HANDLING OF THE RADIATIVE ELECTRON EMISSION MODELING RESULTS BY USE OF THE NEURAL NETWORKS

V. EGOROVA, M. ZHUKOVSKIY

Keldysh Institute of Applied mathematics of RAS
Moscow, Russia
e-mail: eva24372@gmail.com , web page: http://www.keldysh.ru

Summary. Modeling of radiation transport often requires approximation of its results from the detector point set to another 3D point system. In particular, modeling of the radiative electromagnetic field envisages approximation of electron emission simulation results from the radiation transport detector system to a differential grid used for the solution of the Maxwell equations. The approximation of functions in the 3D geometry is a non-trivial problem. An approach based on usage of the neural networks is developed for the solution of the approximation problem in question. The multilayer perceptron is chosen for the construction of the neural network. Network training is worked out by applying the algorithm of error backpropagation. The elaborated method is applied for the approximation of the 3D data calculated by Monte Carlo modeling of electron emission generated by X-ray radiation from the boundary surfaces of irradiated object. The results of the modeling are demanded to be transferred from the given detector point system to the set of the points on the 3D grid for solution of the electromagnetic problem. The approximation is obtained as the response of the constructed neural network. The results of approximation show applicability of the neural networks for solving of the approximation problems in question.

1 INTRODUCTION

The effectiveness of the mathematical modeling of many physical phenomena has greatly increased during some years due to the rapid development of the supercomputers [1-[3] and modern paralleling technology [4]. Among the actual investigations are the interaction of laser radiation with matter; the particle fluxes transport; the radiation propagation in technical objects of complex geometry [5-[14] and others. The world known codes are developed for numerical simulation of the radiation transport processes (MCNP [15], Geant-4 [16], PENELOPE [17], EGSnrc [18] etc.).

The statistical simulation by the use of Monte Carlo method is applied in various fields of the computational physics [5,[7-[11]. The method is convenient and usable for solving the complex boundary problems and allows the high-performance calculation by the use of supercomputers with heterogeneous architecture [7,[8, [11]. The effectiveness of parallelization of the Monte Carlo calculations can reach 100% and its scalability is infinite.

The mathematical modeling often requires to solve the approximation tasks as a part of numerical simulation [6, [10, [19,[20]. For instance, the problem of appropriate treatment of the modeling results occurs during simulation of the radiation transport.

Let us consider the radiative electron emission problem [7,[8]. The photon propagation through matter produces fast electron fluxes. These electrons can leave an object being under photon radiation. Thus, the electron fluxes appear outside and in interior cavities of the

2010 Mathematics Subject Classification: 97M50, 93A30.
Key words and Phrases: Radiative Electron Emission, Statistical Modeling, Neural Network, 3D-approximation

investigated object. The scheme of the emission process is presented in fig. 1.

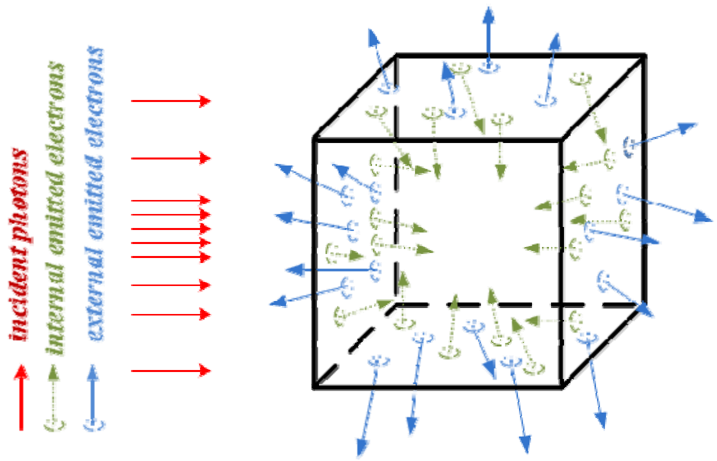


Figure 1: Radiative electron emission process

Modeling of the electron emission processes requires solving the complex boundary-value problems of the photon-electron cascade transport in 3D geometry.

Modeling of radiative electron emission includes the following stages:

− simulating the photon transport in the objects of complex inner structure with accounting of 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 of 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;

− modeling of emitted electrons registration by detecting system.

The algorithms of statistical simulation of electron emission processes are created by developing the weight versions of the Monte Carlo method. The discrete detector system is used for modeling of the registration of the generated electron fluxes.

The results of electron fluxes computing can play the role of initial data for the modeling of the radiative electromagnetic field, for instance. The electromagnetic field is described by the Maxwell equations. The approximation of the computed electron flux data from the mentioned detector system to the differential grid being used for the solution of the Maxwell equations is a non-trivial problem.

The technology of neural networks [21,[22] is used for the solution of the approximation task in question. The multilayer perceptron is chosen for the neural network construction. The network training is worked out by using the algorithm of error backpropagation [22]. The approximation is obtained as the response of constructed neural network.

2 THE PROBLEM STATEMENT

The modeling of the radiation electron emission consists of two stages:

- the statistical simulation of photon-electron transport in an object;
- the evaluation of the flux density of electrons leaving the boundaries of irradiated object.

The surface oriented description of objects is used for modeling of radiation transport [9]. The discrete description of the boundary surfaces of irradiated object is implemented by the triangulation (fig. 2).

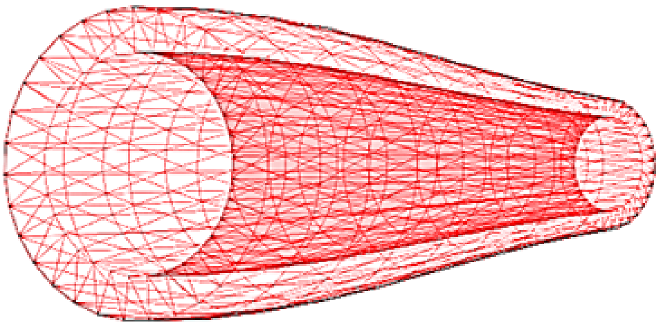


Figure 2: Triangulation of the boundary surfaces

The model of the detector system is worked out for evaluation of the flux density of electrons leaving the boundary surfaces of irradiated object. An example of the model is depicted in fig. 3.

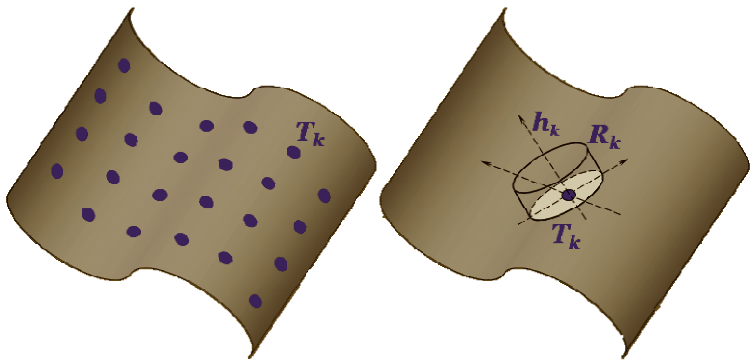


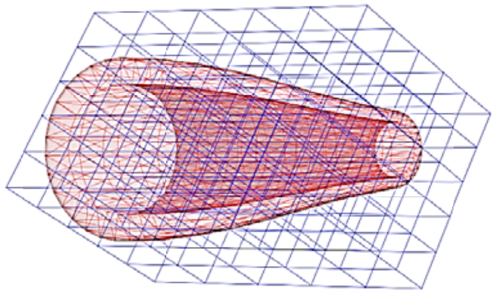
Figure 3: An example of the detector system

A set $\{T_k\}_{k=1}^{K}$ of detectors T_k consists of K different (generally speaking) detectors. Every disk detector (T_k) has a radius (R_k) and a height (h_k) [7]. Every detector of the system belongs to some triangle of corresponding surface after its triangulation.

Thus, statistical evaluation of the electron fluxes is carried out by the use of described discrete detector system.

The results of some physical process computing play often the role of initial data for another phenomenon. Let us consider the generation of the radiative electromagnetic field (REMF) inside and outside the irradiated object [10].

Self-consistent REMF is described by the Maxwell equations. Numerical solution of these equations requires creation of the differential grid constructed by the use of a rectangular grid in Cartesian coordinate system [10]. An example of the grid is presented in fig. 4.



The problem of approximation of electrical current density computed in the points of the set $\{T_k\}_{k=1}^{K}$ to the cells of rectangular electrodynamical grid is actual in that case.

This problem can be formulated as followed.

Let region $\Omega \in \mathbb{R}^3$ be the domain of the function $f(\mathbf{r}) = f(x,y,z), \mathbf{r} \in \Omega$ and sets $Q_N = \{\mathbf{r}_n\}_{n=1}^{N} \in \Omega, Q_M = \{\mathbf{r}_m\}_{m=1}^{M} \in \Omega$ are known. Let $f(Q_N)$ be known. It is required to find $f(Q_M)$ by approximating the $f(Q_N)$ from the set Q_N to the set Q_M.

The neural network technique is applied for solving this problem.

It should be noted that Q_N is called training set (TS), and Q_M is called destination set (DT).

3 THE APPROXIMATION ALGORITHM

A neural network consists of a set of formal neurons. Neurons are connected to each other by some method. Network has layers and every layer has a few neurons. There are input layer and output one. The rest of layers are hidden. An example of neural network topology is presented in fig. 5.

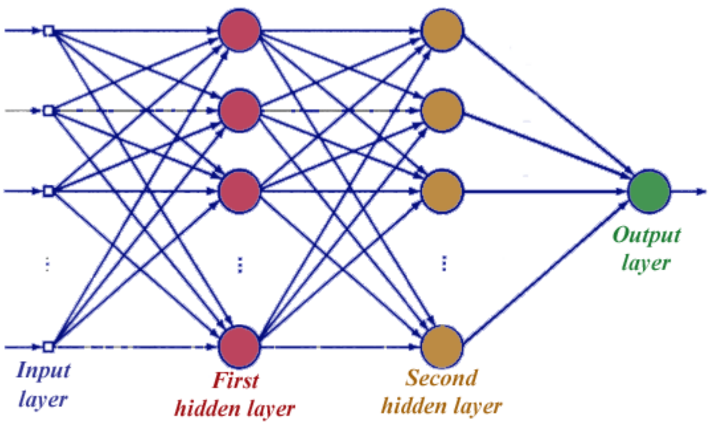


Figure 5: Neural network with two hidden layers

Input information is applied for the entrance of the input layer neurons. Output information is created by neurons of the output layer (the network response). Every neuron of previous layer gives a signal to every neuron of the next layer.

An operation scheme of formal neuron is depicted in fig. 6.

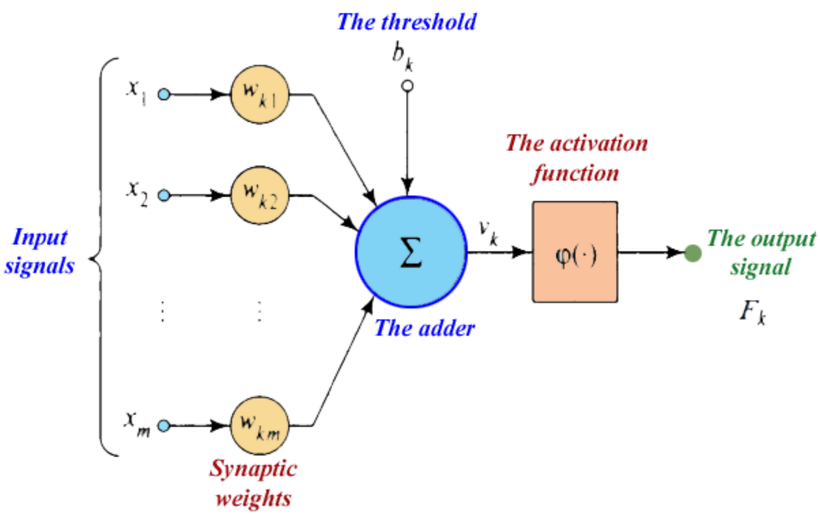


Figure 6: Operating model of some neuron of the layer number *k*

The function $\varphi(t)=\dfrac{1}{1+e^{-t}}$ is chosen as an activation function. The output signal of k^{th} layer is $F_k=\varphi\left(\sum_{i=1}^{m} w_{ki}x_i+b_k\right)$, where w_{ki} are synaptic weights and b_k are thresholds [21].

Let $F(\mathbf{r})$ be an approximation function having to be constructed by use of a neural network as continuous mapping $F:\Omega\in\mathbb{R}^3\Rightarrow\mathbb{R}^1$ (see section 2).

The general approach of discussed method is presented in fig. 7.

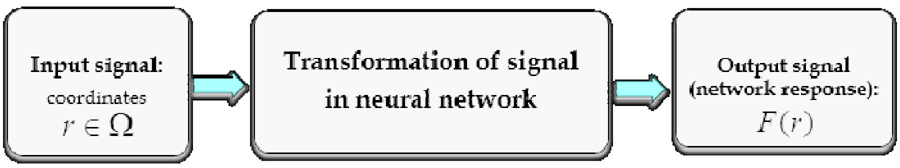


Figure 7: The general scheme of the method

The training set Q_N and $f(Q_N)$ are employed for creating the neural network by applying the algorithm of error backpropagation [21, 22].

The goal of the algorithm is to minimize the mean-square error *E*

$$E=\frac{1}{2N}\sum_{i=1}^{N}\left[f(r_i)-F(r_i)\right]^2, r_i\in Q_N$$

The minimizing process is carried out by the gradient descent method.
The network response and the error *E* are calculated in the forward direction. The correction of the synaptic weights (w_{ki}) is carried out in back direction:

$\Delta w_{ij}=-\eta\dfrac{\partial E}{\partial w_{ij}};\Delta b_i=-\eta\dfrac{\partial E}{\partial b_i}$, $\eta\in(0,1)$ is called the rate of network training [21].

4 THE EXAMPLE OF SOLVING THE APPROXIMATION PROBLEM

Let us consider an object having the form of a truncated cone with aluminum wall 5 mm of thickness. The object is irradiated by X-ray plane flux of 100 keV energy. The flux density $f(Q_N)$ of emitted electrons in the points of the detector set Q_N (fig. 8) is the result of the statistical modeling of the process in question.

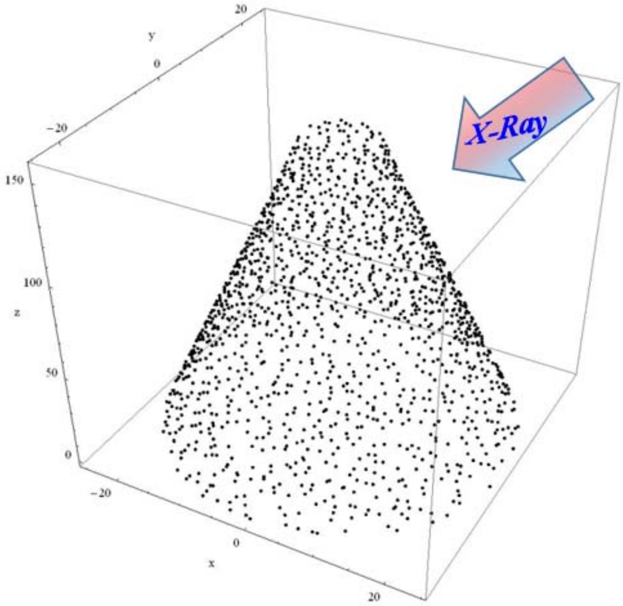


Figure 8: The set of the detector points

The process of network construction is described below.

One hidden layer having 5 neurons is chosen as an initial network topology. Then the mean-square error E is calculated on the training set Q_N. Neurons and layers are added untill the error reaches specified level (the chosen level of the error is 2%).

Firstly the neurons are added to the first hidden layer. The second layer is added when the network error is still more than specified value and is not decreasing by rising of neurons of the first layer (fig. 9).

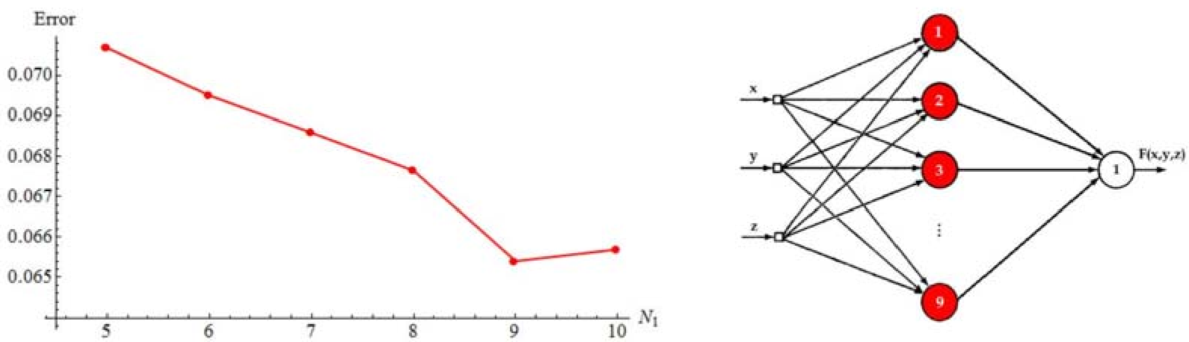


Figure 9: The process of configuration of the first hidden layer

Then the other layers are configurated (fig. 10, 11).

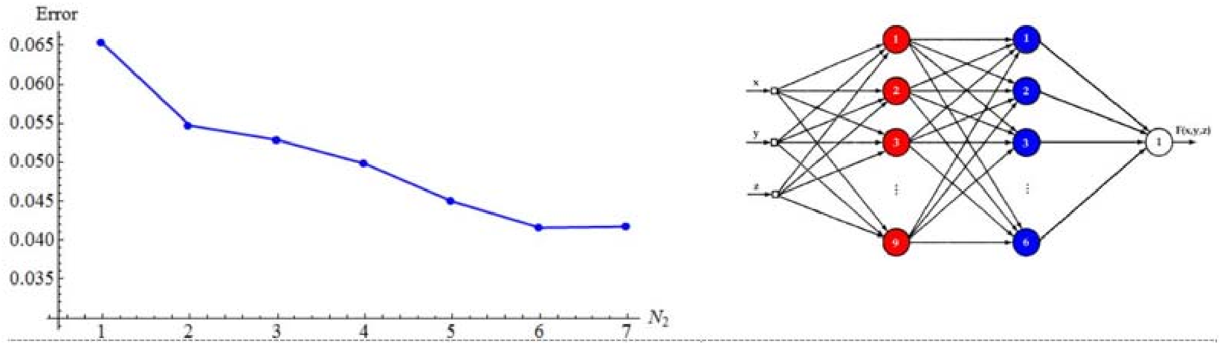


Figure 10: The process of configuration of the second hidden layer

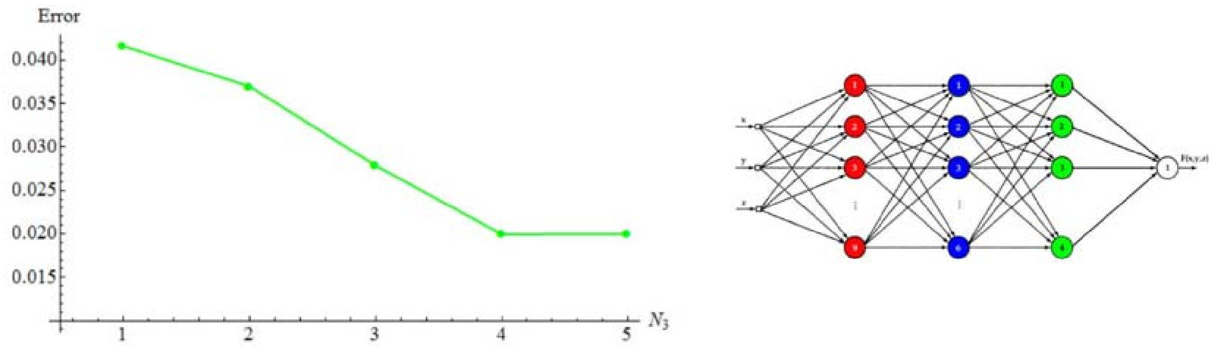


Figure 11: The process of configuration of the third hidden layer

Total process of the network configuration is presented in fig. 12.

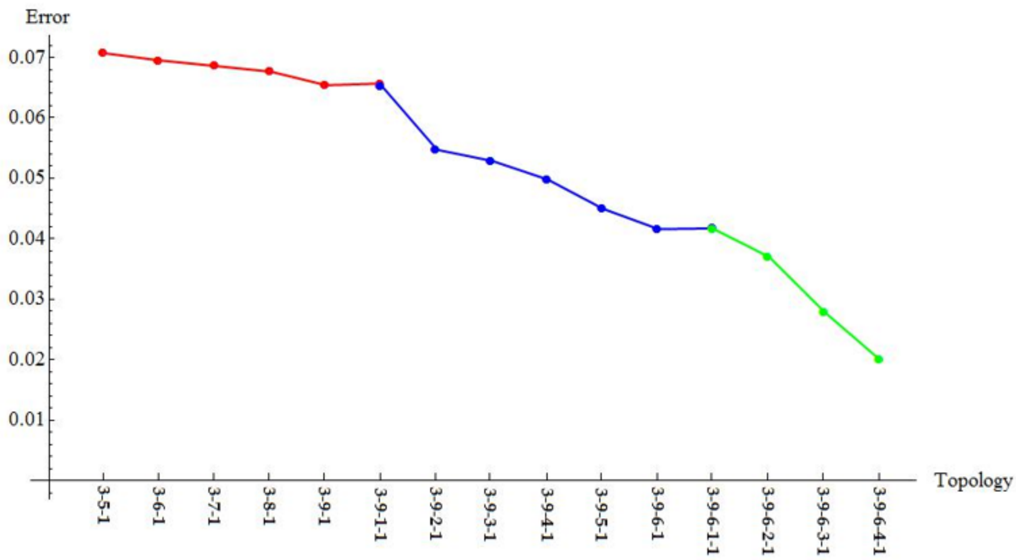


Figure 12: The total process of the network configuration

Thus, the resulting neural network has three hidden layers having 9, 6 and 4 neurons accordingly. The network is depicted in fig. 13.

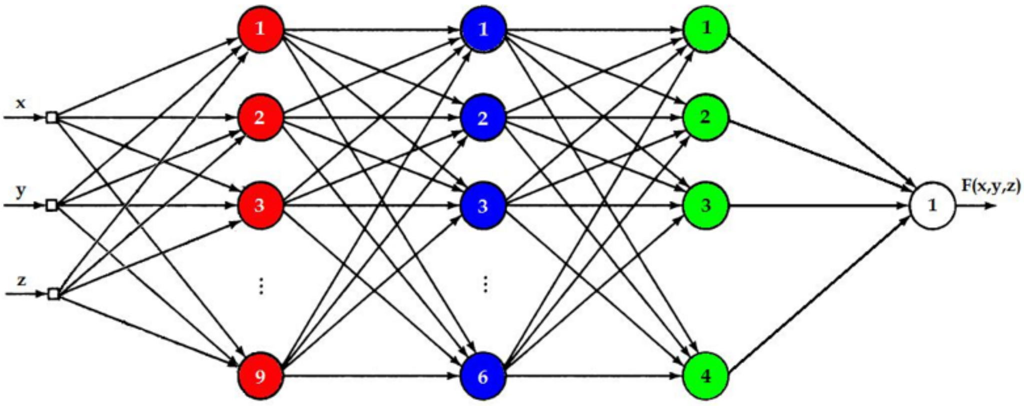


Figure 13: Final configuration of the network

Then the approximation (network response) $F(\mathbf{r}), \mathbf{r} \in Q_M$, is obtained by application of constructed network (fig. 13). The destination set Q_M is the set of points in edges of electrodynamic differential grid (fig. 4). The training set and destination one are presented in fig. 14.

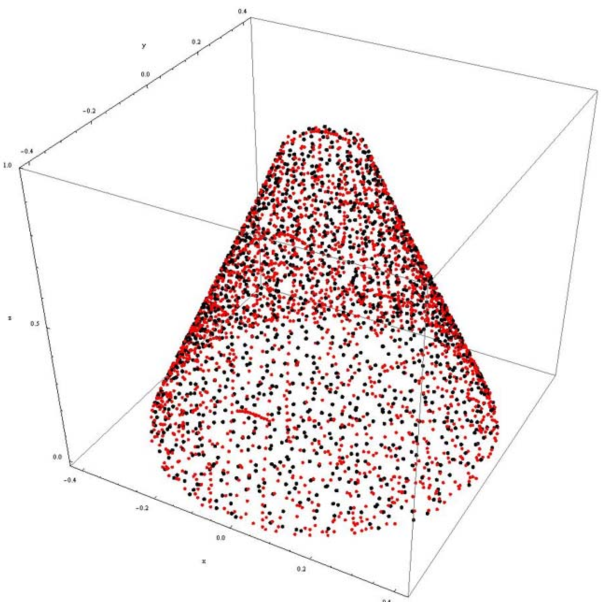


Figure 14: Training set (black points) and destination set (red points)

A visual evaluating of approximation quality is carried out using the following approach. A random point r_0 is chosen from the training set (reference point).

The distance R from r_0 to the axis OZ is calculated. A circle of radius R is constructed in a plane perpendicular to the axis OZ. A uniform angle grid $\{\theta_j\}_{j=1}^{J} = \left\{\theta_1 = \frac{2\pi}{J},...,\theta_J = 2\pi\right\}$ is created on the circle.

Two points nearest to every point of the grid $\{\theta_j\}_{j=1}^{J}$ are found. One point belongs to the training set and second one belongs to the destination set. Thus, we have two arrays $A_J \in Q_N$, $B_J \in Q_M$ and two arrays $f(A_J)$, $F(B_J)$ accordingly.

Then the symmetrization of the arrays $f(A_J)$ and $F(B_J)$ is carried out because the approximated function is symmetrical with respect to the axis XOZ a priori:

$$f_s = \left(f + flip(f)\right)/2; \quad F_s = \left(F + flip(F)\right)/2.$$

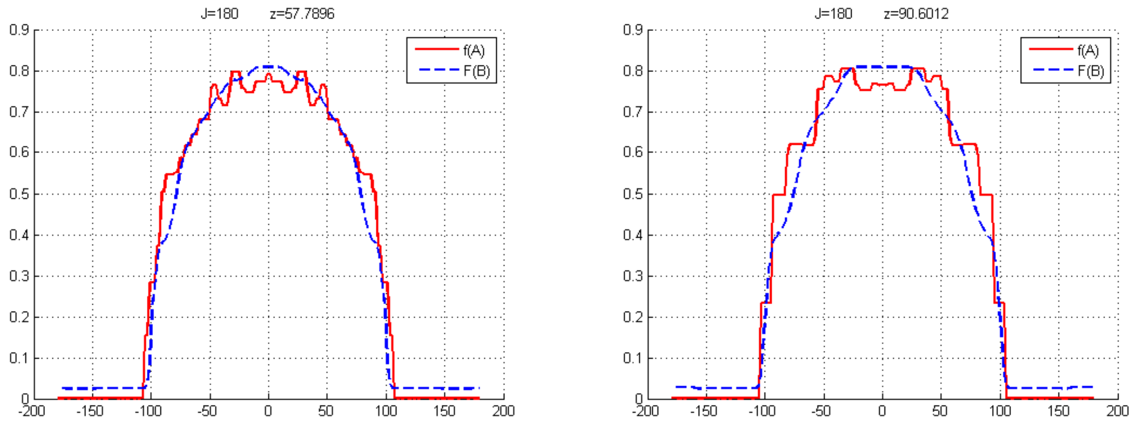


Figure 15: Left picture – $z(r_0)$~58, right picture - $z(r_0)$~91

Some results of visualization are presented in fig. 15 for various r_0. Presented results demonstrated satisfactory quality of required approximation. In addition, smoothing properties of the developed method are shown in the fig. 15. It is significant for the statistical modeling because of existing the non-physical fluctuations.

5 CONCLUSION

Results obtained in the present paper show applicability of the neural network technology for the solution of the problem of processing of the radiation transport modeling results by means of the developed approach to 3D function approximation. The presented method gives the opportunity to use the results of numerical solution of the transport problems in EMF tasks as a current source. Moreover, the elaborated technique allows smoothing the simulation results fluctuations generated by Monte Carlo application.

Further development of the developed approach is planned for solving the vector-function approximation problems in 6D space (space of coordinates and pulses). The input layer will have 6 neurons and output one will have 3 neurons in this case. It is actual, for instance, in numerical modeling of radiation particle velocities. The results of the method development will be presented later.

The work was partially supported by RFBR grant **№ 15-01-03027**.

REFERENCES

[1] Top500 Supercomputers, URL: http://top500.org/.
[2] Yang Xue-Jun et al. "The TianHe-1A Supercomputer: Its Hardware and Software", *Journal of computer science and technology*, **26**(3), 344-351 (2011).
[3] http://www.intel.ru/content/www/ru/ru/processors/xeon/xeon-phi-detail.html.
[4] http://www.nvidia.ru/object/cuda-parallel-computing-ru.html.
[5] G.Z. Lotova, M.A. Marchenko, G.A. Mikhailov, S.V. Rogazinskii, S.V. Ukhinov, V.A. Shklyaev, "Numerical statistical modelling algorithms for electron avalanches in gases", *Russian Journal of Numerical Analysis and Mathematical Modelling*, **29** (4) 251–263 (2014).
[6] I.P. Tsygvintsev, V.A. Gasilov, A.YU. Krukovskiy, V.G. Novikov, I.V. Popov. "Three-dimensional modeling of the laser radiation absorption", *Mathematica Montisnigri*, **XXVII**, 135-152 (2013).
[7] M.E. Zhukovskiy, M.B. Markov, S.V. Podoliako and R.V. Uskov, "Hybrid Parallelization of Computing the Electron Fluxes produced by Photon Radiation", *Mathematica Montisnigri*, **XXXI**, 43-53 (2014).
[8] M. E. Zhukovskiy and R. V. Uskov, "Hybrid Parallelization of the Algorithms of Radiation Cascade Transport Modeling", *Mathematical Models and Computer Simulations*, **7** (6), 601–610 (2015).
[9] M. Zhukovskiy, S. Podoliako, G.-R. Jaenisch, C. Bellon, "Monte-Carlo-Simulation und CAD - Strahlungsausbreitung an realen Bauteilgeometrien", *Materialpruefung*, 47(4), 210-218 (2005)
[10] M.E. Zhukovskiy, M.B. Markov, "Modeling the radiative electromagnetic field", *International Journal of Computing Science and Mathematics*, **2** (1), 46-59 (2008).
[11] A. V. Berezin, A. S. Vorontsov, M. E. Zhukovskiy, M. B. Markov, and S. V. Parot'kin, "Particle Method for Electrons in a Scattering Medium", *Computational Mathematics and Mathematical Physics*, **55** (9), 1534–1546 (2015).
[12] V.I. Mazhukin, A.V. Shapranov, A. A. Samokhin, A.Y. Ivochkin, "Mathematical modeling of non-equilibrium phase transition in rapidly heated thin liquid film", *Mathematica Montisnigri*, **XXVII**, 65-90 (2013).
[13] V.I. Mazhukin, A.A. Samokhin, M.M. Demin, A.V. Shapranov, "Modeling of nanosecond laser vaporization and explosive boiling of metals", *Mathematica Montisnigri*, **XXIX**, 68-90 (2014).
[14] V.I. Mazhukin, A.V. Shapranov, A.V. Mazhukin, O.N. Koroleva, "Mathematical formulation of a kinetic version of Stefan problem for heterogeneous melting/crystallization of metals", *Mathematica Montisnigri*, **XXXVI**, 58-77 (2016).
[15] D. B. Pelowitz, ed., "MCNPX User's Manual, Version 2.6.0", *Los Alamos National Laboratory report LA-CP-07-1473,* (2008).
[16] S. Agostinelli et al, "GEANT4—a simulation toolkit", *Nucl. Instr. Meth. Phys. Res.*, **A506** (3), 250–303 (2003).
[17] Salvat, J.M. Fernández-Varea and J. Sempau, *PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon Transport*, OECD NEA Data Bank/NSC DOC (2011)/5 (OECD Nuclear Energy Agency, Issy-les-Moulineaux), (2011).
[18] I. Kawrakow, E. Mainegra-Hing, D.W.O. Rogers, F. Tessier, B.R.B. Walters, "The EGSnrc Code System: Monte Carlo Simulation of Electron and Photon Transport", *NRCC Report PIPS-701,* (2009).

[19] O.N. Koroleva, A.V. Mazhukin , V.I. Mazhukin, P.V. Breslavskiy, “Approximation of Fermi-Dirac integrals of different orders used to determine the thermal properties of metals and semiconductors”, *Mathematica Montisnigri*, **XXXV**, 37-54 (2016).
[20] O.B. Feodoritova, N.D. Novikova, V.T. Zhukov, “Multigrid method for diffusion equations based on adaptive smoothing”, *Mathematica Montisnigri*, **XXXVI**, 14-25 (2016).
[21] Simon Haykin, “Neural Networks - A Comprehensive Foundation, Second Edition”, *Pearson Education, Inc., Reprint*, (2005).
[22] S. Saarinen, R.B. Bramely and G. Cybenko, “Neural NetWorks, backpropagation and automatic differentiation in Automatic Differentiation of Algorithms: Theory, Implementation and Application”, *A. Griewank and G.F. Corliss, eds., Philadelphia: SIAM*, 31-42 (1992).

Received December 15, 2016