Abstract: We extend the fundamental solutions method into the case of the Cauchy problem for the systems of heat equations on the real axis. We use an approach the fundamental solution of which is replaced by fundamental matrix. Vector function approximation problem appears by using a weighted sum of the fundamental kernel matrices. A weighted sum is understood as the sum of product for the fundamental kernel matrices and the unknown weighted vector coefficients. Setting weighted vector coefficients, center and window width of each Gaussian carried out by the method of least squares. We consider one more way of vector function approximation. This method consists in the fact that we replace the vector Cauchy problem into n disjoint Cauchy problems, then we find an approximation of each scalar problem and the solution of a vector problem. Vector Cauchy problem for the heat equation on the real line with n division points to a multilayer medium is solved. Initial conditions are approximated by a weighted sum of the fundamental kernel matrices satisfying conjugate conditions. The fundamental matrix on the right infinite interval is chosen to be the fundamental matrix for single occasion. The fundamental matrix is uniquely determined by conjugate conditions on the remaining intervals.

Key Words: fundamental solution, fundamental matrix, kernel basis function, Gaussian, approximation of functions

1. Introduction

The method of approximation with basic functions plays an important role in
most of the areas concerning computational science and technology. Approximation of data is an important component in the processing and numerical solving of differential equations. Traditionally, in approximation, coordinate functions are used as the basis, such as polynomial and trigonometric functions. At present, radial basis functions (RBF) are popular for approximating data and solving boundary value problems described by partial differential equations [1], [2], [3], [4].

The feature of RBF method is that, they are built in terms of one variable — distance. RBF method has obvious advantages over the traditional polynomial basic functions. A special case that concerns the method of RBF approximation is the method of fundamental solutions (MFS) using fundamental solutions as basis functions.

The Cauchy problem for the heat equation on the real axis has the form

\[ \begin{align*}
  u_t &= a^2 u_{xx}, \quad x \in (-\infty, \infty), \quad 0 < t \leq T, \\
  u(0, x) &= f(x).
\end{align*} \tag{1} \]

We consider the fundamental basis functions, the kernels of which are generated from the fundamental solution of the heat equation. The fundamental solution also known as the heat kernel which is the solution of the heat equation corresponding to the initial condition of the initial point source of the heat in a known position at the point \( y \). The heat kernel is a solution of the Cauchy problem

\[ \begin{align*}
  u_t &= a^2 u_{xx}, \quad x \in (-\infty, \infty), \quad 0 < t \leq T, \\
  u(0, x) &= \delta(x - y),
\end{align*} \tag{2} \]

A point source of heat at the point \( y \) is given by the Dirac function \( \delta(x - y) \). The Heat kernel as a solution of problem (1) has the form:

\[ G(t, x - y) = \frac{1}{2a\sqrt{\pi t}} \exp \left(-\frac{(x - y)^2}{4a^2t}\right). \]

### 2. Fundamental Solution as Gaussian

If we choose \( a = \frac{1}{2} \), then the fundamental solution with accuracy is up to a multiplier \( \frac{1}{2\sqrt{\pi t}} \) is leading to Gaussian [1]. And \( y \) is considered as a center, \( \sqrt{t} \) is the width of Gaussian. Multiplier \( \frac{1}{2\sqrt{\pi t}} \) we will refer to the corresponding weighted coefficient. The heat kernels can be used to find the general solution of the heat equation. You can get a general solution of the Cauchy problem...
for one-dimensional heat equation by applying the convolution. The solution of the homogeneous Cauchy problem (1) gives the integral formula that is called Poisson integral

\[
\begin{align*}
u(t, x) &= \frac{1}{2a\sqrt{\pi t}} \int_{-\infty}^\infty \exp\left(-\frac{(x - y)^2}{4a^2 t}\right) f(y) dy, \quad (3)
\end{align*}
\]

To calculate the integral in (3), we apply the quadrature formula (Mysovskih, 1981). A quadrature formula is any simple formula approximating a single integral,

\[
\int_{-\infty}^{\infty} g(y) \, dy \approx \sum_{j=1}^{N} c_j g(y_j), \quad (4)
\]

where \(x_j\) — nodes of the quadrature formula, and \(c_j\) — coefficients of the quadrature formula. In quadrature formulas there is a huge amount of views: Gauss, Chebyshev, Simpson, etc., but any of them has the form (4). For the right part of formula (3) the quadrature formula will take the form

\[
\begin{align*}
u(t, x) &\approx \frac{1}{2a\sqrt{\pi t}} \sum_{j=1}^{N} \exp\left(-\frac{(x - y_j)^2}{4a^2 t}\right) w_j, \\
w_j &= f(y_j) c_j.
\end{align*}
\]

Given that for small values of \(t\) the equality is true \(u(t, x) \approx f(x)\) we will obtain, for sufficiently small \(t\), the approximate formula,

\[
\begin{align*}
f(x) &\approx \frac{1}{2a\sqrt{\pi t}} \sum_{j=1}^{N} \exp\left(-\frac{(x - y_j)^2}{4a^2 t}\right) w_j.
\end{align*}
\]

The problem of finding the best values for \(x_j\) — nodes of the quadrature formula, and \(w_j\) — coefficients, as well as the choice of the optimal value of \(t\), leads to the problem of approximating the function by Gaussians. Thus, the fundamental solutions of the heat equation are used as fundamental functions.

3. Approximation of the Cauchy Problem Solution by Gaussians

Next, we will consider a more general problem - the Gaussian approximation with a variable width of window \(\sqrt{t}\), i.e. in the form

\[
\begin{align*}
f(x) &\approx \frac{1}{2a\sqrt{\pi t_j}} \sum_{j=1}^{N} \exp\left(-\frac{(x - y_j)^2}{4a^2 t_j}\right) w_j, \quad (5)
\end{align*}
\]
The approximation problem (5) is well studied. There are standard algorithms for solving it, [1].

Let the approximations of the initial condition be found by the weighted sums of Gaussians,

\[
f(x) \approx \sum_{k=1}^{N} \frac{1}{2a\sqrt{\pi\tau_k}} \exp \left( -\frac{(x - y_k)^2}{4a^2\tau_k} \right) w_k,
\]

then it would be possible to write out the solution of the Cauchy problem (1) in the form

\[
u(t, x) \approx \sum_{k=1}^{N} \frac{1}{2a\sqrt{\pi(t + \tau_k)}} \exp \left( -\frac{(x - y_k)^2}{4a^2(t + \tau_k)} \right) w_k.
\]

(6)

Remark. Formula (6) is obtained without any computation, based on the uniqueness theorem for solving the Cauchy problem:

First, the right part in (6) is presenting a solution of heat equation, as a linear combination of fundamental solutions,

Secondly, from (6) it follows that,

\[
u(0, x) \approx \sum_{k=1}^{N} \frac{1}{2a\sqrt{\pi(\tau_k)}} \exp \left( -\frac{(x - y_k)^2}{4a^2(\tau_k)} \right) w_k \approx f(x).
\]

Thus, the heat equation is performed precisely, and the initial condition is fulfilled with a given accuracy. In fact, the right part of formula (6) satisfies the heat equation as a linear combination of fundamental solutions. The initial condition is satisfied by construction. From the Poisson formula, it follows that if approximation of the initial condition is found with a given accuracy \(\varepsilon\) in a uniform metric,

\[
\max_x |f(x) - \sum_{k=1}^{N} \frac{1}{2a\sqrt{\pi\tau_k}} \exp \left( -\frac{(x - y_k)^2}{4a^2\tau_k} \right) w_k| < \varepsilon
\]

then with same accuracy \(\varepsilon\) the approximation of the Cauchy problem solution will be obtained with a uniformed time \(t\).

\[
\max_x \left| u(t, x) - \sum_{k=1}^{N} \frac{1}{2a\sqrt{\pi(t + \tau_k)}} \exp \left( -\frac{(x - y_k)^2}{4a^2(t + \tau_k)} \right) w_k \right| < \varepsilon, \forall t > 0.
\]
4. Results and Discussions

4.1. Vector Cauchy Problem on the Real Axis

In this work we extend the fundamental basis function method [6] to the case of Cauchy problem for the systems of heat equations on the real axis

\[ u_t' = A^2 u_{xx}, x \in (-\infty, \infty), 0 < t \leq T, \]
\[ u(0, x) = f(x), \]

(7)

here \( A \) — square matrix of size \( m \times m \), \( f(x) \) — a given vector-function of size \( m \times 1 \), \( u(t, x) \) — unknown vector-function of size \( m \times 1 \). Thus, we consider \( m \)-component problem. We will notice that if the matrix \( A \) is a diagonal one, then we obtain \( m \) non-coupled Cauchy problems.

Systems of differential equations arise in the modeling of several parameters, related to each other. For example, in the problems of thermopaste (temperature + elasticity) and thermoplasticity. The most common are two-component models, three component models sometimes [7]. We apply an approach, the fundamental solution of which is replaced by a fundamental matrix,

\[ G(t, x, y) = \frac{A^{-1}}{2\sqrt{\pi t}} \exp \left( -\frac{(x-y)^2}{4t} A^{-2} \right). \]

Matrix \( A^{-1} \) is the inverse of the matrix \( A \). The function of the matrix is usually defined as a series for the exponent,

\[ \exp(A) = \sum_{j=0}^{\infty} \frac{A^j}{j!}, \]

If the known eigenvalues of the matrix \( A \) are simple then each element of the matrix \( \exp(A) \) is calculated as a linear combination of the exponential function of eigenvalues. (Computations can be carried out automatically in Maple or Malab)

There arises the problem of approximating the vector-function \( f(x) \) with the help of weighted sum of kernel fundamental matrices

\[ f(x) \approx \sum_{k=1}^{N} G(t_k, x, y_k) w_k. \]

(8)
We choose the sampling points $x_j, j = 1, ..., K$ then we minimize the square deviation (standard deviation (SD)) of the vector-function

$$
\sum_{j=1}^{K} \left\| f(x_j) - \sum_{k=1}^{N} G(t_k, x_j, y_k) w_k \right\|^2.
$$

The norm of the vector is defined as $\|f\|^2 = \sum_{k=1}^{m} \|f_k\|^2$, $f_k$ — k-th coordinate of vector f. Thus, we have the well-known problem of minimizing the error functional. Note that each Gaussian matrix depends on $m + 2$ parameters ($m$—the number of unknowns, $A$ — matrix of coefficients to the system of equations in the Cauchy problem (7)). The weighted sum is understood as the sum of the products of kernel fundamental matrices for the unknown weighted vector coefficients $w_k$.

The setting of the weighted vector coefficients, centers and width of windows for each ones of Gaussians is performed by the method of least squares.

**Remark.** Usually, when solving vector problems, each component of the vector function $f(x)$ is getting approximated separately. Through this, it’s required to setup the $3Nm$ parameters. We approximate the vector function $f(x)$ immediately. This requires setting up the $N(2 + m)$ parameters. So for the two-component systems it is required to compute parameters in one and a half times less. Let the approximations of the initial conditions be found by the weighted sums of the matrix Gaussians,

$$
f(x) \approx \sum_{k=1}^{N} \frac{a^{-1}}{2a \sqrt{\pi \tau_k}} \exp \left(-\frac{(x - y_k)^2}{4 \tau_k a^{-2}}\right) w_k,
$$

then it would be possible to write out immediately the solution of the vector Cauchy problem (7)

$$
u(t, x) \approx \sum_{k=1}^{N} \frac{a^{-1}}{2a \sqrt{\pi (t + \tau_k)}} \exp \left(-\frac{(x - y_k)^2}{4(t + \tau_k) a^{-2}}\right) w_k.
$$

In fact, the right part of formula (10) satisfies the system of heat conduction equations as a linear combination of the matrix fundamental solutions. The initial condition is satisfied by construction.

### 4.2. Vector Cauchy Problem for the Heat Equation on the Real Axis with Division Points for a Multilayer Medium

Since the 80-s, the interest for study in the composite materials has increased. Mathematically, multicomponent models of physical fields in a multilayered
medium lead to the need for considering separate systems of partial differential equations (that is, systems whose coefficients vary from a layer to a layer). As an example, we consider a vector-separated system of heat equations

\[ u_{it} = A_i^2 u''_{ixx}, x \in (l_{i-1}, l_i), 0 < t \leq T, \]
\[ i = 1, \ldots, n + 1; l_0 = -\infty, l_{n+1} = \infty \] (10)

by initial conditions

\[ u_i(0, x) = f_i(x), x \in (l_{i-1}, l_i), \]
\[ i = 1, \ldots, n + 1 \] (11)

and by the vector conjugate conditions at the points of conjugation

\[ u_i(t, l_i) = u_{i+1}(t, l_i), \]
\[ \Lambda_i u'_{i,x}(t, l_i) = \Lambda_{i+1} u'_{i+1,x}(t, l_i), \quad i = 1, \ldots, n \] (12)

where

\[ \Lambda_i = \begin{pmatrix} \lambda_{i1} & \ldots & 0 \\ \ldots & \ldots & \ldots \\ 0 & \ldots & \lambda_{im} \end{pmatrix}, i = 1, \ldots, n. \]

The initial conditions (10) define the initial state of each component at each of n+1 layers. Vector conjugate conditions (12) argue that all components and their gradients are continuous at each point of conjugation.

4.3. The Error Functional. Gradient Algorithm

The solution of the Cauchy problem (9-11) can be found in the form

\[ u_i(t, x) = \sum_{k=1}^{N} \frac{A_i^{-1}}{2\sqrt{\pi}(t + \tau_k)} \exp \left( -\frac{A_i^{-2}(x - y_k)^2}{4(t + \tau_k)} \right) w_k. \] (13)

The setting of the weighted vector coefficients, the center and width window of each Gaussian are performed using the method of least squares using RBFNN [1]. The error functional I has the form

\[ I = \lambda \sum_{j=1}^{K} \sum_{i=1}^{n+1} \| u_i(0, x_{ij}) - f_i(x_{ij}) \|^2 + \mu_1 \sum_{j=1}^{M} \sum_{i=1}^{n} \| u_i(t_j, l_i) - u_{i+1}(t_j, l_i) \|^2 \\
+ \mu_2 \sum_{j=1}^{M} \sum_{i=1}^{n} \| \Lambda_i u'_{i,x}(t_j, l_i) - \Delta_{i+1} u'_{i+1,x}(t_j, l_i) \|^2, \]
where \(x_{ij} \in (l_{i-1}, l_i)\), \(t_j \in (0, T)\), — sampling points, \(\lambda, \mu_1, \mu_2\) — penalty coefficients, \(K\) — the number of sampling points to the space variable \(x_{ij}\), \(M\) the number of sampling points to a time variable \(t_j\). The number \(n+1\) is the number of layers (a model of a composite body, for example, different alloys of Fe, Ni, Cu, etc.). The second and third terms in the formula for the functional of errors arise from the conjugate conditions (12). The minimum of the error functional is determined by the error gradient algorithm [1].

### 4.4. Comparison of MFS and RBF Methods

The error functional \(I\) for the RBF method [1] has the form

\[
I = \sum_{j=1}^{L} \sum_{i=1}^{n+1} \left| u_{i,t}^j(t_j, x_{ij}) - A_j^2 u_{i,xx}^j(t_j, x_{ij}) \right|^2 \\
+ \lambda \sum_{j=1}^{K} \sum_{i=1}^{n+1} \left| u_i(0, x_{ij}) - f_i(x_{ij}) \right|^2 \\
+ \mu_1 \sum_{j=1}^{M} \sum_{i=1}^{n+1} \left| u_i(t_j, l_i) - u_{i+1}(t_j, l_i) \right|^2 \\
+ \mu_2 \sum_{j=1}^{M} \sum_{i=1}^{n} \left| \Delta_i u_{i,x}^j(t_j, l_i) - \Delta_{i+1} u_{i+1,x}^j(t_j, l_i) \right|^2. \tag{14}
\]

The first addend is equal to zero in the MFS method and, therefore, it is not necessary to calculate the relevant terms in the amount of \((n + 1) \times L\). For the case of small number of layers it is possible to propose an algorithm in which the only second term will remain. We will use the transform operators method (Bavrin et al., 2016). We will choose the approximation for the component of vector functions \(u(t, x)\) in order the conjugate conditions (12) to be satisfied. In formula (14) first, third, and fourth addends will disappear by construction.

### 4.5. MFS and the Transform Operators for a Two-Layer Medium

The solution of the vector Cauchy problem for a two-layer medium (9-11) is determined by the MFS and the method of transform operators (Bavrin et al., 2016).

\[
u_1(t, x) = \sum_{k=1}^{N} \frac{1}{2\sqrt{\pi(t+\tau_k)}} \exp \left( -A_1^2 \frac{(x-y_k)^2-y_k^2}{4(t+\tau_k)} \right) \alpha w_k, \quad x < 0; \\
u_2(t, x) = \sum_{k=1}^{N} \frac{1}{2\sqrt{\pi(t+\tau_k)}} \exp \left( -A_2^2 \frac{(x+y_k)^2-y_k^2}{4(t+\tau_k)} \right) \beta w_k, \quad x > 0, \tag{15}
\]

where

\[
\alpha = \frac{I + A_1^2 \Delta_1^{-1} A_2 A_2^2}{2}, \quad \beta = \frac{I - A_1^2 \Delta_1^{-1} A_2 A_2^2}{2}.
\]
In this case, the transform operators method \cite{8}, means that the approximation of the solution must not be carried out separately for each interval, but immediately on the entire real axis, with the component approximating $u_1$ containing the matrix Gaussian and its reflection with respect to the inner boundary, with some matrix coefficients chosen so that the conjugation conditions would be satisfied. Simply it’s possible to say that, the structure of the component $u_1$ is not an arbitrary, but uniquely determined by the structure of the component $u_2$. The error functional $I$ has the form, 

$$I = \sum_{j=1}^{K} \sum_{i=1}^{n+1} \| u_i(0, x_{ij}) - f_i(x_{ij}) \|^2. \quad (16)$$

The calculation of minimum for functional (16) is to solve the problem of approximating the vector function $f(x)$ by means of matrix-valued Gaussians.

When we use the combination of MFS and the transform operators method the number of sampling points is $2K$, while the number of sampling points in the RBF method is $2L + 2K + 2M$.

The algorithm for solving the vector Cauchy problem for a two-layer medium (10) - (12) consists of two steps:

1) solve the problem of approximation of a vector function by means of matrix-valued Gaussians;
2) write down the solution of problem (10) - (12) according to formulas (15).

4.6. Demonstration of MFS Method in an Example

Suppose, instead of the initial condition $f(x)$ we have on the set of sampling points

$$\tilde{f}(x_i) = \exp \left(-\frac{x_i^2}{4}\right) (x_i^2 - 2) \cdot (1 + 0.1 \cdot \theta_i),$$

where $\theta_i$ -random numbers, $-1 \leq \theta_i \leq 1$. The factor on the right-hand side has a noise component that imitates a 10% error in the data caused by the inaccuracy of the observational data.

The first addend in the right part was chosen for reasons of the possibility of finding the exact solution of the Cauchy problem. The second addend is a noise component that simulates the data errors corresponds to the errors of 10% in the initial conditions caused by the inaccuracy of observations. We use the application of the Curve Fitting Toolbox from Matlab. Let $f_{fit}(x)$ be the approximation of the function $f(x)$ by the 'Gauss2' model (that is, the
approximation is being found as the weighted sum of two Gaussians, the number of Gaussians is chosen experimentally:

\[
\text{fit}(x) = a_1 \exp\left(-\frac{(x-b_1)^2}{c_1^2}\right) + a_2 \exp\left(-\frac{(x-b_2)^2}{c_2^2}\right)
\]

The result is displayed in the form:

Coefficients (with 95% confidence bounds):

\[
a_1 = 2239 \quad b_1 = -0.000151 \quad c_1 = 1.998
\]

\[
a_2 = -2241 \quad b_2 = -0.0001535 \quad c_2 = 1.996.
\]

At the same time, the reliability of the result is estimated at a significant level of 95%. The exact solution \(u(t, x)\) can be found by the method of the Integral Fourier Transform

\[
u(t, x) = \frac{x^2 - 2 - 2t}{(t+1)^2} \exp\left(-\frac{x^2}{4t+4}\right),
\]

RBF approximation \(\text{ufit}(t,x)\) according to formula (6) has the form

\[
\text{ufit} (t, x) = \frac{a_1c_1}{(4t+c_1^2)^{\frac{3}{2}}} \exp\left(-\frac{(x-b_1)^2}{4t+c_1^2}\right) + \frac{a_2c_2}{(4t+c_2^2)^{\frac{3}{2}}} \exp\left(-\frac{(x-b_2)^2}{4t+c_2^2}\right),
\]

\(17\)

---

**Fig. 1. The initial condition and its 'Gauss2' approximation**

Figure 1 shows the graph of the observed initial values. The values were set on the interval \((-10, 10)\) with step 0.01. Here is a graph of its 'Gauss2' approximation. The quality of approximation is high because the initial condition is the second derivative of the Gaussian.
The exact solution and its MFS approximation at time $t = 1$

Figure 2 shows a graph of theoretical values on interval $(-10,10)$ at time $t = 1$. Here is a graph of the RBF approximation by formula (17). Given a 10% error in the initial data, in accordance with the theory, we observe a 10% error in the RBF approximation of the exact solution at time $t = 1$.

### 4.7. Cauchy Problem for Burgers Equation

Here is an attempt to use MFS for nonlinear problems. The most well-known nonlinear model of Burgers equation (Hopf, 1950) is chosen. Cauchy problem for Burgers equation has the form

$$u_t' + uu'_x = \mu u''_{xx}, \quad x \in (-\infty, \infty), \quad 0 < t \leq T,$$

$$u(0, x) = f(x).$$

An important feature of the Burgers equation is the possibility of linearization by Hopf’s substitution

$$u = -2\mu \frac{\partial \ln z}{\partial x},$$
where the function $z$ is the solution of the Cauchy problem for the linear heat equation
\[
\begin{align*}
  z'_t &= \mu u''_{xx}, \quad x \in (-\infty, \infty), \quad 0 < t \leq T, \\
  z(0, x) &= \Psi(x) = \exp \left( -\frac{1}{2\mu} \int_{-\infty}^{x} f(\xi) \, d\xi \right).
\end{align*}
\]

**MFS method for Burgers equation (Hopf,1950)**

We consider the approximation of the initial condition $\Psi(x)$ by the weighted sum of Gaussians
\[
\Psi(x) \approx \sum_{k=1}^{N} \frac{1}{2\mu \sqrt{\pi \tau_k}} \exp \left( -\frac{(x - y_k)^2}{4\mu^2 \tau_k} \right) w_k.
\]

Based on the Hopf’s substitution \cite{9} we conclude,
\[
\begin{align*}
  u(t, x) &\approx \frac{1}{\mu} \sum_{k=1}^{N} \frac{(x-y_k)}{(t+\tau_k) \sqrt{\pi(t+\tau_k)}} \exp \left( -\frac{(x-y_k)^2}{4\mu^2 (t+\tau_k)} \right) w_k. \\
  &\quad \mu \sum_{k=1}^{N} \frac{1}{\sqrt{\pi(t+\tau_k)}} \exp \left( -\frac{(x-y_k)^2}{4\mu^2 (t+\tau_k)} \right) w_k.
\end{align*}
\]

MFS can be applied to the Korteweg-de Vries equation and other nonlinear equations of mathematical physics \cite{10}.

**5. Conclusion**

The method of fundamental solutions in combination with the search for a minimum value of the error functional by the RBFNN method has shown effectiveness in the study of mathematical models for heat and mass transfer. The method is suitable for both of the uncoupled (scalar case) and the uncoupled mathematical models (vector case). The models can be treated as a homogeneous medium, and also as a piecewise homogeneous medium. The method of fundamental solutions in combination with the search for a minimum of the error functional by the RBFNN method can be applied to the study of heat and mass transfer in semi-bounded and unbounded medium. It is hoped that the method will find applications in nonlinear problems related to the Burgers equation. Finally, in the case of domains with plane symmetry, the method can be extended to two or three space variables.
References


