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# The Diffusion Equation with Piecewise Smooth Initial Conditions

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## ABSTRACT

In this paper we consider an initial-value problem for diffusion equation in three dimensional Euclidean space. The initial value is a piecewise smooth function. To solve this problem we apply Fourier transform method and since Fourier integrals of a piecewise smooth function do not converge everywhere, we make use of Riesz summation method.

Keywords: the diffusion equation, Fourier integrals, Riesz summation method, piecewise smooth functions.

AMS 2000 Mathematics Subject Classifications: Primary 42B08; Secondary 42C14.

## INTRODUCTION

The problem which we investigate in this paper is connected with ecology, namely with the spreading of pollution. Suppose that we want to place a new pollution source with a given intensity and we need to predict future ecological situation. Hence one should consider the diffusion equation with piecewise smooth initial conditions in order to study the front of propagation of polluted air.

We consider three dimensional Euclidean space $R^3$ and denote its points by $x=(x_1,x_2,x_3)$ . Let $\Omega\subset R^3$ be a domain where we want to consider our problem. Usually one considers a short time period, such that within this period a polluted air does not reach the boundary of $\Omega$. So we may assume that $\Omega$ is infinitely big and coincides with the whole space $R^3$. If we denote a front of polluted air by $u(x,t)$ and a domain where we place the pollution source by $D$, then in order to calculate $u(x,t)$ we will have the following initial-value problem for the diffusion equation:

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x_1^2}+\frac{\partial^2 u}{\partial x_2^2}+\frac{\partial^2 u}{\partial x_3^2},\ x\in R^3, t>0, \tag{1}$$

$$u(x,0) = f(x), \ \ x \in R^3, \tag{2}$$

where $f(x)$ is a smooth function within the bounded domain D and $f(x) = 0$ otherwise. We denote the boundary of $D$ by $\Gamma$ and suppose that it is smooth. The functions which are smooth on $D \cup \Gamma$ and vanish outside of $D \cup \Gamma$ are said to be *piecewise smooth* functions. It is useful to normalize the functions through dividing their values on the boundary by 2.

If we make use of the Fourier method (the separation of variables method) to solve problem (1) and (2) then we shall have the following formal solution:

$$u(x,t) = \int_{R^3} e^{-t|\xi|^2} g(\xi) e^{i\xi x} \, d\xi, \tag{3}$$

where $g(\xi)$ is an unknown function. Note that function (3) satisfies the diffusion equation. Now we put (3) into the initial condition (2), and formally have

$$u(x,0) = \int_{R^3} g(\xi) e^{i\xi x} \, d\xi = f(x). \tag{4}$$

From the Fourier theory point of view we get $g(\xi) = \hat{f}(\xi)$, where $\hat{f}(\xi)$ is the Fourier transform of $f$ :

$$\hat{f}(\xi) = \left(\frac{1}{2\pi}\right)^3 \int_{R^3} f(\xi) e^{-ix\xi} d\xi.$$

But the point is that we do not know whether or not the integral in (4) converges at every point $x \in R^3$.

Now we may formulate the problem as follows. Let $f(x)$ be an arbitrary piecewise smooth function. Does the following equality

$$\lim_{\lambda \to \infty} \int_{|\xi|^2 < \lambda} \hat{f}(\xi) e^{ix\xi} d\xi = f(x) \tag{5}$$

hold at every point where $f$ is smooth (obviously it does hold in $L_2$ norm by Plancherel's theorem).

Our main goal in this paper is to give a rigorous substantiation for the Fourier method usage to solve diffusion equation with piecewise smooth initial conditions. For this purpose we examine a typical case when the convergence of integral (5) cannot be observed because of the so called the Pinsky phenomenon. Then employing Riesz summation method we show that the problem of divergence can be overcome and finally we present a numerical solution of the corresponding initial-value problem that can be built using the Fast Gauss transform.

## THE PINSKY PHENOMENON

Let $f$ be an arbitrary piecewise smooth function. We investigate the limit

$$\lim_{\lambda\to\infty} \int_{|\xi|^2<\lambda} \hat{f}(\xi) e^{ix\xi} d\xi. \tag{6}$$

In a two-dimensional case, as proved by Il'in (1956) (for further investigations of this question see Alimov (2003)), this limit exists everywhere. However as we can see in simple examples, for higher dimensions this is not the case. The detailed analysis of this limit at $x = 0$ was carried out by Pinsky (1993). We formulate his theorem in three dimensional case.

**Theorem 1.** *Let $f(x)$ be a piecewise smooth function supported on a closed ball $\{x \in R^3 : |x| \le a\}$, $a > 0$. Then limit (6) is equal to $f(0)$ at the origin if and only if*

$$\oint_{|x|=a} f(x)\, d\sigma(x) = 0.$$

This is the first theorem of "if and only if" type that describes the convergence of multiple Fourier integrals (6). It is for this reason that in the mathematical literature this Pinsky's result is called "phenomenal".

As it follows from this theorem, if a piecewise smooth function does not change its sign along ball's boundary, then (6) does not exist at the origin. To examine this we consider a simple function. Let $f(x)$ be the characteristic function of a unit ball normalized along its boundary, i.e. $f(x)=1$, if $|x|<1$; $f(x)=1/2$, if $|x|=1$ and $f(x)=0$ otherwise. In the present case the divergence stated in Theorem 1 can be derived straightforwardly. Indeed

$$\hat{f}(\xi)=\frac{1}{(2\pi)^2}\left(\frac{\cos|\xi|}{|\xi|^2}-\frac{\sin|\xi|}{|\xi|^3}\right) \tag{7}$$

and therefore

$$\int_{|\xi|^2<\lambda}\hat{f}(\xi)d\xi=-\frac{2}{\pi}\int_0^{\lambda}\left[\cos r-\frac{\sin r}{r}\right]dr=1-\frac{2}{\pi}\sin\lambda+o(1),$$

as $\lambda\to\infty$. The oscillation is depicted in Figure 1.

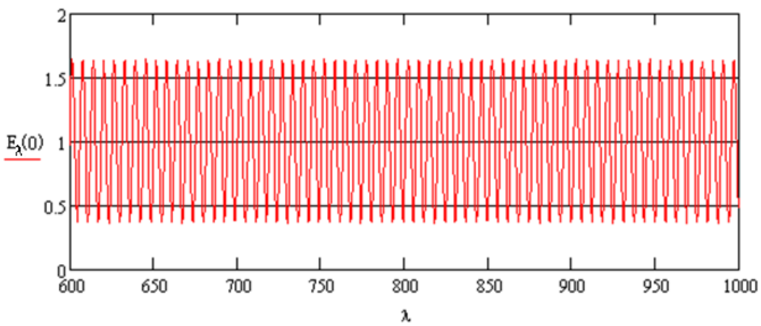


Figure 1: The Fourier Integral divergence at the origin

It is necessary to note that at any other inner point of the ball the convergence of limit (6) does take place. The general behavior of (6) is illustrated in Figure 2 by the example of the points $\{x:|x|=1/2\}$. At this computation result we can see that the corresponding values tend to 1 as $\lambda$ increases.

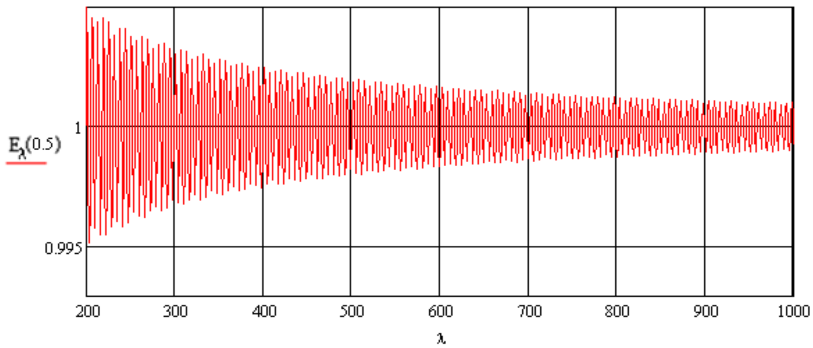


Figure 2: The Fourier Integral convergence by example of the points {x: |x|=1/2}

## THE RIESZ MEANS

If we consider an arbitrary piecewise smooth function, then due to the Pinsky phenomenon, limit (5) does not exist for all points. Therefore we must employ some summation method in order to solve initial-value problem (1) and (2). In this paper we consider the Riesz means of the form

$$E_\lambda^s f(x) = \int\limits_{|\xi|^2<\lambda} \left(1-\frac{|\xi|^2}{\lambda}\right)^s \hat{f}(\xi)e^{i\xi x}\, d\xi.$$

Obviously, the Riesz means of order $s=0$ coincide with ordinary partial integral sums, similar to (5). It is known that the higher the index $s$ the more points there are where $E_\lambda^s f(x)$ converges to $f(x)$. In particular, if $N$ is space dimension and $s>\frac{N-3}{2}$, then $E_\lambda^s f(x)$ uniformly converges to $f(x)$ at any compact domain where $f(x)$ is smooth (see Ashurov (2008)).

Moreover, $E_\lambda^s f(x)$ pointwisely converges at discontinuity points as well (see e.g. Brandolini and Colzani (2000)). Therefore in our three dimensional case the convergence will take place for any positive $s$. Hence the Riesz summation method may be used to solve the initial-value problem (1) and (2).

Let $s=1$ then the Riesz means' convergence for characteristic function at the origin can be shown directly. Recalling (7), we have

$$E_\lambda^1 f(0) = -\frac{2}{\pi}\int_0^\lambda \left(\frac{\cos r}{r^2} - \frac{\sin r}{r^3}\right)\left(1-\frac{r^2}{\lambda}\right) r^2\, dr$$

$$= -\frac{2}{\pi}\int_0^\lambda \left(1-\frac{r^2}{\lambda}\right)\cos r\, dr + \frac{2}{\pi}\int_0^\lambda \frac{\sin r}{r}\left(1-\frac{r^2}{\lambda}\right) dr.$$

Simple calculation shows that the first term is of the form $\text{Const}\times(\cos\lambda - 1)/\lambda$ and the second one is $1-\alpha(\lambda)-(\cos\lambda-1)/\lambda$, where $\alpha(\lambda)\to 0$ as $\lambda\to\infty$. The behavior of the sum as $\lambda$ increases is presented in Figure 3.

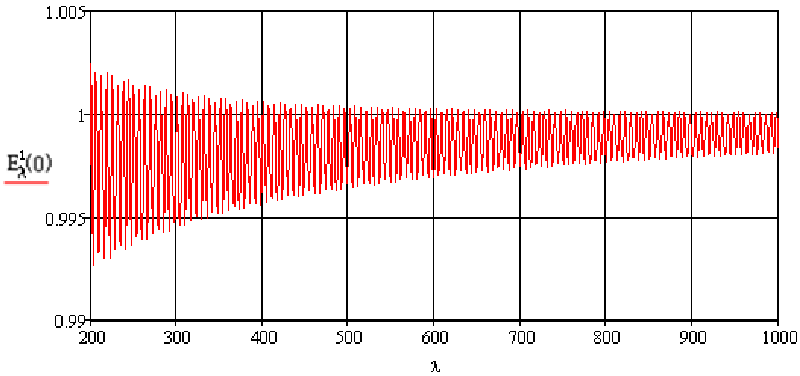


Figure 3: The Riesz means convergence at the origin

## SOLUTION

Now we arrive at to the point where we are able to construct the solution of initial-value problem (1) and (2). As we have seen, we cannot use standard formula (3) with piecewise smooth functions, since it may lead to the divergence of integral partial sums (5).

Therefore we consider the function

$$u_\lambda(x,t) = \int\limits_{|\xi|^2<\lambda} \left(1 - \frac{|\xi|^2}{\lambda}\right) e^{-t|\xi|^2} \hat{f}(\xi) e^{i\xi x}\, d\xi.$$

As it follows from the generalized superposition principle, $u_\lambda(x,t)$ satisfies Equation (1). Now we shall show that the solution can be obtained as

$$u(x,t) = \lim_{\lambda\to\infty} u_\lambda(x,t)$$

We note that the Fourier transform for Gaussian $g_t(x) = e^{-t|x|^2}$ is $\hat{g}_t(\xi) = (2\pi)^{-n} (\pi/t)^{n/2} e^{-|\xi|^2/(4t)}$. Therefore we have

$$u(x,t) = \lim_{\lambda\to\infty} \int\limits_{|\xi|^2<\lambda} \left(1 - \frac{|\xi|^2}{\lambda}\right) (f * \phi_t)(\xi) e^{i\xi x}\, d\xi, \tag{8}$$

where $\phi_t(x) = (4\pi t)^{-n/2} e^{-|x|^2/(4t)}$ if $t > 0$, and $\phi_0(x) = \delta(x)$ is Dirac's function.

It is easy to see that

$$u(x,t) = \lim_{\lambda\to\infty} E_\lambda^1 (f * \phi_t)(x)$$

If $t > 0$ the function $f * \phi_t(x)$ is a smooth function in $R^3$ and as we have mentioned its Riesz means converge uniformly to $f * \phi_t(x)$. Moreover if $t = 0$ then $f * \phi_0(x) = f(x)$ and the corresponding Riesz means also pointwisely converge at each point in $R^3$. Hence $u(x,t)$ defined by (8) satisfies condition (2). This fact proves the validity of Fourier's method for diffusion equation with piecewise smooth initial conditions. Therewith, we have shown that the solution has the following form

$$u(x,t) = \int\limits_{R^3} f(y) \phi_t(x-y)\, dy$$

There are several ways to calculate this type of convolution. Usually one deals with a discretized model

$$u^P(x,t) = \left(\frac{2}{P}\right)^3 \sum_{\|k\|<P} f(k/N)\phi_t(x-k/N)\,,$$

where $\|k\|<P$ is the set $\{k=(k_1,k_2,k_3): |k_j|<P,\, j=1,2,3\}$ .

In this research we employed the Fast Gauss Transform algorithm developed by Greengard and Strain, (1989) with $P = 300$ . The solution (8) for the characteristic function of the unit ball is described by Figure 4 and Table 1.

TABLE 1: The solution $u(x,t)$ for time moments

$T0=0; T1=0.01; T2=0.2; T3=1; T4=5$

| *x* | *T0(x)* | *T1(x)* | *T2(x)* | *T3(x)* | *T4(x)* |
|---|---|---|---|---|---|
| -5 | 0 | 0,0000000001 | 0,0000000002 | 0,0007514067 | 0,0306470985 |
| -4,5 | 0 | 0,0000000022 | 0,0000000034 | 0,0022314433 | 0,0386656875 |
| -4 | 0 | 0,0000000859 | 0,0000001428 | 0,0058975536 | 0,0476408491 |
| -3,5 | 0 | 0,0000002817 | 0,0000060107 | 0,0138794977 | 0,0572540081 |
| -3 | 0 | 0,0000003749 | 0,0001413764 | 0,0291023611 | 0,0671409419 |
| -2,5 | 0 | 0,0000010047 | 0,0018890125 | 0,0543953927 | 0,0768289101 |
| -2 | 0 | 0,0000041382 | 0,0146189413 | 0,0906744905 | 0,0857863342 |
| -1,5 | 0 | 0,0000096637 | 0,0673138337 | 0,1348597700 | 0,0934691179 |
| -1 | 1 | 0,0644142739 | 0,1910925464 | 0,1790223725 | 0,0993745299 |
| -0,5 | 1 | 0,4574745274 | 0,3485861618 | 0,2121654435 | 0,1030953705 |
| 0 | 1 | 0,6141258606 | 0,4237894606 | 0,2245204032 | 0,1043663529 |
| 0,5 | 1 | 0,4574745274 | 0,3485861618 | 0,2121654435 | 0,1030953705 |
| 1 | 1 | 0,0644142739 | 0,1910925464 | 0,1790223725 | 0,0993745299 |
| 1,5 | 0 | 0,0000096637 | 0,0673138337 | 0,1348597700 | 0,0934691179 |
| 2 | 0 | 0,0000041382 | 0,0146189413 | 0,0906744905 | 0,0857863342 |
| 2,5 | 0 | 0,0000010047 | 0,0018890125 | 0,0543953927 | 0,0768289101 |
| 3 | 0 | 0,0000003749 | 0,0001413764 | 0,0291023611 | 0,0671409419 |
| 3,5 | 0 | 0,0000002817 | 0,0000060107 | 0,0138794977 | 0,0572540081 |
| 4 | 0 | 0,0000000859 | 0,0000001428 | 0,0058975536 | 0,0476408491 |
| 4,5 | 0 | 0,0000000022 | 0,0000000034 | 0,0022314433 | 0,0386656875 |
| 5 | 0 | 0,0000000001 | 0,0000000002 | 0,0007514067 | 0,0306470985 |

There are five graphics of $u(x,t)$ for time moments $T0 = 0;\ T1 = 0.01;\ T2 = 0.2;\ T3 = 1;\ T4 = 5$ . Note that the characteristic function *f(x)* is radial, i.e. the function's value at any point depends on the distance from the origin, and therefore a solution of the initial-value problem (1) and (2) will also be radial. Thereby, Figure 4 can be considered as the projection of $u(x,t)$ values to any $x$-coordinate.

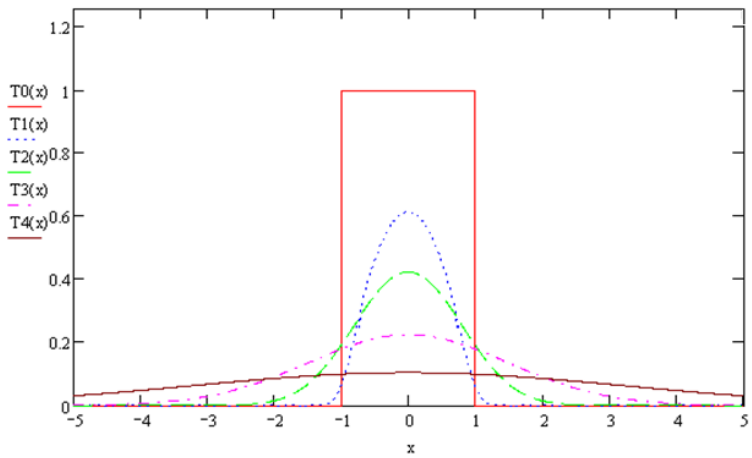


Figure 4: The solution for indicator function for the moments
T0 = 0, T1= 0.01, T2= 0.2, T3= 1, T4= 5

## CONCLUSIONS

We studied the diffusion equation with piecewise smooth initial conditions and gave a rigorous substantiation for the Fourier method usage to solve diffusion equation with piecewise smooth initial conditions. For this purpose we examined a typical case when the convergence of the Fourier integral could not be observed. Employing Riesz summation method we then showed that the problem of divergence could be overcome and finally presented the solution of the corresponding initial-value problem using the Fast Gauss transform.

According to Table 1 and Figure 4, there is a particular moment $t$ for every coordinate $x$ when the value $u(x,t)$ reaches its peak. For points $x : |x| \leq 1$ it is of course the moment $t = 0$ while for the points $1 < |x| \leq 2$ the function reaches its maximum value between $t = 1$ and $t = 5$ . These peak values are important in the context of the application of the solution. For example, we may assume that the units of measurement are chosen in such a way that 0.1 units of pollution in the air may cause hazardous effects on human's health. Then we can see that in this simple model at the distance of 2 the concentration of polluted air does not exceed its critical value and therefore this distance can be considered as a safe one.

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