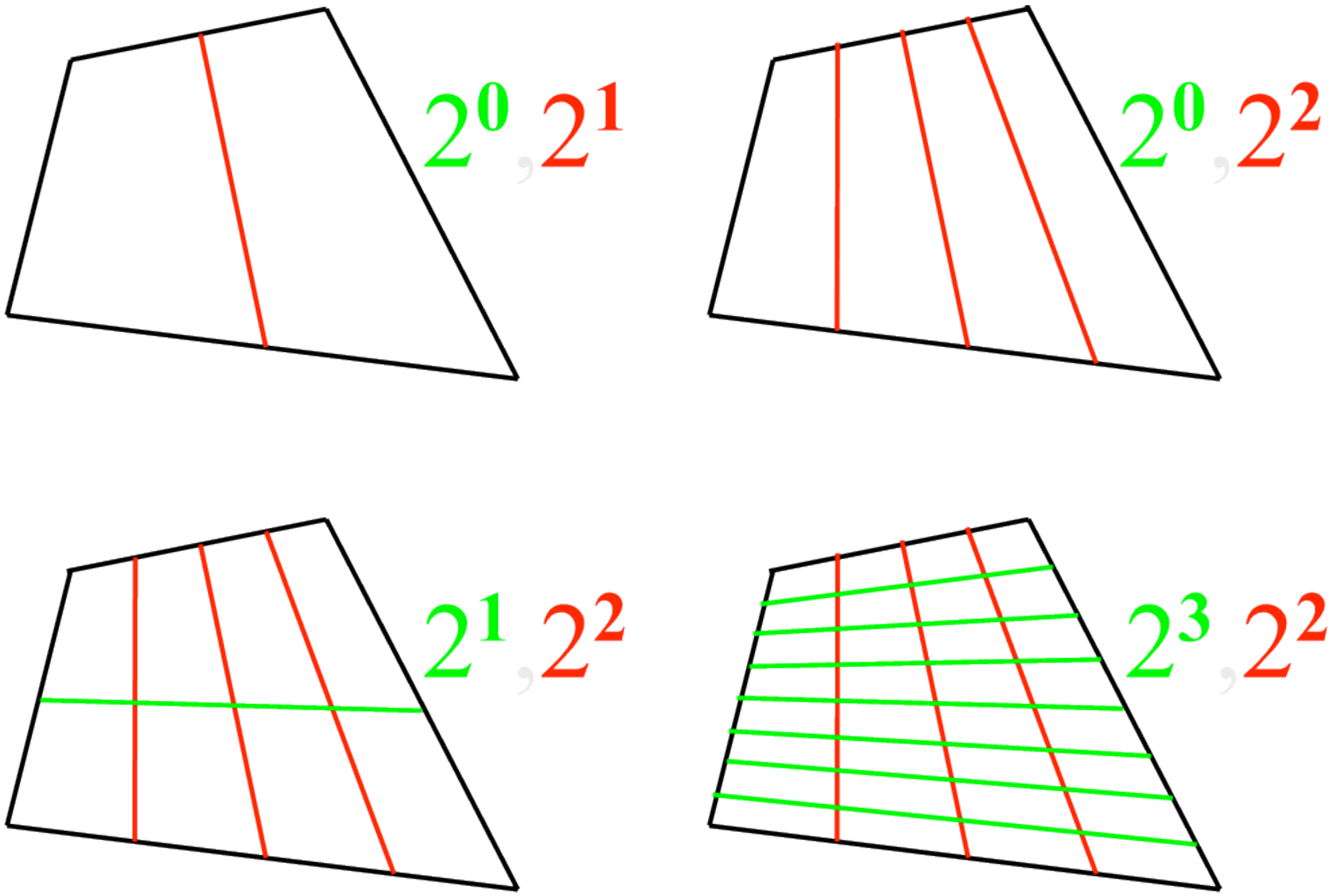
Development of criteria for and algorithms of partitioning a reference energy grid into smaller energy ranges (groups) at those space points and those ranges of the reference energy grid, where the solution in energy variable undergoes significant changes.

An adaptive grid is generated at the beginning of time step basing on the analyzed distribution of the solution function over the reference grid obtained during the previous time step.

The solution functions are interpolated from the old grid to the new one. During reconstruction of the adaptive grid, re-interpolation of the grid values is performed by normalized conservative integration with weights.

The order of resolving space cells during point-to-point computation is determined on the reference grid. With an adaptive grid present in a cell, the subsystem of equations corresponding to the transport equation approximation on the adaptive grid of the given cell has to be solved.

Different refinements in space variables



Adaptive grid generation criteria

$$Div_{rel} = \max\left(\frac{|T_{rad} - T_{rad}^{left}|}{T_{rad} + T_{rad}^{left}}, \quad \frac{|T_{rad} - T_{rad}^{right}|}{T_{rad} + T_{rad}^{right}}\right)$$

$$OrdAdapt = \begin{cases} [F(Div_{rel})], & Div_{rel} \in [0;\ 1) \\ MaxAdapt, & Div_{rel} = 1 \end{cases} \qquad F(x) = x^{l} \cdot (MaxAdapt + 1), \quad \begin{cases} l = 1 \\ l >> 1 \end{cases}$$

$$I_{\mu_{m-1/2}} = \int_0^{\pi} \varepsilon\left(t^n, r_{P_0}, z_{P_0}, \mu_m, \varphi\right)\ d\varphi \approx \sum_{q=1}^{q_m} \varepsilon^{n}_{m-1/2,q-1/2,P_0} \Delta\varphi_{q-1/2} = I_{m-1/2}$$

$$I_{m-1/2}^{j-1/2} = \sum_{q=1}^{q_m} \varepsilon^{n}_{m-1/2,j-1/2,q-1/2,P_0} \Delta\varphi_{q-1/2}, \quad j = 1,\ldots,k_m \qquad I_{m-1/2}^{\max} = \max_{1\le j\le k_m} I_{m-1/2}^{j-1/2}, \quad I_{m-1/2}^{\min} = \min_{1\le j\le k_m} I_{m-1/2}^{j-1/2}$$

$$Div_{rel}^{m-1/2} = Div_{rel}^{m} = \frac{|I_{m-1/2} - I_{m+1/2}|}{I_{m-1/2} + I_{m+1/2}} \qquad I_{m-1/2} / I_{m+1/2} = K^n \qquad Div_{rel}^{m-1/2} = \frac{K^n - 1}{K^n + 1}$$

$$OrdAdapt = \begin{cases} \left[\dfrac{1}{\ln K} \ln \dfrac{1 + Div_{rel}^{m-1/2}}{1 - Div_{rel}^{m-1/2}}\right], & Div_{rel}^{m-1/2} \in \left[0; \dfrac{K^{OrdMax} - 1}{K^{OrdMax} + 1}\right), \\ OrdMax, & Div_{rel}^{m-1/2} \in \left[\dfrac{K^{OrdMax} - 1}{K^{OrdMax} + 1};\ 1\right], \end{cases}$$

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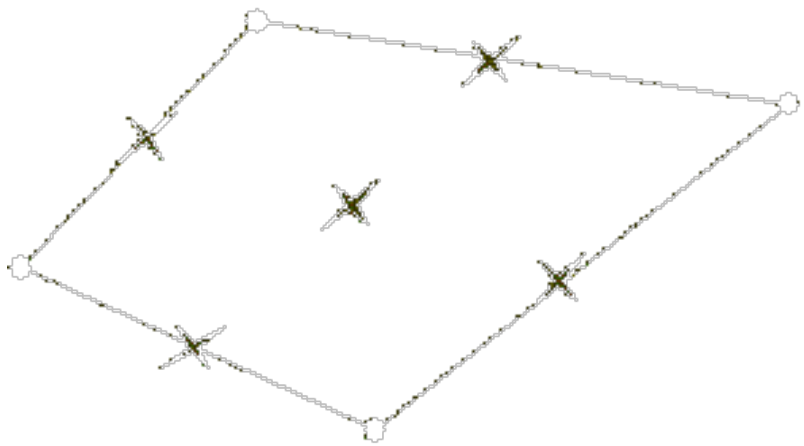
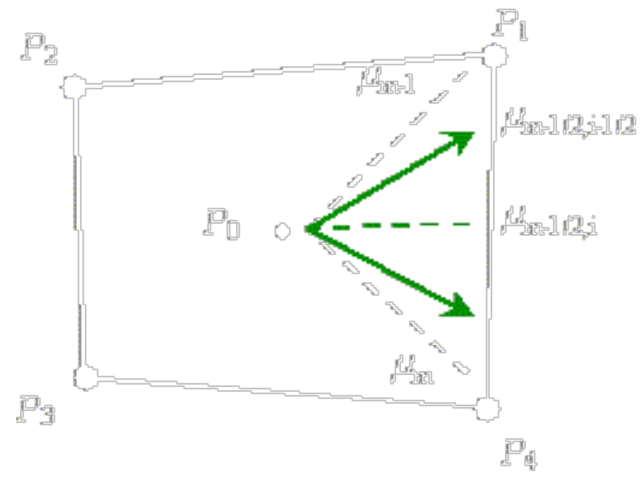
Re-interpolation of grid values at the centers of cells



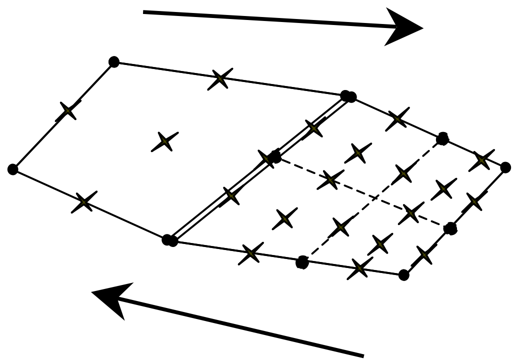


$$F = \frac{1}{m}\sum_i F_i m_i$$

$$\{\mu^{i}_{m-1/2}\}\Big|_{i=1}^{\bar{s}_m+1} \rightarrow \{\mu^{j}_{m-1/2}\}\Big|_{j=1}^{\bar{k}_m+1}$$

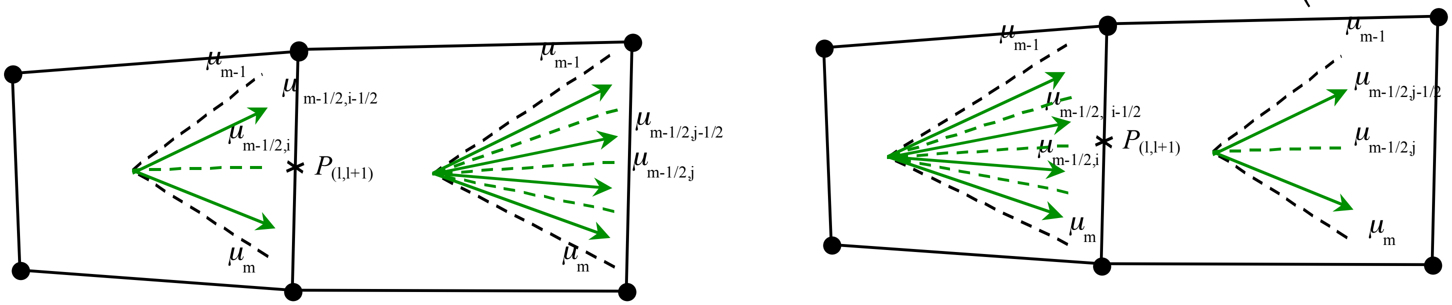
$$\varepsilon_{m-1/2,j-1/2} = \frac{1}{\Delta\mu_{j-1/2}} \cdot \sum_{i=(j-1)\cdot\bar{s}_m/\bar{k}_m+1}^{j\cdot\bar{s}_m/\bar{k}_m} \varepsilon_{m-1/2,i-1/2}\Delta\mu_{i-1/2},\ j = 1,\ldots,\bar{k}_m$$

Re-interpolation of values on edges of cells



$$F = \frac{1}{R}\sum_i F_i R_i$$

$$\varepsilon_{m-1/2,j-1/2,P(l,l+1)} = \varepsilon_{m-1/2,i-1/2,P(l,l+1)},\ j = 1,\ldots,\bar{k}_m,\ i = \mathrm{int}\left(\frac{j-1}{\bar{k}_m / \bar{s}_m}\right)+1$$



$$R_{j-1/2,P(l,l+1)}\varepsilon_{m-1/2,j-1/2,P(l,l+1)} = \frac{1}{\Delta\mu_{m-1/2}^{j-1/2}} \sum_{i=(j-1)\cdot\bar{s}_m/\bar{k}_m+1}^{j\cdot\bar{s}_m/\bar{k}_m} \varepsilon_{m-1/2,i-1/2,P(l,l+1)} R_{i-1/2,P(l,l+1)} \Delta\mu_{m-1/2}^{i-1/2}, \quad j = 1,\ldots,\bar{k}_m$$

Computational Techniques

Computations for convergence

Selection of the reference grid and the adaptability level

Computations using an adaptive grid

Comparison between results and running times

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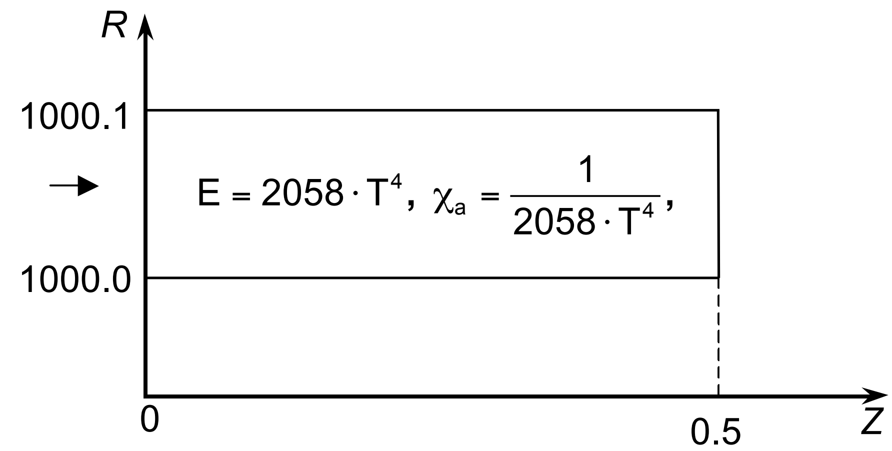
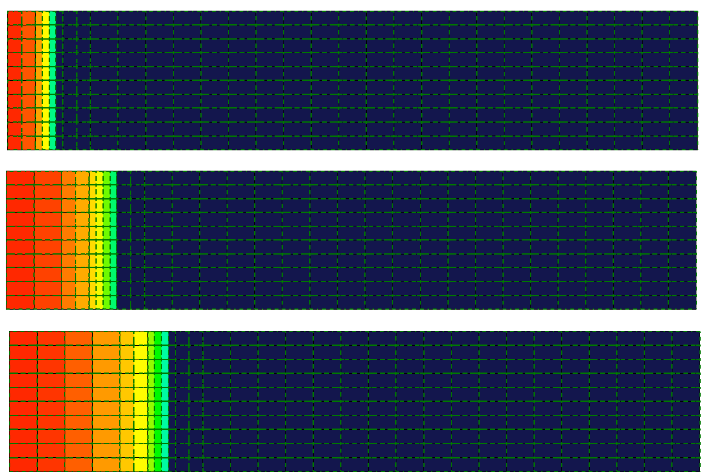
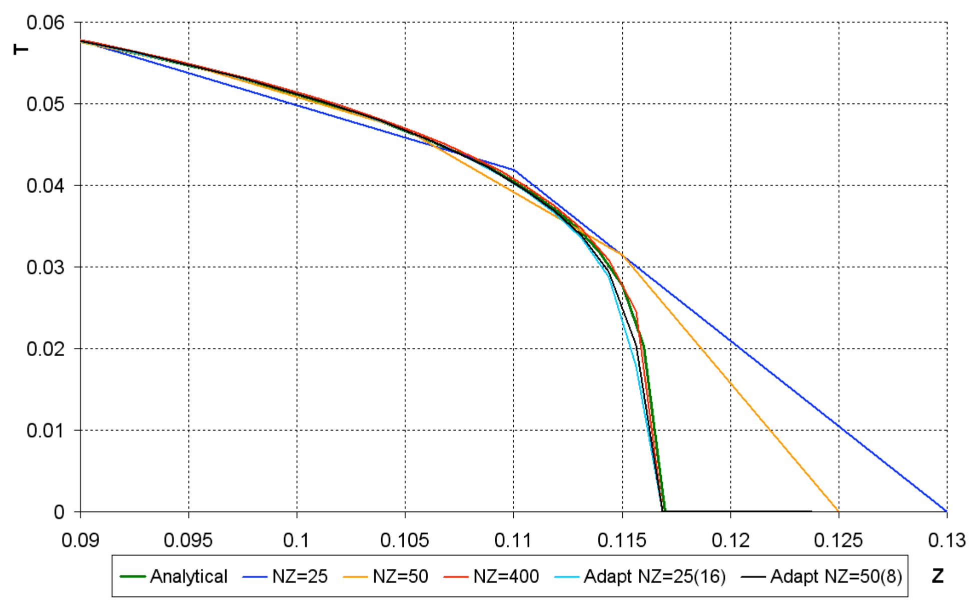
Task 1D

$$\varepsilon(0,\mu,t) = \frac{ct}{c + (cC_1\mu + 1)},\ \mu > 0,\ C_1 = -0.85903205\ldots$$







Ratio between running times:
NZ=400 to Adapt NZ=25(16) :: 9

Ratio between running times:
NZ=400 to Adapt NZ=50(8) :: 5.6

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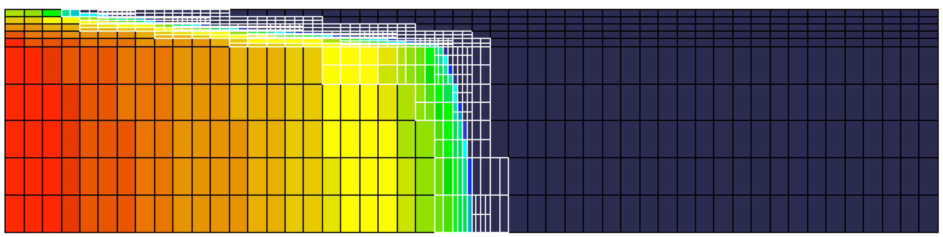
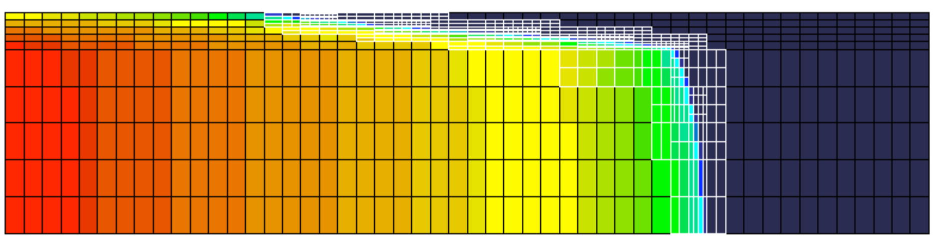
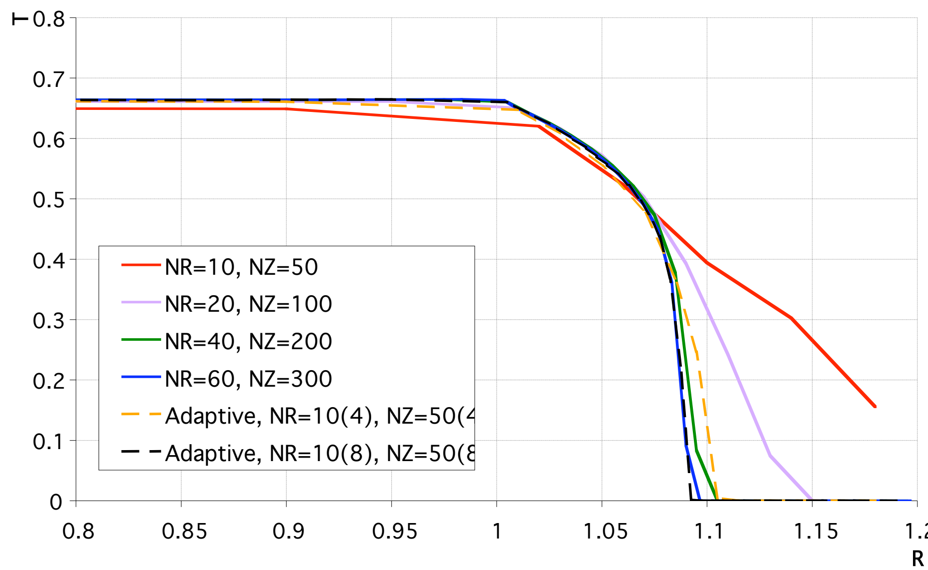
Task 2D

$$\chi_a = \frac{A}{T^3}$$

$$E = 0.81 \cdot T$$







Ratio between running times: NR=40, NZ=200 to Adapt NR=10(4), NZ=50(4) :: 8.9

Ratio between running times: NR=60, NZ=300 to Adapt NR=10(8), NZ=50(8) :: 4.8

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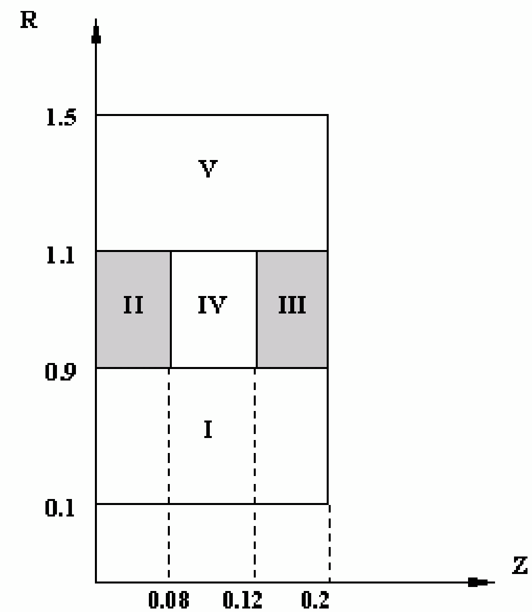
Slit benchmark problem



On the surface (R=0.1, 0<=Z<=0.2) isotropic energy flux equal to one is given.

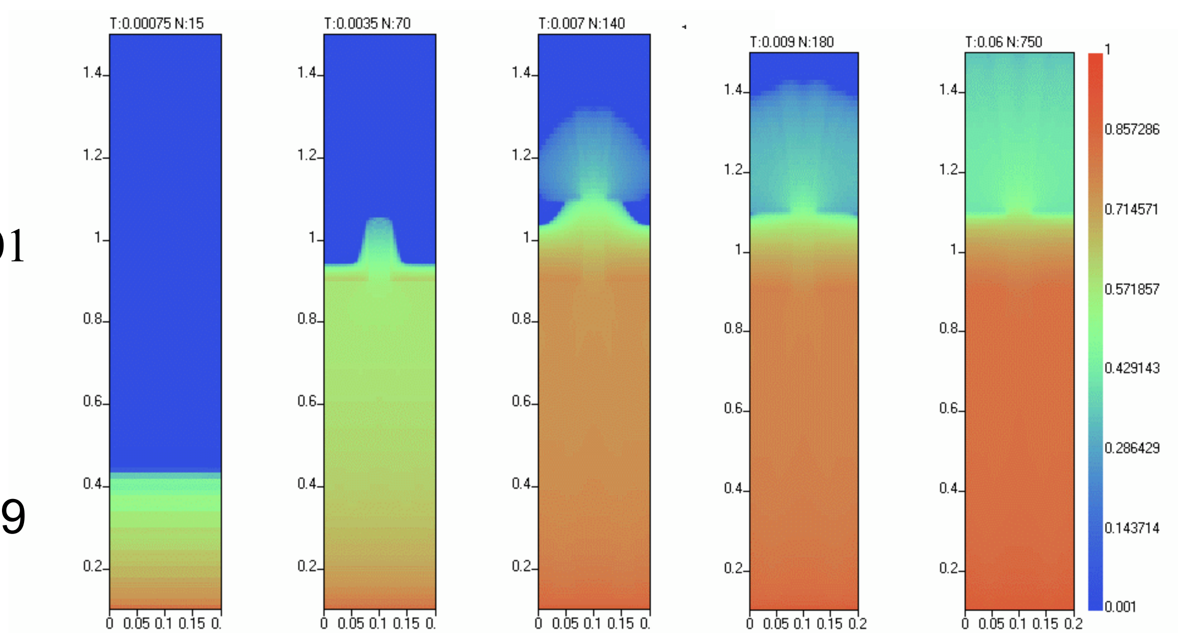
On a side surfaces (Z=0 and Z=0.25) the “specular reflection” boundary condition is given.

On the other surface the “free surface” boundary condition (zero coming-in flux) is given.

$$\chi_a = \frac{A}{T^3} \qquad \chi_s = 0 \qquad T_0 = 0.001$$

Domains I, III, V (transparent), A=0.1374

Domains II,IV (dense), A=50.89



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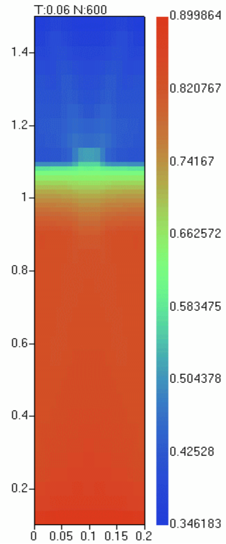
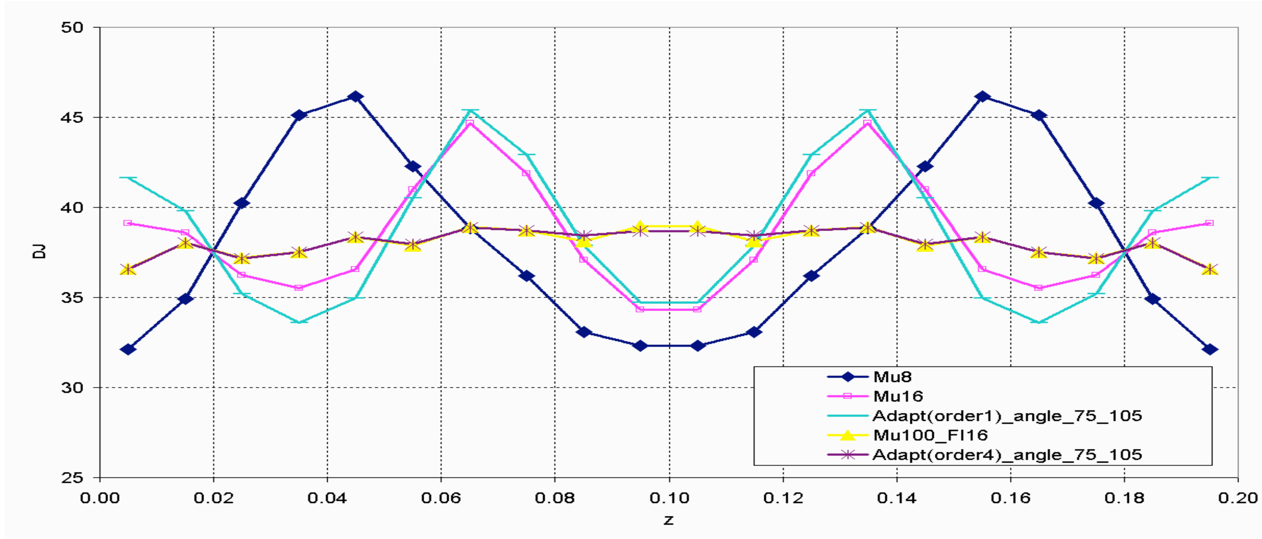
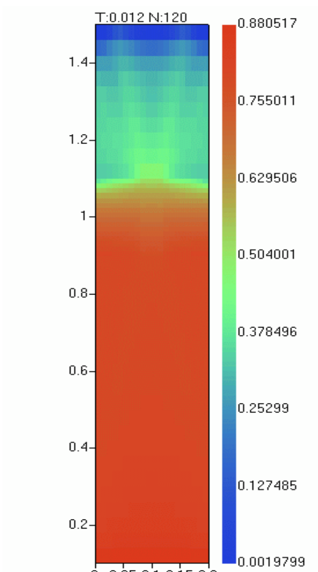
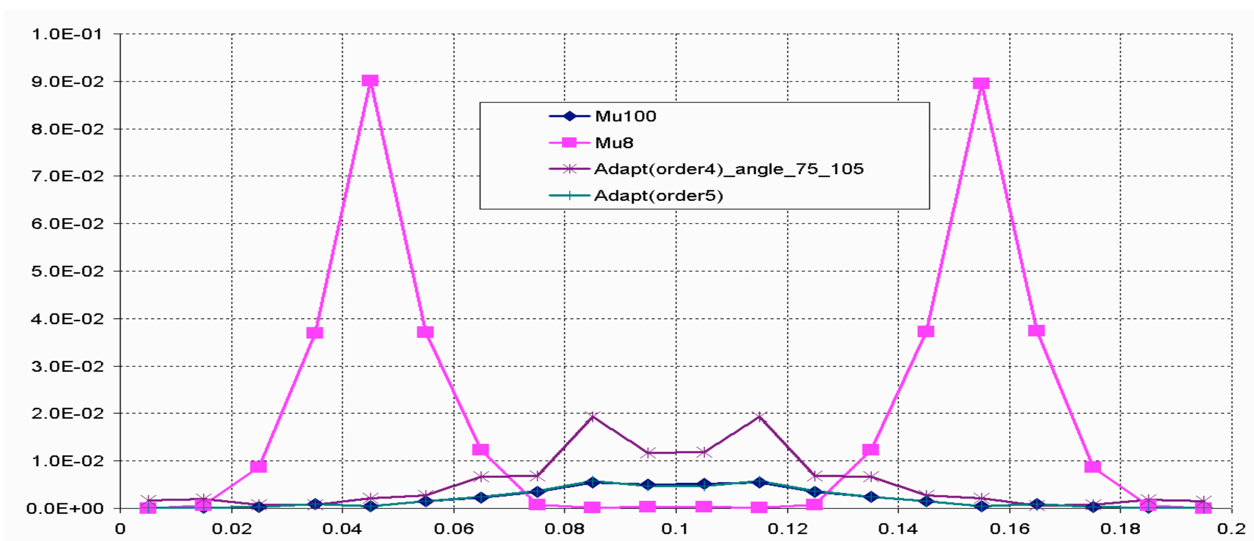
One-side flow for R=1.5 Time=0.06





One-side flow for R=1.5 Time=0.012





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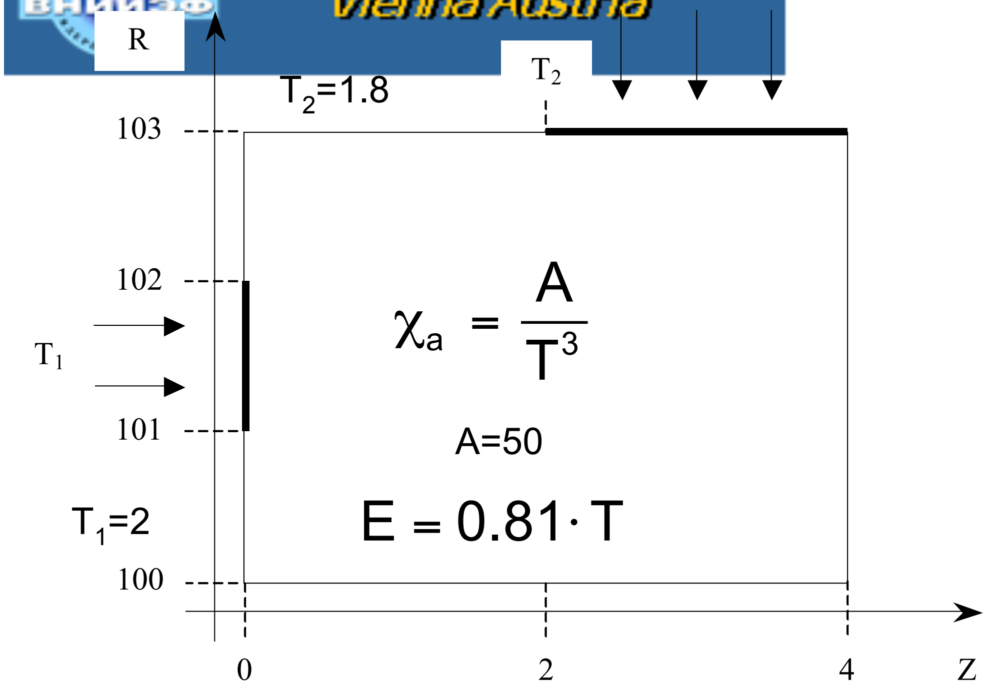
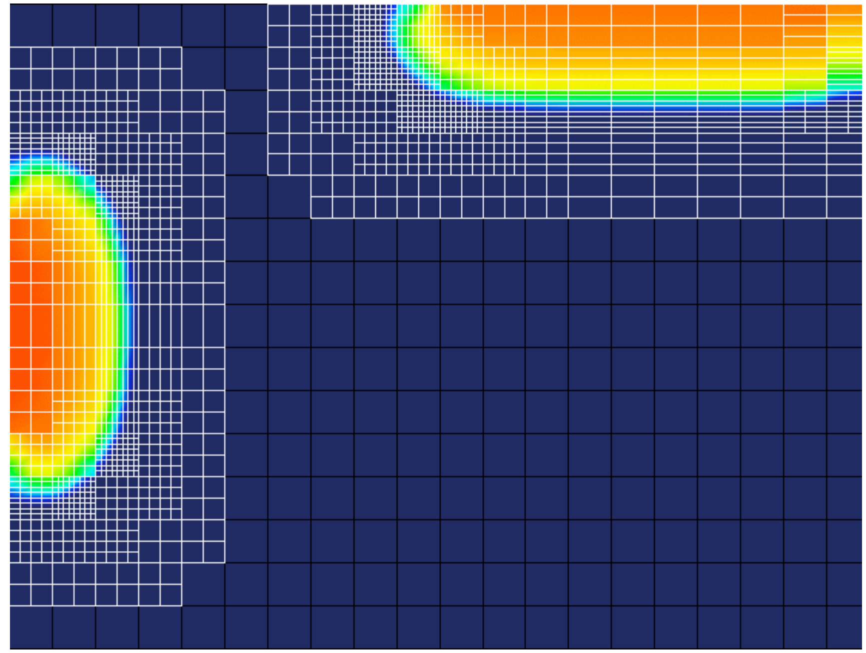
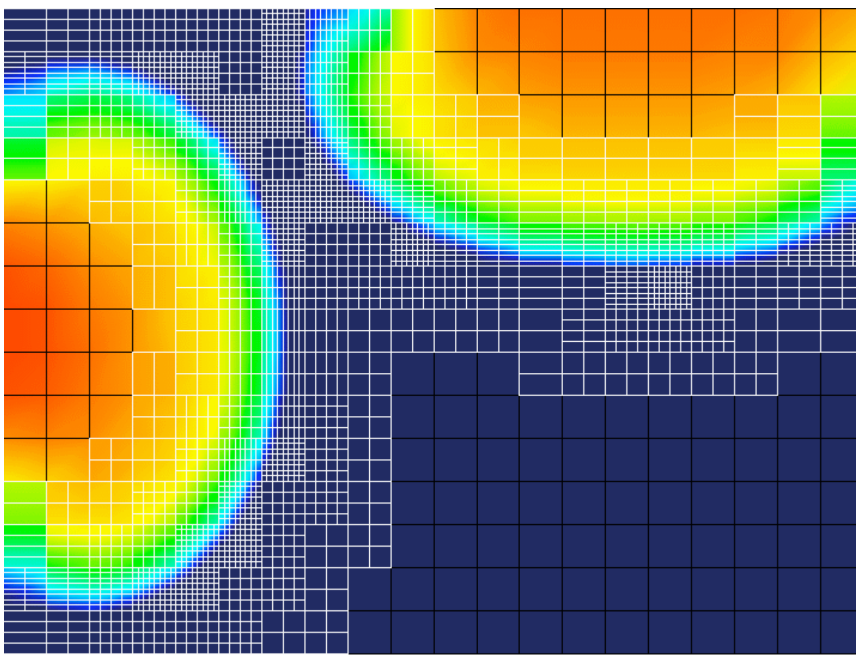
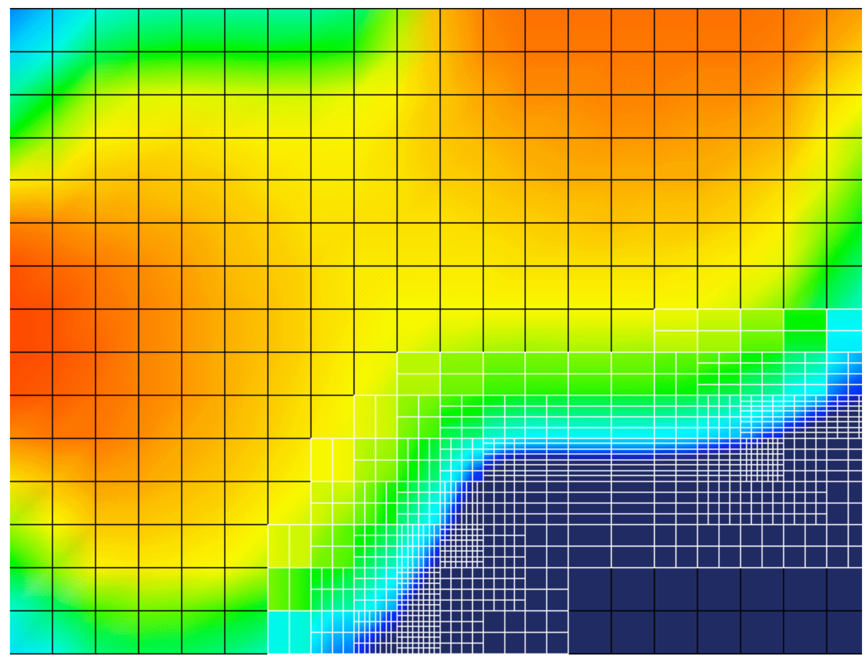
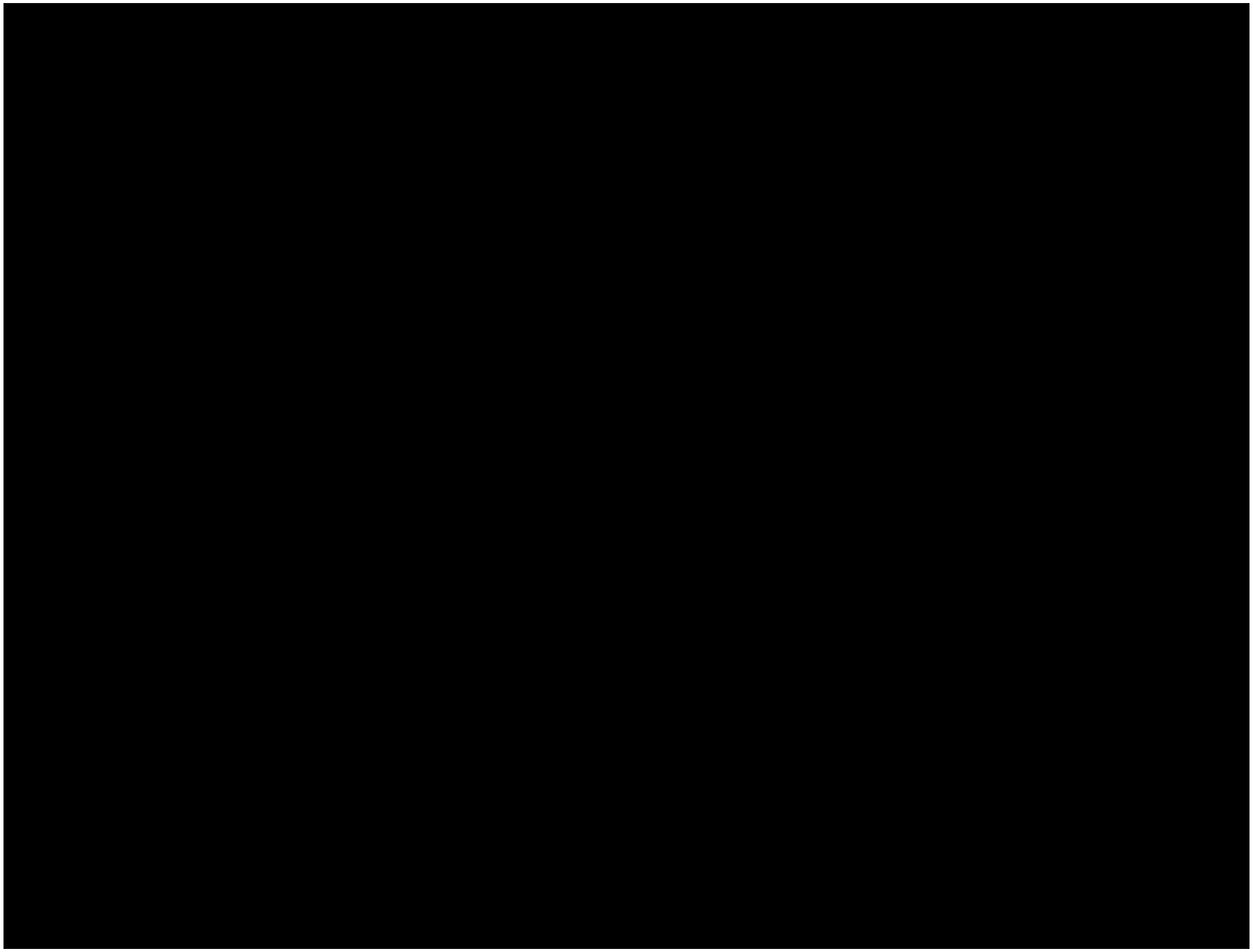
Task 4





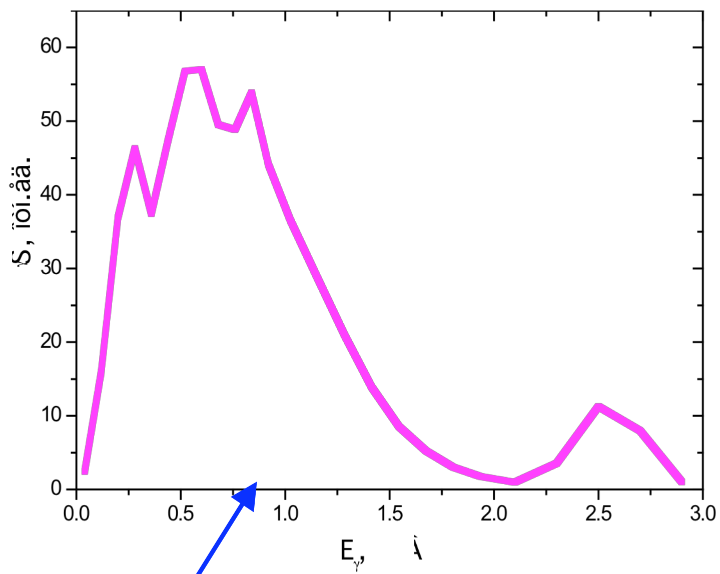




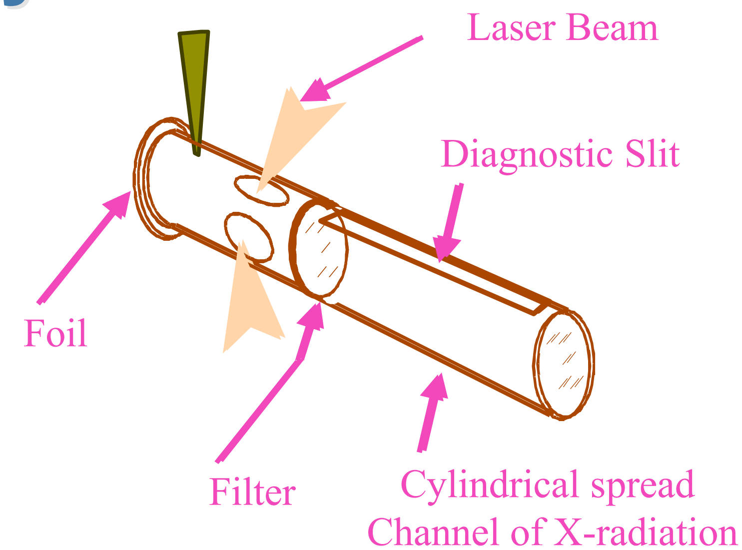


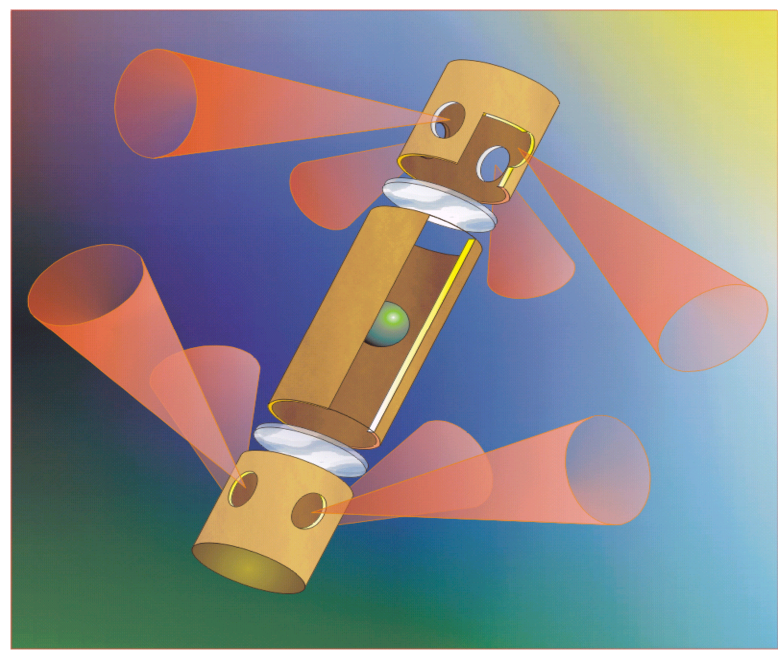
ILLUMINATOR target's cylindrical channel

25 energy groups;
96 flight directions (S_{12});



X-radiation spectrum





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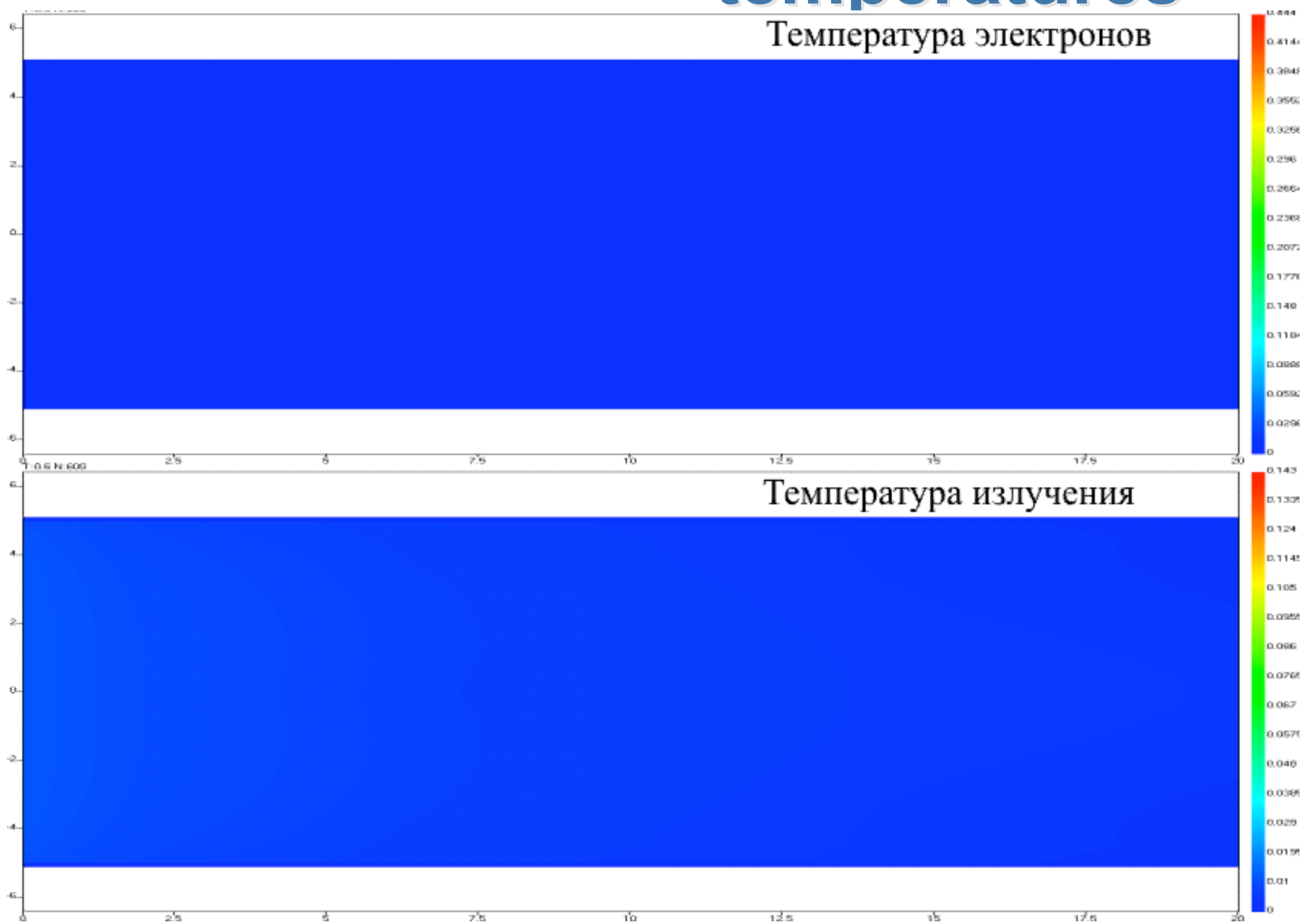
Space distributions of temperatures



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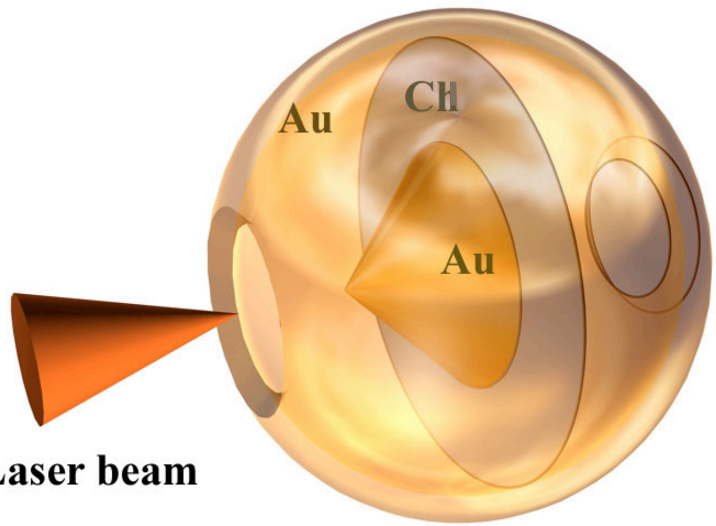
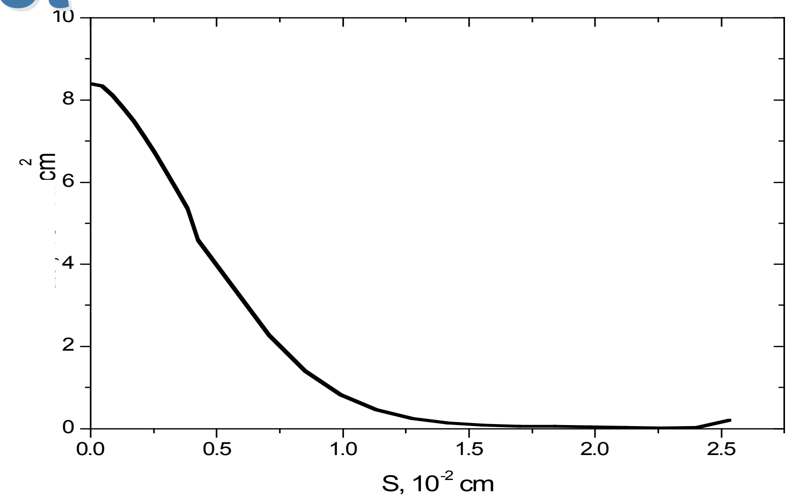
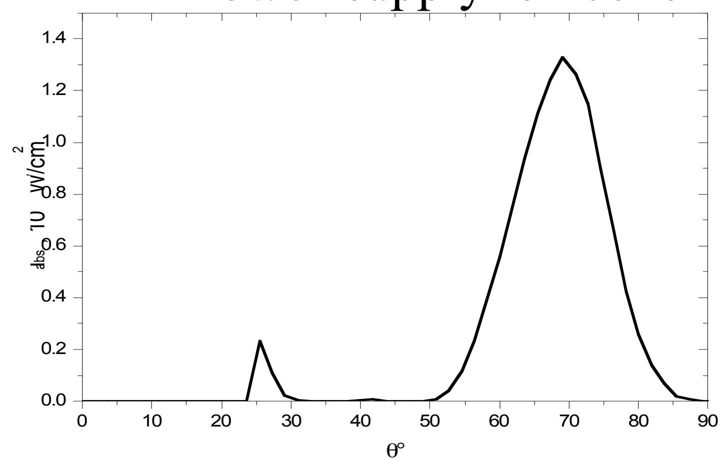
HOHLRAUM "labyrinth" target





Power-supply on cone



Power-supply on inside of case

10 energy groups;
96 flight directions (S_{12});

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Spatial distribution

substance temperature	radiation temperature