Journal of Computational and Applied Mathematics 453 (2025) 116153

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Enhancing interpolation and approximation error estimates using a novel Taylor-like formula

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ARTICLE INFO

Keywords:
Taylor's theorem
Taylor-like formula
Interpolation error
Finite differences scheme
Error estimate
Heat equation

ABSTRACT

In this paper, we present an approach to enhance interpolation and approximation error estimates. Based on a previously derived first-order Taylor-like formula, we demonstrate its applicability in improving the P_1-interpolation error estimate. Following the same principles, we have also developed a novel numerical scheme for the heat equation that provides a better error estimate compared to the classical implicit finite differences scheme. Numerical illustrations confirm this behavior.

1. Introduction

Even today, improving the accuracy of approximation continues to pose a challenge in the field of numerical analysis. In this context, we recently derived a novel first-order Taylor-like formula in [1]. The aim of this formula was to obtain a reduced remainder compared to the one obtained with the traditional Taylor formula. This result was achieved by "transferring" the numerical weight of the remainder to the main part of the expansion. Extension to second order were also proposed in [2], in the same spirit as what can be found in [3] for quadrature formula

From a mathematical perspective, the root of these issues can be found in Rolle's theorem and in Lagrange and Taylor's theorems, (see for instance [4,5]), basically due to an unknown point in the remainder of the Taylor expansion. As a result, most of the error estimates concentrate on the *asymptotic behavior* of the error, for instance, in finite element methods, as the mesh size tends to zero.

In this context, various approaches have been proposed to identify ways of enhancing the approximation accuracy. For instance, in the realm of numerical integration, we refer the reader to [6,7] or [8], along with the references cited therein. From a different perspective, because of the lack of information, heuristic methods have been explored, basically based on a probabilistic approach, see for instance [9–12] or [13–15]. This makes possible to compare different numerical approaches, for instance for a fixed mesh size, see [16].

However, accurately estimating the upper bounds of error estimates and developing methods to enhance these upper bounds remain significant challenges. In this context, we proposed in [17] a refined first-order expansion formula in $\mathbb{R}^n$, to obtain a reduced remainder compared to the one obtained by usual Taylor's formula, and we investigated some related properties. Similar problems have been considered in the past years, and are often referred to as the perturbed (or corrected) quadrature rules, see for instance [7] or [8]. In other instances, authors obtained in [18,19] or [20] the trapezoid inequality by the difference between the supremum and the infimum bounds of the first derivative.

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https://doi.org/10.1016/j.cam.2024.116153
Received 23 October 2023; Received in revised form 7 July 2024
Available online 25 July 2024

In this paper, we address error estimates related to interpolation and approximation based on our new Taylor-like formula. We will demonstrate that the interpolation error estimate can be enhanced, even within the broader class of Sobolev spaces $W^{1,1}$. Additionally, we explore how finite differences schemes can be improved (in terms of precision), by using our approach.

The paper is organized as follows. In Section 2, we recall the first-order Taylor-like formula proposed in [1]. Then, we consider classical applications of the new Taylor expansion. In Section 3, we show how it can improve the P_1-interpolation error estimate. In Section 4, we use it to derive a new numerical scheme for the heat equation. We also provide numerical illustrations to verify the theoretical analysis. Concluding remarks follow.

2. A new first order expansion formula

To begin with, let us recall the first order Taylor-like formula we derived in [1]. To this end, we consider an integer n in $\mathbb{N}^*$, $(a,b) \in \mathbb{R}^2$, $a < b$, and a function $f \in C^2(]a,b[)$. We have

Theorem 2.1. *Let f be a real mapping defined on $[a,b]$ which belongs to $C^2([a,b])$, such that: $\forall x \in [a,b], -\infty < m_2 \leqslant f''(x) \leqslant M_2 < +\infty$. Then, we have the following first order expansion:*

$$f(b) = f(a) + (b-a)\left(\frac{f'(a)+f'(b)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f'\left(a + k\frac{(b-a)}{n}\right)\right) + (b-a)\epsilon^{(1)}_{a,n+1}(b), \tag{1}$$

where :

$$|\epsilon^{(1)}_{a,n+1}(b)| \leqslant \frac{(b-a)}{8n}(M_2 - m_2). \tag{2}$$

This result is optimal in the sense that the weights involved in the linear combination of f' at the equally spaced points $a+k\frac{(b-a)}{n}$ guarantee the remainder $\epsilon^{(1)}_{a,n+1}(b)$ to be minimum.

The particular case of (1) when $n = 1$ will be also considered in the sequel. In this case, we have:

$$f(b) = f(a) + (b-a)\left(\frac{f'(a)+f'(b)}{2}\right) + (b-a)\epsilon_{a,2}(b)\,. \tag{3}$$

Above, the remainder $\epsilon_{a,2}(b)$ satisfies the following inequality:

$$\frac{(b-a)}{8}(m_2 - M_2) \leqslant \epsilon_{a,2}(b) \leqslant \frac{(b-a)}{8}(M_2 - m_2).$$

This result can be compared with the well-known first order Taylor's formula [21], that we recall here for completeness. With the same notations, we have:

$$f(b) = f(a) + (b-a)f'(a) + (b-a)\epsilon_{a,1}(b),$$

where:

$$\frac{(b-a)}{2}m_2 \leqslant \epsilon_{a,1}(b) \leqslant \frac{(b-a)}{2}M_2.$$

In the following of the paper, we will consider two applications where formulas (1) and (3) will be involved. In Section 3 we will show how (1) can be used to improve the P_1-interpolation error estimate. In Section 4, we will apply (3) to develop a new numerical scheme for the heat equation, with a smaller upper bound in the approximation error estimate compared to the one associated with the classical implicit finite differences scheme.

3. Improving the $W^{1,1}$ interpolation error estimate

The first application we have in mind is related to the interpolation error estimate. Now, numerous partial differential equations are not well posed for any integer m in $H^m(\Omega)$ but in a more general class of Sobolev spaces, namely, $W^{m,p}(\Omega), (m,p) \in \mathbb{N}^{*2}$, and in particular in the space $W^{1,1}(\Omega)$, where Ω denotes a given non empty open domain in $\mathbb{R}^d$.

It is for example the case of the Laplace equation with a given right-hand side $f \in L^p(\Omega), (p \neq 2)$. Indeed, in that case, the solution u to the associated variational formulation belongs to $W^{1,p}(\Omega), (p \neq 2)$, if the domain Ω is regular enough. Other cases may be found for example in [22–24].

In the sequel, we consider for $\Omega =]0,1[$, the functional framework based on the Sobolev space $W^{1,1}(]0,1[)$ defined by:

$$W^{1,1}(]0,1[) = \left\{ u :]0,1[\to \mathbb{R},\ u \in L^1(]0,1[)\,;\, u' \in L^1(]0,1[) \right\},$$

where u' is the weak derivative of u in $L^1(]0,1[)$, see [25].

Using this framework, we will derive in this section a new interpolation error estimate based on the new Taylor-like formula (1). More precisely, we consider a given real function u defined on the interval $[0,1]$ which belongs to $C^2([0,1]) \subset W^{1,1}(]0,1[)$.

We also introduce a mesh on $[0,1]$ defined by: $(x_i)_{i=0,\dots,N+1}$ such that $x_0 = 0$ and $x_{N+1} = 1$. Moreover, we define the mesh size h by: $h = \max_{i=0,\dots,N} h_i$, where $h_i = x_{i+1} - x_i, (i = 0,\dots,N)$.

Finally, we consider the P_1-interpolation polynomial u_I of u which satisfies:

$$\forall i \in \{0, \dots, N+1\},\ u_I(x_i) = u(x_i),$$
$$\forall x \in [x_i, x_{i+1}], u_I \in P_1([x_i, x_{i+1}]),$$

where $P_1([x_i, x_{i+1}])$ is the space of polynomials of degree at most 1 defined on $[x_i, x_{i+1}]$. We also introduce the following notations: For any $u \in W^{1,1}(]0,1[)$, we denote by $\|.\|_{1,1}$ the standard norm defined by:

$$\|u\|_{1,1} = \|u\|_{0,1} + \|u'\|_{0,1},$$

where the norm $\|u\|_{0,1}$ is defined by:

$$\|u\|_{0,1} = \int_0^1 |u(x)|\, dx.$$

We first derive the classical interpolation error estimate based on the standard Taylor formula:

Lemma 3.1. *Let u be in $C^2([0,1])$ and u_I the corresponding P_1-interpolation polynomial. Then, the standard Taylor formula leads to the following interpolation error estimate:*

$$\|u - u_I\|_{1,1} \le (h + h^2)\|u''\|_\infty, \tag{4}$$

where $\|u''\|_\infty = \operatorname{ess\,sup}_{x\in[0,1]} |u''(x)|$.

Proof. We recall the classical first order Taylor formula [1] given by:

$$u(x_{i+1}) = u(x_i) + h_i u'(x_i) + h_i \epsilon^{(T)}, \tag{5}$$

with:

$$|\epsilon^{(T)}| \le \frac{h_i}{2}\|u''\|_\infty. \tag{6}$$

- We begin by evaluating the L^1-norm of the derivative, that is $\|u' - u'_I\|_{0,1}$.
We have:

$$\|u' - u'_I\|_{0,1} = \int_0^1 |u'(x) - u'_I(x)|\, dx = \sum_{i=0}^{N} \int_{x_i}^{x_{i+1}} |u'(x) - u'_I(x)|\, dx.$$

Then, given that u'_I is constant on $[x_i, x_{i+1}]$, by the help of (5), we get:

$$\forall \in [x_i, x_{i+1}] : u'_I(x) = \frac{u(x_{i+1}) - u(x_i)}{h_i} = u'(x_i) + \epsilon^{(T)}.$$

As a consequence, using (6) and Fubini's theorem [25], we can derive the following sequence of inequalities:

$$\begin{aligned}
\int_{x_i}^{x_{i+1}} |u'(x) - u'_I(x)|\, dx &= \int_{x_i}^{x_{i+1}} |u'(x) - u'(x_i) - \epsilon^{(T)}|\, dx && (7)\\
&\le \int_{x_i}^{x_{i+1}} |u'(x) - u'(x_i)|\, dx + \frac{h_i^2}{2}\|u''\|_\infty\\
&= \int_{x_i}^{x_{i+1}} \left| \int_{x_i}^{x} u''(t) dt \right| dx + \frac{h_i^2}{2}\|u''\|_\infty\\
&\le \int_{x_i}^{x_{i+1}} \int_{x_i}^{x} |u''(t)| dt\, dx + \frac{h_i^2}{2}\|u''\|_\infty\\
&\le \int_{x_i}^{x_{i+1}} |u''(t)| \left(\int_t^{x_{i+1}} dx \right) dt + \frac{h_i^2}{2}\|u''\|_\infty\\
&= \int_{x_i}^{x_{i+1}} (x_{i+1} - t)|u''(t)|\, dt + \frac{h_i^2}{2}\|u''\|_\infty \le h_i^2\|u''\|_\infty. && (8)
\end{aligned}$$

By summing over i between 0 and N, and using that $\sum_{i=0}^{N} h_i = 1$, we finally get:

$$\|u' - u'_I\|_{0,1} \le \left(\sum_{i=0}^{N} h_i^2 \right) \|u''\|_\infty \le h\|u''\|_\infty\,. \tag{9}$$

- Let us now evaluate the L^1-norm $\|u - u_I\|_{0,1}$. First of all, we remark that we have, for all $x \in [x_i, x_{i+1}]$,

$$|u(x) - u_I(x)| = \left| \int_{x_i}^{x} \left(u'(t) - u'_I(t) \right) dt \right|. \tag{10}$$

Then,

$$|u(x) - u_I(x)| \leq \int_{x_i}^{x} |u'(t) - u_I'(t)|\, dt \leq \int_{x_i}^{x_{i+1}} |u'(t) - u_I'(t)|\, dt. \tag{11}$$

So, by using inequalities (7)–(8), we get that

$$\forall \in [x_i, x_{i+1}],\ |u(x) - u_I(x)| \leq h_i^2 \|u''\|_\infty.$$

It remains now to integrate this inequality on $[x_i, x_{i+1}]$ to obtain that

$$\int_{x_i}^{x_{i+1}} |u(x) - u_I(x)| \leq h_i^3 \|u''\|_\infty,$$

and summing over all values of i between 0 and N, this yields

$$\|u - u_I\|_{0,1} \leq h^2 \|u''\|_\infty. \tag{12}$$

Finally, by combining inequalities (9) and (12), we get the interpolation error estimate (4). ■

Now, let us derive the interpolation error estimate obtained by using the Taylor-like formula (1), instead of the standard Taylor formula.

Theorem 3.2. *Let u be in $C^2([0,1])$ and u_I the corresponding P_1-interpolation polynomial. Then, the Taylor-like formula (1) leads to the following interpolation error estimate:*

$$\|u - u_I\|_{1,1} \leq \frac{(h + h^2)}{2} \|u''\|_\infty + \frac{(h + h^2)}{8n}(M_2 - m_2), \forall n \in \mathbb{N}^*. \tag{13}$$

In particular, when n goes to $+\infty$, we get:

$$\|u - u_I\|_{1,1} \leq \frac{(h + h^2)}{2} \|u''\|_\infty. \tag{14}$$

Proof. Here also, we begin by evaluating the L^1-norm of the derivative, that is $\|u' - u_I'\|_{0,1}$. By the help of (1)–(2), setting $a = x_i, b = x_{i+1}$, we obtain that

$$\int_{x_i}^{x_{i+1}} |u'(x) - u_I'(x)|\, dx = \int_{x_i}^{x_{i+1}} \left| u'(x) - \left(\frac{u'(x_i) + u'(x_{i+1})}{2n} + \frac{1}{n} \sum_{k=1}^{n-1} u'\left(x_i + k\frac{h_i}{n} \right) + \epsilon_n \right) \right| dx.$$

Writing now $u'(x)$ in the integral as

$$u'(x) = \frac{1}{2n} u'(x) + \frac{1}{2n} u'(x) + \frac{1}{n} \sum_{k=1}^{n-1} u'(x),$$

enables us to derive the following estimate:

$$\int_{x_i}^{x_{i+1}} |u'(x) - u_I'(x)|\, dx \leq I_1 + I_2 + I_3 + \frac{h_i^2}{8n}(M_2 - m_2), \tag{15}$$

where we set:

$$\begin{aligned}
I_1 &= \frac{1}{2n} \int_{x_i}^{x_{i+1}} |u'(x) - u'(x_i)|\, dx, \\
I_2 &= \frac{1}{2n} \int_{x_i}^{x_{i+1}} |u'(x) - u'(x_{i+1})|\, dx, \\
I_3 &= \frac{1}{n} \sum_{k=1}^{n-1} \int_{x_i}^{x_{i+1}} |u'(x) - u'(x_k')|\, dx,
\end{aligned} \tag{16}$$

with: $x_k' = x_i + k\frac{h_i}{n}$.

Implementing the same techniques we used in (7)–(8), that is, based on Fubini's theorem, we get for I_1 and I_2:

$$I_1 \leq \frac{1}{2n} \int_{x_i}^{x_{i+1}} (x_{i+1} - t)|u''(t)|\, dt \leq \frac{h_i^2}{4n} \|u''\|_\infty, \tag{17}$$

$$I_2 \leq \frac{1}{2n} \int_{x_i}^{x_{i+1}} (t - x_i)|u''(t)|\, dt \leq \frac{h_i^2}{4n} \|u''\|_\infty. \tag{18}$$

Concerning the estimate of I_3, the treatment is based on the same principles but it has to be adapted. We proceed as follows.

Having x_k' which belongs to the open interval $]x_i, x_{i+1}[$, we first split the integral in (16) as

$$\int_{x_i}^{x_{i+1}} |u'(x) - u'(x_k')|\, dx = \int_{x_i}^{x_k'} \left| \int_{x_k'}^{x} u''(t)\, dt \right| dx + \int_{x_k'}^{x_{i+1}} \left| \int_{x_k'}^{x} u''(t)\, dt \right| dx. \tag{19}$$

Then, by using Fubini's theorem on each term separately, we get the two following inequalities:

$$\int_{x_i}^{x'_k} \left| \int_{x'_k}^{x} u''(t)\,dt \right| dx \le \int_{x_i}^{x'_k} (t-x_i)|u''(t)|\,dt,$$

and

$$\int_{x'_k}^{x_{i+1}} \left| \int_{x'_k}^{x} u''(t)\,dt \right| dx \le \int_{x'_k}^{x_{i+1}} (x_{i+1}-t)|u''(t)|\,dt,$$

which enables us to get from (19)

$$\begin{aligned}
\int_{x_i}^{x_{i+1}} |u'(x)-u'(x'_k)|\,dx &\le \int_{x_i}^{x'_k}(t-x_i)|u''(t)|\,dt + \int_{x'_k}^{x_{i+1}}(x_{i+1}-t)|u''(t)|\,dt,\\
&\le \left[\int_{x_i}^{x'_k}(t-x_i)\,dt + \int_{x'_k}^{x_{i+1}}(x_{i+1}-t)\,dt\right]\|u''\|_\infty,\\
&\le \left[\frac{(x'_k-x_i)^2}{2} + \frac{(x_{i+1}-x'_k)^2}{2}\right]\|u''\|_\infty. \qquad (20)
\end{aligned}$$

Then, using that $x'_k \in]x_i, x_{i+1}[$, we can write it as a affine combination of x_i and x_{i+1}, namely:

$$x'_k = tx_i + (1-t)x_{i+1}, (0 < t < 1).$$

Thus, (20) can be written as

$$\int_{x_i}^{x_{i+1}} |u'(x)-u'(x'_k)|\,dx \le \frac{1}{2}\left(2t^2-2t+1\right)h_i^2\,\|u''\|_\infty \le \frac{h_i^2}{2}\,\|u''\|_\infty, \qquad (21)$$

and by summing on k between 0 and $n-1$, (16) leads to:

$$I_3 \le \left(\frac{n-1}{2n}\right) h_i^2\,\|u''\|_\infty. \qquad (22)$$

Finally, by the help of inequalities (17), (18) and (22), the estimate (15) gives

$$\begin{aligned}
\int_{x_i}^{x_{i+1}} |u'(x)-u'_I(x)|\,dx &\le \left[\frac{1}{4n}+\frac{1}{4n}+\frac{n-1}{2n}\right] h_i^2\,\|u''\|_\infty + \frac{h_i^2}{8n}(M_2-m_2),\\
&\le \frac{h_i^2}{2}\|u''\|_\infty + \frac{h_i^2}{8n}(M_2-m_2). \qquad (23)
\end{aligned}$$

Now, by summing on i between 0 to N, we get the following estimate for the L^1-norm of the derivative:

$$\|u'-u'_I\|_{0,1} \le \frac{h}{2}\|u''\|_\infty + \frac{h}{8n}(M_2-m_2). \qquad (24)$$

Let us now evaluate the L^1-norm, that is $\|u-u_I\|_{0,1}$.

Like in the previous proof, (see (10)–(11)), we can write, for all $x \in [x_i, x_{i+1}]$,

$$|u(x)-u_I(x)| \le \int_{x_i}^{x} |u'(t)-u'_I(t)|\,dt \le \int_{x_i}^{x_{i+1}} |u'(t)-u'_I(t)|\,dt.$$

Then, due to estimate (23), this inequality becomes

$$|u(x)-u_I(x)| \le \frac{h_i^2}{2}\|u''\|_\infty + \frac{h_i^2}{8n}(M_2-m_2).$$

Now, integrating on x which belongs to $[x_i, x_{i+1}]$ leads to

$$\int_{x_i}^{x_i+1} |u(x)-u_I(x)|\,dx \le \frac{h_i^3}{2}\|u''\|_\infty + \frac{h_i^3}{8n}(M_2-m_2).$$

Finally, we sum over all values of i between 0 to N and we get that

$$\|u-u_I\|_{0,1} \le \frac{h^2}{2}\|u''\|_\infty + \frac{h^2}{8n}(M_2-m_2). \qquad (25)$$

In these conditions, the $W^{1,1}$-norm of the P_1-interpolation error can be obtained by adding inequalities (24) and (25), that is

$$\|u-u_I\|_{1,1} \le \frac{h+h^2}{2}\|u''\|_\infty + \frac{h+h^2}{8n}(M_2-m_2), \forall n \in \mathbb{N}. \qquad (26)$$

By letting n going to $+\infty$ in (26), we obtain estimate (14). ■

Remark 1. To appreciate the improvement between the two errors estimates (4) and (13), let us consider the asymptotic case, namely error estimate (14) when the number of points n goes to infinity. In that case, the upper bound is half that of (4).

In other words, for a large number of points n where the last term in (4) is negligible, the size of the interval containing the interpolation error using the Taylor-like formula is halved.

Significant consequences in terms of mesh size and implementation efficiency arise when we generalize these results to other Sobolev spaces, see [26].

Remark 2. We can observe the impact of Theorem 3.2 in various contexts, including the Lagrange finite element error estimate. Indeed, in [26], we propose an extension of Theorem 3.2 to $W^{1,p}$ Sobolev spaces for $p > 1$. In these cases, based on Banach-Nečas-Babuška Theorem applied to reflexive Banach spaces [27], and due to the generalized Céa's lemma (again, see [27]), we can improve the classical Lagrange finite element approximation error by enhancing the interpolation error of Theorem 3.2.

Remark 3. At first sight, estimate (14) that shows the $W^{1,1}$ error is not "usual" in the norm sense, since the right-hand side contains the L^∞ norm of the second derivative. However, it is very common in the framework of Taylor formulas and their applications to the finite element method, see for instance [28] or [29]. In this context, it is classically assumed that the functions have "sufficient" regularity, typically C^2 or C^3 depending on the need. Hence, it is preferred to establish error estimates with right-hand sides containing the L^∞ norm of the second or third derivative. Eventually, one can replace these norms when the solution $u \in H^2$ instead of C^2, even if, very often, we have to assume the solution to be in C^2 to prove regularity result (i.e. that the weak solution coincides with the strong one), see among others [25]. Note also that the central point here is not the norm used in the right-hand side, but the value of the constant involved in the standard Taylor formula compared to the one obtained with our new approach. Moreover, the convergence is slower if the solution is less regular [27]: assuming here that the right-hand side belongs to C^2 is to make comparison with the "best possible case" for the classical Taylor formula.

To end this section, let us summarize the different steps that outline how, from the Taylor-like formula (1), we can derive a new numerical scheme.

Stepwise algorithm:

- Derive a Taylor-like formula (1) by introducing a set of degrees of freedom (points and weights) to minimize the resulting remainder (see [1]).
- Minimize of the corresponding remainder and compute the optimal points and weights.
- Derive interpolation error estimates in $W^{1,1}$, either by implementing the standard Taylor's formula, or by using the new Taylor-like formula.
- Compare the two corresponding upper bounds to show the decreased value obtained with the new Taylor-like formula.
- Derive of an improved finite difference scheme by approximating a first order partial derivative using the Taylor-like formula (see Section 4).

In the next section, we provide an illustration of the last step, i.e. derivation of an improved scheme.

4. Enhancing finite differences schemes discretization

In this section, we give another application of the new Taylor-like formula (3). We first consider an implicit finite differences scheme to approximate the heat equation. Then, we will show how we can improve the error bound of the error estimate, without deteriorating neither the consistency error and the order of convergence, nor the stability.

More precisely, we will derive with (3) a new implicit finite differences scheme, that is first-order in time and second-order in space. In addition, it will be unconditionally stable, as the standard implicit finite differences scheme, but the upper bound of the error estimate will be two times smaller than the standard one.

4.1. Derivation of the scheme

To begin with, let us introduce the one dimensional heat equation defined as follows: consider a function $u(x,t)$ defined on $I \times [0,T]$, solution to:

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t), \quad (x,t) \in I \times [0,T], \tag{27}$$

where I is a given open subset of $\mathbb{R}$, (bounded or not), and T a given positive real number.

We add this equation with an initial condition, namely $u(x,t=0) = u_0(x)$, where $u_0(x)$ is a given regular function (for instance bounded in $\mathbb{R}$.) When I is a bounded subset of $\mathbb{R}$, says $I = [a,b]$, $a < b$, $a,b \in \mathbb{R}$, we also add boundary conditions, and we have $u(x=a,t) = l_1(t)$ and $u(x=b,t) = l_2(t)$, where l_1, l_2 denote given functions of t.

We also introduce a constant time step $k \equiv \Delta t$ and the corresponding discrete time $t^{(n)}$, defined by: $t^{(n)} = nk, (n \in \mathbb{N})$, as well as a constant mesh size $h \equiv \Delta x$ and the nodes of the mesh $x_j = jh, (j \in \mathbb{Z})$. Finally, we denote by $\tilde{u}_j^{(n)}$ an approximation of solution u to Eq. (27) at a given point $(x_j, t^{(n)})$, that is, $\tilde{u}_j^{(n)} \simeq u(x_j, t^{(n)})$.

Let us now remind the standard implicit scheme [30], that we denote $(\mathbf{FD}_1)$:

$$(\mathbf{FD}_1) \qquad \frac{\tilde{u}_j^{(n+1)} - \tilde{u}_j^{(n)}}{k} = \frac{\tilde{u}_{j-1}^{(n+1)} - 2\tilde{u}_j^{(n+1)} + \tilde{u}_{j+1}^{(n+1)}}{h^2}, \quad \forall (j,n) \in J \times \mathbb{N}, \tag{28}$$

where J denotes the total number of space nodes used in the space domain I.

It is well known [30] that the finite differences scheme $(\mathbf{FD}_1)$ is first-order in time and second-order in space. Indeed, introducing $m_2, M_2 \in \mathbb{R}$ the lower and upper bounds of the second derivative in time of u, that is

$$\forall t \in [0,T],\ m_2 \leqslant \frac{\partial^2 u}{\partial t^2}(.,t) \leqslant M_2\,, \tag{29}$$

and using the classical Taylor formula, we readily get that

$$\frac{\partial u}{\partial t}(x, t^{(n+1)}) = \frac{u(x,t^{(n+1)}) - u(x,t^{(n)})}{k} + \epsilon_n^{(T)}, \tag{30}$$

where

$$|\epsilon_n^{(T)}| \leq \frac{k}{2}\max(|m_2|, |M_2|). \tag{31}$$

Finally, introducing $u_j^{(n+1)} \equiv u(x_j, t^{(n+1)})$, the exact values of u at the point $(x_j, t^{(n+1)})$ and the same at the point $(x_j, t^{(n)})$, the well-known approximation of $\frac{\partial u}{\partial t}$ at $(x_j, t^{(n+1)})$ is given by

$$\frac{\partial u}{\partial t}(x_j, t^{(n+1)}) \simeq \frac{u_j^{(n+1)} - u_j^{(n)}}{k}\,. \tag{32}$$

Now, let us introduce another approximation of the first-order partial derivative $\frac{\partial u}{\partial t}$, for a solution u to Eq. (27) which is C^2 in time, by using the new Taylor-like formula (3).

So, let us set in (3) $a = t^{(n)}$ and $b = t^{(n+1)}$. Then, for any given $x \in I$, we get:

$$u(x, t^{(n+1)}) = u(x, t^{(n)}) + \frac{k}{2}\left(\frac{\partial u}{\partial t}(x, t^{(n)}) + \frac{\partial u}{\partial t}(x, t^{(n+1)})\right) + k\epsilon_n,$$

where the remainder ϵ_n satisfies here

$$|\epsilon_n| \leq \frac{k}{8}(M_2 - m_2). \tag{33}$$

Then, by the help of (27), we obtain that

$$\frac{\partial u}{\partial t}(x, t^{(n+1)}) = \frac{2}{k}\left(u(x,t^{(n+1)}) - u(x,t^{(n)})\right) - \frac{\partial^2 u}{\partial x^2}(x, t^{(n)}) - 2\epsilon_n, \tag{34}$$

that leads to the following approximation of $\frac{\partial u}{\partial t}$ at the point $(x_j, t^{(n+1)})$:

$$\frac{\partial u}{\partial t}(x_j, t^{(n+1)}) \simeq \frac{2}{k}\left(u_j^{(n+1)} - u_j^{(n)}\right) - \frac{u_{j-1}^{(n)} - 2u_j^{(n)} + u_{j+1}^{(n)}}{h^2}\,. \tag{35}$$

This approximation is clearly of the first order in time and of the second order in space.

Now, we want to compare the error bounds obtained by the approximations (32) and (35) of the time partial derivative. First, remark that the quantity involved in approximation (32) is $\epsilon_n^{(T)}$, whereas $2\epsilon_n$ is involved in approximation (35).

Moreover, assuming that $0 \leq m_2 \leq M_2$ and setting $\Lambda \equiv M_2 - m_2, (\Lambda \geq 0)$, we have:

$$|2\epsilon_n| \leq \frac{k}{4}\Lambda \leq \frac{k}{2}\max\left(|m_2|, |m_2 + \Lambda|\right) = \frac{k}{2}(m_2 + \Lambda).$$

Consequently, approximation (35) leads to an upper bound necessary smaller than that of (32).

The minimum gain that can be observed corresponds to $m_2 = 0$, and in this case, the error bound for approximation (35) is two times smaller than that of (32). Moreover, as m_2 increases, the error bound related to (35) decreases at least twice.

We are now in position to derive the main result of this section. So, for all $(j,n) \in J \times \mathbb{N}$, let us denote by $(\mathbf{FD}_2)$ the finite differences scheme defined by

$$(\mathbf{FD}_2) \qquad -\frac{k}{2h^2}\tilde{u}_{j-1}^{(n+1)} + \left(1 + \frac{k}{h^2}\right)\tilde{u}_j^{(n+1)} - \frac{k}{2h^2}\tilde{u}_{j+1}^{(n+1)} = \frac{k}{2h^2}\left(\tilde{u}_{j-1}^{(n)} + \tilde{u}_{j+1}^{(n)}\right) + \left(1 - \frac{k}{h^2}\right)\tilde{u}_j^{(n)}. \tag{36}$$

Hence, we have the following result:

Theorem 4.1. *The implicit scheme ($\mathbf{FD}_2$) is consistent with heat equation (27). It is first-order accurate in k (time) and second-order accurate in h (space), that is in $O(k)$ and $O(h)^2$. Moreover, for $m_2 \geq 0$, the error estimate bound in k is at least two times smaller that of the classical implicit finite differences scheme. Finally, when the open set of integration I is equal to $\mathbb{R}$, the scheme ($\mathbf{FD}_2$) is unconditionally stable.*

Proof. Consistency and order of convergence in space and in time were proved above when we introduced the scheme ($\mathbf{FD}_2$).

To learn the stability of the scheme, and check the necessary stability condition, we introduce as usual the amplitude coefficient A defined by $\tilde{u}_j^{(n)} = A^n e^{ipx_j}$, where p is a given real parameter.

Then, replacing this expression of $\tilde{u}_j^{(n)}$ in the scheme ($\mathbf{FD}_2$), we get, after some elementary trigonometrical transformations, that the coefficient A is equal to

$$A = \frac{1-X}{1+X}, \quad \text{where} \quad X = \frac{2k}{h^2}\sin^2\left(\frac{ph}{2}\right). \tag{37}$$

Given that $X \geq 0$, we obtain that $|A| \leq 1$, and the necessary stability condition is always fulfilled.

Finally, when the open set of integration I is equal to $\mathbb{R}$, the scheme ($\mathbf{FD}_2$) is unconditionally stable, since the necessary condition becomes a sufficient one [30]. ■

Remark 4. The application proposed here to the approximation of the heat equation has to be viewed as an example. Clearly, the new Taylor-like formula can be applied in various contexts and for different equations, depending on the specific requirements. Depending on their needs, readers can choose how to adapt formula (1) in a same manner as proposed here.

4.2. Numerical illustration

In this subsection, we propose numerical simulations to verify the theoretical analysis. We have intentionally chosen a simple example, where the exact solution is known, that will help us to check numerically the relevance of the error bounds we derived.

Note that the two schemes we implemented here have the same approximation order. Our goal is to assess the effective precision of each scheme by verifying that a smaller constant in the error estimates results in better effective accuracy for a given mesh size.

Hence, we consider the heat Eq. (27) in the bounded domain $I = [-1, 1]$, and we take a final time $T = 2$. The initial condition we consider consists in a constant initial temperature, namely $u(x, t = 0) = 1, \forall -1 \leq x \leq 1$. For the boundary conditions, we take a homogeneous Dirichlet condition on $x = \pm 1$, that is $u(x = -1, t) = u(x = 1, t) = 0$.

With these conditions, we can easily determine the analytical solution $u(x, t)$ of (27), which can be expressed by considering both the initial and the boundary conditions:

$$u(x,t) = \sum_{n\geq 1} a_n \cos(b_n x)\exp(-b_n^2 t)\,, \tag{38}$$

where the coefficients a_n and b_n are given by

$$a_n = \frac{4}{\pi}\frac{(-1)^{n-1}}{2n-1}, \qquad b_n = (2n-1)\frac{\pi}{2}.$$

With this data, we implement the classical implicit scheme ($\mathbf{FD}_1$) and the new scheme ($\mathbf{FD}_2$), and then compare them to the exact solution (38). Since the solution is given as a series, we will compute it by considering a sufficiently large number of terms, typically such as 100 terms. Additionally, considering the symmetry of the solution at the point $x = 0$, we can reduce the computational domain to the interval $[0, 1]$ by imposing a symmetry condition at $x = 0$ of the form $\frac{\partial u}{\partial x} = 0$. Practically, we implemented the schemes ($\mathbf{FD}_1$) and ($\mathbf{FD}_2$) using the package FreeFem++ [31] to compute the approximations.

As a first test case, we consider solutions obtained by both schemes compared to the exact solution for a given time $0 < t_0 < T$. It is worth noting that, theoretically, both schemes have the "same precision", in the sense that they are both first-order accurate in time and second-order accurate in space. However, ($\mathbf{FD}_2$) has a smaller constant than ($\mathbf{FD}_1$). In Fig. 1, we plot these solutions as a function of x ($x \in [0, 1]$ using the symmetry of the solution), obtained on the same mesh for two different times, $t_0 = \frac{T}{2}$ and $t_0 = \frac{4T}{5}$. In this example, we use a time step $k = 5.10^{-2}$ and a mesh size $h = 4.10^{-2}$. As shown in this figure, the new scheme is more precise than the classical one, indicating its best precision is due to the smaller constant.

The second numerical case aims to assess the behavior of the effective errors of each scheme in comparison to the upper bound. To achieve this, we consider the same dataset as before and, using the known exact solution, we first compute the lower and upper bounds m_2 and M_2 of $\frac{\partial^2 u}{\partial t^2}(\cdot, t)$ as introduced in (29). Under these conditions, for the classical scheme ($\mathbf{FD}_1$), we can compute, for a given $x \in [-1, 1]$, the bound $\frac{k}{2}\max(|m_2|, |M_2|)$ of the error $|\epsilon_n^{(T)}|$. For simplicity, we denote $\mathcal{M}_2 = \max(|m_2|, |M_2|)$. Following the theoretical study above, we know that the absolute value of the remainder $|\epsilon_n^{(T)}|$ is bounded by $\frac{k}{2}\mathcal{M}_2$.

Now, considering the expression (32) that approximates $\frac{\partial u}{\partial t}(\cdot, t)$, we can also examine, for each $x \in [-1, 1]$ (or in $[0, 1]$ using the symmetry), the relative position of this approximation to the upper bound $\frac{k}{2}\mathcal{M}_2$. So, we define the quantity

$$|\epsilon_{n,h}^{(T)}| = |\frac{\partial u}{\partial t}(x_j, t^{n+1}) - \frac{u_j^{(n+1)} - u_j^{(n)}}{k}|$$

that approximates $|\epsilon_n^T|$ introduced in (30). Indeed, for a small enough k, $\frac{u_j^{(n+1)} - u_j^{(n)}}{k}$ is close from $\frac{\partial u}{\partial t}(x_j, t^{n+1})$, so that $|\epsilon_{n,h}^{(T)}|$ is also bounded by $\frac{k}{2}\mathcal{M}_2$.

Now, following the same approach for the new scheme ($\mathbf{FD}_2$), from the expression (35), we can introduce the quantity

$$|\epsilon_{n,h}| = \frac{1}{2}|\frac{\partial u}{\partial t}(x_j, t^{(n+1)}) - \left(\frac{2}{k}\left(u_j^{(n+1)} - u_j^{(n)}\right) - \frac{u_{j-1}^{(n)} - 2u_j^{(n)} + u_{j+1}^{(n)}}{h^2}\right)|$$

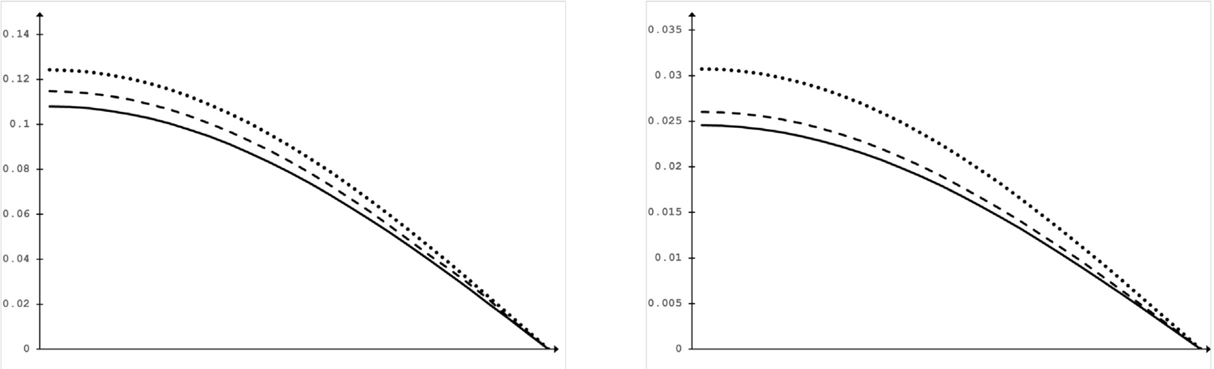

Fig. 1. Comparison of the exact solution u (solid line) as a function of x ($x \in [0,1]$), with the ones obtained with the new scheme FD2 (dashed line) and the classical scheme FD1 (dotted line), for two different times. Left: at time $t_0 = \frac{T}{2}$. Right: at time $t = \frac{4T}{5}$.

that approximates $|\epsilon_n|$ introduced in (33), for small enough k and h. In these conditions, $|\epsilon_{n,h}|$ is bounded by $\frac{k}{8}(M_2 - m_2)$. Also using the quantity $\mathcal{M}_2$ introduced above, we have

$$\frac{k}{8}(M_2 - m_2) \le \frac{k}{4}\mathcal{M}_2.$$

We computed, for the different values of x, $|\epsilon_{n,h}^{(T)}|$ and the related bound $\frac{k}{2}\mathcal{M}_2$ for the classical scheme (**FD**$_1$). Similarly, we computed $|\epsilon_{n,h}|$ and the related bound $\frac{k}{4}\mathcal{M}_2$ for the new scheme (**FD**$_2$). The results we obtained are summarized in Table 1, each line corresponding to a different values of x.

In the first column, we give the values of the upper bound $\frac{k}{2}\mathcal{M}_2$ that have to be compared to the second column, namely the values of the approximate error $|\epsilon_n^T|$. In the same way, the third column gives the values of the upper bound $\frac{k}{4}\mathcal{M}_2$, to be compared to the last one, that is, the values of $|\epsilon_{n,h}|$.

Firstly, it can be observed that, as expected, the values of $|\epsilon_{n,h}^{(T)}|$ (second column) are lower for each value of x (each line) than those of the first column. Similarly for the second scheme, the values of $|\epsilon_{n,h}|$ (fourth column) are lower than those of the third column. By the way, it can be noted that the values of $|\epsilon_{n,h}|$ are much smaller than their upper bound, due to the fact that the quantity $\frac{k}{4}\mathcal{M}_2$ overestimates the true value $\frac{k}{8}(M_2 - m_2)$.

More significantly, we observe that for each x, the value $|\epsilon_{n,h}^{(T)}|$ is almost always (except in one case) greater than the bound $\frac{k}{4}\mathcal{M}_2$ of the scheme (**FD**$_2$). This indicates that the improvement provided by the scheme (**FD**$_2$) indeed corresponds to better accuracy than what (**FD**$_1$) can achieve, even though they are of the same order. If the error of (**FD**$_1$) had also been smaller than $\frac{k}{4}\mathcal{M}_2$, we would have concluded that the scheme (**FD**$_2$) provides a better estimation, but numerically does not offer (or not significantly) better accuracy than the classical scheme. The fact that $|\epsilon_{n,h}^{(T)}|$ is greater than the upper bound of scheme (**FD**$_2$), and significantly above $|\epsilon_{n,h}|$ in practice, demonstrates that the improvement in the constant does indeed correspond to a better accuracy of the new scheme.

We illustrate this behavior in Fig. 2, where we plot, depending on x, the values of the four columns of Table 1. The two solid lines represent the values of the bounds $\frac{k}{2}\mathcal{M}_2$ (the highest) and $\frac{k}{4}\mathcal{M}_2$ (the lowest). One can see that the curve representing $|\epsilon_{n,h}^{(T)}|$ (black dashed line), related to the scheme (**FD**$_1$), almost always lies between these two curves. On the contrary, the curve representing $|\epsilon_{n,h}|$ (gray dashed line), is much lower than the one depicting $\frac{k}{4}\mathcal{M}_2$.

5. Conclusion

In this paper we have proposed a way to enhance interpolation and approximation error estimates. Based on a new Taylor-like formula, we show how it can be applied to improve first, the P_1-interpolation error estimate, then, to propose new numerical schemes yielding to smaller upper bounds in the corresponding error estimate.

In the first part, considering that numerous partial differential equations are well-posed within the general class of Sobolev spaces $W^{m,p}(\Omega), (m,p) \in \mathbb{N}^{*2}$, and particularly in the space $W^{1,1}(\Omega)$, we initially consider this framework, where we proved new interpolation error estimates.

In a second part, we have considered another application of the new Taylor-like formula. Turning out our attention to the analysis of a classical implicit finite differences scheme used to discretize the heat equation, we showed how we can enhance the upper bound of the error estimate, while maintaining the consistency error and the order of convergence at the same level, together with the stability as well. Numerical illustrations have been proposed to compare the resulting new scheme compared to the classical implicit finite differences scheme.

This new first-order Taylor-like formula could also find applications in various other contexts. For example, we can develop new schemes for different types of partial differential equations or ordinary differential equations, as well as tackle more general problems within the Sobolev spaces $W^{m,p}(\Omega)$ when $p > 1$.

***Homages*:** The authors want to warmly dedicate this research to pay homage to the memory of Professors André Avez and Gérard Tronel who largely promote the passion of research and teaching in mathematics of their students.

Table 1
Comparison between $|\epsilon_{n,h}^{(T)}|$ (second column) and his upper bound (first column) for the scheme (**FD$_1$**), and similarly, between $|\epsilon_{n,h}|$ (fourth column) and his upper bound (third column) for (**FD$_2$**). Each line corresponds to a value of x.

$\frac{k}{2}\mathcal{M}_2$	$\lvert\epsilon_{n,h}^{(T)}\rvert$	$\frac{k}{4}\mathcal{M}_2$	$\lvert\epsilon_{n,h}\rvert$
0.605	0.447	0.302	0.086
0.633	0.455	0.316	0.085
0.675	0.465	0.337	0.050
0.722	0.476	0.361	0.055
0.763	0.485	0.381	0.038
0.785	0.486	0.392	0.041
0.772	0.508	0.386	0.027
0.709	0.699	0.354	0.030
0.583	0.402	0.291	0.021
0.383	0.304	0.191	0.025
0.341	0.286	0.170	0.019
0.431	0.420	0.215	0.026
0.664	0.474	0.332	0.023
1.120	0.910	0.560	0.028
1,86	1.184	0.793	0.027
2.023	0.928	1.011	0.024
2.390	1.242	1.195	0.023
2.644	1,56	1.322	0.051
2.751	2.294	1.375	0.125
2.685	2.040	1.342	0.154
2.436	2.221	1.218	0.165
2.011	1.871	1.005	0.574
1.434	1.202	0.717	0.592
0.746	0.714	0.373	0.257

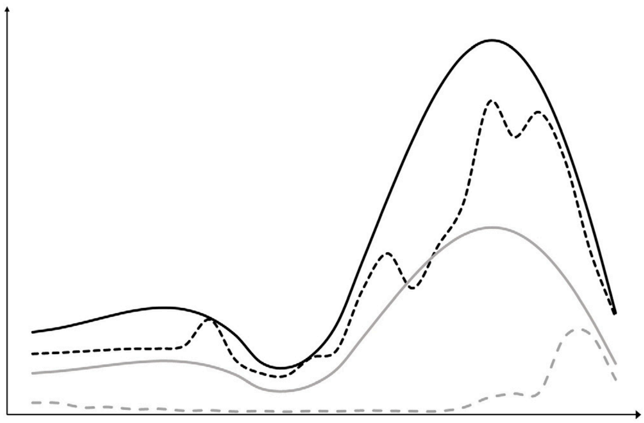

Fig. 2. Representation of the four columns of Table 1 as a function of x. The curve $|\epsilon_{n,h}^{(T)}|$ (black dashed line) almost always lies between the two solid lines $\frac{k}{2}\mathcal{M}_2$ (upper) and $\frac{k}{4}\mathcal{M}_2$ (lower). The curve $|\epsilon_{n,h}|$ (gray dashed line) is always much lower than $\frac{k}{4}\mathcal{M}_2$.

Data availability

No data was used for the research described in the article.

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