Hermite Interpolation Approach to High-Order Approximation of Heat Equations

Chinedu Nwaigwe and Azubuike Weli

Abstract

It is usually desirable to approximate the solution of mathematical problems with high-order of accuracy and preferably using compact stencils. This work presents an approach for deriving high-order compact discretization of heat equation with source term. The key contribution of this work is the use of Hermite polynomials to reduce second order spatial derivatives to lower order derivatives. This does not involve the use of the given equation, so it is universal. Then, Taylor expansion is used to obtain a compact scheme for first derivatives. This leads to a fourth-order approximation in space. Crank-Nicholson scheme is then applied to derive a fully discrete scheme. The resulting scheme coincides with the fourth-order compact scheme, but our derivation follows a different philosophy which can be adapted for other equations and higher order accuracy. Two numerical experiments are provided to verify the fourth-order accuracy of the approach.

Index Terms

Compact schemes, Heat Equation, Hermite interpolation, high-order schemes.

I. Introduction

This work is concerned with using the Hermite interpolation polynomial to derive a fourth order compact numerical scheme for the following heat conduction problem:

$$\begin{aligned} &\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + f(x,t), \quad x \in (a,b) \subset \mathbb{R}, \\ &u(x,0) = g(x), \quad x \in [a,b]; \\ &u(0,t) = q_L(t), u(1,t) = q_L(t), \quad t \geq 0, \end{aligned} \tag{1}$$

where, $f : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ and q_L, q_R are given functions of t and $k > 0$. In the above problem k represents the thermal conductivity, f the heat source/sink term, g the initial heat distribution and q_L, q_R are the left and right boundary conditions respectively. Although the above problem is linear, for general cases of the functions f, g, q_L and q_R the exact solution may be difficult (if not impossible) to find in closed form. Hence, numerical methods are reliable means of approximating the solution in the general case.

Among the many methods to numerically approximate the solution of heat equations, the finite difference method stands out due to its simplicity and mathematical ’richness’ - there is a lot of literature dealing with the analysis of the methods - making them more reliable to use. There are two types of these methods, explicit and implicit methods. Due to stability considerations explicit methods use smaller time steps compared to implicit methods; this makes explicit schemes slower than their implicit versions. But most importantly, to obtain high order (like fourth order) accuracy, explicit methods (and even classical implicit methods) require large computational stencils like $\{x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}\}$ at a grid point x_i where x_{i-2}, x_{i-1} are the left neighbors of x_i and x_{i+1}, x_{i+2} are the right neighbors. Higher order accuracy would require even more neighbors on both sides of x_i, see [1] for example. Such large stencils lead to inefficient schemes in terms of both CPU time and memory usage. For these reasons, compact finite difference schemes [2], [3], [4] have been proposed to give implicit schemes with high accuracy on smaller stencils. This saves both CPU time and computer memory.

It is proven that compact schemes give better accuracy than noncompact implicit schemes [4]. Hence, many studies have been focused on developing and applying compact schemes to solve diverse problems. For example, Dlamini and coworkers [5] applied compact finite difference relaxation method (CFDRM) to solve unsteady boundary layer problems. Compact scheme is used in solving coupled Burgers’ equation in [6]. Also, [7] proposes two high order finite difference schemes for solving two-dimensional linear parabolic equations where fourth order compact schemes were considered. Also, [8] derived the compact theta scheme for the linear initial-boundary value problems, while [9] formulated a fourth order compact scheme that satisfies the Lie symmetry. Shukla and Zhong [10] used simple polynomial interpolation to derive arbitrarily high-order compact schemes for the first derivative and tridiagonal compact schemes for the second derivative. Compact finite difference ideas are also

ISSN: 2736-5484
DOI: http://dx.doi.org/10.24018/ejmath.2023.4.1.208
Published on February 25, 2023.
C. Nwaigwe is with the Mathematics Department, Rivers State University, Nigeria (e-mail: nwaigwe.chinedu@ust.edu.ng).
A. Weli is with the Mathematics Department, Rivers State University, Nigeria (e-mail: weli.azubuike@ust.edu.ng).

being exploited for quasi-linear and nonlinear problems involving gamma equation [11], elliptic and parabolic equations [12], parabolic equations [13], [14], [15] and convection-diffusion equations [16], [17].

In this paper, we show how to derive fourth order compact finite difference scheme for heat equation via Hermite Interpolation Polynomial, and use some numerical examples to test the scheme. Unlike other studies in this direction (example [10]) which used complicated tools, here our derivation is simple to understand and extend to other problems. The numerical scheme is formulated in section II while numerical examples are provided and discussed in section III. Concluding remarks are made in section IV.

II. Numerical Scheme

Let $N_x > 0$ be a positive integer, $h = 1/N_x$ the mesh size, $M = N_x + 1$ the number of mesh points, Δt the time step size be given, $x_i = ih$ for $0 \le i \le N_x$, and $t^n = n\Delta t$ for $n \ge 0$. We want the approximation $u_i^n \approx u(x_i, t^n)$.

The first target is to derive a discrete version of (1) at mesh point x_i.

A. Spatial Discretization of the Problem

By discretizing in space alone we obtain

$$\left.\frac{\partial u}{\partial t}\right|_i = \alpha \left.\frac{\partial^2 u}{\partial x^2}\right|_i + f_i. \tag{2}$$

The goal of this subsection is to express the first term on the right hand side of (2) in terms of the solution values at the grid points. To this end, we will use the Hermite Interpolating polynomial to derive the finite difference scheme. Let us first define the computational stencil for point(x_i) namely:

$$I_i = \{x_{i-1}, x_i, x_{i+1}\}.$$

Since the points in I_i are all global coordinates, we need to define a local coordinate on I_i, given a

$$\varepsilon = \varepsilon(x) = x - x_i \text{ for all } x \in I_i. \tag{3}$$

This transforms the points in $I_i = \{x_{i-1}, x_i, x_{i+1}\}$ to the local coordinates $E_i = \{\varepsilon_0, \varepsilon_1, \varepsilon_2\}$ where $\varepsilon_0 = x_{i-1} - x_i = -h, \varepsilon_1 = x_i - x_i = 0$, and $\varepsilon_2 = x_{i+1} - x_i = h$. So that we have the local points:

$$E_i = \{-h, 0, h\}.$$

To be consistent with the local point notations, we also use $U_0(t), U_1(t), U_2(t)$ to denote the solution $u_{i-1}(t), u_i(t), u_{i+1}(t)$ respectively, that is at points x_{i-1}, x_i, x_{i+1} respectively. Similarly, we use the symbols $W_0(t), W_1(t), W_2(t)$ to denote the first derivative of the solution at grid points x_{i-1}, x_i, x_{i+1} respectively. Hence we can construct the following local table (see Table I) for the solution U and its first derivative W in I_i as follows:

TABLE I
Solution and Its Derivatives at Local Stencil Points. t Is Fixed

ε	$-h$	0	h
$u(\varepsilon, t)$	$U_0(t)$	$U_1(t)$	$U_2(t)$
$u'(\varepsilon, t)$	$W_0(t)$	$W_1(t)$	$W_2(t)$

Having constructed the Table I, we assume that the solution satisfies the Hermite polynomial in each stencil, that is
We assume:

$$U(x,t) \approx H(x,t) = \sum_{k=0}^{2} U_k(t) F_k(\varepsilon_k) + \sum_{k=0}^{2} W_k(t) G_k(\varepsilon_k), \tag{4}$$

where

$$\begin{aligned} F_k(\varepsilon) &= [L_k(\varepsilon)]^2 \left[1 - 2L_k'(\varepsilon_k)(\varepsilon - \varepsilon_k)\right], \\ G_k(\varepsilon) &= [L_k(\varepsilon)]^2 (\varepsilon - \varepsilon_k), \quad k = 0, 1, 2, \end{aligned} \tag{5}$$

with

$$\begin{aligned} L_0(\varepsilon) &= \frac{\varepsilon^2 - \varepsilon h}{2h^2} \Rightarrow L_0'(\varepsilon_0) = \frac{-3}{2h} \text{ and } L_0''(\varepsilon) = \frac{1}{h^2}. \\ L_1(\varepsilon) &= \frac{h^2 - \varepsilon^2}{h^2}, \Rightarrow L_1'(\varepsilon_1) = 0 \text{ and } L_1''(\varepsilon) = \frac{1}{h^2}. \\ L_2(\varepsilon) &= \frac{\varepsilon^2 + h\varepsilon}{2h^2}, \Rightarrow L_2'(\varepsilon_1) = 0 \text{ and } L_2''(\varepsilon_2) = \frac{3}{2h}. \end{aligned} \tag{6}$$

Hence,

$$\begin{aligned} F_0(\varepsilon) &= \frac{(\varepsilon^2-\varepsilon h)^2(8h+6\varepsilon)}{8h^5}, \\ F_1(\varepsilon) &= \frac{(\varepsilon^2-h^2)^2}{h^4}, \\ F_2(\varepsilon) &= \frac{(\varepsilon^2+h)^2(8h-6\varepsilon)}{8h^5}, \end{aligned} \tag{7}$$

and

$$\begin{aligned} G_0(\varepsilon) &= \frac{(\varepsilon^2-\varepsilon h)^2(\varepsilon+h)}{4h^4}, \\ G_1(\varepsilon) &= \frac{(h^2-\varepsilon^2)^2\varepsilon}{h^4}, \\ G_2(\varepsilon) &= \frac{(\varepsilon^2+\varepsilon h)^2(\varepsilon-h)}{4h^4}. \end{aligned} \tag{8}$$

Putting all these together, we arrive at a fourth approximation of $u(t)$ in the stencil as

$$\begin{aligned} U(\varepsilon,t) \approx H(\varepsilon,t) = &\left(\frac{\varepsilon^2-\varepsilon h}{2h^2}\right)^2\left(\frac{8h+6\varepsilon}{2h}\right)U_0(t) + \frac{(\varepsilon^2-h^2)^2}{h^4}U_1(t) \\ &+ \frac{(\varepsilon^2+h)^2(8h-6\varepsilon)}{8h^5}U_2(t) + \frac{(\varepsilon^2-\varepsilon h)^2(\varepsilon+h)}{4h^4}W_0(t) \\ &+ \frac{(h^2-\varepsilon^2)^2\varepsilon}{h^4}W_1(t) + \frac{(\varepsilon^2+\varepsilon h)^2(\varepsilon-h)}{4h^4}W_2(t). \end{aligned} \tag{9}$$

This is a polynomial representation of the solution in the stencil. It has fourth order of accuracy. One can easily confirm that $H(\varepsilon=-h,t)=U_0(t), H(\varepsilon=0,t)=U_1(t), H(\varepsilon=h,t)=U_2(t)$.

The first derivative with respect to ε is

$$\begin{aligned} \frac{\partial H(x,t)}{\partial x} = &\frac{U_0(t)}{8h^5}[2(2x-h)(x^2-xh)(8h+6x)6(x^2-xh)^2] \\ &+ \frac{U_1(t)}{h^4}[4x(x^2-h^2)] \\ &+ \frac{U_2(t)}{8h^5}[(8h+6x)2(2x+h)(x^2+xh)-6(x_2+xh)^2] \\ &+ \frac{W_0(t)}{4h^4}[(x+h)2(2x-h)(x^2-xh)+(x^2+xh)^2] \\ &+ \frac{W_1(t)}{h^4}[(x^2-h^2)^2+4x(x^2-h^2)] \\ &+ \frac{W_2(t)}{4h^4}[2(2x+h)(x^2+xh)(x-h)+(x^2+xh)^2]. \end{aligned} \tag{10}$$

It is also easy to confirm that

$$\left.\frac{\partial H}{\partial \varepsilon}\right|_{(\varepsilon=\varepsilon_k,t)} = W_k(t) \qquad \forall k=0,1,2.$$

Evaluating the second derivative at grid point i, that is $\left.\frac{\partial^2 H}{\partial \varepsilon^2}\right|_{(\varepsilon=\varepsilon_1,t)}$ one obtains

$$\begin{aligned} \left.\frac{\partial^2 H(\varepsilon,t)}{\partial \varepsilon^2}\right|_{(\varepsilon=\varepsilon_1,t)} &= \frac{U_0(t)}{8h^5}[2[0+h^2(8h)+6\times 0]+0] \\ &+ \frac{U_1(t)}{h^4}[4h^2] + \frac{U_2(t)}{8h^5}[2[0+0+8h^3]-12[0]] \\ &+ \frac{W_0(t)}{4h^4}[2[0+0+h^3]+0] + \frac{W_1(t)}{h^4}[0] + \frac{W_2(t)}{4h^4}2[0-h^3+0]+0 \\ &= \frac{2U_0(t)}{h^2} + \frac{4U_1(t)}{h^2} + \frac{2U_2(t)}{2h} + \frac{W_0(t)}{h^2} + \frac{W_2(t)}{2h} \\ &\frac{2U_0(t)-4U_1(t)+2U_2(t)}{h^2} + \frac{W_0(t)-W_2(t)}{2h}. \end{aligned} \tag{11}$$

Transforming back to global variables (u_i, u_i', etc), the approximation (11) gives the following formulation.

$$\left.\frac{\partial^2 u(x,t)}{\partial x^2}\right|_i = \frac{2}{h^2}(u_{i+1}(t) - 2u_i(t) + u_{i+1}(t)) + \frac{u_{i-1}'(t) - u_{i+1}'(t)}{2h} \tag{12}$$

where

$$u_i' = \left.\frac{\partial u}{\partial x}\right|_i .$$

Remark II.1. *Equation* (15) *is the major contribution of this work. One can see that it has reduced second order derivatives to lower order derivatives. Below we suggest one way to use Taylor series and the given equation to obtain a semi-discrete scheme - discrete in space but continuous in time.*

From Taylor series expansion, we obtain:

$$\begin{aligned}\frac{u_{i+1}' - u_{i-1}'}{2h} &= \left.\frac{\partial^2 u}{\partial x^2}\right|_i + \frac{h^2}{3!}\left.\frac{\partial^4 u}{\partial x^4}\right|_i + \frac{h^4}{5!}\left.\frac{\partial^6 u}{\partial x^6}\right|_i + O(h^6)\\ &= \left.\frac{\partial^2 u}{\partial x^2}\right|_i + \frac{h^2}{6}\frac{\partial^2}{\partial x^2}\left.\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_i + O(h^4)\\ &= \left.\frac{\partial^2 u}{\partial x^2}\right|_i + \frac{1}{6}\left[\left.\frac{\partial^2 u}{\partial x^2}\right|_{i+1} - 2\left.\frac{\partial^2 u}{\partial x^2}\right|_i + \left.\frac{\partial^2 u}{\partial x^2}\right|_{i-1}\right] + O(h^4). \end{aligned} \tag{13}$$

This leads to the relationship:

$$\frac{u_{i+1}' - u_{i-1}'}{2h} = \frac{1}{6}(u_{i+1}'' + 4u_i'' + u_{i-1}'') + O(h^4) \tag{14}$$

Putting (14) into (15), we get

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_i = \frac{2}{h^2}(u_{i+1} - 2u_i + u_{i+1}) - \frac{1}{6}(u_{i+1}'' + 4u_i'' + u_{i-1}''). \tag{15}$$

Using the right hand side of (15) to replace $\left.\frac{\partial^2 u}{\partial x^2}\right|_i$ in (2), we obtain

$$\begin{aligned}\left.\frac{\partial u}{\partial t}\right|_i &= \alpha \left.\frac{\partial^2 u}{\partial x}\right| + f_i(t)\\ &= 2\alpha\frac{(u_{i+1} - 2u_i + u_{i-1})}{h^2} - \frac{\alpha}{6}(u_{i+1}'' + 4u_i'' + u_{i-1}'') + f_i + O(h^4)\\ &= 2\alpha\frac{(u_{i+1} - 2u_i + u_{i-1})}{h^2}\\ &- \frac{1}{6}\left(\left.\frac{\partial u}{\partial t}\right|_{i-1} - f_{i-1} + 4\left.\frac{\partial u}{\partial t}\right|_i - 4f_i + \left.\frac{\partial u}{\partial t}\right|_{i+1} - f_{i+1}\right) + f_i. \end{aligned} \tag{16}$$

Simplifying this leads to the semi-discrete scheme:

$$\begin{aligned}\frac{10}{6}\left.\frac{\partial u}{\partial t}\right|_i + \frac{1}{6}\left.\frac{\partial u}{\partial t}\right|_{i-1} + \frac{1}{6}\left.\frac{\partial u}{\partial t}\right|_{i+1} =& 2\alpha\frac{(u_{i+1} - 2u_i + u_{i-1})}{h^2}\\ &+ \frac{1}{6}\left(f_{i-1} + 10f_i + f_{i+1}\right) + O(h^4) \end{aligned} \tag{17}$$

This is the semi-discrete scheme - discrete in space but continuous in time. We apply the Crank-Nicholson time integrator to obtain the fully discrete scheme below.

B. Fully Discrete Scheme - Crank-Nicholson Time Integration

Using Crank-Nicholson integration, we obtain

$$\begin{aligned}\frac{10}{6\Delta t}(u_i^{n+1} - u_i^n) + \frac{1}{6\Delta t}(u_{i-1}^{n+1} - u_{i-1}^n) + \frac{1}{6\Delta t}(u_{i+1}^{n+1} - u_{i+1}^n)\\ = \frac{\alpha(u_{i+1}^{n+1} + u_i^{n+1} + u_{i-1}^{n+1})}{h^2} + \frac{1}{12}(f_{i-1}^{n+1} + 10f_i^{n+1} + f_{i+1}^{n+1})\\ + \frac{\alpha(u_{i+1}^n + u_i^n + u_{i-1}^n)}{h^2} + \frac{1}{12}(f_{i-1}^n + 10f_i^n + f_{i+1}^n). \end{aligned} \tag{18}$$

Or

$$\begin{aligned}\left(1-6\alpha\frac{\Delta t}{h^2}\right)u_{i-1}^{n+1}+\left(10+12\alpha\frac{\Delta t}{h^2}\right)u_{i}^{n+1}+\left(1-6\alpha\frac{\Delta t}{h^2}\right)u_{i+1}^{n+1}\\ =\left(1-6\alpha\frac{\Delta t}{h^2}\right)u_{i-1}^{n}+\left(10+12\alpha\frac{\Delta t}{h^2}\right)u_{i}^{n}\\ +\left(1-6\alpha\frac{\Delta t}{h^2}\right)u_{i+1}^{n}+\frac{\Delta t}{2}\Big[(f_{i-1}^{n+1}+f_{i-1}^{n})\\ +10(f_{i}^{n+1}+f_{i}^{n})+(f_{i+1}^{n+1}+f_{i+1}^{n})\Big].\end{aligned} \tag{19}$$

This is the fully discrete scheme which is implemented for the heat problem (1). Numerical experiments are provided in the next section to verify the correctness and convergence of this scheme.

III. Numerical Results

We now present some numerical experiments to demonstrate the accuracy and convergence of the scheme presented above. The scheme is implemented in a C++ code written and maintained by the first Author. It does all the necessary linear algebra calculations with the help of the Eigen C++ library [18]. The examples here are derived via the method of manufactured solutions [19], [20], [21]. The error is computed in l_2-norm and the experimental order of convergence is computed using the formula (see [22], [23])

$$EOC=\frac{\ln\left(\frac{e_h}{e_{h/2}}\right)}{\ln 2}, \tag{20}$$

where e_h and $e_{h/2}$ are the errors (in l_2-norm) of the solutions computed on a mesh of step sizes h and $h/2$ respectively.

Problem 1: We consider the problem:

$$\begin{aligned}\frac{\partial u}{\partial t}&=\frac{1}{\pi^2}\frac{\partial^2 u}{\partial x^2}\quad \forall\, x\in(0,1),\, t>0,\\ u(0,t)&=0, u(1,t)=0,\quad t\geq 0,\\ u(x,0)&=-sin(\pi x)\quad x\in[0,1],\end{aligned} \tag{21}$$

whose exact solution is $u(x,t)=-e^{-t}sin(\pi x)$.

The numerical solution of this problem is computed on a sequence of grids with $M=6\times 2^p$ mesh points, for $p=0,1,\cdots,5$ and the results are outputted after $t=0.1$. The results are displayed in Table II. It can be seen that the error vanishes as the mesh size vanishes, showing that the method converges for this particular problem. Equally worthy of note is that the experimental order of convergence is four which is the same as the theoretical order of convergence as derived in the previous section. This verifies the correctness and validity of the formulation.

TABLE II
Experimental Order of Convergence for Problem 1. *EOC* Is the Computed Order of Convergence

M	$Error$	EOC
6	1.92511e-05	-
12	1.19209e-06	4.01338
24	7.43129e-08	4.00373
48	4.64178e-09	4.00086
96	2.89982e-10	4.00064
192	1.77779e-11	4.02781

1) Example 2: The second example is

$$\begin{aligned}\frac{\partial u}{\partial t}&=\frac{\partial^2 u}{\partial x^2}-(x+t^2)sin(\pi x)+2\pi t cos(\pi x)\quad \forall\, x\in(0,1),\, t>0,\\ u(0,t)&=0, u(1,t)=0,\quad t\geq 0,\\ u(x,0)&=sin(\pi x)\quad x\in[0,1],\end{aligned} \tag{22}$$

whose exact solution is $u(x,t)=e^{-xt}sin(\pi x)$.

The solution of this problem is approximated on a sequence of grids with $M=6\times 2^p$ mesh points, for $p=0,1,\cdots,6$. The errors and EOC on each mesh is recorded in Table III. One can also see that the numerical solution converges to the exact solution and does so with fourth order of convergence. This also verifies the method and its implementation.

TABLE III
EXPERIMENTAL ORDER OF CONVERGENCE FOR PROBLEM 2. EOC IS THE COMPUTED ORDER OF CONVERGENCE

M	$Error$	EOC
6	0.000135932	-
12	8.42054e-06	4.01283
24	5.25185e-07	4.00302
48	3.28072e-08	4.00074
96	2.05019e-09	4.00018
192	1.2813e-10	4.00007
384	8.0259e-12	3.9968
768	5.36471e-13	3.90309

IV. CONCLUSION

A simple approach to derive a fourth order (in space) compact scheme is presented for heat equation with source term. The approach assumes that the solution within a stencil is given by a Hermite polynomial which enables us to express second derivative in terms of lower derivatives. Taylor series and Crank-Nicholson scheme are applied to derived the fully discrete scheme. Numerical examples are also presented to verify the formulation and the results show that
(i) the scheme converges to the exact solution and
(ii) it is fourth order of convergence.
We recommend that the approach be applied to other PDEs and even in higher dimensions.

ACKNOWLEDGMENT

We thank the reviewers for the suggestions that improved the work.

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