UDC 530.1

PARTICLE TRANSFER MODELLING IN NONLINEAR SYSTEMS BY MONTE-CARLO METHOD

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Program complex, which implements Monte-Carlo method for modeling of particle transfer in systems which parameters depends of particle flux, is developed. Complex is oriented on computations of parameters of different astrophysical objects, and parameters of perspective nuclear systems. Approach to modeling process, is described in article. Test results are presented. Problem definitions from areas of neutron physics and astrophysics are presented. The work was supported by the Russian Foundation for Basic Research (grant № 09-08-13746-ofi-c).

Keywords: Monte-Carlo method, modeling, particle transfer, particle flux, perspective nuclear systems.

Problem of definition

Statistical modeling of particle transfer process is prevalent method, that operates with problems of computation of neutron flux in nuclear systems and photon fluxes in astrophysics and physics of planetary atmospheres.

Mathematical model of the particle transfer process is transfer equation:

$$\frac{\partial \Phi(\vec{r},\vec{\upsilon})}{\partial t} + \vec{n}\nabla\Phi(\vec{r},\vec{\upsilon}) + \sigma_{tot}(\vec{r},|\vec{\upsilon}'|)\Phi(\vec{r},\vec{\upsilon}) = \sum_i \int_V \nu^i(\vec{r},|\vec{\upsilon}'|)\sigma^i(\vec{r},|\vec{\upsilon}'|)\omega^i(\vec{\upsilon},\vec{\upsilon}';\vec{r})\Phi(\vec{r},\vec{\upsilon}')d\vec{\upsilon}' + f_0(\vec{r},\vec{\upsilon}), \quad (1)$$

where $\Phi(\vec{r},\vec{\upsilon})$ - particle flux density at point $\vec{r}$, with speed $\vec{\upsilon}$, $\vec{n} = \vec{\upsilon}/|\vec{\upsilon}|$ - flux direction, $\sigma^i(\vec{r},|\vec{\upsilon}'|)$ - cross sections of different types of interaction, $\sigma_{tot}(\vec{r},|\vec{\upsilon}'|)$ - total interaction cross section, $\omega^i(\vec{\upsilon},\vec{\upsilon}';\vec{r})$ angle-energy distributions, $\nu^i(\vec{r},|\vec{\upsilon}'|)$ average numbers of particles that survives in reaction, or being produced by reaction, $f_0(\vec{r},\vec{\upsilon})$ - particle source distribution, a V - volume of modeling area.

Software that implements statistical modeling method of particle transfer, usually, oriented on solving of problems that has no dependence of modeling system parameters of particle flux density. However systems that have dependences of it's characteristics of flux, or some values that depends of flux, are more rule than exception. Transfer equation in such systems is nonlinear:

$$\frac{\partial \Phi(\vec{r},\vec{\upsilon})}{\partial t} + \vec{n}\nabla\Phi(\vec{r},\vec{\upsilon}) + \sigma_{tot}(\vec{r},|\vec{\upsilon}'|,P(\vec{r},\vec{\upsilon}))\Phi(\vec{r},\vec{\upsilon}) = \sum_i \int_V \nu^i(\vec{r},|\vec{\upsilon}'|,P(\vec{r},\vec{\upsilon}))\sigma^i(\vec{r},|\vec{\upsilon}'|,P(\vec{r},\vec{\upsilon}))\omega^i(\vec{\upsilon},\vec{\upsilon}';\vec{r},P(\vec{r},\vec{\upsilon}))\Phi(\vec{r},\vec{\upsilon}')d\vec{\upsilon}' + f_0(\vec{r},\vec{\upsilon},P(\vec{r},\vec{\upsilon})), \quad (2)$$

where $P(\vec{r},\vec{\upsilon})$ - ensemble of parameters that depends on flux. This dependence is a set of additional conditions:

$$P(\vec{r},\vec{\upsilon}) = \mathrm{B}(\Phi(\vec{r},\vec{\upsilon})). \quad (3)$$

In bounds of this work we discuss only systems where parameter is temperature of medium $T(\vec{r})$, and dependence has integral character during to particle spectrum:

$$T(\vec{r}) = \frac{1}{4\pi}\int_{\mathrm{E}} \mathrm{B}(\Phi(\vec{r},\vec{\upsilon}))d\vec{\upsilon}, \quad (4)$$

where E - vector field of velocities.

In amount of different cases we can bring the problem to the linear case. Thereto, dependence of medium parameters: σ_{tot}, ν^i, σ^i, ω^i must be weak enough to neglect, and dependence of source parameters must be linear $f_0\left(\vec{r},\vec{\upsilon},T(\vec{r})\right)=f'(\vec{r},\vec{\upsilon})T(\vec{r})$. That case is typical for problems of atmosphere temperature spatial distribution computations in some astrophysical systems, where main process is radiative heat transfer, and amount of gas component is low [1].

Problems with dependence of parameters of temperature presence are more common, and requires another solutions. Some of this problems are, for example, problems of determination of nuclear reactors of temperature conditions, or temperature fields in circumstellar clouds with high gas content [1,2].

Usual way of solving of such problems is using of iterative process, which correspond consecutive solving of equations (2) and (4).

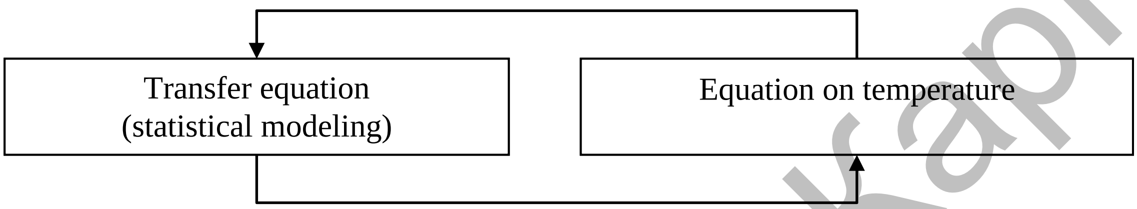

Fig.1. Iterative process

To determine temperature in such problems, we need to calculate energy release distribution, and solve the problem of heat transfer. Because of high computation cost, there is a need in using of supercomputing.

Examples of the modeling systems

One of the examples is a problem of temperature parameters calculation in facility for nuclear spent fuel transmutation, with gas dynamical trap (GDT) based neutron source. System is presented extensive source of 14 MeV neutrinos, surrounded by fuel blanket with spent fuel. In model length of neutron source geometry of blanket and fuel consist can be various. In the purpose of safety, it is necessary, for hole system, to be subcritical (neutron multiplication coefficient must be less then one).

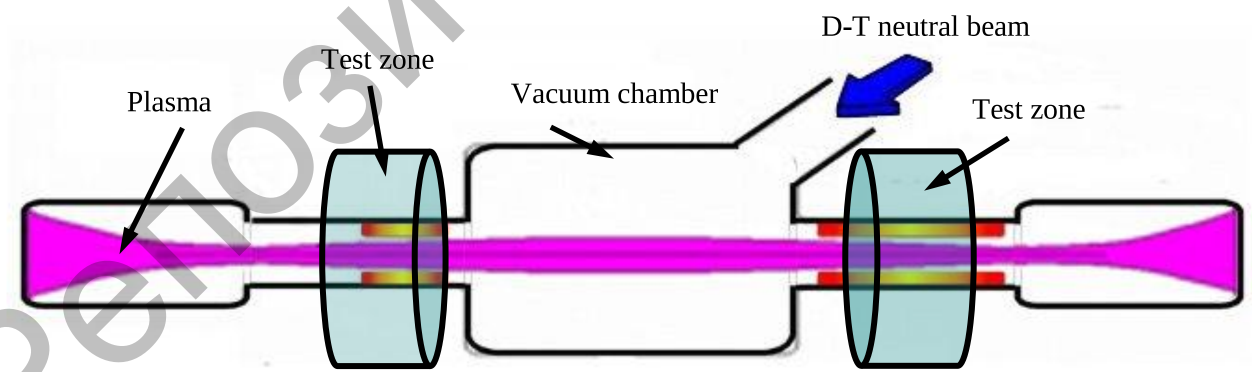

Fig.2. Scheme of nuclear spent fuel transmutation facility

Another example is problem of calculation of spatial temperature distribution in circumstellar clouds. Heat transfer in such systems has main role, due to low medium density and high spatial scale. Among numerous of systems of that type, there are systems with height or low presence of gas. The cloud around Vega system refers to the first type, dust cloud around β -Fig star, to the second.

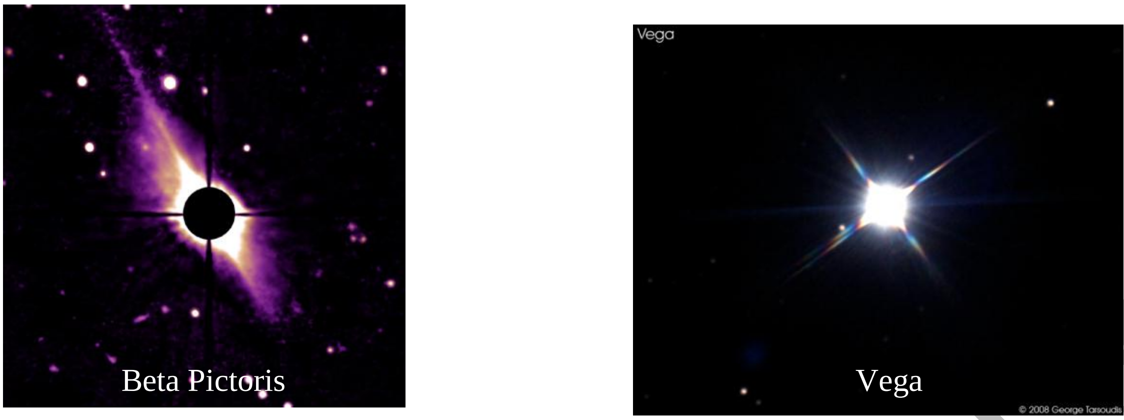

Fig.3. Examples of circumstellar clouds

Modeling methods

Program complex that allows to model particle transfer process in systems with temperature dependence of medium parameters, was built. Modules for modeling of neutron and photon trajectories in different conditions was developed. Data for modeling of photon behavior in astrophysical systems consists of absorption cross sections subject to temperature and wavelength from HITRAN and HITEMP databases, and optical characteristics of aerosols, derived from Mie approach.

Neutron data processing module is oriented to work with multigroup neutron constant systems, and with systems of evaluated neutron data.

Part of group data processing was done by PREPRO code, with ENDF-VII (Evaluated Nuclear Data File) in ENDF-6 format as input data. ENDF database is commonly used for calculation of parameters of nuclear and thermonuclear systems. Neutron data processing module allows to calculate macroscofig data with different medium temperature density and composition one.

Calculation results

Test calculation of systems with spherical geometry in one group approach was done. Results of test calculations show that all modules work correct. Calculations of temperature distributions and parameters of out light in dust and gas-dust clouds of β-Pic and Vega. Results are in good agreement with known estimations and experimental data [3,4].

Testing of correctness of neutron process modeling was based on calculation of benchmarks from International handbook of evaluated criticality safety Benchmark experiments. This base is oriented to testing software for neutron calculations in area of reactor modeling. Calculations of benchmarks hmf-001(Godiva), hmf-002(Tuballoy-Oralloy assemblies), hmf-003, pmf-001(Jezebel), pmf-008, imf-004, and imf-005, are in good agreement with database values. Spectrums of hmf-001(Godiva) and pmf-001(Jezebel) are shown in fig. 4.

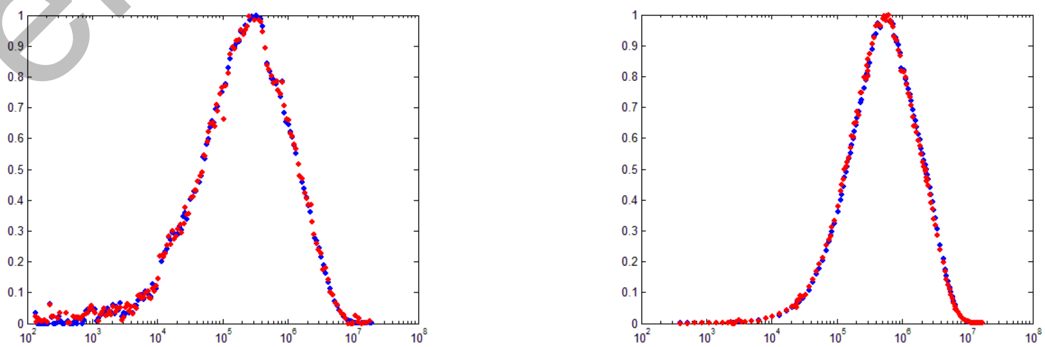

Fig. 4. Spectrums of normalized neutron flux of assemblies Jezebel (right) and Godiva (left) on energy

Choice of benchmark cases caused by it's ability to show possible errors in neutron data block. Calculation of multiplication coefficient of fuel blanket with plutonium, minor actinides oxygen and magnesium for transmutation facility was done. Blanket configurations are close to configurations for European accelerator driven system for transmutation EFIT (Europian Facility for Industrial Transmutation)[5].

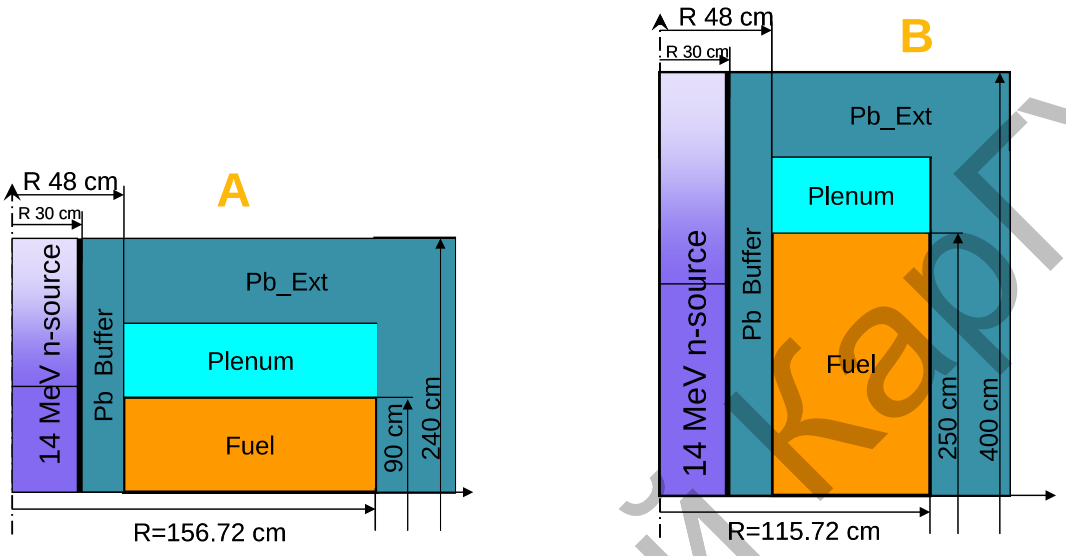

Fig.5. Configuration of fuel blanket

Two variants of homogenized structure of blanket are shown on fig. 5 Multiplication coefficients are $k_{eff}^{A} = 0.969 \pm 0.001$ and $k_{eff}^{B} = 0.980 \pm 0.001$ respectively, and are in good agreement with results of other codes.

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