An adapted plane waves method for heat conduction problems

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Abstract

In this paper we construct a new set of basis functions for the numerical solution of nonhomogeneous heat conduction problems with Dirichlet boundary conditions and null initial data. These functions can be seen as Newtonian potentials of plane waves for the heat equation and satisfy a null initial condition. Density results for adapted waves will be established and several numerical simulations will be presented in order to discuss the accuracy and feasibility of the proposed method. An application of the method for heat problems with non null initial temperature will also be discussed.

Key words Heat equation, Meshfree methods, Method of particular solutions, Plane waves method.
AMS subject classifications 35K05, 65N35

1 Introduction

The heat equation is one of the most studied partial differential equation and have many applications in engineering problems and in some areas of applied mathematics such as mathematical finance. For the latter, one of the most well known example is the modelling of pricing problems for a derivative product. For instance, in the context of European options for the Black-Scholes equation this leads to Cauchy problems for the heat equation (eg. [26]) and more generally to partial integro-differential equation for the heat equation (eg. [10]) when the underlying dynamics are driven by Lévy processes.

Classical numerical methods for the heat equation include mesh based methods such as the finite difference method, finite element method and boundary integral methods like the boundary element method (BEM). BEM is usually a very efficient method for homogeneous problems but require domain integrations for nonhomogeneous problems. This can be circumvent for instance by decomposing the solution as a sum of a particular solution and a solution of an homogenenous problem (eg. [19]) or by using the so called radial integration method (eg. [1] and [27]).

Meshfree methods, on the other hand, don't require the construction of a mesh nor integration techniques for improper integrals. Approximations with radial basis functions for the strong formulation of the problem were implemented in [8] while weak formulations with reproducing kernel methods and local methods can be found in [9] and [11], respectively. A comparison between meshless methods for both strong and weak formulations can be found in [22].

Other popular meshfree methods are based on superpositions of fundamental solutions of the differential equation governing the BVP (eg. [5]). Since fundamental solutions centred at source points placed in the exterior of the domain satisfy the homogeneous differential equation, this method is well suited for homogeneous BVP problems. For instance in [7], [13], [14], [15] and [16] the authors study such fundamental solutions techniques for homogeneous heat BVPs. Finally we mention some hybrid mesh-meshfree techniques for heat problems. Here we cite the works [6], [17] and [24] where iterative methods combining finite differences in time with meshfree methods for the spatial variable were analysed and implemented.

In this paper we construct new basis functions for the approximation of nonhomogeneous heat problems with null initial condition and Dirichlet boundary conditions. These basis functions are globally defined and have the property of satisfy null initial condition. BVPs with null initial condition appear in inverse source problems but applications of the proposed method go beyond numerics for the heat equation. In fact, since the heat kernel is the density function of a multivariate normal distribution, the adapted waves method can also be applied to devise a control variate for the Monte Carlo integration method with respect to the Gaussian measure (see [25] for variance reduction techniques via basis functions).

An extension to problems with non null initial conditions is also discussed. Here, we propose a decomposition of the solution as a sum of a function, u_p, satisfying both the homogeneous heat equation and the initial condition and a function, v, solution to a nonhomogeneous problem with null initial condition. By applying classical separation of variables we show that we can consider an approximation for u_p using superposition of basis functions satisfying Helmholtz equations for many frequencies. Here, well known methods such as the plane waves method (see [2] for such method on manifolds) or the fundamental solutions for Helmholtz problems depicted in [3] can be applied.

The solution to the second problem, v, is approximated using the adapted waves functions. We justify this procedure by establishing boundary density results for these functions and present several numerical simulations to show the effectiveness of the method.

The paper is organized as follows: In section 2 we establish some notation and introduce the studied BVP for the heat equation. Then, in section 3 we discuss the decomposition of the solution that splits the problem in the computation of u_p and v. In section 3.1 we introduce the adapted plane waves method and in 4 we establish the corresponding density results. These results justify both boundary approximation methods using adapted waves and also approximation for the solution v. In section 5 we present these two numerical algorithms and in section 6 we show several numerical simulations.

2 Preliminaries for the heat equation

Let $\Omega \subset \mathbb{R}^n$ be a open, bounded simply connected domain with regular boundary $\Gamma = \partial\Omega$ and consider the parabolic cylinder

$$\Omega_T := \Omega \times]0, T[, \quad T > 0$$

as the domain of heat propagation. Let

$$\Sigma = \Gamma \times]0, T[$$

and consider the initial value problem for the heat equation with Dirichlet boundary condition

$$\begin{cases} (\partial_t - \Delta_x) u(x,t) = f(x,t), & (x,t) \in \Omega_T \\ u(x,0) = u_0(x), & x \in \Omega \\ u(x,t) = g(x,t), & (x,t) \in \Sigma \end{cases} \tag{1}$$

together with the compatibility condition

$$u_0(x) = g(x, 0), \quad x \in \Gamma. \tag{2}$$

Here, Δ_x denotes the Laplace operator in the variable $x = (x_1, \ldots, x_n)$, that is

$$\Delta_x u = (\partial_{x_1,x_1} + \ldots + \partial_{x_n,x_n})u.$$

When u_0 belongs to $H^1(\Omega)$, $u_0|_\Gamma$ is a element in the trace space $H^{1/2}(\Gamma)$ and the above compatibility condition should be understood in the trace sense.

We suppose that the source term f belongs to the space $L^2(\Omega_T) = L^2(0, T, L^2(\Omega))$, that is, for almost every $t \in [0, T]$ fixed, $f(x, t) \in L^2(\Omega)$ and

$$||f(\bullet, t)||_{L^2(\Omega)} \in L^2(0, T).$$

Accordingly to [18] when the initial data $u_0 \in H^1(\Omega)$ satisfies the compatibility condition (2) and the Dirichlet data g is a element in $H^{3/2,3/4}(\Gamma) = L^2(0, T, H^{3/2}(\Gamma)) \cap H^{3/4}(0, T, L^2(\Gamma))$ then (1) is well posed with solution

$$u \in H^{2,1}(\Omega_T) = L^2(0, T, H^2(\Omega)) \cap H^1(0, T, L^2(\Omega)).$$

Higher regularity results can be obtained when the input data (f, u_0, g) is more regular and appropriate compatibility conditions are considered (eg. [18]).

3 Decomposition of the solution

In order to approximate the solution of the linear problem (1) using a collocation method, we consider a set of basis functions φ_k and write

$$u \approx \tilde{u} = \sum_{k=1}^{N} \alpha_k \varphi_k.$$

We then compute the coefficients α_k by imposing the following conditions

$$\left\{ \begin{array}{ll} (\partial_t - \Delta_x)\tilde{u}(x^{(j)}, t_j) = f(x^{(j)}, t_j), & (x^{(j)}, t_j) \in \Omega_T \\ \tilde{u}(y^{(j)}, 0) = u_0(y^{(j)}), & y^{(j)} \in \Omega \\ \tilde{u}(z^{(j)}, s_j) = g(z^{(j)}, s_j), & (z^{(j)}, s_j) \in \Sigma \end{array} \right. ,$$

in some chosen domain and boundary points $(x^{(j)}, t_j)$, $(z^{(j)}, s_j)$.

However, this system may become very large even when considering the heat equation in one or two dimensional spatial variables. One possibility to circumvent this problem is to consider a decomposition of the solution of (1) as a sum of two functions that can be approximated with less computational effort. Here, we consider the decomposition

$$u = u_p + v$$

where u_p is a particular solution for the problem

$$\begin{cases} (\partial_t - \Delta_x)u_p(x,t) = 0, & (x,t) \in \Omega_T \\ u_p(x,0) = u_0(x), & x \in \Omega \end{cases} \tag{3}$$

and v is the solution of the following problem with null initial data

$$\begin{cases} (\partial_t - \Delta_x)v(x,t) = f(x,t), & (x,t) \in \Omega_T \\ v(x,0) = 0, & x \in \Omega \\ v(x,t) = g(x,t) - u_p(x,t), & (x,t) \in \Sigma \end{cases} . \tag{4}$$

Regarding the approximation for a particular solution u_p we can consider a separation of variables for u_p,

$$u_p(x,t) = \psi(x)e^{-t\kappa^2}$$

where κ is some positive real number. Imposing the homogeneous heat equation $(\partial_t - \Delta_x)u_p = 0$ in Ω_T we arrive at the following Helmholtz problem for ψ,

$$(\Delta_x + \kappa^2)\psi = 0 \text{ in } \Omega.$$

If the initial data u_0 satisfies the Helmholtz equation for a given wavenumber κ^2 then we can take $\psi = u_0$ and the function

$$u_p(x,t) = u_0(x)e^{-t\kappa^2}$$

satisfies (3). Moreover, let

$$u_0(x) \approx \tilde{u}_0(x) = \sum_k \alpha_k \psi_{\xi^{(k)}}(x), \;\; \xi^{(k)} = (\xi_1^{(k)}, \ldots, \xi_n^{(k)}) \in \mathbb{R}^n \tag{5}$$

with coefficients $\alpha_k \in \mathbb{C}$ computed so that

$$\tilde{u}_0(x^{(k)}) = u_0(x^{(k)})$$

on some collocation points $x^{(k)} \in \Omega$. If the basis functions $\psi_{\xi^{(k)}}$ satisfy

$$(\Delta_x + |\xi^{(k)}|^2)\psi_{\xi^{(k)}} = 0 \text{ in } \Omega$$

then,

$$\tilde{u}_p(x,t) = \sum_k \alpha_k \psi_{\xi^{(k)}}(x) e^{-t|\xi^{(k)}|^2}$$

satisfies the homogeneous heat equation in Ω_T and

$$\tilde{u}_p(x,0) = \tilde{u}_0(x) \approx u_0(x).$$

Hence, we can consider $\tilde{u}_p$ as an approximation for a function satisfying (3).

For instance, we can consider the approximation (5) using plane waves basis functions

$$\psi_\xi(y) = e^{iy\cdot\xi}, \;\; y \in \mathbb{R}^n, \; \xi \in \mathbb{R}^n$$

and take $\xi^{(k)}$ in a ball $B(0,R) = \{\xi \in \mathbb{R}^n : |\xi| < R\}$ or we can also consider an approximation for u_0 in terms of fundamental solutions for the Helmholtz equations in non-resonance frequencies. These are well known methods that can be found in the literature (eg. [3]) and henceforth we shall only address the numerical solution for the heat equation with null initial data, meaning that we shall consider (4) with $u_p \equiv 0$.

3.1 Adapted Plane Waves method

In this section we propose a method for the solution of (4) relying on functions with prescribed null initial condition. The main ideia is to construct basis functions φ, that, for some given ψ, satisfy the Cauchy problem

$$\begin{cases} (\partial_t - \Delta_x)\varphi(x,t) = \psi(x,t), & (x,t) \in \mathbb{R}^n \times \mathbb{R}^+ \\ \varphi(x,0) = 0, & x \in \mathbb{R}^n \end{cases}. \tag{6}$$

Formally, such function φ can be given by

$$\varphi(x,t) = \int_0^t \int_{\mathbb{R}^n} \psi(y,s)\Phi(x-y,t-s)dyds \tag{7}$$

where

$$\Phi(x,t) = \begin{cases} (4\pi t)^{-\frac{n}{2}} e^{-\frac{|x|^2}{4t}}, & t > 0 \\ 0, & t < 0 \end{cases}$$

is a fundamental solution for the heat equation (eg. [12]). For some density functions ψ, this convolution can be explicitly computed. Let $\xi \in \mathbb{R}^{n+1}$ and define the complex valued function

$$z(\xi) = \xi_1^2 + \ldots + \xi_n^2 + \xi_{n+1} i.$$

Given plane waves

$$\psi_\xi(x,t) = e^{i(x,t)\cdot\xi} \tag{8}$$

with $(x,t) \in \mathbb{R}^n \times \mathbb{R}$ define

$$\varphi_\xi(x,t) = \frac{1}{z(\xi)}\psi_\xi(x,t)(1 - e^{-tz(\xi)}), \ \ \xi \neq 0. \tag{9}$$

Clearly $\varphi_\xi(x,0) = 0$ and we have

$$\Delta_x \varphi_\xi(x,t) = -(\xi_1^2 + \ldots + \xi_n^2)\varphi_\xi(x,t),$$

$$\partial_t \varphi_\xi(x,t) = i\xi_{n+1}\varphi_\xi(x,t) + \frac{\overline{z(\xi)}}{|z(\xi)|^2}\psi_\xi(x,t)z(\xi)e^{-tz(\xi)}$$

therefore

$$(\partial_t - \Delta_x)\varphi_\xi(x,t) = z(\xi)\varphi_\xi(x,t) + \psi_\xi(x,t)e^{-tz(\xi)} = \psi_\xi(x,t)$$

and φ_ξ satisfies (6) for the source term ψ_ξ. We call the function φ_ξ an adapted wave function. In Figure 1 we plot a two dimensional adapted plane wave function.

Remark 3.1. When $\psi_0 \equiv 1$ the corresponding adapted function is

$$\varphi_0(x,t) = t.$$

This can be seen by a direct computation or by taking the limit

$$\varphi_\xi(x,t) = \psi_\xi(x,t)\frac{1 - e^{-tz(\xi)}}{z(\xi)} \underset{\xi \to 0}{\to} \psi_0(x,t)t = t.$$

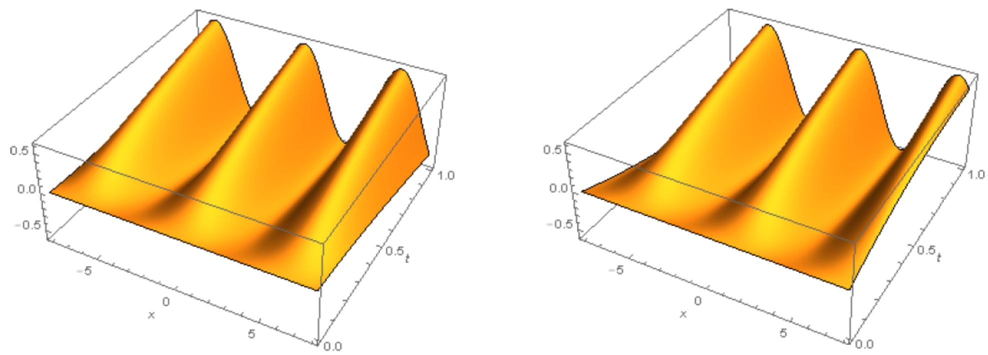

Figure 1: Left: Real part of the two dimensional adapted wave function $\varphi_{(1,1)}$. Right - Imaginary part of the same function.

Remark 3.2. When $tz(\xi) \approx 0$, the computational evaluation of $1 - e^{-tz(\xi)}$ is affected by subtractive cancellation. Hence, for computational purposes, we should consider instead a truncation of

$$\varphi_\xi(x,t) = \psi_\xi(x,t) \sum_{k=1}^{\infty} \frac{z(\xi)^{k-1}}{k!} t^k. \tag{10}$$

Remark 3.3. There are several choices for pairs (φ_ξ, ψ_ξ). For instance, if we consider Laplace functions,

$$\psi_{i\xi}(x,t) = e^{-(x,t)\cdot\xi}$$

then the pair $(\varphi_{i\xi}, \psi_{i\xi})$ satisfies (6).

Moreover, for fundamental solutions $\Phi(x-y,t)$, the corresponding adapted function is $t\Phi(x-y,t)$ since

$$\begin{cases} (\partial_t - \Delta_x) t\Phi(x-y,t) = \Phi(x-y,t) \\ t\Phi(x-y,t)|_{t=0} = 0 \end{cases}.$$

Remark 3.4. For the heat equation with diffusion coefficient $\alpha > 0$, the adapted wave function is

$$\varphi_\xi^\alpha(x,t) = \frac{1}{z_\alpha(\xi)} \psi_\xi(x,t)(1 - e^{-tz_\alpha(\xi)})$$

with

$$z_\alpha(\xi) = \alpha(\xi_1^2 + \ldots + \xi_n^2) + \xi_{n+1} i,$$

meaning that the pair $(\varphi_\xi^\alpha, \psi_\xi)$ satisfies

$$\begin{cases} (\partial_t - \alpha\Delta_x)\varphi_\xi^\alpha(x,t) = \psi_\xi(x,t) \\ \varphi_\xi^\alpha(x,0) = 0 \end{cases}$$

with ψ_ξ a plane wave defined by (8).

4 Main results for the adapted waves method

In this section we establish some density results. We start with the following density result on the whole domain of propagation Ω_T.

Lemma 4.1. *The set of functions defined by (8),*

$$\{\psi_\xi|_{\Omega_T} : \xi \in O\},$$

where $O \subset \mathbb{R}^{n+1}$ is open, spans a dense subspace in $L^2(\Omega_T)$.

Proof. Let $f \in L^2(\Omega_T)$ such that

$$\int_0^T \int_\Omega f(x,t)\psi_\xi(x,t)dxdt = 0, \ \ \forall \xi \in O.$$

Denote by $\tilde{f} \in L^2(\mathbb{R}^{n+1})$ the extension of f by zero to the whole space $\mathbb{R}^{n+1}$. Then

$$0 = \int_0^T \int_\Omega f(x,t)\psi_\xi(x,t)dxdt = \mathcal{F}(\tilde{f})((-2\pi)^{-1}\xi) = 0, \ \ \forall \xi \in O. \tag{11}$$

On the other hand, since $\tilde{f}$ has compact support, the Fourier transform of $\tilde{f}$, $\mathcal{F}(\tilde{f})$, is analytic. Hence, by uniqueness of analytic continuation, condition (11) implies $\mathcal{F}(\tilde{f})(\xi) = 0$ in the whole $\mathbb{C}^{n+1}$ (eg. [4]) hence $\tilde{f} = 0$ and $f = 0$ follows. □

Remark 4.2. For a compactly supported function $\tilde{f} \in L^2(\mathbb{R}^{n+1})$, the two-sided Laplace transform $\mathcal{L}(\tilde{f})(\xi) = \mathcal{F}(\tilde{f})(i\xi)$ is also analytic. Hence, when

$$\mathcal{L}(\tilde{f})(\xi) = 0, \quad \xi \in O$$

then $\mathcal{F}(\tilde{f}) = 0$ in the whole complex space $\mathbb{C}^{n+1}$. In particular, from above lemma, $f = 0$ and we also have a density result for Laplace basis functions

$$\psi_{i\xi}(y) = e^{-y\cdot\xi}, \ \ y = (x,t) \in \Omega_T, \ \ \xi \in O.$$

We now establish boundary density results for the adapted waves.

Let $\tilde{O}$ be some open bounded domain such that $\overline{\tilde{O}} \subset \mathbb{R}^n \setminus \{0\}$, $\tilde{\xi} = (\tilde{\xi}_1, \ldots, \tilde{\xi}_n) \in \tilde{O}$ and define the linear bounded operator

$$\mathcal{A} : L^2(\tilde{O}) \to L^2(0,T,L^2(\Gamma)), \ f \mapsto \mathcal{A}(f)(x,t) = \int_{\tilde{O}} \varphi_\xi(x,t) f(\tilde{\xi})d\tilde{\xi}, \ \ (x,t) \in \Sigma, \ \xi = (\tilde{\xi}_1, \ldots, \tilde{\xi}_n, 0) \in \mathbb{R}^{n+1}.$$

with kernel φ_ξ defined by (9). We start by computing the adjoint of $\mathcal{A}$.

Lemma 4.3. *The adjoint of $\mathcal{A}$ is the operator $\mathcal{A}^* : L^2(0,T,L^2(\Gamma)) \to L^2(\tilde{O})$,*

$$g \mapsto \mathcal{A}^*(g)(\tilde{\xi}) = \int_0^T \int_\Gamma \overline{\varphi}_\xi(x,t)g(x,t)dS_xdt = \int_0^T \int_\Gamma \varphi_{-\xi}(x,t)g(x,t)dS_xdt.$$

Proof. We have, by Fubini's theorem,

$$
\begin{aligned}
\langle \mathcal{A}(f), g\rangle_{L^2(0,T,L^2(\Gamma))\times L^2(0,T,L^2(\Gamma))} &= \int_0^T \int_\Gamma \left(\int_{\tilde{O}} \varphi_\xi(x,t) f(\tilde{\xi}) d\tilde{\xi} \right) \overline{g}(x,t) dS_x dt \\
&= \int_{\tilde{O}} f(\tilde{\xi}) \left(\int_0^T \int_\Gamma \varphi_\xi(x,t) \overline{g}(x,t) dS_x dt \right) d\tilde{\xi} \\
&= \int_{\tilde{O}} f(\tilde{\xi}) \left(\overline{\int_0^T \int_\Gamma \overline{\varphi}_\xi(x,t) g(x,t) dS_x dt} \right) d\tilde{\xi} \\
&= \left\langle f, \int_0^T \int_\Gamma \overline{\varphi}_\bullet(x,t) g(x,t) dS_x dt \right\rangle_{L^2(\tilde{O})}.
\end{aligned}
$$

□

Theorem 4.4. *Let $\tilde{O}$ be the annulus $\tilde{O} = B_{r_2}(0) \setminus \overline{B}_{r_1}(0) \subset \mathbb{R}^n$, with $0 < r_1 < r_2$ and suppose that for any $\tilde{\xi} \in \tilde{O}$, $|\tilde{\xi}|$ is not an eigenfrequency for the Laplace–Dirichlet problem in Ω. Then, the operator $\mathcal{A}^*$ is injective and in particular $\mathcal{A}$ has dense range in $L^2(0,T,L^2(\Gamma))$.*

Proof. The condition that $|\tilde{\xi}|$ is not an eigenfrequency for the Laplace-Dirichlet problem in Ω means that if u solves

$$
\begin{cases} (\Delta + |\tilde{\xi}|)u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma = \partial\Omega \end{cases}
$$

then $u = 0$.

We claim that for $g \in L^2(0,T,L^2(\Gamma))$ such that

$$
\mathcal{A}^*(g)(\tilde{\xi}) = \int_0^T \int_\Gamma \varphi_\xi(x,t) g(x,t) dS_x dt = 0, \quad \forall \tilde{\xi} \in \tilde{O} \tag{12}
$$

we must have $g = 0$. Applying Fubini's theorem to the integral in (12) gives

$$
\begin{aligned}
0 &= \int_0^T \int_\Gamma \varphi_\xi(x,t) g(x,t) dS_x dt = \int_\Gamma \int_0^T \varphi_\xi(x,t) g(x,t) dt dS_x \\
&= \int_\Gamma \left(\psi_\xi(x,0) \int_0^T (1 - e^{-t|\tilde{\xi}|^2}) g(x,t) dt \right) dS_x.
\end{aligned}
$$

On the other hand, for any $\tilde{\xi}$ in $\partial B_r(0)$, $r \in]r_1, r_2[$ the above equation can be written as

$$
\int_\Gamma \left(e^{irx\cdot d} \int_0^T (1 - e^{-tr^2}) g(x,t) dt \right) dS_x = 0, \quad \forall d \in \mathbb{R}^n : |d| = 1. \tag{13}
$$

Since the set of plane waves

$$
\left\{ e^{rix\cdot d}|_{x\in\Gamma} : |d| = 1 \right\}
$$

spans a dense subspace in $L^2(\Gamma)$ when r is not an eigenfrequency for the Laplace–Dirichlet problem in Ω (eg. [23]) then, from (13), follows

$$\left\| \int_0^T (1-e^{-tr^2}) g(\bullet,t)dt \right\|_{L^2(\Gamma)} = 0.$$

Hence

$$\int_0^T e^{-tr^2} g(x,t)dt = \int_0^T g(x,t)dt$$

for almost every $x \in \Gamma$ and this equation can be written as

$$\mathcal{L}(\tilde{g}(x,\bullet))(r^2) = \int_0^T g(x,t)dt, \tag{14}$$

where $\tilde{g}(x,t)$ is the extension of $g(x,t)$ by zero, to the whole $\mathbb{R}$. Since r belongs to an open interval and the right hand side of (14) is (for fixed x) a constant then by analytic continuation the above identity holds in $\mathbb{C}$ and in particular, taking the inverse Fourier transform,

$$\tilde{g}(x,t) = \int_0^T g(x,s)ds\delta(t), \tag{15}$$

where δ is the Dirac delta distribution centered at the origin. However, $\tilde{g}(x,\bullet) \in L^2(\mathbb{R})$ hence (15) implies $\int_0^T g(x,s)ds = 0$. We now conclude from (14) that

$$\mathcal{L}(\tilde{g}(x,\bullet))(s) = 0, \quad \forall s \in \mathbb{C}$$

and the claim follows from remark 4.2. □

Remark 4.5. We emphasize that for this boundary density result we are considering source points in a n dimensional space contained in the plane $x_{n+1} = 0$. Note also that the heat source term is approximated using source points in $\mathbb{R}^{n+1}$. This is important when dealing only with the approximation for boundary data because in such situation we obtain a dimensional reduction for the source space.

5 Numerical Algorithms

Our density results lead to two algorithms. One for the approximation of boundary functions using adapted waves (Algorithm 1) and the second for nonhomogeneous heat problem with null initial condition (4) (Algorithm 2).

Algorithm 1 (Boundary data approximation with adapted waves)

1. Consider collocation points $(x^{(j)}, t_j) = (x_1^{(j)}, \ldots, x_n^{(j)}, t_j),\ j = 1, \ldots,\ N$ on $\Gamma \times [0,T]$
2. Consider source points $\xi^{(k)} = (\tilde{\xi}_1^{(k)}, \ldots, \tilde{\xi}_n^{(k)}, 0),\ k = 1, \ldots,\ M$
3. Define the approximation $\tilde{g}(x,t) = \sum_{k=1}^{M} \alpha_k \varphi_{\xi^{(k)}}(x,t)$ to the Dirichlet data $g \in L^2(0,T,L^2(\Gamma))$
4. Compute the coefficients α_k by solving the linear system $\tilde{g}(x^{(j)}, t_j) = g(x^{(j)}, t_j)$.

Algorithm 2 (approximation with adapted waves for problem (4))

1. Consider boundary collocation points $(x_\Gamma^{(j)}, t_j) = (x_{1\Gamma}^{(j)}, \ldots, x_{n\Gamma}^{(j)}, t_j),\ j = 1, \ldots,\ N_1$ on $\Gamma \times [0, T]$ and vonsider domain collocation points $(x_\Omega^{(j)}, t_j) = (x_{1\Omega}^{(j)}, \ldots, x_{n\Omega}^{(j)}, t_j),\ j = 1, \ldots,\ N_2$ in the domain $\Omega \times]0, T[$

2. Consider source points $\xi^{(k)} = (\xi_1^{(k)}, \ldots, \xi_n^{(k)}, \xi_{n+1}^{(k)}),\ k = 1, \ldots,\ M$ in some open set $\mathcal{O} \subset \mathbb{R}^{n+1}$.

3. Define the approximation $\tilde{v}(x,t) = \sum_{k=1}^{M} \beta_k \varphi_{\xi^{(k)}}(x,t)$ to the solution (4).

4. Compute the coefficients β_k by solving the linear system

$$\begin{cases} (\partial_t - \Delta_x)\tilde{v}(x_\Omega^{(j)}, t_j) = \sum_{k=1}^{M} \beta_k \psi_{\xi^{(k)}}(x_\Omega^{(j)}, t_j) = f(x_\Omega^{(j)}, t_j) \\ \tilde{v}(x_\Gamma^{(j)}, t_j) = g(x_\Gamma^{(j)}, t_j) - u_p(x_\Gamma^{(j)}, t_j) \end{cases}$$

Note that for long-time simulations (eg. [20] and [21]) both methods will lead to very large systems of equations because we are considering time direction as an additional space dimension. In this case, we should perform first a time transformation $t \mapsto \tau(t) = \frac{t}{T} : [0, T] \to [0, 1]$ which will lead to a heat equation in variables (x, τ) with diffusion coefficient $T > 0$ for which the adapted waves discussed in Remark 3.4 can be applied.

6 Experimental results

In this section we present several numerical examples for the proposed algorithms. We start with algorithm 1 for one dimensional problems.

Example 1

We present a numerical simulation to illustrate algorithm 1 for the boundary data

$$\begin{cases} u(0,t) = -t^2 \sin(3\pi(t - 0.4)) \\ u(1,t) = \log(t^2 + 1)\cos(\pi t) \end{cases}, \quad t \in [0, 1]$$

We consider 1500 uniformly distributed sources $\tilde{\xi}_j \in O =]-20, 20[$. In order to reduce oscillations near $t = 0$ we consider 1000 uniformly distributed collocation points on $\{0\} \times [0, 0.5]$ and 100 collocation points on $\{0\} \times]0.5, 1]$. The same strategy was applied for collocation points on $\{1\} \times [0, 1]$. Figure 2 shows the absolute boundary error. Additionally we computed the RMS error

$$RMS_\Gamma = \sqrt{\frac{\sum_{j=1}^{2000} |\tilde{g}(0, t_j) - u(0, t_j)|^2 + |\tilde{g}(1, t_j) - u(1, t_j)|^2}{4000}}$$

on some uniformly distributed points $t_j \in [0, 1]$. The computed RMS error for this example was 3.9×10^{-7}.

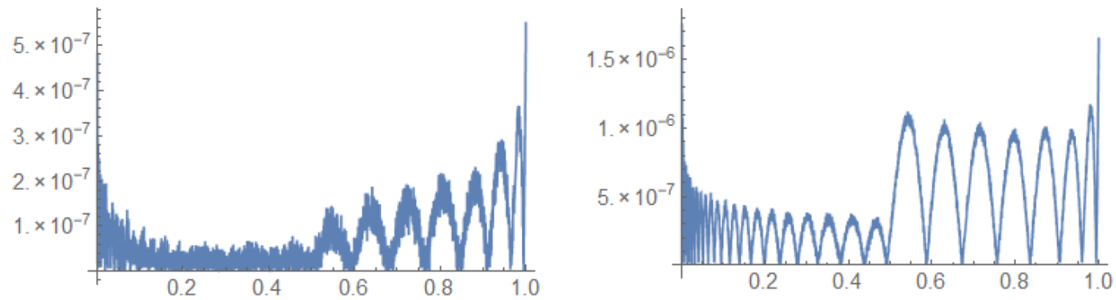

Figure 2: On the top: absolute error $|\tilde{g}(0,t) - u(0,t)|$ for the boundary approximation. On the bottom the same but for $|\tilde{g}(1,t) - u(1,t)|$.

Example 2

Here we consider the numerical approximation for the heat conduction problem (1) applying algorithm 2. The domain of propagation is the unit square $\Omega_T =]0,1[^2$ and the solution is

$$u(x,t) = t \ \mathrm{sech}(x^3 + t^2),$$

meaning that $f = (\partial_t - \Delta_x)u$, $g_0(t) = u(0,t) = t \ \mathrm{sech}(t^2)$, $g_1(t) = u(1,t) = t \ \mathrm{sech}(1+t^2)$ and $u(x,0) = 0$. 1500 source points uniformly distributed over $]-20,20[^2$ were considered whilst the domain collocation points were 1680. In order to avoid instabilities near the boundary, these points were uniformly distributed in the domain $[-0.3, 1.3]^2$. On the boundary, we choose 240 uniformly distributed collocation point. This means that the total number of collocation points is 1920. Figure 3 shows the absolute error for the approximation.

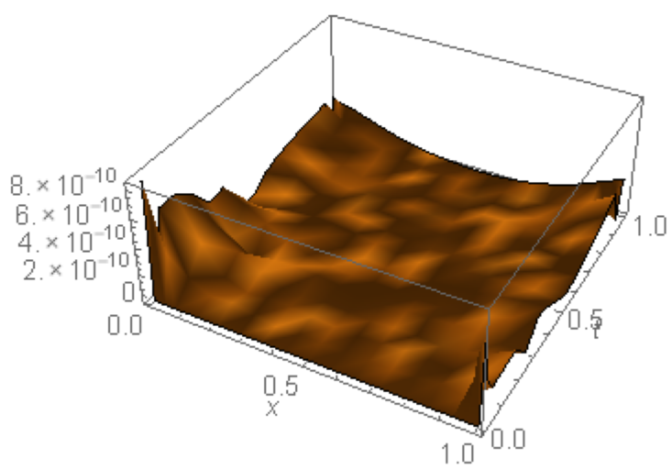

Figure 3: Domain error $|\tilde{v}(x,t) - u(x,t)|$.

We also compute the RMS error

$$RMS_\Omega = \sqrt{\frac{\sum_{j=1}^{10200} |\tilde{v}(x^{(j)}, t_j) - u(x^{(j)}, t_j)|^2}{10200}}.$$

The computed error for this example was 9.9×10^{-11}.

Example 3

In this example we present numerical results for algorithm 1 on three dimensional surfaces. The surface here considered is the cylindrical surface

$$\Sigma = \partial B(0,1) \times \left]0, \frac{1}{2}\right[= \left\{x \in \mathbb{R}^2 : |x| = 1\right\} \times \left]0, \frac{1}{2}\right[$$

and the function to be approximated is

$$g(x,t) = \sin(t)\sqrt{x_1^2 + \cos(x_2) + t}, (x,t) \in \Sigma.$$

We considered 2000 collocation points on the surface $\partial B(0,1) \times [0, 0.8]$ and several sets of source points $\tilde{\xi}$ (see Figure 4, left and right plots, respectively).

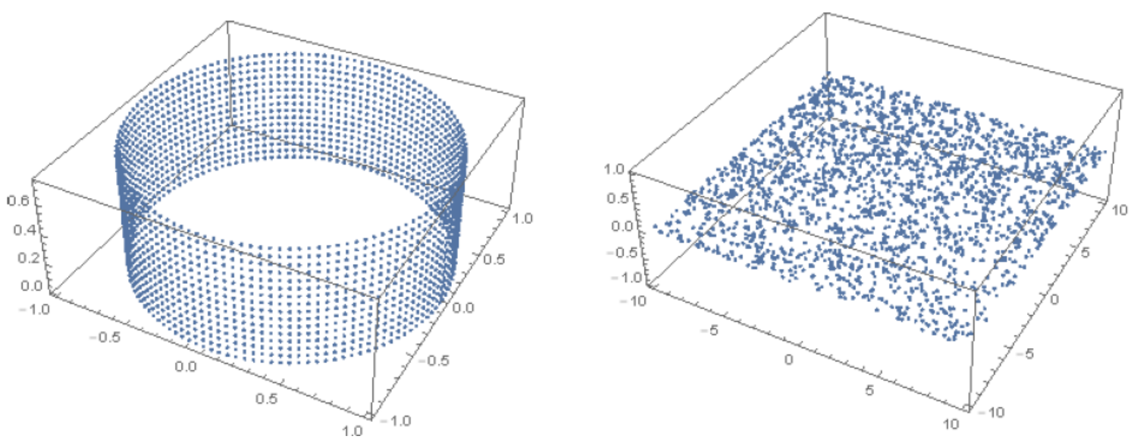

Figure 4: Distribution of boundary collocation points (left plot) and source points $\tilde{\xi}$ (right plot).

First, we took 1000 source points uniformly distributed in the square $[-10, 10]^2$. Computational time for this method was 13 seconds.

However, oscillations near $t = 0$ due to subtractive cancellation yields poor reconstruction results as we can see in Figure 5, left plot. Instead, we now consider adapted waves as in (10), with series truncation at the 7th term. The corresponding results are now much better (see Figure 5, right plot) with an increase of 2 seconds in computational time.

We now test the variation of the RMS error with respect to the number of sources and frequency values, $|\tilde{\xi}|^2$. The results, using the same truncated waves, are presented in Table 1. As we can see in this table increasing the number of sources and frequencies does not provide better RMS values.

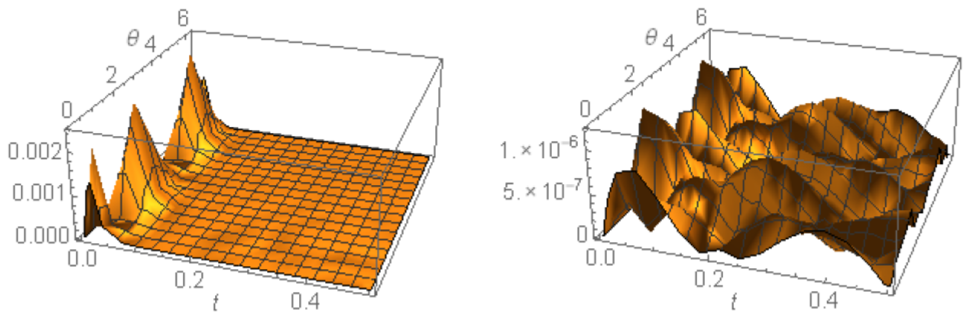

Figure 5: Absolute error for $|\tilde{g}(\cos\theta, \sin\theta, t) - g(\cos\theta, \sin\theta, t)|$ using adapted waves (left plot) and series representation (10), truncated at the 7th term.

number of source points	500	1000	1500	2000
RMS error	2.2×10^{-7}	1.1×10^{-7}	1.8×10^{-6}	3.0×10^{-6}

Table 1: RMS error for the approximation of g, using adapted waves truncated at the 7th term. Second and third columns are for sources $\xi \in [-5, 5]^2$. Last columns are for $\xi \in [-10, 10]^2$.

Finally, we show the evolution of the RMS error as a function of the number of terms in the truncation of series (10). For this example we obtained decreasing error up to 7 terms (see Figure 6). When considering 9 terms we obtained a slight error increase. This is due to an increase sensitivity of higher order terms with respect to perturbations in the coefficients.

Example 4

In this example we present some simulations for a two dimensional problem in a domain with non smooth boundary.

The domain of propagation is $\Omega_T = \Omega \times \left]0, \frac{1}{2}\right[$ with

$$\Omega = B_1^1(0) = \left\{x \in \mathbb{R}^2 : |x_1| + |x_2| < 1\right\}.$$

The heat source and initial condition are both null and the Dirichlet boundary data is (see Figure 7)

$$g(x, t) = 10(1 - \cos(t)) \sin(x_1^3 x_2), \quad x \in \Gamma = \partial\Omega, t \in \left[0, \frac{1}{2}\right].$$

We parametrize the non smooth surface $\Gamma \times [0, \frac{1}{2}]$ by

$$r(s,t) = \begin{cases} (1 + 2s, -1 + |1 + 2s|, t) & (s,t) \in [-1, 0] \times [0, \frac{1}{2}] \\ (2s - 1, 1 - |2s - 1|, t) & (s,t) \in [0, 1] \times [0, \frac{1}{2}] \end{cases}.$$

First we to apply algorithm 1 just for the approximation of g. We considered 2000 collocation points (see Figure 8) and 1000 uniformly distributed sources in $[-5, 5]^2$.

We obtained a maximum absolute error of the order 4×10^{-6} and the corresponding error plot is presented in Figure 9. The computed RMS error was 10^{-7}.

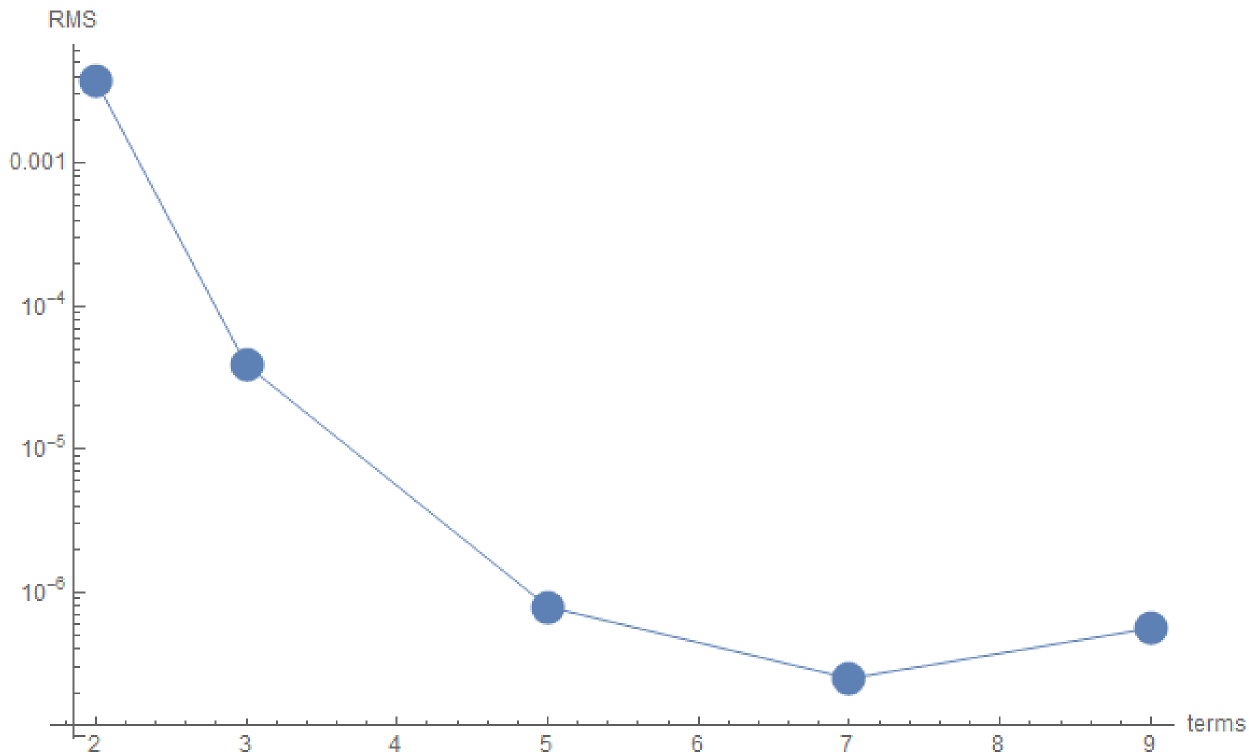

Figure 6: RMS error as a function of the number of truncation terms in (10). Here we considered 500 uniformly distributed points in $[-5, 5]^2$.

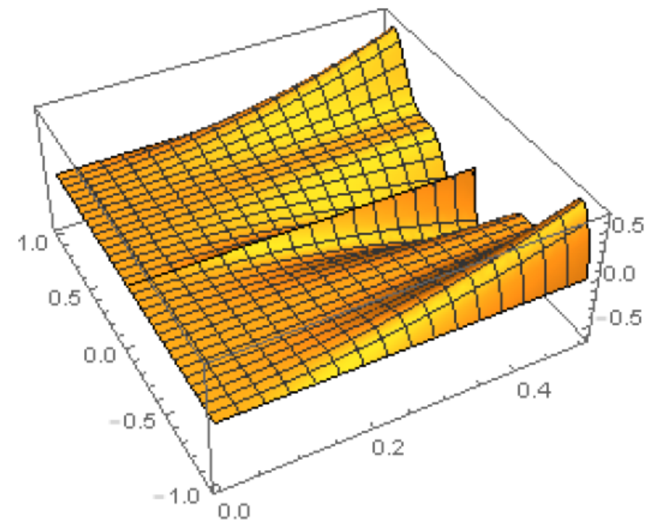

Figure 7: Plot of the function $g(r(s,t))$, $(s,t) \in [-1,1] \times [0, \frac{1}{2}]$.

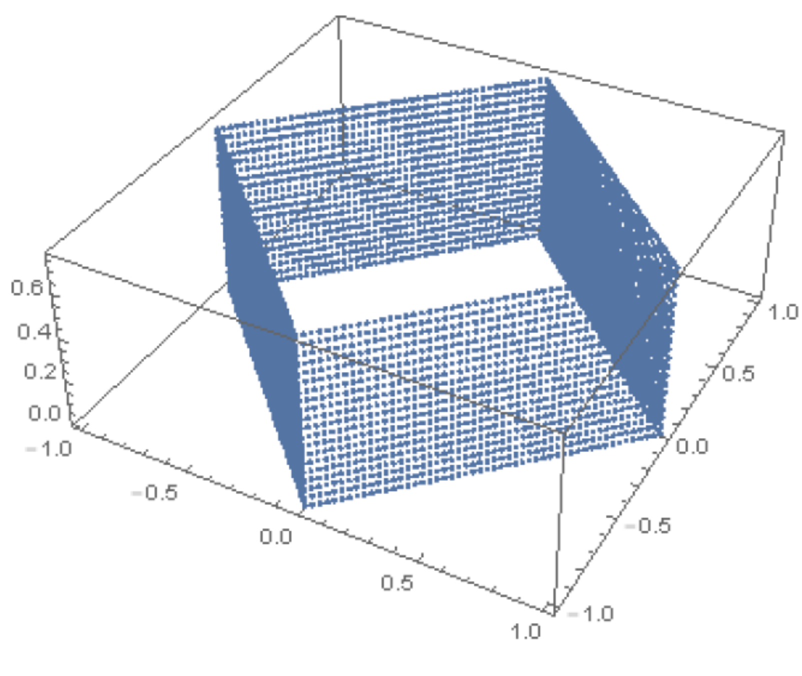

Figure 8: Distribution of collocation points over Σ.

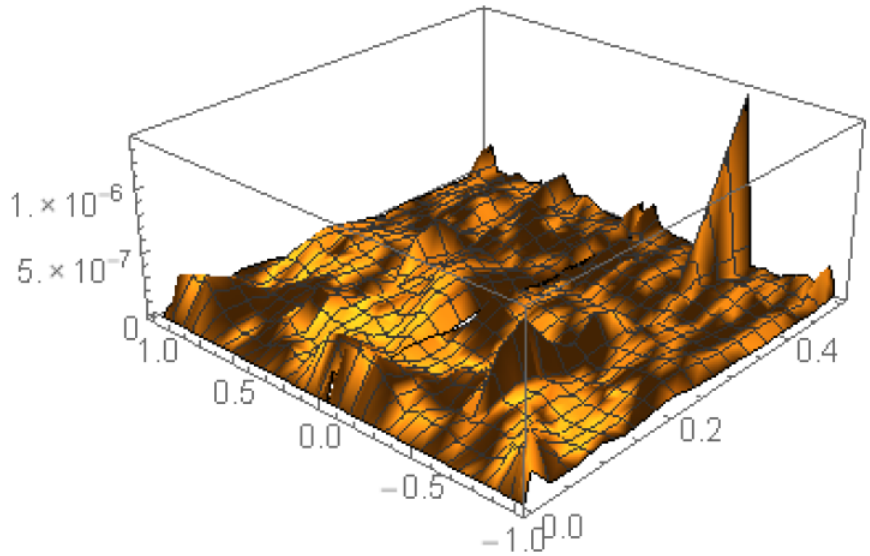

Figure 9: Absolute error on the surface $\Gamma \times \left[0, \frac{1}{2}\right]$.

We now apply algorithm 2 in order to approximate the solution of the heat problem. A total number of 3500 collocation points on the domain Ω_T and surface Σ were considered. The number of source points were 1000, placed in the cube $[-5, 5]^3$.

In this setting, the RMS boundary error increases to 10^{-3}. For the approximation of the source term we obtained similar error values. We show the absolute error plot at time $t = \frac{1}{2}$ in Figure 10.

7 Conclusions

We presented a collocation method with new basis functions for heat conduction problems. The main advantage of this method is that the basis functions satisfy null initial condition and can be linearly combined to obtain an approximation for both source and boundary data. We established density results regarding these functions and two related methods were proposed and tested: one for the approximation of the Dirichlet data and the other for the whole heat problem. Overall we obtained good numerical results.

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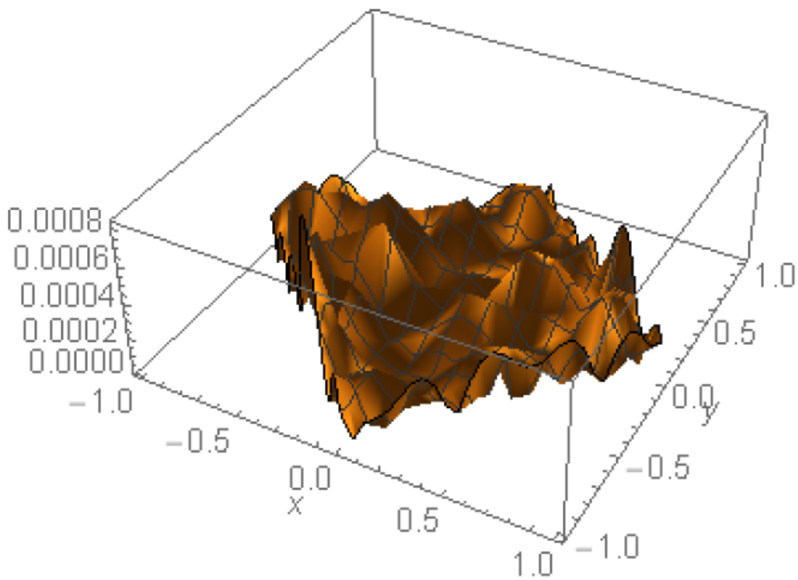

Figure 10: Absolute error for the approximation of f at $t = \frac{1}{2}$.

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