# Meshless Kernel Techniques for the Heat Equation 

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#### Abstract

Using the heat equation as a simple example, we give a rigid theoretical analysis of the Method of Lines, implemented as a meshless method based on spatial trial spaces spanned by translates of positive definite kernels. In addition, we provide a class of positive definite kernels that allow to solve the heat equation for scattered initial data by kernel-based interpolation or approximation, avoiding time intergation completely. Some numerical illustrations are given as well.


## 1 Introduction

(SecIntro) There are plenty of application papers in which kernels or radial basis functions are successfully used for solving partial differential equations by meshless methods. The usage of kernels is typically based on spatial interpolation at scattered locations, writing the trial functions "entirely in terms of nodes" [2]. For stationary partial differential equations, the discretization can take pointwise analytic derivatives of the trial functions to end up with a linear system of equations. This started in [6] and was pursued in the following years, including a convergence theory in [9. There are also variations that use weak data, like the Meshless Local Petrov-Galerkin method [1] with a convergence theory in [11]. For the potential equation, there are special kernels that allow the use of trial functions that satisfy the differential equation exactly [10, 5].

For time-dependent partial differential equations, meshless kernel-based methods were similarly based on a fixed spatial interpolation, but now the coefficients are time-dependent, and one obtains a system of ordinary differential equations for these. This is the well-known Method of Lines, and it turned to be experimentally useful in various cases (see e.g. [14, 7, 4, 13]). However, a rigid analysis of its behavior seems to be still missing. Furthermore, there are no known meshless kernel-based methods so far that allow the use of trial functions that satisfy the differential equation exactly.

For the simple case of the heat equation, this paper provides both an analysis of the Method of Lines and a construction of kernels that generate trial functions solving the heat equation. To this end, we start with basics on kernels, then describe the Method of Lines and analyze it. After this, we turn
to kernels satisfying the heat equation and provide a simple interpolatory method that avoids time integration at all. Some numerical examples are provided as well.

## 2 Kernel-Based Space Discretization

(SecKBSD) A kernel is a symmetric function

$$
K: \Omega \times \Omega \rightarrow \mathbb{R}
$$

on some spatial domain $\Omega \subset \mathbb{R}^{d}$. The kernel usually is assumed to be positive definite, i.e. for all selections of finite point sets $X=\left\{x_{1}, \ldots, x_{n}\right\} \subset \Omega$, the $n \times n$ kernel matrices $A=A(X)$ with entries $K\left(x_{j}, x_{k}\right), 1 \leq j, k \leq n$ are symmetric and positive definite. Standard examples are radial basis functions like the Gaussian

$$
K(x, y)=\exp \left(-\|x-y\|_{2}^{2}\right) \text { for all } x, y \in \mathbb{R}^{d}
$$

or the compactly supported Wendland function

$$
K(x, y)=\left\{\begin{array}{cc}
\left(1-\|x-y\|_{2}\right)^{4}\left(1+4\|x-y\|_{2}\right) & \|x-y\|_{1} \leq 1 \\
0 & \|x-y\|_{1} \geq 1
\end{array}\right.
$$

for all $x, y \in \mathbb{R}^{d}$ with $d \leq 3$.
The standard way to use kernels for solving time-dependent partial differential equations is to introduce a fixed space discretization via finite spatial point sets $X=\left\{x_{1}, \ldots, x_{n}\right\} \subset \Omega$ and to generate spatial trial functions via translates of a kernel $K$ in the form
(eqsa)

$$
\begin{equation*}
s(x):=\sum_{j=1}^{n} \alpha_{j} K\left(x, x_{j}\right), x \in \Omega . \tag{1}
\end{equation*}
$$

Interpolation of a spatial function $f: \Omega \rightarrow \mathbb{R}$ on the given point set $X$ is done by solving the system

$$
s\left(x_{k}\right)=\sum_{j=1}^{n} \alpha_{j} K\left(x_{k}, x_{j}\right)=f\left(x_{k}\right), 1 \leq k \leq n
$$

involving the $n \times n$ kernel matrix $A$ with entries $K\left(x_{j}, x_{k}\right), 1 \leq j, k \leq n$ which is positive definite for all positive definite kernels.

For further use we note that one can construct a Lagrange basis $u_{1}(x), \ldots, u_{n}(x)$ of the span of the functions $K\left(\cdot, x_{j}\right), 1 \leq j \leq n$ via solving the system (equKA)

$$
\begin{equation*}
u(x)=K(x) A^{-1} \tag{2}
\end{equation*}
$$

where we use the notation

$$
u(x):=\left(u_{1}(x), \ldots, u_{n}(x)\right), K(x)=\left(K\left(x, x_{1}\right), \ldots, K\left(x, x_{n}\right)\right) .
$$

Here and in what follows, indices running over functions will be column indices, while indices running over points will be row indices. In particular, it is convenient to introduce the column-valued evaluation operator defined as

$$
E(f):=\left(f\left(x_{1}\right), \ldots, f\left(x_{n}\right)\right)^{T} \text { for all } f: \Omega \rightarrow \mathbb{R},
$$

and application of this operator to a row of $m$ functions $v_{1}, \ldots, v_{m}$ should generate the $n \times m$ matrix with entries $v_{j}\left(x_{k}\right)$ with $1 \leq j \leq m$ for the columns and $1 \leq k \leq n$ for the rows. In particular, the kernel matrix then is $A=E(K(x))$ and the Lagrange property simply follows from

$$
E(u(x))=E\left(K(x) A^{-1}\right)=E(K(x)) A^{-1}=A A^{-1}=I_{n \times n} .
$$

Using the Lagrange basis, the representation (1, eqsa) of an interpolant to a function $f$ turns into

$$
s(x)=\sum_{j=1}^{n} u_{j}(x) f\left(x_{j}\right)=u(x) E(f), x \in \Omega
$$

which is "entirely in terms of nodes" as required for meshless methods [2], belytschko-et-al:1996-1.

If $L$ is a linear spatial differential operator, and if the kernel $K$ is sufficiently smooth to allow application of $L$, an advantage of kernel-based spatial discretizations is that

$$
(L s)(x)=\sum_{j=1}^{n}\left(L u_{j}\right)(x) f\left(x_{j}\right)=L u(x) E(f), x \in \Omega
$$

is explicitly available and again "entirely in terms of nodes". The required derivatives $L u_{j}$ of the Lagrange basis functions $u_{j}$ come from (2, equKA) via solving

$$
(L u)(x)=(L K)(x) A^{-1}
$$

provided that one can explicitly evaluate the action of $L$ on $K$.

## 3 Method of Lines

(SecMOLgen) With these notations concerning spatial functions and their derivatives, we now turn to modeling time-dependent functions $v(x, t)$ where the spatial argument $x$ varies in $\Omega$. One can always interpolate values $v\left(x_{k}, t\right)$ of $u(x, t)$ at all times $t$ to get an interpolant
(eqsvE)

$$
\begin{equation*}
s(x, t)=\sum_{j=1}^{n} v\left(x_{j}, t\right) u_{j}(x)=u(x) E(u(\cdot, t)) \tag{3}
\end{equation*}
$$

in terms of the Lagrange basis. This can be seen as a superposition of a separation of variables. The action of a spatial linear operator $L$ then is

$$
(L s)(x, t)=\sum_{j=1}^{n} v\left(x_{j}, t\right)\left(L u_{j}\right)(x)=(L u)(x) E(v(\cdot, t)),
$$

again separating the time variation from the space variation.
A linear evolution equation

$$
u_{t}(x, t)=(L u)(x, t), x \in \Omega, t \geq 0
$$

with a starting function $u_{0}$ on $\Omega$ with

$$
u(x, 0)=u_{0}(x) \text { for all } x \in \Omega
$$

can then be modeled by substituting (3, eqsvE) and discretizing the spatial variable to the points $x_{1}, \ldots, x_{n}$. This leads to

$$
\begin{aligned}
s_{t}\left(x_{k}, t\right) & =(L s)\left(x_{k}, t\right) & & 1 \leq k \leq n, t \geq 0 \\
s\left(x_{j}, 0\right) & =u_{0}\left(x_{j}\right), & & 1 \leq j \leq n,
\end{aligned}
$$

i.e. the whole problem is posed discretely in space, but continuously in time. The seond part is just interpolation of the initial function, while the first takes the form

$$
\frac{\partial}{\partial t} v\left(x_{k}, t\right)=\sum_{j=1}^{n} v\left(x_{j}, t\right)\left(L u_{j}\right)\left(x_{k}\right), 1 \leq k \leq n, t \geq 0
$$

which is a linear system of ordinary differential equations

$$
y_{k}^{\prime}(t)=\sum_{j=1}^{n} y_{j}(t)\left(L u_{j}\right)\left(x_{k}\right), 1 \leq k \leq n, t \geq 0
$$

for unknowns $y_{k}(t)$ having the meaning $y_{k}(t)=v\left(x_{k}, t\right)$ for an approximate solution $v(x, t)$ of the problem. The initial values are

$$
y_{j}(0)=u_{0}\left(x_{j}\right), 1 \leq j \leq n .
$$

This is the classical Method of Lines in the simplest linear case without additional boundary conditions. It is easy to generalize to nonlinear problems of the form

$$
u_{t}(x, t)=F(t, u(x, t),(L u)(x, t)),
$$

leading to a nonlinear system

$$
y_{k}^{\prime}(t)=F\left(t, \sum_{j=1}^{n} y_{j}(t) u_{j}\left(x_{k}\right), \sum_{j=1}^{n} y_{j}(t)\left(L u_{j}\right)\left(x_{k}\right)\right)
$$

of ODEs, and it is also easy to incorporate multiple spatial differential operators.

Additional time-dependent boundary conditions of the form

$$
u(z, t)=u_{B}(z, t) \text { for all } z \in \Gamma:=\partial \Omega, t \geq 0
$$

can also be handled. One discretizes them to

$$
v\left(x_{n+i}, t\right)=u_{B}\left(x_{n+i}, t\right), 1 \leq i \leq m
$$

for a choice of boundary points $x_{n+1}, \ldots, x_{n+m}$. These are added to the spatial interpolation problem, avoiding coalescence with the points $x_{1}, \ldots, x_{n}$. The trial functions are again specified in the form (3, eqsvE), but they split into

$$
\begin{aligned}
s(x, t) & =\sum_{j=1}^{n} v\left(x_{j}, t\right) u_{j}(x)+\sum_{i=1}^{m} v\left(x_{n+i}, t\right) u_{n+i}(x) \\
& =\sum_{j=1}^{n} v\left(x_{j}, t\right) u_{j}(x)+\sum_{i=1}^{m} u_{B}\left(x_{n+i}, t\right) u_{n+i}(x)
\end{aligned}
$$

being still entirely in terms of values at the nodes. Since we form the Lagrange basis with respect to all points $x_{1}, \ldots, x_{n+m}$, the first sum vanishes on the boundary points $x_{n+1}, \ldots, x_{n+m}$, while the second attains the correct boundary values there. The resulting ODE system then is the inhomogeneous system

$$
y_{k}^{\prime}(t)=\sum_{j=1}^{n} y_{j}(t)\left(L u_{j}\right)\left(x_{k}\right)+\sum_{i=1}^{m} u_{B}\left(x_{n+i}, t\right) L\left(u_{n+i}\right)(x)
$$

in the linear case, for $1 \leq k \leq n$ and all $t \geq 0$.
In numerical experiments, this technique was reported to work well (see e.g. [14, 7, 4, 13]), but a thorough mathematical analysis of its behavior is still missing, since one has to fight stability properties [8]. We shall supply a thorough analysis for a simple special case, the heat equation.

## 4 Method of Lines for Heat Equation

(SecMOL) Consider

$$
u_{t}=u_{x x}
$$

on $(x, t) \in[0,1] \times[0, \infty)$ under boundary conditions

$$
\begin{aligned}
u(x, 0) & =u_{0}(x), x \in[0,1] \\
u(0, t) & =u_{0}(0)=0, t \geq 0 \\
u(1, t) & =u_{0}(1)=0, t \geq 0
\end{aligned}
$$

defined by a smooth function $u_{0}$ on $[0,1]$ vanishing at both ends. By standard transformations, any heat equation problem with constant boundary values can be brought into this form.

For simplicity, we discretize [0, 1] by

$$
\begin{equation*}
0=x_{0}<x_{1}<\ldots<x_{n+1}=1 \tag{4}
\end{equation*}
$$

using equidistant points $x_{j}=j h, 0 \leq j \leq n+1$ with distance $h=1 /(n+1)$, but any other discretization (4), eqxdist) with fill distance

$$
h:=\sup _{x \in[0,1]} \min _{1 \leq j \leq n}\left|x-x_{j}\right|
$$

will do. Let $K$ be a smooth positive definite symmetric kernel on $\mathbb{R}$ and let $u_{0}, \ldots, u_{n}$ be the Lagrange basis for interpolation using translates of $K$ in the points $x_{0}, \ldots, x_{n+1}$. Note that $u_{1}, \ldots, u_{n}$ will automatically satisfy the zero boundary conditions at $x_{0}$ and $x_{n+1}$.

We use interpolatory trial functions

$$
s(x, t)=\sum_{j=1}^{n} s\left(x_{j}, t\right) u_{j}(x)
$$

vanishing at $x=0$ nd $x=1$ and interpolate the starting function $u_{0}$ by requiring

$$
s\left(x_{k}, 0\right)=u_{0}\left(x_{k}\right), 1 \leq k \leq n .
$$

The Method of Lines uses functions

$$
y(x, t)=\sum_{j=1}^{n} y_{j}(t) u_{j}(x)
$$

with $y\left(x_{j}, t\right)=y_{j}(t)$ and poses the linear ODE system

$$
y_{k}^{\prime}(t)=\sum_{j=1}^{n} y_{j}(t) u_{j}^{\prime \prime}\left(x_{k}\right), 1 \leq k \leq n
$$

with starting values

$$
y_{k}(0)=s\left(x_{k}, 0\right)=u_{0}\left(x_{k}\right), 1 \leq k \leq n .
$$

Introducing the matrix-vector notation for values at the points $x_{1}, \ldots, x_{n}$ as in the previous section, we get the linear first-order system

$$
\begin{equation*}
y^{\prime}(t)=U^{\prime \prime} y(t) \tag{5}
\end{equation*}
$$

with the solution

$$
y(t)=\exp \left(U^{\prime \prime} t\right) y(0) .
$$

The solution satisfies

$$
y_{t}\left(x_{k}, t\right)=y_{x x}\left(x_{k}, t\right), 1 \leq k \leq n
$$

by construction, since

$$
\begin{aligned}
y_{t}\left(x_{k}, t\right) & =\sum_{j=1}^{n} y_{j}^{\prime}(t) u_{j}\left(x_{k}\right) \\
& =y_{k}^{\prime}(t) \\
& =\sum_{j=1}^{n} y_{j}(t) u_{j}^{\prime \prime}\left(x_{k}\right), 1 \leq k \leq n \\
& =y_{x x}\left(x_{k}, t\right), 1 \leq k \leq n .
\end{aligned}
$$

## 5 Error Analysis

(SecEA) We introduce the interpolant $v(x, t)$ to the true solution $u(x, t)$ at the points $x_{0}, \ldots, x_{n+1}$ for all $t$. This is

$$
v(x, t)=\sum_{j=1}^{n} u\left(x_{j}, t\right) u_{j}(x)
$$

and we use it to insert the true solution into the ODE system for the Method of Lines. Then

$$
\begin{aligned}
u_{t}\left(x_{k}, t\right) & =u_{x x}\left(x_{k}, t\right) \\
& =\sum_{j=1}^{n} u\left(x_{j}, t\right) u_{j}^{\prime \prime}\left(x_{k}\right)+u_{x x}\left(x_{k}, t\right)-\sum_{j=1}^{n} u\left(x_{j}, t\right) u_{j}^{\prime \prime}\left(x_{k}\right) \\
& =\sum_{j=1}^{n} u\left(x_{j}, t\right) u_{j}^{\prime \prime}\left(x_{k}\right)+u_{x x}\left(x_{k}, t\right)-v_{x x}\left(x_{k}, t\right) .
\end{aligned}
$$

Introducing vectors for values at the $x_{k}$ again, we get

$$
u^{\prime}(t)=U^{\prime \prime} u(t)+\left(u_{x x}-v_{x x}\right)(t)
$$

and

$$
(u-y)^{\prime}(t)=U^{\prime \prime}(u-y)(t)+\left(u_{x x}-v_{x x}\right)(t)
$$

Since the discrete starting values $(u-y)(0)$ are zero, the standard formula for inhomogeneous linear first-order systems yields

$$
\begin{equation*}
(u-y)(t)=\int_{0}^{t} \exp \left(U^{\prime \prime}(t-s)\right)\left(u_{x x}-v_{x x}\right)(s) d s \tag{6}
\end{equation*}
$$

This is an exact formula for the error at the discrete points.
We shall use a smooth positive definite translation-invariant kernel $K$ on $\mathbb{R}$ with positive Fourier transform $\hat{K}$ and some order $m>1 / 2$ in the sense (eqkerord)

$$
\begin{equation*}
\int_{\mathbb{R}} \hat{K}(\omega)\left(1+|\omega|^{2}\right)^{m} d \omega<\infty . \tag{7}
\end{equation*}
$$

It will be reproducing in a "native" Hilbert space of at least continuous functions which is contained in Sobolev space $W_{2}^{m}(\mathbb{R})$. Then we can get (equvbound)

$$
\begin{equation*}
\|u(\cdot, t)-v(\cdot, t)\|_{L_{2}[0,1]} \leq C h^{m}\|u(\cdot, t)\|_{K} \tag{8}
\end{equation*}
$$

since we can also assume by standard results on the heat equation that the solution is smooth enough to lie in the spatial native space of the kernel for all times. Similarly,

$$
\left\|u_{x x}(\cdot, t)-v_{x x}(\cdot, t)\right\|_{L_{2}[0,1]} \leq C h^{m-2}\|u(\cdot, t)\|_{K} .
$$

The corresponding result for $L_{\infty}$ errors in 1D is

$$
\begin{equation*}
\left\|u_{x x}(\cdot, t)-v_{x x}(\cdot, t)\right\|_{L_{\infty}[0,1]} \leq C h^{m-2-1 / 2}\|u(\cdot, t)\|_{K} \tag{9}
\end{equation*}
$$

All of this follows from standard literature on kernel-based methods, see e.g. [15].

## 6 Bounding the Exponential

The remaining problem now is to bound the matrix exponential

$$
\exp \left(U^{\prime \prime} t\right) c=\sum_{n=0}^{\infty} \frac{t^{n}}{n!}\left(U^{\prime \prime}\right)^{n} c
$$

somehow, e.g. via

$$
\left\|\exp \left(U^{\prime \prime} t\right) c\right\|_{2} \leq \sum_{n=0}^{\infty} \frac{t^{n}}{n!} \rho\left(U^{\prime \prime}\right)^{n}\|c\|_{2}
$$

where $\rho$ is the spectral radius.
A special way to deal with the matrix exponential is to use that the matrix $U^{\prime \prime}$ will be negative definite. In fact, if $A$ is the standard kernel matrix for the given points, and $A^{\prime \prime}$ is the same, but with second derivatives of the kernel, we can use that $u \mapsto-u_{x x}$ is elliptic, thus $-A^{\prime \prime}$ will be positive definite. But $U^{\prime \prime}$ is the major part of $A^{-1} A^{\prime \prime}$ after dropping the outer rows and columns. This implies that $U^{\prime \prime}$ is negative definite. Thus the matrix exponential decays for increasing time, and can be bounded by a constant when looking at the integral (6, equyt). By Cauchy-Schwarz, the final error bound on data then is

$$
\begin{equation*}
\left|u\left(x_{j}, t\right)-y\left(x_{j}, t\right)\right| \leq \sqrt{t} C h^{m-2}\left(\int_{0}^{t}\|u(\cdot, t)\|_{K}^{2} d t\right)^{1 / 2} \tag{10}
\end{equation*}
$$

Theorem 6.1. If the Method of Lines is carried out using a kernel of order $m$ in the sense of (7, eqkerord), the error on the discretization points and up to all fixed times will be given by (10, eqMOLbound).

Since the true solution is $C^{\infty}$ and vanishes for increasing $t$ due to its standard series representation based on separation of variables, we know that the second factor in (10, eqMOLbound) is uniformly bounded.

The error outside the data can be bounded by a-posteriori analysis, using the Lagrange basis again. Writing

$$
y(x, t)=\sum_{j=1}^{n} u_{j}(x) y\left(x_{j}, t\right)
$$

and making use of the fact [3] that the Lagrange basis functions are uniformly bounded if the distribution of spatial data points is not too irregular, we have (eqMOLboundglob)

$$
\begin{align*}
|v(x, t)-y(x, t)| & =\left|\sum_{j=1}^{n} u_{j}(x)\left(v\left(x_{j}, t\right)-y\left(x_{j}, t\right)\right)\right| \\
& =\left|\sum_{j=1}^{n} u_{j}(x)\left(u\left(x_{j}, t\right)-y\left(x_{j}, t\right)\right)\right|  \tag{11}\\
& \leq C n \sqrt{t} h^{m-2} \\
& \leq C \sqrt{t} h^{m-3}
\end{align*}
$$

for the global error between the interpolant $v$ to the true solution and the solution $y$ via the Method of Lines. The error between the true solution $u$ and its interpolant $v$ has the better bound (8, equvbound). This implies
Theorem 6.2. If the Method of Lines is carried out using a kernel of order $m$ in the sense of (7, eqkerord), the error on the discretization points and up to all fixed times will be of order $\mathcal{O}\left(\sqrt{t} h^{m-3}\right)$.

Note that there is no CFL condition here, since there is no time step. At this point, it is assumed that the ODE system induced by the Method of Lines is solved exactly, and propagation of roundoff is ignored. Any ODE solver has to cope with the linear system (5, eqyU) somehow, and since we shall see in the next section that $U^{\prime \prime}$ has negative eigenvalues of absolute value $\mathcal{O}\left(h^{2}\right)$, the ODE system will be hard to integrate with good quality if $h$ is small. All instability issues are shifted back to the ODE system when using the Method of Lines, but there is a CFL condition behind the scene, as we shall see in the next section.

## 7 Time Stepping Techniques

(SecTST) Using the above spatial discretization, and using the notation $w(x, t)$ for our approximate solution, a variation of a forward Euler timestepping method would then be

$$
\frac{w\left(x_{k}, t+\Delta t\right)-w\left(x_{k}, t\right)}{\Delta t}=w_{x x}\left(x_{k}, t\right)=\sum_{j=1}^{n} w\left(x_{j}, t\right) u_{j}^{\prime \prime}\left(x_{k}\right) .
$$

It still has a time discretization, but the space discretization is hidden in the exact differentiation of the spatial interpolant. In our vector notation, it is

$$
E(w(\cdot, t+\Delta t))=\left(I+U^{\prime \prime} \Delta t\right) E(w(\cdot, t))
$$

Its stability can thus be analyzed via linear algebra, and the algorithm is the same as a forward Euler step for the linear ODE system

$$
w^{\prime}(t)=U^{\prime \prime} w(t)
$$

we encountered before. We shall have to analyze the spectrum of $U^{\prime \prime}$ for asserting stability, and this will follow below.

By standard approximation results like (9, eqinfdiffbnd) for kernel-based methods, we get

Theorem 7.1. For kernels with orders $m>5 / 2$, the forward Euler method (and others discretizing the spatial second derivative in the same way) will be consistent of order $m-5 / 2$.

Note that for stable methods the consistency order will be the convergence order.

To check stability and to get a CFL condition, we need
Theorem 7.2. (TheSpecBound) The spectral radius of $U^{\prime \prime}$ satisfies

$$
\rho\left(U^{\prime \prime}\right) \leq C h^{-2}
$$

if spatial discretization is done with $m>5 / 2$.

Proof: If $\lambda$ is an eigenvalue of $U^{\prime \prime}$ with eigenvector $c$, then

$$
\begin{aligned}
U^{\prime \prime} c & =\lambda c \\
\sum_{j=1}^{n} u_{j}^{\prime \prime}\left(x_{k}\right) c_{j} & =\lambda c_{k}, 1 \leq k \leq n
\end{aligned}
$$

and the function

$$
s_{\lambda}(x):=\sum_{j=1}^{n} c_{j} u_{j}(x)
$$

satisfies

$$
s_{\lambda}^{\prime \prime}\left(x_{k}\right)=\lambda s_{\lambda}\left(x_{k}\right), 1 \leq k \leq n
$$

and vanishes on both $x_{0}=0$ and $x_{n+1}=1$. We invoke the "sampling" inequality

$$
\left\|s^{\prime \prime}\right\|_{\infty,[0,1]} \leq C\left(h^{m-5 / 2}\|s\|_{m}+h^{-2}\|s\|_{\infty, X}\right) \text { for all } s \in W_{2}^{m}[0,1]
$$

from [16] for $m>5 / 2$ and normalize $s$ to satisfy $\|s\|_{m}=1$. Then

$$
\begin{aligned}
\left|\lambda \| s_{\lambda}\left(x_{k}\right)\right| & \leq\left\|s^{\prime \prime}\right\|_{\infty,[0,1]} \\
& \leq C h^{-2}\|s\|_{\infty, X} .
\end{aligned}
$$

Picking $k$ with $\left|s_{\lambda}\left(x_{k}\right)\right|=\|s\|_{\infty, X}$ yields the assertion.
Thus, for Euler time-stepping in the ODE system (5, eqyU), a spectral radius of order $h^{-2}$ means that there must be a CFL condition of the form

$$
\Delta t \leq C(\Delta x)^{2}
$$

as is to be expected.


Figure 1: Absolute error

We close this section by an example. Figure 1 shows the absolute error for the case with the exact solution

$$
u(x, t)=\sin (\pi x) \exp \left(-\pi^{2} t\right)
$$

using the Method of Lines for 15 equidistant spatial points, using the $C^{4}$ Wendland kernel. Note that there is a sharp increase of errors close to the boundary right after the start of the integration. For illustration, see Figure


Figure 2: Errors at startup and first time step

2 giving the initial error of about 0.00004 and the error after the first time step at $t=0.001$, which is roughly 0.01 . This unexpected effect is observable for various other cases as well. It turns out that we missed the additional conditions

$$
u_{t}(0, t)=0=u_{x x}(0, t), u_{t}(1, t)=0=u_{x x}(1, t)
$$

forcing the second spatial derivative of the solution to be zero at the boundary for all times. Our interpolants should have incorporated this condition. This teaches us the lesson that the trial space should always be as close to the solution space as possible. But since we present an even better trial space in the next section, we refrain from repairing the above case.

## 8 Direct Heat Kernel Techniques

For our special problem, solutions in series form are given by

$$
u(x, t)=\sum_{k=1}^{\infty} c_{k} \sin (k \pi x) \exp \left(-k^{2} \pi^{2} t\right)
$$

when the initial function has the series expansion

$$
u_{0}(x)=u(x, 0)=\sum_{k=1}^{\infty} c_{k} \sin (k \pi x)
$$

with at least

$$
\sum_{k=1}^{\infty} c_{k}^{2} \leq \infty
$$

To apply kernel techniques directly, we can go over to kernels (ewheatkerser)

$$
\begin{equation*}
K(x, y, t):=\sum_{k=1}^{\infty} \lambda_{k} \sin (k \pi x) \sin (k \pi y) \exp \left(-k^{2} \pi^{2} t\right) \tag{12}
\end{equation*}
$$

with positive summable weights $\lambda_{k}$. By standard arguments concerning expansion kernels, we get

Theorem 8.1. (TheKerPosDef) Each such kernel satisfies the heat equations

$$
K_{t}(x, y, t)=K_{x x}(x, y, t)=K_{y y}(x, y, t)
$$

and the boundary conditions

$$
K(0, y, t)=K(x, 0, t)=K(1, y, t)=K(x, 1, t)
$$

for all $x, y \in[0,1]$. Furthermore, they are positive definite on $\Omega=[0,1]$ for all $t \in \mathbb{R}$.

Now one can take a set $X=\left\{x_{1}, \ldots, x_{n}\right\} \subset(0,1)$ of scattered points and interpolate the starting function $u_{0}$ by solving
(eqheatkersys)

$$
\begin{equation*}
u_{0}\left(x_{j}\right)=\sum_{k=1}^{n} \alpha_{k} K\left(x_{j}, x_{k}, 0\right), 1 \leq j \leq n \tag{13}
\end{equation*}
$$

for coefficients $\alpha_{1}, \ldots, \alpha_{n}$. Then the function

$$
s(x, t):=\sum_{k=1}^{n} \alpha_{k} K\left(x, x_{k}, t\right)
$$

will satisfy the heat equation and the boundary conditions. This yields a much better trial space, and avoids numerical integration completely. Due to the maximum principle, the error for all positive times is bounded by the $L_{\infty}$ interpolation error $\left\|s(\cdot, 0)-u_{0}\right\|_{\infty}$ at startup. A theoretical analysis of this error requires an application of kernel interpolation theory to $K(x, y, 0)$, which can be done using periodicity and Fourier expansions. We leave details of this to another paper.

The choice of the weights in the kernel series (12, ewheatkerser) will depend on the smoothness of the starting function $u_{0}$, since kernel interpolation theory [15, 12] tells us that the smoothness of the kernel $K(x, y, 0)$ should be not lower than the smoothness of the function supplying the data. And since


Figure 3: Kernel with weights $1 / n$ !
the smoothness of the functions generated by trigonometric series is related to the decay of the coefficients, the smoothness of $K(x, y, 0)$ is controlled by decay of the $\lambda_{k}$. We focus on a simple example here.

The choice $\lambda_{k}=1 / k$ ! gives a series which generates an analytic kernel plotted in Figure 3, It has an explicit representation

$$
\begin{aligned}
4 K(x, y, 0)=-\exp (\exp (\pi(x+y))) & +\exp (\exp (-\pi(x+y))) \\
-\exp (\exp (\pi(x-y))) & -\exp (\exp (-\pi(x-y)))
\end{aligned}
$$

which unfortunately suffers from severe cancellation. But the rapid convergence of the series (12, ewheatkerser) allows to sum the series up until the limit of double precision is reached, i.e. at $k=19$. This will, however, lead to inevitable rank loss in (13, eqheatkersys) for more than $n=19$ data points. Nonetheless, and in particular if the initial function $u_{0}$ is very smooth, there usually are good projections of the right-hand side into the column space of the matrix, leading to unexpectedly good results. Figure 4 shows an example for the starting function $u_{0}(x)=1-2|x-0.5|$ using only 13 points. The error is bounded by the visible difference of the starting function and its first interpolant.

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Figure 4: Solution of heat equation
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