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HYBRID PARALLELIZATION OF COMPUTING THE ELECTRON FLUXES PRODUCED BY PHOTON RADIATION

M. ZHUKOVSKIY[*], M. MARKOV[*], S.PODOLYAKO[*] AND R. USKOV[*]

[*] Keldysh Institute for Applied mathematics of RAS
Moscow, Russia
e-mail: zhuk@kiam.ru, web page: http://www.keldysh.ru

Summary. Principles of Monte Carlo simulating the radiative electron emission by use of supercomputers having the heterogeneous architecture are considered. Questions of calculation parallelization with application of graphical processors as arithmetical co-processors are discussed. A technique of effective distribution of calculation between central processor and graphical one is worked out. Developed weight modification of Monte Carlo method meant for computing by use of NVIDIA© CUDA is described. Some results of modeling of electron emission from aluminum plate being under photon radiation are represented.

Keywords. Mathematical modeling, electron transport, CUDA technology, hybrid parallelization

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Key words and Phrases: Mathematical Modeling, Bremsstrahlung, Hybrid Parallelization.

1 INTRODUCTION

The photon propagation through matter produces fast electron fluxes. These electrons can leave an object being under photon radiation. As a result the processes of radiative electron emission occur outside and in interior cavities of the investigated object. Accounting the electron emission is significant when carrying out different experiments with ionizing radiation, for instance during non-destructive testing of materials. Modeling of perspective X-ray sources and development of modern detectors of radiation is impossible without correct taking into account the radiative electron emission.

Investigation of electron emission processes requires solving the complex boundary tasks of radiation transport in 3D problem statements. The Monte Carlo method is effective method of solution of the mentioned problems. However application of this method for modeling radiation transport in objects with complex geometrical structure requires huge computational burden and presupposes the use of multiprocessors computers including hybrid supercomputers as well. Modeling of the electron emission is more complex because of the small parameter of the task. Namely, the photon path up to its absorption is much bigger than electron path up to its thermalization.

The algorithms of radiative electron emission modeling on hybrid computers with use of NVIDIA© CUDA technology are considered in the paper.

2 CONCEPT OF MODELING OF RADIATIVE ELECTRON EMISSION

Physical models of electron transport are developed usually on the basis of complex theories describing the average characteristics of investigated processes, for instance, theory of multiple scattering[1], Landau theory of energy losses[2] etc. Implementation of such models implies working up the algorithms with complex logic stipulated by necessity of applicable conditions control of the used approximations when computing. In addition it is often required to carry out iteration procedures when the choice of model parameters is impossible a priori. It should be noted that these models are hardly fit hybrid computers architecture because of their own complex inner logic.

On the other hand computing systems with traditional architecture do not allow detail studying the physical processes under enough full models developed without conventional statements. These models taking into account every interaction between particle and matter give possibility to investigate processes under study in detail.

Therefore the modeling of particle transport is carried out by authors of the paper within the bounds of the model of individual collisions[3] (MIC). This model has simple inner logic and it is much more effective when it is implemented for hybrid computers in comparison with widely used models based on the embedded trajectories idea[4,5].

The basis of the MIC is a distribution of particles parameters changing in the course of the processes being simulated. The distribution is determined in the following way.

Let x be the values of ξ characterizing the state of the particle (e.g. energy loss or angle of scattering). If the distribution density of this value in the current physical process (normalized by 1) $f(x)$ is known, then, the distribution of this value $F(x)$ is determined by the integral $F(x)=\int_{-\infty}^{x} f(t)dt$. The value $F(x)$ is equal to the probability of inequality $\xi < x$. In order to simulate (play) the random value ξ the inverse function technique[6] is used. Namely: $x = F^{-1}(\gamma), \gamma \in (0,1)$, $F^{-1}(\gamma)$ is the function inverse to $F(x)$, γ is uniformly distributed in $(0,1)$.

The probability distribution density $f(x)$ is constructed by cross-section data[7] handling: $f(x) = \frac{1}{\sigma}\frac{\partial \sigma}{\partial x}$; where σ and $\frac{\partial \sigma}{\partial x}$ are the cross-section and differential cross-section of the processes in question.

Modeling of radiative electron emission includes next stages:

- Simulating the photon transport in the objects of complex inner structure with accounting the processes of elastic and inelastic interaction between X-rays and matter;
- Modeling of generation of fast electron fluxes produced due to photo absorption and Compton scattering of X- rays in the object;
- Simulating the electron transport in matter with taking into account the various collision processes up to leaving the electron from the object or up to the fast electron thermalization. The base feature of the electron transport is the significant difference between range photon path and electron distance (up to three orders);
- Modeling of registration of emitted electrons by detecting system.

The algorithms of statistical simulation of electron emission processes are created by developing the weight versions of the Monte Carlo method. As mentioned above the photon path up to its absorption is much bigger than electron path up to its thermalization. A direct statistical simulation of electron emission is ineffective under these conditions as far as the fraction of electrons able to reach boundary surfaces of the object is very low.

The following way is worked out for increasing the photon trajectory worth. First of all, energy E_e of photo or Compton electrons produced by current photon is played. Secondly, the stopping path $L_e(E_e)$ of the electron is calculated. Then a segment of possible electron appearance is constructed so that the electron can leave object. It is supposed that an electron can leave the object if the distance between it and bound of the object is not bigger than L_e. Length of the segment is chosen in agreement with beforehand calculated L_e as shown on the fig.1 (segment AC).

A point of photo absorption or Compton scattering is then played according to formula:

$$x = \frac{1}{\mu_{ph}} \ln\left[1 - \gamma\left(1 - \exp\left\{-\mu_{ph}|AC|\right\}\right)\right], \tag{1}$$

in (1): x is the distance between A and point of the photon interaction; γ is uniformly distributed in $(0,1)$ random number; $\mu_{ph}(E_{ph})$ is the total attenuation coefficient (total macroscopic cross section) of the photon.

Initial statistical weight w_e^0 of produced electron is defined as $w_e^0 = w_{ph} \cdot p_{\text{int}}(E_{ph}) \cdot p_e(L_e)$, where: w_{ph} is current weight of photon; $p_{\text{int}}(E_{ph})$ is probability of producing the electron by the photon of energy E_{ph}; $p_e(L_e)$ is probability of the electron production on the segment AC. The probability $p_e(L_e)$ is equal to

$$p_e(L_e) = \exp(-\mu_{ph}OA) - \exp(-\mu_{ph}OC) = \exp(-\mu_{ph}OA)\left(1 - \exp(-\mu_{ph}AC)\right). \qquad (2)$$

First factor in right part of (2) is the probability of photon to reach the point A. Second one is the probability of electron production on segment AC under the condition that the photon has reached the point A.

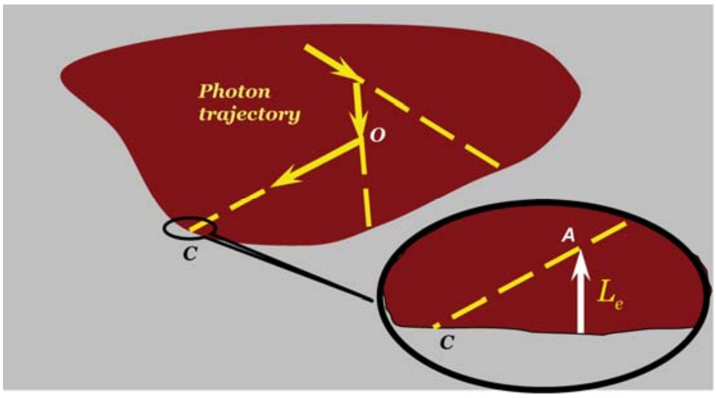


Fig.1. Scheme of modeling of radiative electron emission

The processes of both electrons production are considered on every section of every photon trajectory. Thus, the rare event of production of electron capable to leave the object is simulated by the developed weight algorithm considerably decreasing the results variance. The trajectory of produced electron is computed up to its leaving the object or up to its thermalization by use of the Monte Carlo method coupled with MIC being mentioned above.

After two electron trajectories completion the photon trajectory is continued from the point O. The new point O' of interaction is played and then new direction and energy of the photon are played. The following way is applied in order to increase the information value of the photon trajectory.

It is stated that the photon does not leave an object during a priori defined number n_{coll} of collisions. After every scattering its statistical weight is decreased by the probability p_{rm} of the remaining in the object: $w'_{ph} = w_{ph} \cdot \left[1 - \exp(-\mu_{ph}s)\right]$; w_{ph}, w'_{ph} are weights of the photon before and after scattering respectively; s is the distance from the point of interaction up to the object boundary ($s = OC$ on the fig.1). Moreover, it is supposed that the photon is not absorbed by the matter of the object. The photon weight is decreased in that case by the survival probability $p_{sr} = 1 - p_{ab}$; $w''_{ph} = w'_{ph} \cdot p_{sr}$; p_{ab} is the probability of the photo absorption. After n_{coll} collisions the photon trajectory is simulated via the analog computation. Number n_{coll} can be specified for instance in agreement with the criterion of the weight smallness.

It is important to note that the electrons produced at the point O' are ignored even through O' belong to corresponding segment $A'C'$ (see above).

The developed methods are sufficiently homogeneous. Therefore they can be easy parallelized including the application of graphical processors due to independence of particle trajectories.

The main features of the described algorithm implementation for hybrid computers are considered in the paper below.

3 IMPLEMENTATION OF DEVELOPED ALGORITHM FOR HYBRID COMPUTERS

It is necessary to take into account a number of features of using the graphical processors as arithmetical co-processors.

1. Graphical processor (GPU) is very useable for performing the huge number of arithmetical calculations. A lot of logical operations can sufficiently decrease performance of the graphical processor though.
2. The RAM memory space available to GPU is not large. The NVIDIA© CUDA technology 4.0 gives possibility to use RAM of central processor (CPU). However it leads to significant decrease of the graphical processor speed.
3. Load balancing between CPU and GPU is the key for effective usage of hybrid computer.

Algorithms of simulating the radiation transport in matter based on the Monte Carlo method have large number of independent threads. Such algorithms can be well parallelized by use any parallel computational architecture including the computer having poor data access synchronization techniques (hybrid computers with nodes including CPU and graphical processors as well). At the same time the algorithms in question require huge amount of arithmetical calculations. These circumstances make well suitability of the algorithms for implementation for hybrid computers.

Approaches to application of NVIDIA© CUDA technology for solving the problems of X-ray transport through the multicomponent objects[8] are developed by the authors of this paper. Algorithms of statistical modeling of electron transport for carrying out the numerical experiment on hybrid computers using NVIDIA© CUDA technology[9] are worked out as well. The effectiveness of mentioned implementation is caused by relatively uniform density of calculations on any stage of the algorithms.

Radiative electron emission modeling method has not the calculation density homogeneity. Therefore it is impossible to develop effective direct application of the parallelization ways[8,9]. It is necessary to distribute calculation charge between CPU and GPU and to carry out load balancing for optimization of computing.

Let us consider the computational scheme of the emission modeling (fig.2). The sequence of stages is the following.

- The tracing of object (finding of intersection points of a ray along current motion direction of a photon with boundaries of the object homogeneous parts) is carried out in compliance with ray-tracer algorithm[10].
- Modeling of Compton and photo electrons production inside the corresponding segment AC (see fig.1).
- Simulation of the electron trajectory up to its leaving the object or up to its thermalization.

- Registration of the electron if it reaches boundary of the object.
- Continuation of the photon trajectory.

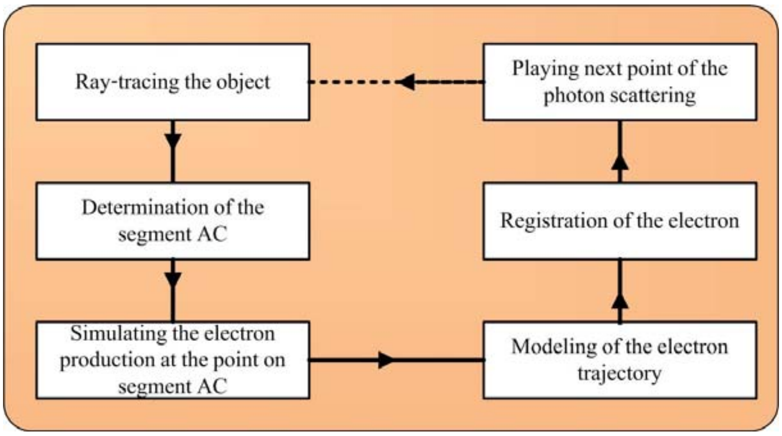


Fig.2. Calculation scheme of the electron emission modeling

Different parts of the computing scheme have different calculation density. Therefore it is necessary in some parts of the algorithm to rely on GPU and for remainder - on CPU. Namely, parts of high computational density are executed on GPU and parts of relatively low computational density are executed on CPU.

Investigations of the computing load on every stage of the electron emission modeling allow estimating the relative calculation density of different parts of the algorithm. Analysis of developed method has shown that simultaneous modeling of the photon trajectories and produced electrons leads to strongly nonuniform computational density on different stages of algorithm. Parts of low density (simulating the interaction between photons and matter, electron production processes) alternate with parts of high density (tracing the object, simulating the electron trajectories).

Results of the analysis have allowed distributing the computational load among the central processors and the graphical ones.

3.1 Ray-tracing the object

The goal of tracing the multicomponent object is to compute points of intersection of the ray along the photon motion direction with homogeneous parts of the object. Corresponding task is solved in two stages.

- Calculation of points coordinates of the intersection of the photon ray with envelopes bounding the homogeneous components of the object;
- Determination of optical thickness of intersected component along the ray.

The triangulation model is used for description of the complex objects having the piecewise homogeneous structures[10]. In practice the envelopes of homogeneous parts are defined by hundreds of thousand triangles. Therefore the problem of determination of intersection points coordinates requires huge number of arithmetical operations. Counting for mentioned above features of using the hybrid computers this stage is carried out on GPU.

It is known that a computational job for GPU (kernel) consists of group of calculation threads collated to blocks. Blocks are collated to grid.

Two computing kernels are used for executing the first stage of ray tracing. First kernel performs transformation of triangle vertexes to local coordinate system defined by the motion direction of current photon. Grid of this kernel consists of $N_{ph} \times M_v$ array of blocks. Every block is one-dimensional array of 512 threads. Total number of vertexes is $512 \cdot M_v$. Structure of the kernel is represented on figure 3.

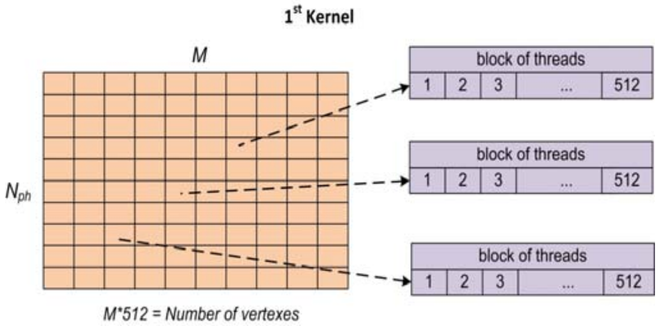


Fig.3. Configuration of first kernel.

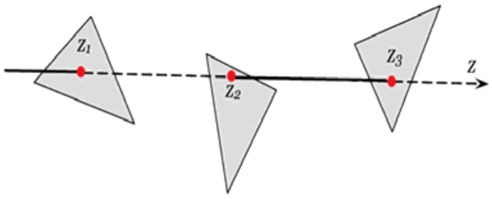


Fig.4. Intersection of triangles by photon ray.

Thus, the pair “photon-vertex” is corresponded to one thread.

Second kernel computes intersection point coordinates along the motion direction of current photons. It is assumed that polar axis z of local coordinate system is coaxial to the photon motion direction (fig.4).

Grid of 2nd kernel consists of N_{ph} blocks. Every block is array of 512 threads. A thread computes array of z by exhaustive searching all of the triangles in accordance with algorithm[10]. Result of 2nd kernel work is N_{ph} of array enclosing the intersection point coordinates. Increasing the computation speed is attained by allocating the desired arrays in shared memory of the blocks. Atomic operations excluding the simultaneous access to the memory are used for synchronization of access to array elements.

The 2nd stage of object tracing is to determine the set of optical thicknesses homogeneous parts of object intersecting by the photon ray. This stage requires substantially executing the logical operations of comparison and rearrangement. Therefore this stage is carried out by use of CPU.

3.2 Modeling of the electron emission

Firstly the segment AC is determined. As mentioned above it is equal to stopping path of electron (production and transport of photo electron is modeled at first and of Compton electron after that or vice-versa).

Using the results of the object tracing and $L_e\left(E_e\right)$ the segment AC is constructed (fig.1). The point of electron production is played according to conditional probability (1). The electron initial motion direction is played then. This part of algorithm is carried out on CPU.

Then trajectories of two produced electrons are followed up to its thermalization or up to leaving the object. Modeling the electron trajectory is computed on GPU by use of MIC[3].

Modeling the electron transport requires reconfiguration of GPU memory (roll-out of object geometry data; roll-in of electron interaction data). Therefore running this modeling of every step of photon trajectory is not effective. The next approach is used for increasing the effectiveness of calculations. Characteristics of produced electrons are saved in electron pool and trajectories of all electrons of the pool are computing all together after filling of the pool.

Electron trajectory modeling is carried out on graphical processor and registration of electron is computed on CPU because of big dimension of electron sample and the GPU memory is not enough for saving the sample.

After finishing the electron transport simulating the photon trajectory is continued from the point O (fig.1). Next point of photon interaction is played and modeling of interaction between photon and matter in the point is computing. Algorithms of solving the corresponding tasks have complex logical structure and therefore are carrying out on CPU.

An analysis of calculation density of different steps of electron emission modeling has allowed distributing the parts of algorithm between central processor and graphical one of a node of hybrid computing system. The distribution of different parts calculation scheme is shown on the figure 5.

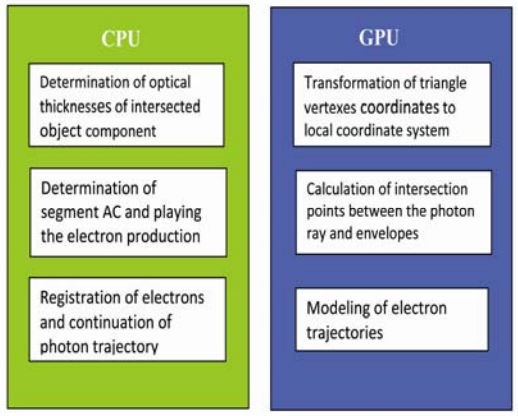
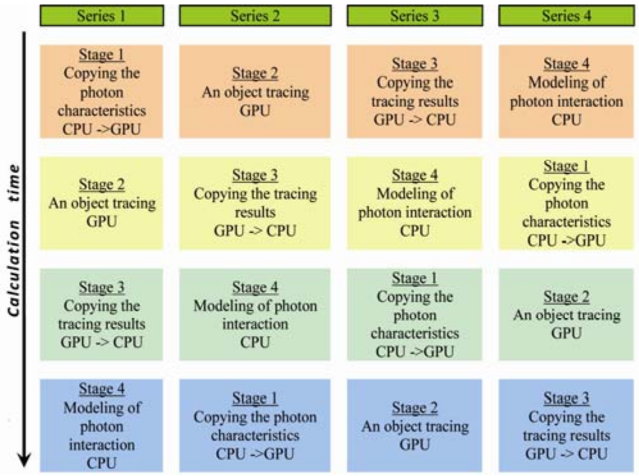


Fig.5. Distribution of parts of computing scheme between CPU and GPU.



Series 1	Series 2	Series 3	Series 4
Stage 1 Copying the photon characteristics CPU ->GPU	Stage 2 An object tracing GPU	Stage 3 Copying the tracing results GPU -> CPU	Stage 4 Modeling of photon interaction CPU
Stage 2 An object tracing GPU	Stage 3 Copying the tracing results GPU -> CPU	Stage 4 Modeling of photon interaction CPU	Stage 1 Copying the photon characteristics CPU ->GPU
Stage 3 Copying the tracing results GPU -> CPU	Stage 4 Modeling of photon interaction CPU	Stage 1 Copying the photon characteristics CPU ->GPU	Stage 2 An object tracing GPU
Stage 4 Modeling of photon interaction CPU	Stage 1 Copying the photon characteristics CPU ->GPU	Stage 2 An object tracing GPU	Stage 3 Copying the tracing results GPU -> CPU

Fig.6. An example of organization computing series for simultaneous loading of CPU and GPU.

The iteration of the computational algorithm (modeling the next step of photon trajectory) is a sequence of calculation stages carrying out either on CPU or on GPU. Independence of photon trajectory modeling gives possibility to compute simultaneously calculations of different series. At that different calculations of the series are on the different stages. Thus, computing is carried out at the same time on both CPU and GPU. The fact allows increasing the effectiveness of hybrid computers application. An example of simultaneous loading of central processor and graphical one is represented on figure 6.

4 RESULTS OF MODELING

Two experiments were carried out for analysis of developed method capabilities: computational experiment with aluminum plate irradiated by X-ray (and its comparison with MCNP[11]) and natural experiment with aluminum plate irradiated by ^{137}Cs source of gamma rays.

4.1 Computational experiment

Configuration of the experiment is next. The photon flux is falling normally on aluminum plate. Energy of incident photons is E_0, thickness of the plate is h. Energy spectra of emitted from irradiated surface of the plate and from rear one are measured.

Calculations are carried out for two variants. Electron emission modeling results are represented on figures 7-10. Results of MCNP computing are shown for comparison.

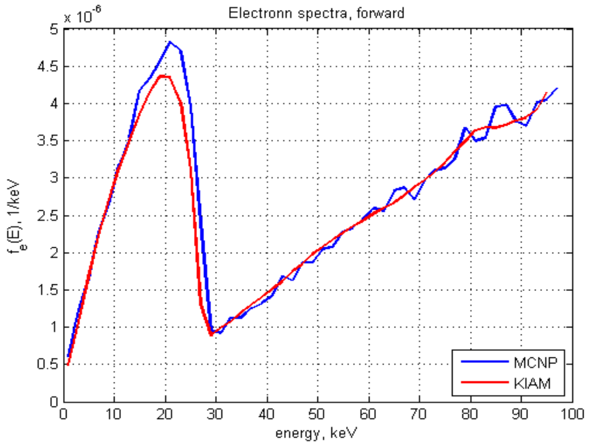


Fig.7. Spectra of electrons emitted from rear surface of the aluminum sample

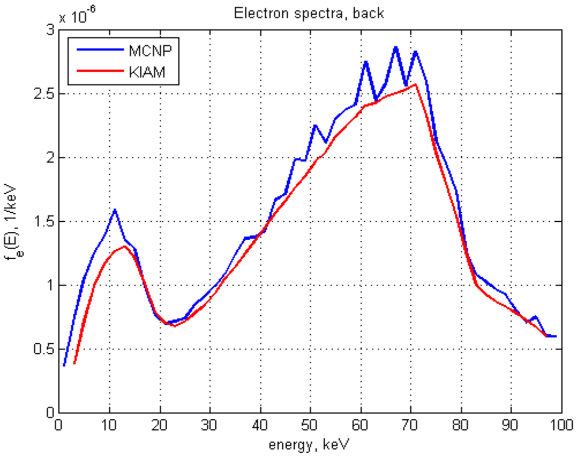


Fig.8. Spectra of electrons emitted from irradiated surface of the aluminum sample

Electron spectra on fig. 7 and 8 are obtained for $E_0 = 100\,keV$ and $h = 1cm$. Red line - results computed by described in the paper method (KIAM – Keldysh Institute for Applied Mathematics), blue line – by MCNP.

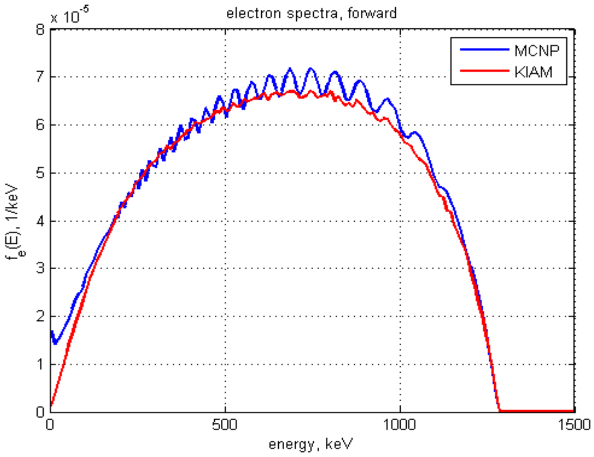


Fig.9. Spectra of electrons emitted from rear surface of the aluminum sample

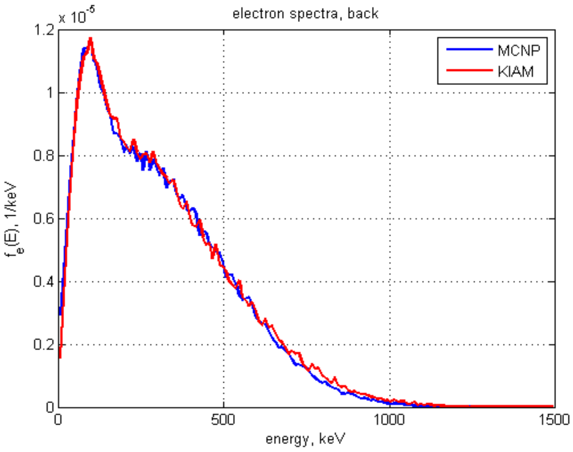


Fig.10. Spectra of electrons emitted from irradiated surface of the aluminum sample

Electron spectra pictured on fig. 9 and 10 are obtained for $E_0 = 1500\,keV$ and $h = 4cm$. Represented figures demonstrate satisfactory fit of results.

4.2 Modeling of experiment with ^{137}Cs source

Scheme of experiment is shown on fig. 11. An aluminum plate is irradiated by photons emitted from ^{137}Cs source. Measurements of radiation are carried out with use of silicon detector. Measured value is number of pulses $F(E)$, E is radiation energy deposit in detector.

It is obvious that a contribution in the measured value is made by emitted electrons and transmitted photons as well.

Next experimental technique is used for obtaining the emitted electrons contribution $F_e(E)$. Firstly the photon contribution $F_{ph}(E)$ is measured by performing the experiment without sample. Then the experiment with sample is carried out (measured value $F(E)$). Thus, $F_e(E)$ is calculated as:

$$F_e(E) = F(E) - F_{ph}(E). \tag{3}$$

Suggested experimental technique is reasonable when next conditions are fulfilled:

1. Gamma-radiation attenuation when passing through the sample is insignificant;
2. Contribution of scattered gamma-radiation is negligible in comparison with electron one;
3. Relative electron distribution in detector is appreciably larger than measurement error.

As shown in the paper[12] the conditions 1 – 3 are satisfied for ^{137}Cs as source and for the sample of 2 mm Al.

The comparison of computed data and experimental measurements are represented on the figure 12.

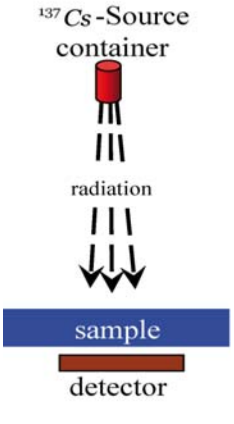


Fig.11. Scheme of the experiment

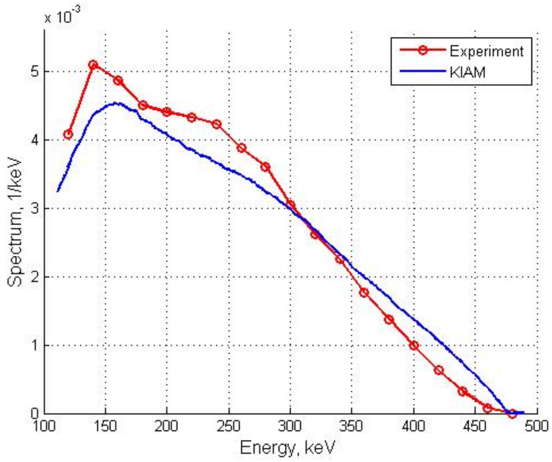


Fig.12. Energy deposit distribution. Red line – experiment; blue one – calculations.

5 CONCLUSION

Developed method is applicable for computing the characteristics of electron fluxes emitted from surfaces of objects being under radiation by use of hybrid supercomputers.

Constructed algorithms based on the Monte Carlo method modifications are effective for mathematical modeling of X-ray and electron transport on calculating systems with heterogeneous architecture. The significant feature of the method is the effective distribution of calculation between central processor and graphical one.

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