EASC 2015

Radiative Transfer Modeling at HPC's Using Self-Ajoint Transport Equation

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Subject

A new parallel technique of three-dimensional radiative transfer modeling.

Report outline

1. Modern studies of extreme states of hot dense matter in laboratory and natural conditions: fundamental research, development of small-scale technologies, biomedical applications etc.
2. Goal - development of software for predictive modeling of high-density energy plasmas.

3. Meeting the challenges relating:
   (a) effective using of HPC systems (clusters, hybrid architectures)
   (b) Adequate accounting for a set of non-linear processes (high-temperature plasma "multiphysics"): multiscale structures, strong coupling of hydrodynamic, thermal and radiative processes.
4. How to benefit from the advent of new high-performance systems
5. Problems related to commonly used models of radiative/absorbing hot matter.
6. Description of the proposed technique.
7. Some results and discussions

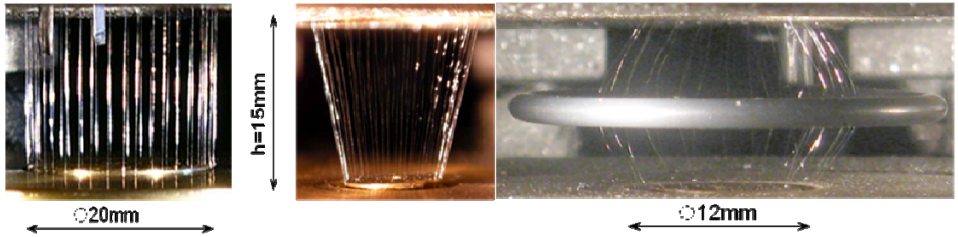
An example of HEDP studies:

A pulsed power device (multi MA electric current generator) produces fast Z-pinch by evaporating a multiwire array made of thin 6-7 micron tungsten wires. An ablating material is ionized and is accelerated by a magnetic field to a velocity of about 400-500 kilometers per second. The electric pulse lasts about 100 nanoseconds. The imploded plasma jets form a dense hot Z-pinch. When plasma jets decelerate at the axis of the system its kinetic energy rapidly converses into the thermal one. The conversion produces a high-power (milti-TW) soft X-ray pulse.

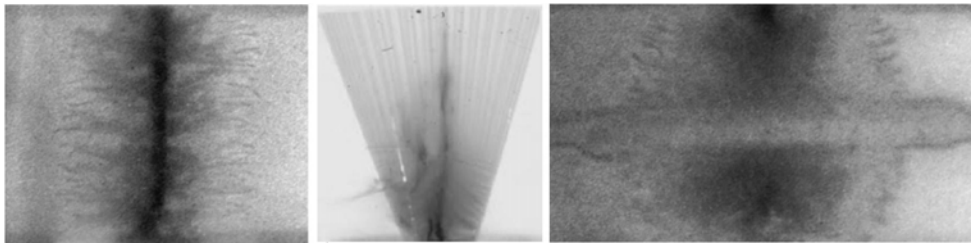
ANGARA-5-1 facility (TRINITI, Moscow)

CURRENT PULSE: 4 MA, 600 KJ, rise time 90 ns.
X-ray PULSE: energy 30-100 kJ, duration 6-10 ns.
LOAD:
Wire arrays (Al, W, Mo, Cu) 40-200 wires, ∅ 4-10μm

Multiwire arrays before experiment



X-ray photographs after implosion



The HPC functionality makes it possible to reproduce 3D radiation field with the desired precision.

Radiation transport equation (TE)

Stationary equation for the spectral intensity of the radiation $I_\nu\left(\vec{r},\Omega\right)d\nu d\Omega = h\nu c\cdot f\left(\vec{r},\nu,\Omega,t\right)d\nu d\Omega$, where f is the photon distribution function dependent on the position vector $\vec{r}$, frequency ν, the ray direction Ω, and time t, is the following:

$$\ell_\nu\left(\vec{r}\right)\left(\Omega\ \nabla\right)I_\nu\left(\vec{r},\Omega\right)+I_\nu\left(\vec{r},\Omega\right)=J_\nu\left(\vec{r}\right),$$

where ℓ_ν is the free path, $\chi = 1/\ell_\nu$ is opacity (inverse value of the mean) free path, and J_ν is the emissivity. The optical properties of the matter strongly depend on its temperature and density as well as on the photons frequency ν.

Specific radiation energy is computed as $U=\frac{1}{c}\int_0^{4\pi}\int_0^{\infty} I d\nu d\Omega$,

and specific radiation energy flux is $\vec{W}=\int_0^{4\pi}\int_0^{\infty} I d\nu \Omega d\Omega$.

The radiation source term in the energy balance equation is $Q_{Rad}=-\operatorname{div}\vec{W}$.

Multigroup approximation

Optical properties are strongly dependent on density and temperature, and vary between different frequency bands of the emitted/absorbed photons. A good practical assumption is that the emissivity primarily depends on a thermodynamic state of a substance, and almost has no dependence on the radiative intensity**.**

Proper accounting of optical properties: the entire frequency band is divided into M spectral intervals or groups: $\nu_1=0<...<\nu_i<...<\nu_M<\infty$ ν, wherein $\ell_\nu = \ell_i$, $J_\nu = J_i$ ~const when $\nu_i<\nu<\nu_{i+1}$ $(i=1\div M)$. The equation (1) is solved for each group. Having the radiative intensity distribution over space and angle variables one can calculate the radiative heat transfer, radiative losses or contributions into the energy balance of a plasma. The average values $I_i = \int_{\nu_i}^{\nu_{i+1}} I_\nu d\nu$ are used in the calculations, with their sum providing the desired spectral integral. For correct calculation of the energy balance we need, as a rule, just a few tens of spectral bands. In situations where the principal studied object is the emitted radiation spectrum essentially more fine spectrum representation may be required, i.e. for more precise analysis we may need several hundred or even thousand spectral groups. Calculations for some spectral group are implemented independently from the others.

A good occasion in view of parallel implementation: the calculation formulas for different spectral groups are identical and differ only in the values of emissivity and opacity coefficients.

New technique development: background.

"Diffusion" model of radiation (DM)

DM is one of the most popular techniques of computing the thermal radiation transfer in HEDP studies.

A usual way to reduce the dimension of the problem is to use the first P1 approximation of the spherical harmonic expansion for the radiation transport equation (TE)

$$-\mathrm{div}\frac{c\cdot\ell}{3}\mathrm{grad}U+\frac{c}{\ell}U=\frac{c}{\ell}J\ .$$

The equation connecting the flux and the density of radiation is obtained with the assumption of the angular isotropy of the radiations field: $\vec{W}=\frac{c\cdot\ell}{3}\mathrm{grad}U$.

Radiation energy term may be computed as $Q_{Rad}=\frac{c}{\ell}(J-U)$.

DM includes the approximate dependence of the radiation flux on a temperature gradient and exact energy balance equation. The last ensures a wide range of the model applicability. However, the validity of DM is justified only for states close to LTE, therefore DM is not applicable to radiation fields with significant anisotropy. Modifications of the "gradient" approximation to the radiation flux through the semi-empirical correction factors (e.g., Eddington tensor, interpolations of a mean free photon propagation path between LTE and non-LTE models) make the diffusion model significantly depending on specific conditions.

Direct solution of the transport equation. Method of characteristics (“ray-tracing”).

The general solution of the transport equation (TE) can be used to calculate the radiation intensity along the characteristics - "rays" $\vec{\Omega}$. The direct solution of the transport equation is not very difficult to obtain directly:

$$\frac{\partial I_\nu}{\partial S} + \chi_\nu \cdot I_\nu = \chi_\nu \cdot I_{\nu p}\,,\; I_\nu \mid_{S=S_0} = I_\nu \mid_r = I_\nu^*.$$

General solution to TE has the appearance:

$$I_\nu(s) = I_\nu^* \cdot \exp\left\{-\int_{S_0}^{S} \chi_\nu(s')ds'\right\} + \int_{S_0}^{S} I_{\nu p}(s') \cdot \chi_\nu(s') \cdot \exp\left\{-\int_{S_1}^{S} \chi_\nu(s'')ds''\right\} ds$$

A curse of dimensionality: 3D in space and 2D in angular variables. Getting a good quality of numerical solution requires a great number of characteristics Ω in each computational point: all pairs of cells in the computational domain should be linked by rays of different families (directions defined by angular variables). Otherwise one can encounter the lack of accuracy caused by a "beam effect" (numerical): photons emitted in some intensely radiating subdomain may not affect the energy balance in some other subdomain not reached by appropriate ray. Experimental evaluation conducted for various unstructured computational grids show that acceptable accuracy calculation of grid-characteristic method is very costly. In addition, the corresponding algorithm does not scale well in the case of the parallel solution of a general system of equations of radiation plasmodynamics geometric domain decomposition.

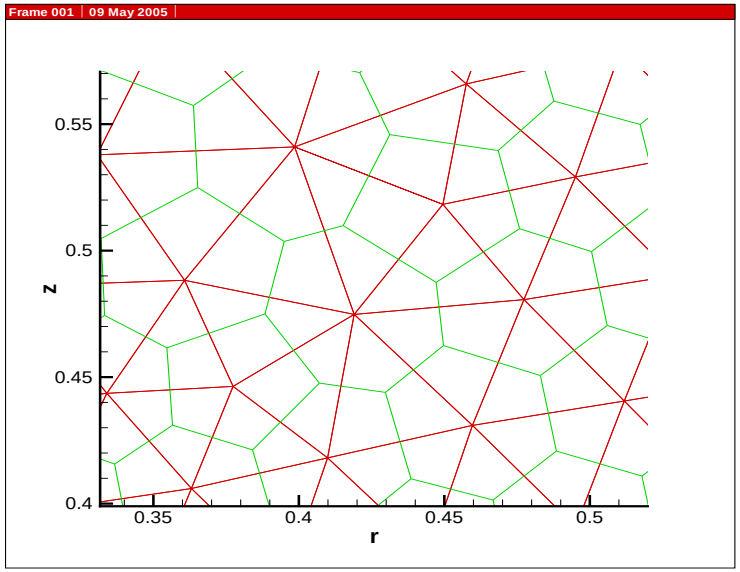
Numerical experiments conducted with for various unstructured computational grids exhibit serious drawbacks of the ray-tracing method:

(a) An acceptable accuracy calculation via the grid-characteristic method is very costly.

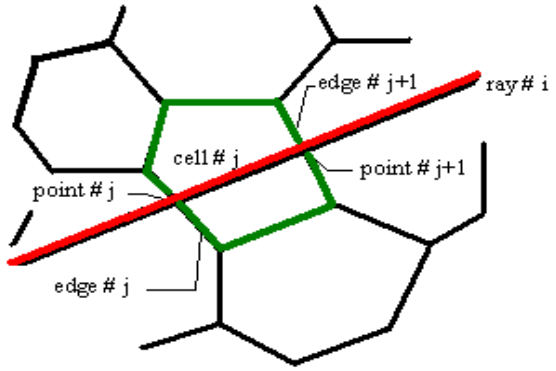
(b) As a characteristic crosses the entire computational domain from one end to the other, the corresponding algorithm shows poor scaling in the case of a domain decomposition approach to calculation of radiation plasmodynamics equations.

Known approaches to solving the radiation problems (methods of spherical harmonic moments discrete ordinates, etc.) to a greater or lesser extent, are also not free from the listed drawbacks. If one needs a reasonably precise accounting of plasma heterogeneity, or the angular distribution of the radiation intensity in coupled problems (radiative gasdynamics), these methods seems to be quite costly .

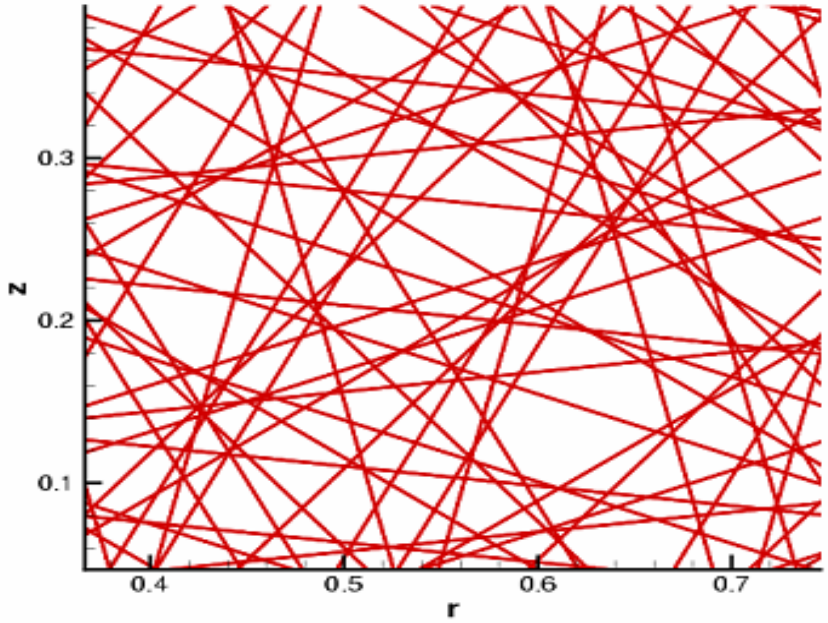
2D triangular mesh and finite volumes
(modified Voronoi diagram)



One ray crossing the FV mesh



A fragment of the characteristic (ray) grid covering computational domain - (12 angle sectors)



Possible way of accounting for radiation anisotropy.
Self-adjoint form of a radiative transfer equation.

Angular non-uniformity of photon distribution function can be accounted in second-order self-adjoint transport equation. Self-adjoint equation for neutron transport was thoroughly examined. V. S. Vladimirov [1951] established a new variational principle for one-velocity transport equation and derived the appropriate boundary conditions. B. N. Chetverushkin [1986] proposed similar approach for radiation transport.

Self-adjoint equation (SA) can be obtained via replacing a photon emissivity function in transport equation (TE) according the following formula $I(\vec{r},\mathbf{\Omega}) = \varphi(\vec{r},\mathbf{\Omega}) - \frac{1}{\chi(\vec{r})}(\mathbf{\Omega}\nabla)\varphi(\vec{r},\mathbf{\Omega})$.

An auxiliary function φ is symmetric $\varphi(x,-\mathbf{\Omega}) = \varphi(x,\mathbf{\Omega})$, and satisfies the differential equation

$$-\mathrm{div}\left(\frac{1}{\chi(\vec{r})}\mathbf{D}(\mathbf{\Omega})\,\mathrm{grad}\,\varphi(\vec{r},\mathbf{\Omega})\right) + \chi(\vec{r})\varphi(\vec{r},\mathbf{\Omega}) = \chi(\vec{r})J(\vec{r})$$

where $\mathbf{D}(\mathbf{\Omega}) = \mathbf{\Omega}\otimes\mathbf{\Omega}$ $\left(D_{ij} = \Omega_i\Omega_j\right)$ is a “dyadic” or tensor product of two vectors.

Boundary condition proper to (SA) takes the appearance: $\vec{n}\frac{1}{\chi(\vec{r})}\mathbf{D}(\mathbf{\Omega})\,\mathrm{grad}\,\varphi(\vec{r},\mathbf{\Omega}) - (\mathbf{\Omega}\,\vec{n})\varphi(\vec{r},\mathbf{\Omega}) = 0$,

when $(\mathbf{\Omega}\,\vec{n}) < 0$, $\vec{n}$ is the outward normal to the boundary (zero income flux).

For discretization in the space of angular variables we use quadrature formulas by V.I. Lebedev, developed for calculations on the spherical surfaces which are a set of angular directions $\{\boldsymbol{\omega}_k\}_{k=1}^{N}$ with weights α_k. To construct a difference scheme we assume that within each solid angle, resulting from such partition, a value of φ does not depend on the angular variables.

Thus we get a set of N self-adjoint equations for N variables φ_k with its tensor $\mathbf{D}(\omega_k)$ for each quadrature node ω_k.

Specific radiation energy is calculated by numerical integration by means of these quadrature nodes

$$U(\vec{r}) = \sum_{k=1}^{N} \alpha_k \varphi_k(\vec{r}) \approx \int_{4\pi} I(\vec{r}, \boldsymbol{\Omega}) d\Omega,$$

and radiation flux is calculated as $\vec{W} = \sum_{k=1}^{N} w_k \omega_k \frac{I(\vec{r}, \omega_k) - I(\vec{r}, -\omega_k)}{2} = -\frac{1}{\chi(\vec{r})} \sum_{k=1}^{N} \alpha_k \mathbf{D}(\omega_k) \operatorname{grad} \varphi_k(\vec{r}) \approx \int_{4\pi} \boldsymbol{\Omega} I(x, \boldsymbol{\Omega}) d\Omega$.

The source term in the energy balance equation can be found from the self-adjoint equation without numerical differentiation: $Q_{Rad} = -\operatorname{div} \vec{W} = \chi(\vec{r})\left(J(\vec{r}) - U(\vec{r})\right)$

Additionally, this model allows calculating the intensity of the radiation in the desired direction:

$$I(\vec{r}, \omega_k) = \varphi_k(\vec{r}) - \frac{1}{\chi(\vec{r})} \omega_k \operatorname{grad} \varphi_k(\vec{r}).$$

For the numerical implementation of the model we have to solve a set of (MxN) independent elliptic type equations (M is a number of spectral groups, N is a number of quadrature points on the sphere). The equations are not coupled and are solved independently, which makes good opportunity for parallel computations of various types, e.g. CPU clusters or hybrid CPU/GPU systems. To ensure adequate calculation accuracy the value of M and N can be several tens or even hundreds. A spatial difference approximation to (SA) results in a system of linear equations with a symmetric positive defined matrix, which allows using of effective iteration methods, e.g. those based on Krylov subspaces, or Richardson iterations with optimised Chebyshev set of parameters.

Each of these elliptic equations (EE) has the appearance

$$-\left[\frac{\partial}{\partial x}\frac{1}{\chi}\left(\Omega_x^2\frac{\partial\varphi}{\partial x}+\Omega_x\Omega_y\frac{\partial\varphi}{\partial y}+\Omega_x\Omega_z\frac{\partial\varphi}{\partial z}\right)+\frac{\partial}{\partial y}\frac{1}{\chi}\left(\Omega_x\Omega_y\frac{\partial\varphi}{\partial x}+\Omega_y^2\frac{\partial\varphi}{\partial y}+\Omega_y\Omega_z\frac{\partial\varphi}{\partial z}\right)+\frac{\partial}{\partial z}\frac{1}{\chi}\left(\Omega_x\Omega_z\frac{\partial\varphi}{\partial x}+\Omega_y\Omega_z\frac{\partial\varphi}{\partial y}+\Omega_y^2\frac{\partial\varphi}{\partial z}\right)\right]+\chi\varphi=\chi J,$$

where (Ω_x, Ω_y, Ω_z) are the direction cosines of the corresponding angular direction,

and $\chi(\vec{r})$, $J(\vec{r})$ are individual for each spectral interval.

We use a variant of the known Galerkin method with discontinuous basis functions for the variables defined in the grid cells to discretize this equation. In the case of a regular rectangular grid this procedure provides a difference scheme on a template with 27 nodes. If we use a grid with irregular structure (unstructured) a template includes all cells having a common node with the central cell.

An important feature of our algorithm:

Preliminary transformation of rotation is applied to the elliptic equation (EE): $(\Omega_x, \Omega_y, \Omega_z) \rightarrow (1, 0, 0)$. By means of this transformation we exclude from the equation (EE) mixed derivatives with respect to spatial variables, thereby the structures corresponding to its difference analogue are greatly simplified which significantly contributes to the acceleration of iterative processes of solving the equation (EE).

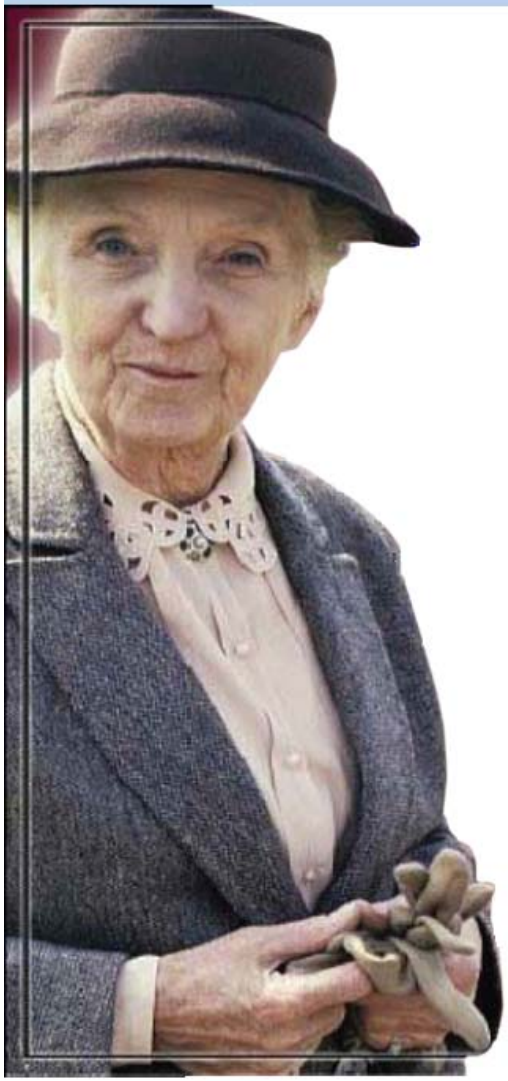
Advantages:

1) Symmetrical self-ajoint equation vs initial unsymmetrical transport equation

2) Scalability of the method is determined by the choice of linear solvers – it's convenient and efficient!!

The technique of radiative transport computation has been implemented as a part of an object-oriented code designed for numerical investigation of magnetogasdynamics problems at massively parallel systems of cluster type.

MARPLE 3D –
Magnetically Accelerated Radiative Plasma Explorer



- **MARPLE MAIN PHYSICS**
- One-fluid two-temperature MHD model + Hall effect + generalized Ohm's law - *A.Bobrova, E.Lazzaro, P.V.Sasorov. Magnetohydrodynamic two-temperature equations for multicomponent plasma. Phys. Plasmas, 12, 2005.*
- Radiative energy transfer: multigroup model, radiation diffusion, self-adjoint equation, Sn- method
  B.N. Chetveruskin, Radiative gas flow problems. Moscow, 1988
- Equations of state, transport and kinetic coefficients, opacity and emissivity coefficients: data tables and/or analytics – code TERMOS (KIAM RAS) - *A.F. Nikiforov, V.G.Novikov, V.B.Uvarov, Birkhauser Verlag, Basel, Berlin, 2005.*
- **MARPLE MAIN NUMERICS**
- 3D (x,y,z) geometry, 3D velocity & EMF vectors
- Unstructured / mixed elements / block computational meshes
- Splitting scheme for RMHD system,
  high-resolution TVD schemes with flux correction (non-dissipative MHD),
  implicit FV / FE schemes (dissipative processes),
  2-nd order predictor-corrector time advanced scheme
- HPC: domain decomposition, MPI / CUDA parallelism

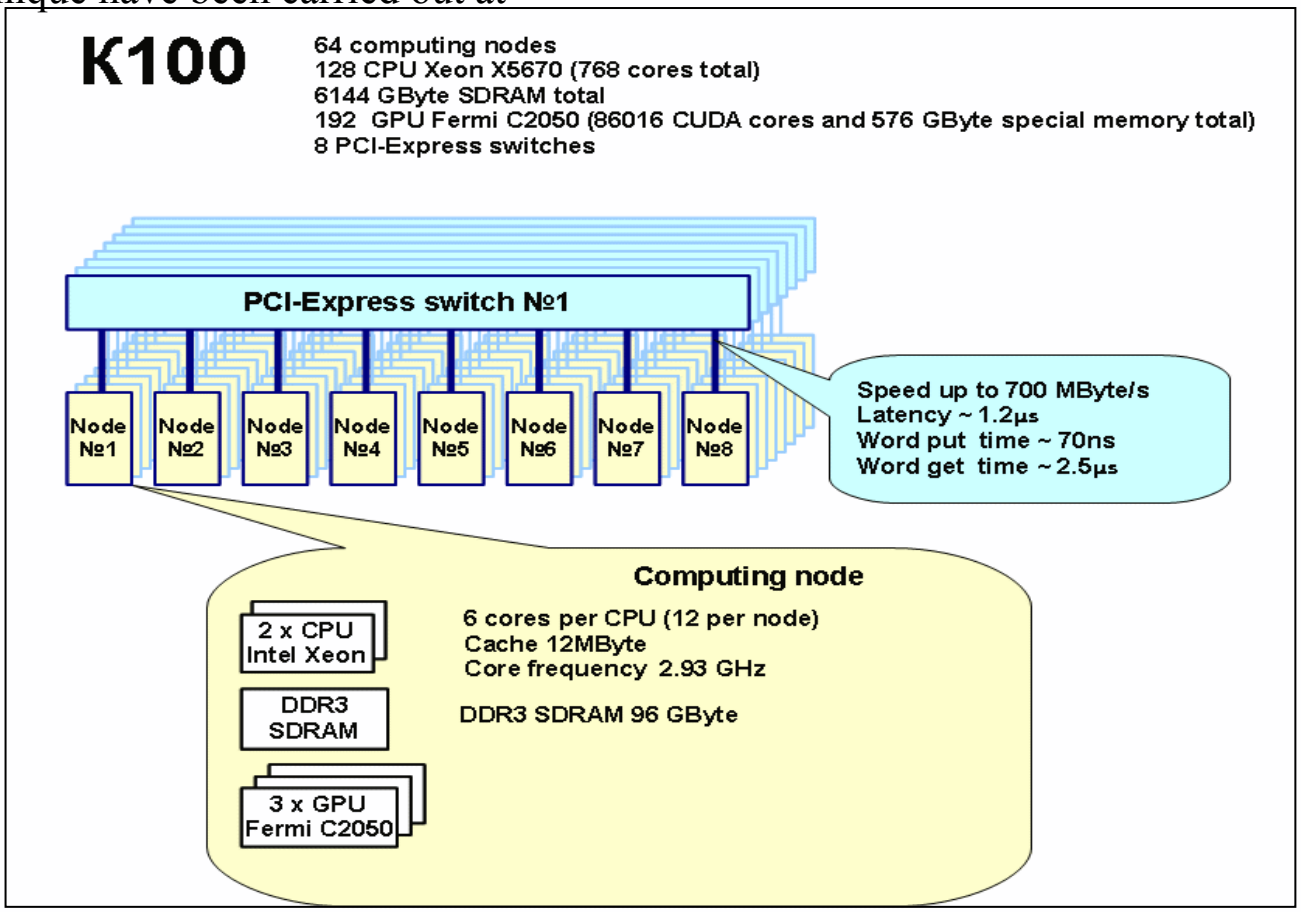
Numerical experiments on testing of the technique have been carried out at

KIAM RAS (Moscow) **K-100**

Scalable GPGPU-based

Hybrid Computing System

(Peak performance ~ 107 TFLOPS)



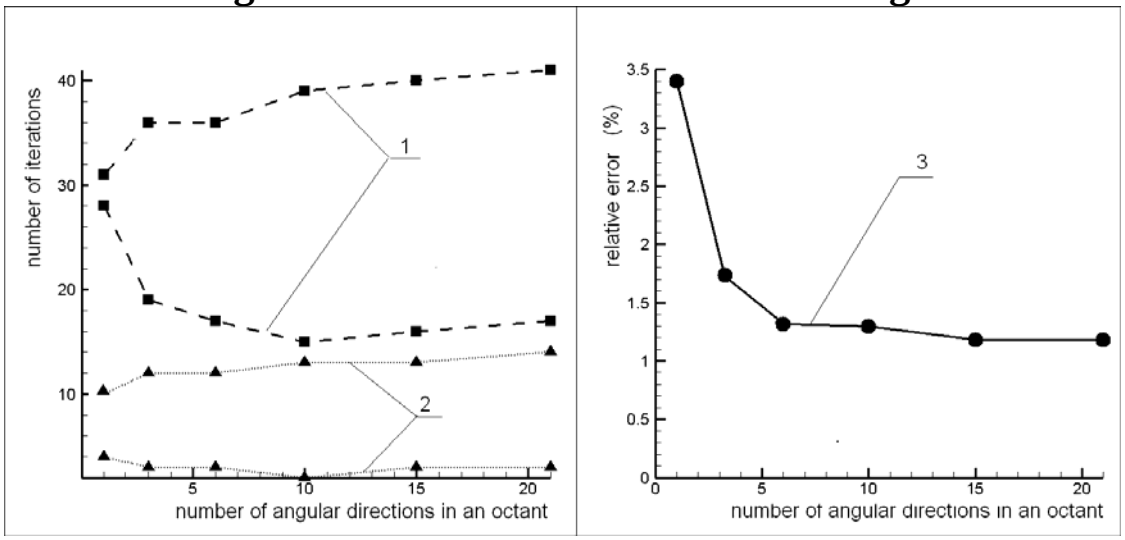
Second-order self-adjoint equation:

- implicit scheme for elliptic-type equation
- solving big linear systems
- acceleration via GPU CUDA linear solvers
- Krylov solvers & Chebyshov iterations
- K100 hybrid parallelism

- Bi-conjugate gradient with stabilization (BiCGStab) method with Least-squares polynomial preconditioner was implemented based on Aztec library (SNL).
- Best performance achieved in configuration 1CPU+1GPU.
- Speedup obtained: 1.5 for the entire linear system solution (1.28 for the first iteration computing the matrix norm).

Accuracy/convergence study with respect to spatial and angular variables were performed using 3D meshes of different element types (tetrahedrons, cubes, triangular prisms). Calculations of integral values (radiation energy per unit volume, radiative flux) were done via quadrature formulas with angular directions varied from 1 to 21 in an octant. For solving appropriate linear equation systems we have used BICGStab - biconjugate gradient method with stabilization, in combination with symmetric Gauss-Seidel preconditioner from Aztec library (SNL).

Convergence of the solutions with increasing number of angular directions



The test problem relates to the radiation produced by an infinite cylinder with constant nonzero emissivity and opacity. Outside the cylinder emissivity and opacity are small. We have calculated radiation intensity and radiation energy flux.

1 - maximum and minimum (depending on direction) the number of iterations of the original form of the equation (EE);

2 - maximum and minimum (depending on direction) after the number of iterations of rotation;

3 - relative error (numerical results versus analytical solution).

Further improvement of the numerical solution accuracy without increasing the number of angular directions can be achieved by refinement of the spatial grid. Owing to the proposed rotation transformation the number of iterations decreased by a factor of 2 and 3 compared with the original equation including cross derivatives.

The proposed method correctly reproduces the limiting cases: completely isotropic radiation (no "beam effect") and propagation of a "laser beam" with the acute δ-shaped angular distribution.

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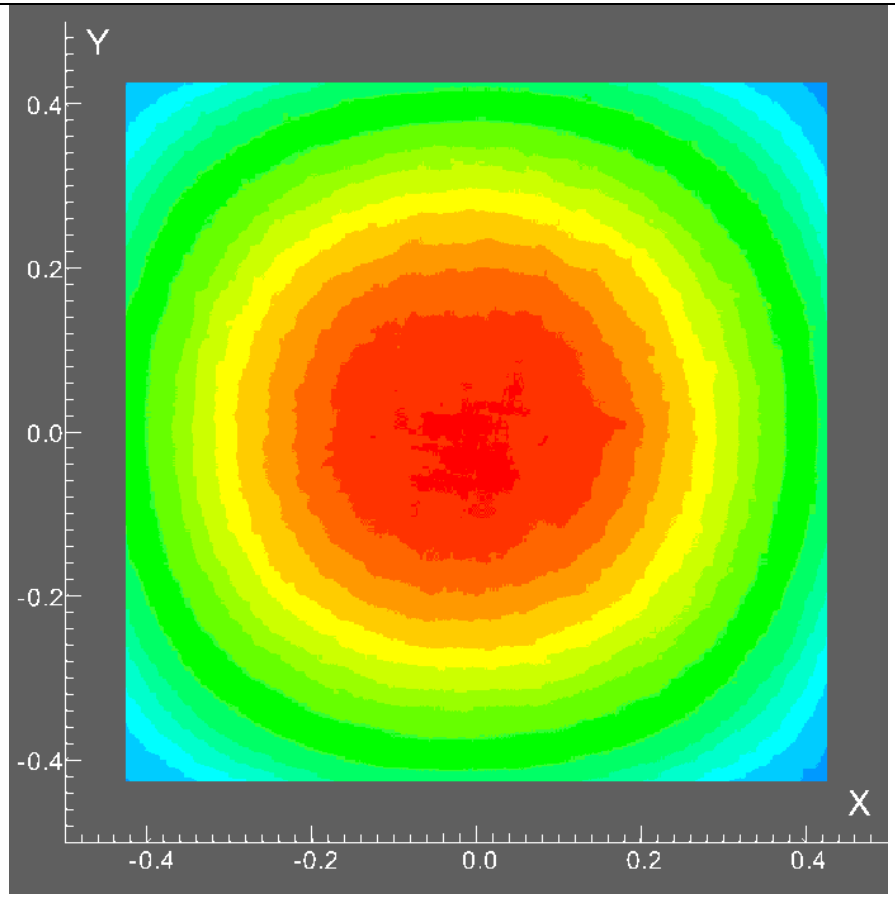
<td> 
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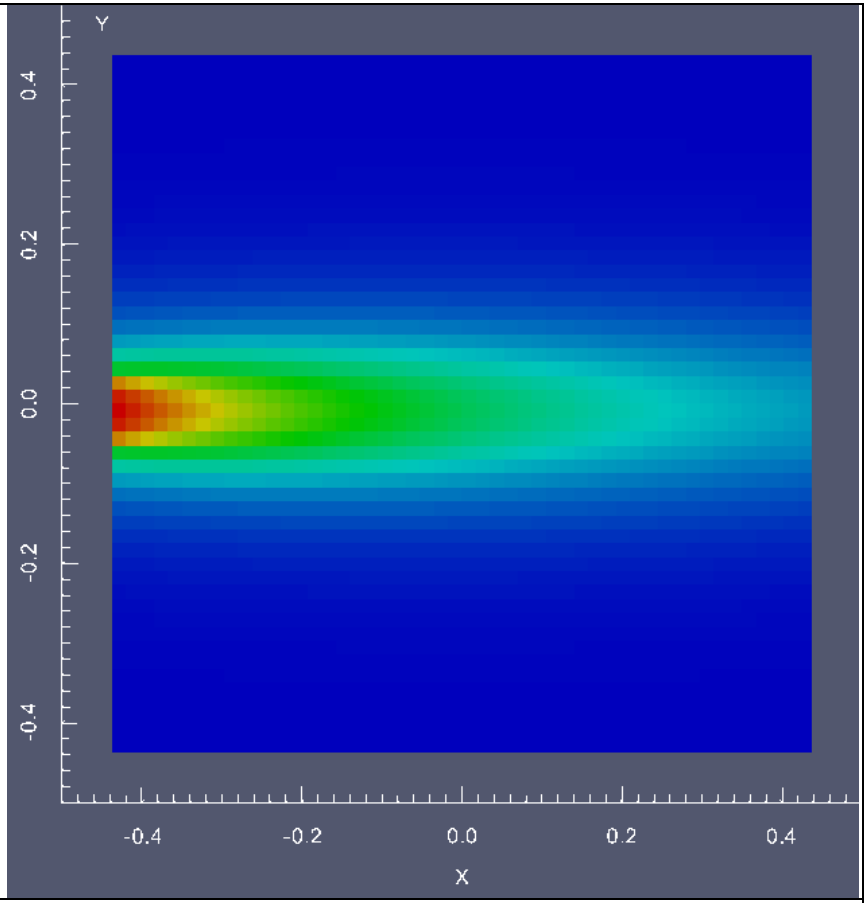
<td> 
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<tr>
<td>Izotropic radiation of a solid sphere. No "beam effect".
R = 0.1;
χ = 10, J = 10 when r < R; χ = 1, J = 0.00025 when r > R.
21 angular directions in an octant.</td>
<td>Laser beam propagation.
χ = 1, J = 0 in the domain.
Incident radiation J = 100 along OX axis
at the boundary in the point (-0.5, 0, 0).</td>
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</table>

Beam propagation in preferential direction

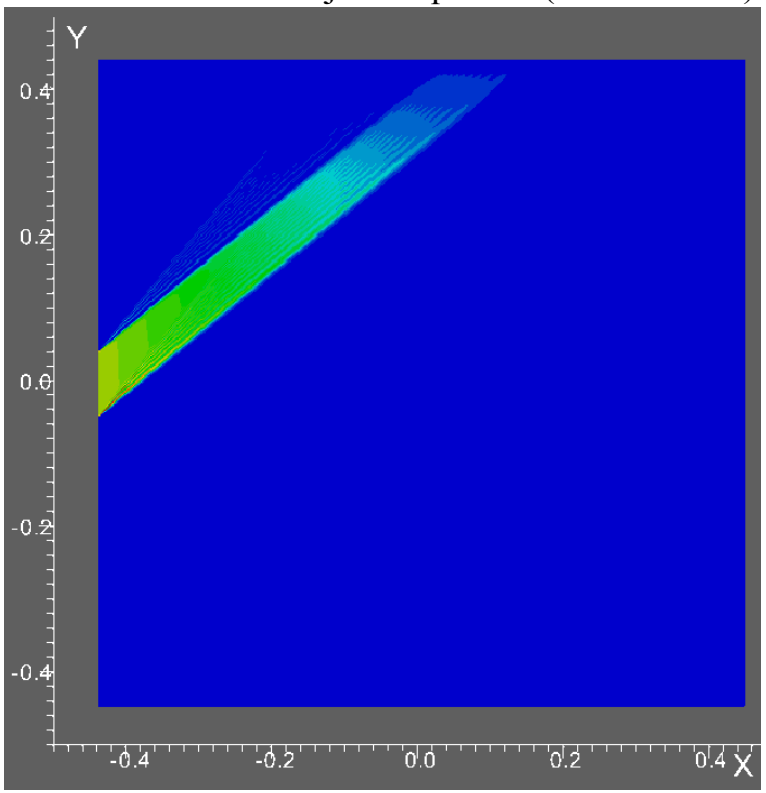
$\chi = 1$, $J = 0$ inside the domain. Incident radiation in the direction $\mathbf{\Omega} = (0.707, 0.707, 0)$:

uniform beam $J = 100$, d = 0.1, center at the boundary point (-0.5, 0, 0).

Cubic mesh 500x500x10 with periodic boundary conditions along OZ axis.

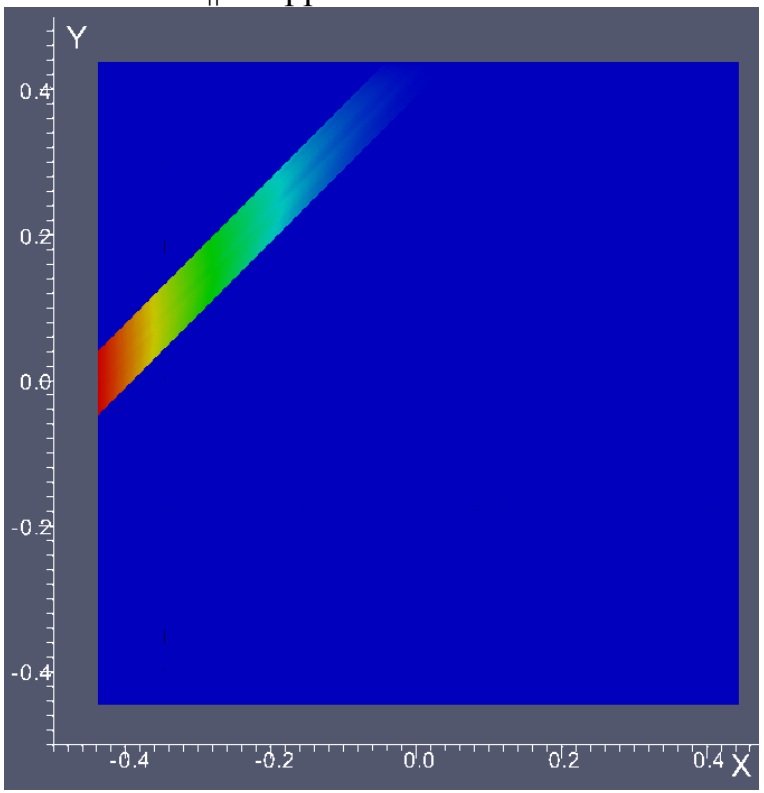
BICGStab with symmetric Gauss-Seidel preconditioner from preconditioner from Aztec library (SNL), resultant residual 10^{-6}.

Initial form of self-adjoint equation (full **D** tensor)



Aztec: 136 iterations in 1.3687 sec.
resultant residual, global:
Euclidean norm = 2.16155e-07 | Chebyshev norm = 1.85093e-08

Rotation OX || **Ω** applied



Aztec: 50 iterations in 0.399258 sec.
resultant residual, global:
Euclidean norm = 4.03083e-07 | Chebyshev norm = 3.19039e-08

In this case the use of the rotation transformation not only reduces the number of iterations, but also eliminates the "numerical diffraction" effect and allows adequate simulating of extremely anisotropic radiation distributions.

Summary

Angular non-uniformity of photon distribution function can be accounted effectively by means of a second-order self-adjoint transport equation.

DG procedure to self-adjoint transport equation leads to a set of (MxN) elliptic-type equations. They may be solved independently giving good opportunity for using of any parallelization paradigm.

Accurate simulation requires the value of tens to hundreds for both M (the number of spectral groups) and N (the number of quadrature points on a sphere).

Spatial discretization yields linear system with a symmetric positive definite matrix allowing application of effective linear solvers.

Numerical experiments demonstrate good scalability at KIAM RAS K-100 scalable GPGPU-based hybrid computing system.

We have obtained robust numerical procedure suitable for multiscale simulations in finely discretized computational domains. It's a promising technique for upcoming exaflop computing.