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Numerical simulations of a coupled conductive-radiative heat transfer model using parallel computing

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Summary. In many problems related to cryopreservation of living cells and tissues, the formation of ice in intra and extracellular liquids plays very important role. There are many models predicting the homogeneous ice nucleation an formation of dendrites. Nevertheless, the application of such models requires fitting parameters and verifications trough measurements of the ice content during freezing. There are different methods for detecting homogeneously nucleated ice and ice dendrites. One of such techniques can be based on the difference in attenuation factors of ice and water under infrared radiation. The paper is devoted to the investigation of a model of the radiative and conductive heat transfer, which can be useful for the reconstruction of the inner properties of media.

The conductive-radiative heat transfer in a layer located between two reflecting and radiating surfaces is considered. This process is described by a nonlinear systems of two differential equations: an equation of the radiative heat transfer and an equation of the conductive heat exchange. The problem is characterized by anisotropic scattering of the medium and by specularly and diffusely reflecting boundaries. An iterative method for solving this problem is applied. For the calculation of solutions of the problem considered, two approaches are used. First, a recursive algorithm based on some modification of the Monte Carlo method is proposed. Second, the diffusion approximation of the radiative transfer equation is utilized. Numerical comparisons of the approaches proposed are done in the case of isotropic scattering.

1 Introduction

The study of the coupled heat transfer [1, 2] where the radiative and conductive contributions are simultaneously taken into account is important for many engineering applications. So, S. Andre and A. Degiovanni [3, 4], J.M. Banoczi and C.T. Kelley [5] and A. Klar and N. Siedow [6] have studied the thermal properties of semi-transparent materials such as glass, polymers, paper, and certain insulating materials in the context of the coupled radiative-conductive model. The mathematical treatment of this nonlinear model is studied in

[7, 8, 9, 10]. In [7], C.E. Siewert and J.R. Thomas Jr. use the simple iteration method and a computationally stable version of the P_N approximation. In work [8], the authors have applied the Newton iteration method instead of the simple iteration procedure. This allows the authors to calculate some numerical examples which are not feasible using the simple iteration method. C.T. Kelley has provided existence and uniqueness theorems for the considered problem in the case of isotropic scattering and non-reflecting boundaries [9]. An analytical version of the discrete-ordinates method along with Hermite's cubic splines and Newton's method to solve a class of coupled nonlinear radiation-conduction heat transfer problems in a solid cylinder is proposed in [10]. Computational details of the method are discussed. The algorithm is implemented to establish high-quality results for various data sets which include some difficult cases.

In the present paper, some iterative algorithm for solving this problem is implemented. For the calculation of solutions of the radiative transfer equation, two ways are used. In the first approach, a recursive algorithm based on some modification of the Monte Carlo method is proposed. This algorithm suits for the application of parallel calculations, and hence it can provide a good accuracy within a reasonable computing time. In the second approach, the diffusion approximation of the radiative transfer equation is used. It is shown that using this approximation give a good description of the solution behavior. A numerical comparison of the proposed approaches is done in the case of isotropic scattering and reflecting boundaries. The calculations are implemented on a computer cluster of the Technical University of Munich using the technology of parallel computing supported by the application programming interface OpenMP.

2 Problem formulation

Let us consider the coupled conductive-radiative heat transfer problem which is formulated as in [7]. The equation of radiation transfer for a homogenous layer is written in the normalized form as

$$\nu f_z(z,\nu) + f(z,\nu) = c\int_{-1}^{1} p(\nu,\nu')f(z,\nu')d\nu' + (1-c)u^4(z), \tag{1}$$

where $f(z,\nu)$ is a normalized density of the radiation flux at the point $z \in [z_1, z_2] \equiv [0, d]$ in the direction which angle cosine with the positive direction of the axis z is $\nu \in [-1, 1]$; c the albedo of single scattering; $p(\nu, \nu')$ the phase function; $u(z)$ the normalize temperature. Introduce the following sets for the definition of boundary conditions: $\Gamma^{\pm} = \{\{z_1 \times (0, \mp 1]\} \cup \{z_2 \times [\pm 1, 0)\}\}$.

We supply equation (1) with the boundary conditions

$$f(z_i,\nu) = h(z_i) + (Bf)(z_i,\nu), \quad i = 1, 2, \quad (z_i,\nu) \in \Gamma^-, \tag{2}$$

where

$$h(z_i) = \varepsilon_i U_i^4, \quad (Bf)(z_i, \nu) = \rho_i^s f(0, -\nu) + 2\rho_i^d \int_0^1 f(0, -\operatorname{sgn}(\nu)\nu')\nu' d\nu'.$$

Here, U_1 and U_2 are normalized temperatures on the boundaries; ρ_i^s and ρ_i^d the coefficients of specular and diffuse reflections, respectively; $\varepsilon_i = 1 - \rho_i^s - \rho_i^d$ the emissivity coefficients for the boundary surfaces.

The equation of the conductive heat transfer is written as

$$u''(z) = \frac{1}{N_c} q'(z), \quad q(z) = \frac{1}{2} \int_{-1}^1 f(z, \nu')\nu' d\nu', \tag{3}$$

where N_c is the conduction-to-radiation parameter [7]. For equation (4), we put the following boundary conditions:

$$u(0) = U_1, \quad u(d) = U_2. \tag{4}$$

For finding the solution of system (1)-(4), we will use a simple iteration method with parameter. According to that, choose an initial approximation of the temperature $u(z)$ (for example, the linear approximation which corresponds to zero value of the right-hand side of (3)) and denote it as $u_0(z)$. Then, substitute $u_0(z)$ into (1) instead of the function $u(z)$, calculate the solution of the problem (1)-(2), and denote it as $f_1(z, \nu)$. Then, by using the function $f_1(z, \nu)$ instead of $f(z, \nu)$, find the right-hand side of (3), calculate the solution of the problem (3)-(4), and denote it as $\tilde{u}_1(z)$. For a certain small value of the parameter α, the term $u_1(z) = \alpha \tilde{u}_1(z) + (1 - \alpha) u_0(z)$ will be the next approximation of $u(z)$. Then, put $u_1(z)$ instead of the function $u(z)$ into equation (1), calculate the next approximation $f_2(z, \nu)$, and so on. Thus, in the kth step, we use the terms $u_{k-1}(z)$ and $\tilde{u}_k(z)$ for determining the next approximation of the function $u(z)$ by the following formula:

$$u_k(z) = \alpha \tilde{u}_k(z) + (1 - \alpha) u_{k-1}(z).$$

The main complexity in the numerical realization of this iterative method is finding the solution of the radiative transfer equation (1). For its treatment, we will mainly use a recursive algorithm based on the Monte Carlo method. As alternative, we will construct a diffusion approximation of equation (1) (P_1 approximation). We will compare the results of these approaches with the numerical data from [7, 8].

3 Solvability of the radiative transfer equation

Let us consider the problem (1), (2). We assume that the function $u(z)$ is non-negative, and $u(z) \in C_b(0, d)$, where $C_b(X)$ is the Banach space of functions bounded and continuous on X with the norm $\|\varphi\|_{C_b(X)} = \sup_{x\in X} |\varphi(x)|$. Also, let $p(\nu,\nu') \in C_b(\Omega \times \Omega)$, where $\Omega = [-1,0) \cup (0,1]$ and

$$\int_{-1}^{1} p(\nu,\nu')d\nu' = 1.$$

Note that the operator $B : C_b(\Gamma^+) \to C_b(\Gamma^-)$ is linear, bounded, nonnegative, and $\|B\| < 1$.

Denote $X = (z_1, z_2) \times \{[-1,0) \cup (0,1]\}$. We define a class $D(X)$ where solutions f of the problem (1)-(2) are sought.

Definition 1. *A function $f(z,\nu)$ belongs to $D(X)$, if the following properties hold:*
1) $f(z,\nu)$ is absolutely continuous in $z \in (z_1, z_2]$ for all $\nu > 0$, and absolutely continuous in $z \in [z_1, z_2)$ for all $\nu < 0$;
2) $\nu f'_z(z,\nu) + f(z,\nu) \in C_b(X)$;
3) $f(z,\nu) \in C_b(\Gamma^-)$.

For further reasoning, we introduce the following function

$$\xi(\nu) = \begin{cases} z_1, \ \nu \in (0,1], \\ z_2, \ \nu \in [-1,0). \end{cases} \tag{5}$$

Thus, the function ξ describes the boundary points of the layer.

Let us assume that $c < 1$ and chouse a constant $\widetilde{c}$ such that $c < \widetilde{c} < 1$. The differential expression $Lf(z,\nu) = \nu f'_z(z,\nu) + \mu(z)f(z,\nu)$ defines a linear operator $L : D(X) \to C_b(X)$. In the space $D(X)$, we introduce the norm:

$$\|\varphi\|_D = \max\left\{\|\varphi\|_{C_b(\Gamma^-)}, \widetilde{c}^{-1} \|L\varphi\|_{C_b(X)}\right\} \tag{6}$$

and notice that the inclusion $D(X) \subset C_b(X)$ holds.

The expressions

$$(A\varphi)(z,\nu) = \frac{1}{\nu} \int\limits_{\xi(\nu)}^{z} \exp\left(-\frac{z-z'}{\nu}\right) \varphi(z',\nu)dz', \tag{7}$$

$$(S\varphi)(z,\nu) = c\int_{-1}^{1} p(\nu,\nu')\varphi(z,\nu')d\nu', \tag{8}$$

$$(Tf)(z,\nu) = (Bf)(\xi(\nu),\nu) \exp\left(-\frac{z-\xi(\nu)}{\nu}\right) + (ASf)(z,\nu) \tag{9}$$

define linear operators $A : C_b(X) \to D(X)$, $S : C_b(X) \to C_b(X)$, and $T : D(X) \to D(X)$.

According to [10], the following statements hold:

Theorem 1. *A function f is a solution of the problem (1),(2), iff it is a solution of the operator equation*

$$f(z,\nu) = f_0(z,\nu) + (Tf)(z,\nu), \tag{10}$$

$$f_0(z,\nu) = \exp\left(-\frac{z-\xi(\nu)}{\nu}\right) h(\xi(\nu)) + (1-c)(Au^4)(z)$$

in the class $D(X)$.

Theorem 2. *Assuming that the inequalities $\|B\| \leq 1$ and $c < 1$ hold, there exists a unique solution of the problem (1),(2) (or of the integral equation (10)) that can be found in the form of the Neumann series*

$$f(z,\nu) = \sum_{k=0}^{\infty} (T^k f_0)(z,\nu) \tag{11}$$

converging in the norm of $C_b(X)$.

Remember that $\|B\| < 1$ in our case, and therefore the conditions of Theorem 2 are satisfied.

4 Recursive algorithm based on the Monte Carlo method

Let us consider the iterative algorithm described in section 2. For computing a solution of the problem (1)-(2) corresponding to a given function $u(z)$, we will describe below a recursive algorithm based on the Monte Carlo method.

We suppose that the conditions of Theorems 2 hold true. Hence, there exists a unique solution of the problems (1)-(2) that can be found in the form of the Neumann series (11). The Monte Carlo method is appropriate for computing the finite sums

$$f_N(z,\nu) = \sum_{n=0}^{N} (T^n f_0)(z,\nu). \tag{12}$$

To implement that, rewrite (12) as the following recurrence relation:

$$f_n(z,\nu) = (Tf_{n-1})(z,\nu) + f_0(z,\nu), \quad n = 1,2,...,N. \tag{13}$$

Let us consider a structure of the operator T (see equation (9)). It contains two summands: the first one describes reflection effects, the second one describes the contribution of scattering effects. Consider the second summand in more detail. Applying simple transformations, we rewrite it in the form

$$I(z,\nu) = c\left(1 - \exp\left(-\frac{z-\xi}{\nu}\right)\right) \times$$

$$\times \int_{\xi}^{z} \int_{-1}^{1} \frac{\exp\left(-(z-z')/\nu\right)}{\nu(1-\exp\left(-(z-\xi)/\nu\right))} p(\nu,\nu') f(z',\nu') d\nu' dz', \tag{14}$$

where $\xi = \xi(\nu)$. According to the Monte Carlo techniques, we can approximate the integral in this expression as the mean value of a random sequence defined by the random variables z' and ν' distributed over the intervals (ξ, z) and $(-1, 1)$ with the densities

$$\frac{\exp(-(z - z')/\nu)}{\nu(1 - \exp(-(z - \xi)/\nu))}, \quad p(\nu, \nu'), \tag{15}$$

respectively. Therefore, the integral (14) is being approximated with the following finite sum:

$$\overline{I}(z, \nu) = \frac{c}{M}\left(1 - \exp\left(-\frac{z - \xi(\nu)}{\nu}\right)\right)\sum_{k=1}^{M} f(z_k, \nu_k).$$

Here, ν_k, z_k, $k = 1, 2, ..., M$ are independent realizations of the random variables z' and ν' distributed over the intervals (ξ, z) and $(-1, 1)$ with the densities (15). Hence, we can approximate the value of the functions $f_n(z, \nu)$, $n = 1, 2, ..., N$, as follows:

$$f_n(z, \nu) \approx \overline{f}_n(z, \nu) = \frac{1}{M}\sum_{k=1}^{M} s_k(z, \nu), \quad \overline{f}_0(z, \nu) = f_0(z, \nu), \tag{16}$$

$$s_k(z, \nu) = \left(B\overline{f}_{n-1}\right)(\xi(\nu), \nu)\exp\left(-\frac{z - \xi(\nu)}{\nu}\right) + \\ + c\left(1 - \exp\left(-\frac{z - \xi(\nu)}{\nu}\right)\right)\overline{f}_{n-1}(z_k, \nu_k) + f_0(z, \nu). \tag{17}$$

Thus, the finite sum (12) can be calculated using the recurrence relations (16), (17).

It should be noted that the above recursive algorithm based on the Monte Carlo method is suitable for the utilization of parallel computing technologies. There are two basic ways for the parallelization of the computing process. First, the calculation of the function f at each point of the layer is performed by a separate thread. Second, the generation of each recursive trajectory of the Monte Carlo method is performed by a separate thread.

5 Implementations of the iterative method

In this section, we consider different approaches to the representation of solutions of the problem (1)-(2), which will allow us to obtain the source term of equation (3) in a convenient form. Let us consider the case of isotropic scattering for certainty. In the first subsection, some modifications of the recursive procedure of the Monte Carlo method are considered. In the second one, a model based on the diffusion approximation of the radiation transfer equation is derived.

5.1 Recursive relations based on the Monte Carlo method for the coupled heat transfer problem

Let us introduce some representations of solutions of the problem (1)-(4) for the implementation of the recursive procedure of the Monte Carlo method.

After integrating equation (3), we obtain

$$u(z) = \sigma \int_0^z q(\zeta) d\zeta + C_1 z + C_2, \tag{18}$$

where $\sigma = 1/N_c$. The constants C_1 and C_2 are defined from the boundary conditions (4):

$$C_1 = d^{-1} \left(U_2 - U_1 - \sigma \int_0^d q(\zeta) d\zeta \right), \quad C_2 = U_1.$$

Then, we can use the Monte Carlo algorithm which is analogous to that described in section 3 for computing the integral summand in the right-hand side of (18). For this end, denote

$$a(z) = \frac{1}{2} \int_0^z \int_{-1}^1 f_N(\zeta, \nu) d\zeta d\nu \approx \frac{1}{2} \int_0^z \int_{-1}^1 f(\zeta, \nu) d\zeta d\nu,$$

where $f_N(z, \nu)$ is defined by (13).

Then, in the first step of the recursive procedure, compute

$$\overline{a}(z) = \frac{z}{M} \sum_{k=1}^{M} \overline{f}_N(z_k, \nu_k), \tag{19}$$

where the random variables z_k and ν_k are uniformly distributed over the intervals $(0, z)$ and $(-1, 1)$, respectively. The following computation of $\overline{f}_n(z, \nu)$, $n = 1, 2, ..., N$, is implemented on the base of formulas (16) and (17).

The *next modification* of the recursive relations is based on different analytical representations of solutions of the coupled heat transfer problem (1)-(4). According to [9], we obtain from equation (1):

$$q'(z) = (1 - c) \left(2u^4(z) - \int_{-1}^1 f(z, \nu) d\nu \right).$$

After substitution of this expression into (3) and the integration, we obtain

$$u(z) = \sigma(1 - c) \int_0^z \int_0^\zeta \left(2u^4(x) - \int_{-1}^1 f(x, \nu') d\nu' \right) dx d\zeta + C_1 z + C_2. \tag{20}$$

The constants C_1 and C_2 are defined from the boundary conditions (4) as follows:

$$C_1 = d^{-1}\left(U_2 - U_1 + \sigma(1-c)\int_0^d\int_0^\zeta\left(2u^4(x) - \int_{-1}^1 f(x,\nu')d\nu'\right)dxd\zeta\right),$$

$$C_2 = U_1.$$

Now, we use the recursive Monte Carlo algorithm for the calculation of the integral of f in the right-hand side of equation (20). For this end, denote

$$b(z) = \frac{1}{2}\int_0^z\int_0^\zeta\int_{-1}^1 f_N(x,\nu)d\nu dxd\zeta \approx \frac{1}{2}\int_0^z\int_0^\zeta\int_{-1}^1 f(x,\nu)d\nu dxd\zeta,$$

where $f_N(z,\nu)$ is defined by (13).

In the first step of the recursive procedure, calculate

$$\overline{b}(z) = \frac{z}{M}\sum_{k=1}^{M} x_k \overline{f}_N(z_k,\nu_k), \tag{21}$$

where the random variables x_k, z_k, ν_k are uniformly distributed over the intervals $(0,z)$, $(0,x_k)$ and $(-1,1)$, respectively. The following calculation of $\overline{f}_n(z,\nu)$, $n=1,2,...,N$, is implemented using formulas (16), (17).

Thus, two kinds of recursive relations based on the Monte Carlo method are proposed. The proposed approaches allow us to avoid the instability that occurs due to differentiating the term $q(z)$ in the right-hand side of equation (4).

5.2 Diffusion approximation for the coupled heat transfer problem

In conclusion, we consider an approach based on a diffusion approximation (also named P_1 approximation) [11]. We represent the function $f(z,\nu)$ by the sum of the two first summands in the Fourier expansion in Legendre polynomials:

$$f(z,\nu) \simeq \phi_0(z) + \nu\phi_1(z). \tag{22}$$

It gives us the following approximation of equation (1):

$$-\phi_0''(z) + 3(1-c)\phi_0(z) = 3(1-c)u^4(z), \tag{23}$$

There are different approaches to the derivation of the boundary conditions for the diffusion approximation (23). Exemplary discussions of this issue can be found in the book [12]. In the present work, we choose the following way: substitute the expansion (22) into the boundary conditions (2) instead of the function $f(z,\nu)$ and integrate (2) over all incoming directions ν of the layer. This yields

$$\varepsilon_1\phi_0(0) - \frac{1}{2}\left(1 + \rho_1^s + \frac{4}{3}\rho_1^d\right)\phi_0'(0) = \varepsilon_1 U_1^4, \tag{24}$$

$$\varepsilon_2\phi_0(d)+\frac{1}{2}\left(1+\rho_2^s+\frac{4}{3}\rho_2^d\right)\phi_0'(d)=\varepsilon_2 U_2^4. \tag{25}$$

Equation (3) is rewritten as follows

$$u''(z)=-\widetilde{\sigma}\phi_0''(z),\quad \widetilde{\sigma}=\frac{1}{3N_c}. \tag{26}$$

Note that the function $\phi_0(z)$ is interpreted here as the function $f(z,\nu)$ averaged over all directions ν.

From equation (26), we obtain

$$u(z)=-\widetilde{\sigma}\phi_0(z)+C_1 z+C_2. \tag{27}$$

The constants C_1 and C_2 are defined from the boundary conditions (4) as follows:

$$C_1=d^{-1}(U_2-U_1+\widetilde{\sigma}(\phi_0(d)-\phi_0(0))),$$

$$C_2=U_1+\widetilde{\sigma}\phi_0(0).$$

Thus, the coupled problem (1)-(4) is reduced to the system of equations (23)-(25), and (27).

In the next section, we present the results of numerical experiments based on the above proposed approaches.

6 Numerical experiments

Numerical experiments are carried out for two problems considered by C.E. Siewert and J.R. Thomas in [7, 8] where the simple iteration procedure [7] and Newton's iteration method [8] combined with a computationally stable version of the P_N approximation have been used. In both cases, the following values of parameters are taken: $c=0.9$, $d=3$, $U_1=1$, $\rho_1^s=0.1$, $\rho_1^d=0.2$, $\varepsilon_1=0.7$, $U_2=0.5$, $\rho_2^s=0.3$, $\rho_2^d=0.1$, and $\varepsilon_2=0.6$. The difference between the two considered problems consists in the value of the conduction-to-radiation parameter N_c. The calculations are implemented for N_c equals 0.05 and 0.00001. The last value of N_c corresponds to the case of high-temperature transfer.

Figure 1 presents the following approximations of the temperature $u(z)$ ($N_c=0.05$): first, computed on the basis of the Monte Carlo recursive algorithm (16),(17), and (19); second, computed on the basis of the diffusion approximations (23)-(25), and (27); and third, obtained by C.E. Siewert and J.R. Thomas [7]. For the implementation of the Monte Carlo method, the following values are taken: the number of the summands of the Neumann series, $N=14$; the number of the generated trajectories, $M=10000$. The diffusion approximation is implemented with the Maple 9.5. For both approaches, 20 steps of the iterative algorithm are used. The parameter α of the simple iteration method is chosen to be equal 0.5. As it can be seen, all approximations are close enough to each other.

In experiments presented in Figure 2, all the parameters are the same as in the previous case excepting for $N_c = 0.00001$. This corresponds to higher temperatures compared with the previous case. In the implementation of the numerical method, 500 steps of the iterative procedure are used. The parameter α of the simple iteration method is chosen to be equal 0.0001. It is seen that the deviation of the temperature curves is more essential than in Figure 1. Nevertheless, the diffusion approximation describes the behavior of the temperature properly. Thus, it can be successfully applied to various heat transfer problems which are not require obtaining very high accuracy.

Figure 3 shows numerical experiments that demonstrate the convergence of the iterative procedure based on the Monte Carlo method when $N_c = 0.00001$. The plots correspond to 50 steps, 150 steps and 500 steps of the iterative procedure, respectively.

Figure 4 shows numerical experiments ($N_c = 0.00001$) that demonstrate an instability of the iterative procedure based on the Monte Carlo method. This instability occurs in the case of insufficient number of the trajectories, $M = 2000$. The plots correspond to 300 and 900 steps of the iterative procedure. A similar effect is observed in the case of utilizing the diffusion approximation when few decimal places were used in the computation.

The presented calculations are implemented on a computer cluster of the Technical University of Munich using the technology of parallel computing supported by the application programming interface OpenMP

7 Conclusion

The different approaches for computing solutions of nonlinear coupled radiative-conductive heat transfer problems are considered. Recursive procedures based on the Monte Carlo method are proposed. The advantage of this approach is the high accuracy of the algorithms and the possibility of using parallel computing technologies.

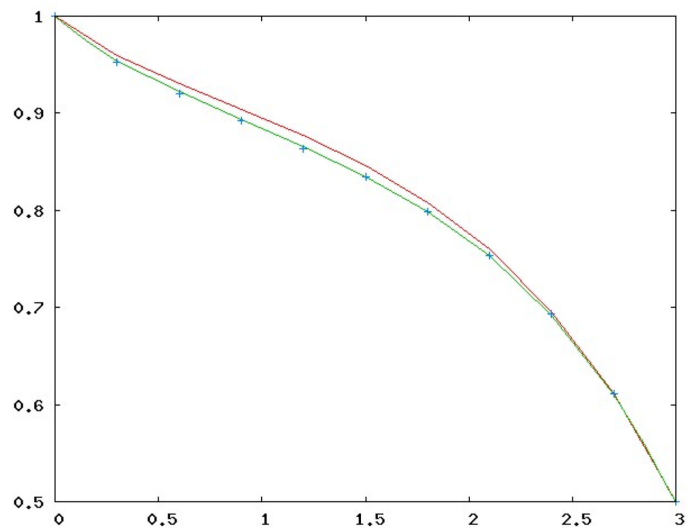

Fig. 1. The results of numerical simulation for $N_c = 0.05$ after 20 steps of the iterative algorithm based on the Monte Carlo method (red); diffusion approximation (green); comparison with Siewert's data (+).

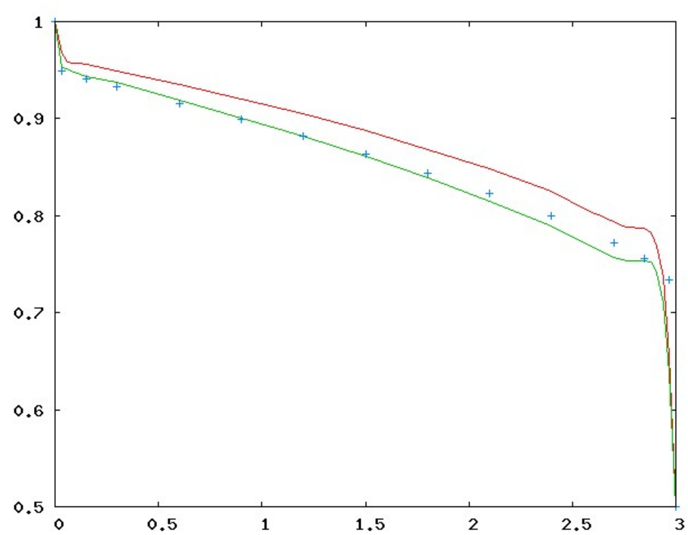

Fig. 2. The results of numerical simulation for $N_c = 0.00001$ after 500 steps of the iterative algorithm based on the Monte Carlo method (red); diffusion approximation (green); comparison with Siewert data (+).

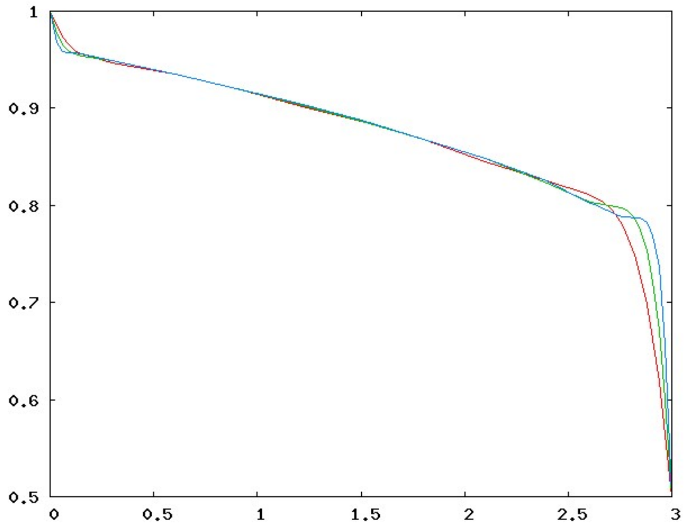

Fig. 3. The numerical experiments, $N_c = 0.00001$, demonstrating a convergence of the iterative procedure based on the Monte Carlo method. The plots correspond to 50 steps (red), 150 steps (green) and 500 steps (blue) of the iterative procedure.

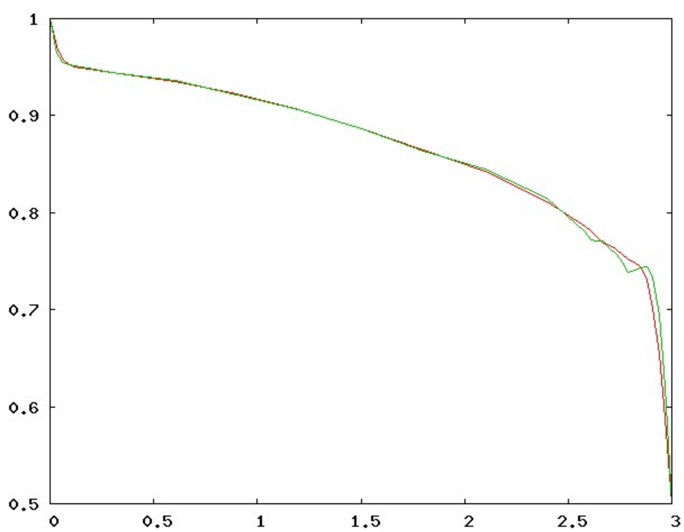

Fig. 4. The numerical experiments, $N_c = 0.00001$, demonstrating instability of the iterative procedure based on Monte Carlo method. This instability occurs in the case of insufficient number of trajectories. The plots correspond to 300 steps (red) and 900 steps (green) of the iterative procedure.

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